

Electronic Supplementary Material

Microhydration of Small Protonated Polyaromatic Hydrocarbons: A First Principles Study

**Muthuramalingam Prakash,^{*,†} K. Rudharachari Maiyelvaganan,^{†,#} N. Giri Lakshman,^{†,#},
C. Gopalakrishnan,^{†,#}, Majdi Hochlaf^{*,‡}**

[†] Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603203, Chengalpattu District, Tamil Nadu, India.

[‡] Université Gustave Eiffel, COSYS/IMSE, 5 Bd Descartes, 77454, Champs Sur Marne, France.

[#] *These authors contributed equally to this work.*

* Authors for correspondence

M. P.: Phone: +91 44 2741 6230. Email: M.P.: prakashspm@gmail.com & prakashm4@srmist.edu.in;

ORCID: orcid.org/0000-0002-1886-7708;

M. H.: email: majdi.hochlaf@univ-eiffel.fr; ORCID: orcid.org/0000-0002-4714737-7978

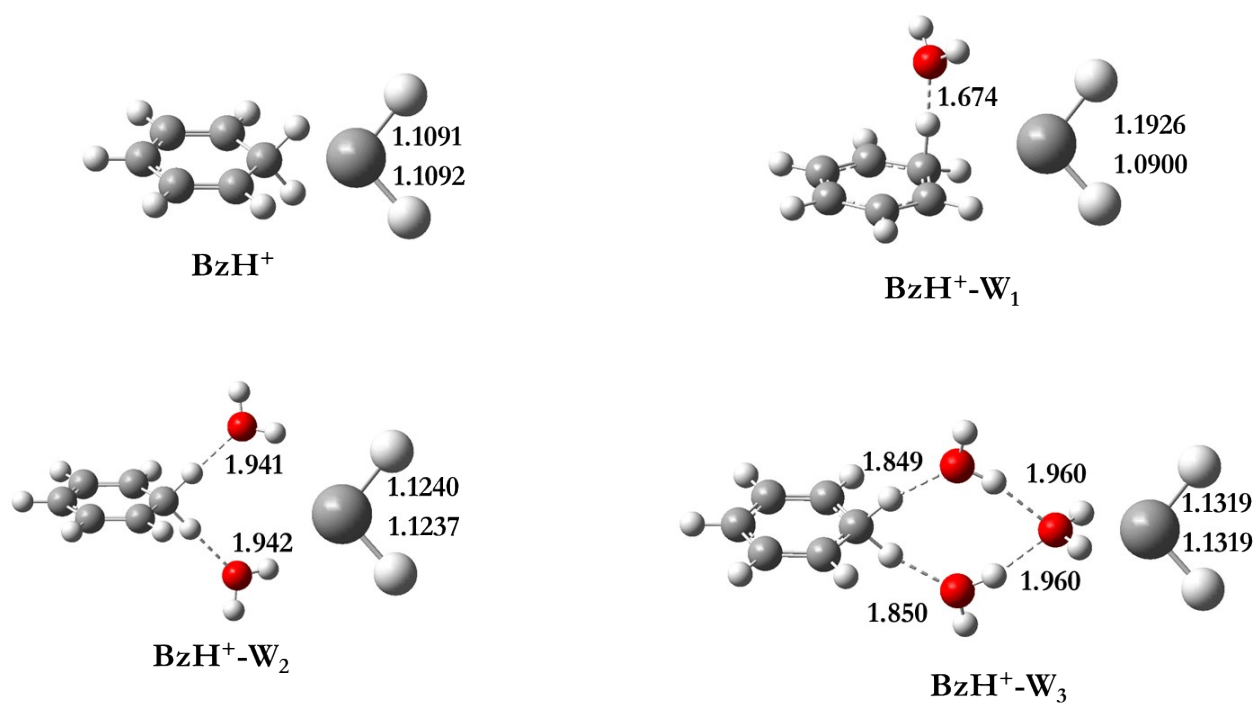


Figure S1: Optimized structures of BzH⁺, and BzH⁺-W_{*n*}, (*n* = 1 – 3) clusters at MP2/6-311++G^{**}. Close view of the sp³ C-H bond distances (before and after hydration) and the intermonomer distances (in Å) are given.

Table S1: Optimized equilibrium structures of protonated BzH^+-W_n ($n = 1 - 3$) clusters and their different isomers at MP2/6-311++G** level. The calculated total energy (E_T) and their relative energies (E_R) are provided. Most stable isomers are in bold letter. These isoemers are given based on the mode of interaction

BzH^+-W_n	E_T (a.u)	E_R (a.u)	E_R (kcal/mol)
$\text{BzH}^+-\text{W}_{1a}$ (C-H \cdots O)	-308.16771	0.009847	6.17
$\text{BzH}^+-\text{W}_{1b}$ (O-H$\cdots$$\pi$)	-308.17756	0	0
$\text{BzH}^+-\text{W}_{1c}$ (O-H \cdots π)	-308.17599	0.00157	0.98
$\text{BzH}^+-\text{W}_{2a}$ (C-H \cdots O)	-384.45717	0.0389441	24.43
$\text{BzH}^+-\text{W}_{2b}$ (O-H$\cdots$$\pi$)	-384.49611	0	0
$\text{BzH}^+-\text{W}_{3a}$ (C-H \cdots O)	-460.75523	0.0506862	31.80
$\text{BzH}^+-\text{W}_{3b}$ (O-H$\cdots$$\pi$)	-460.80591	0	0
$\text{BzH}^+-\text{W}_{3c}$ (O-H \cdots π)	-460.79994	0.0059776	3.75

of atoms within BzH^+-W_n ($n = 1 - 3$) clusters

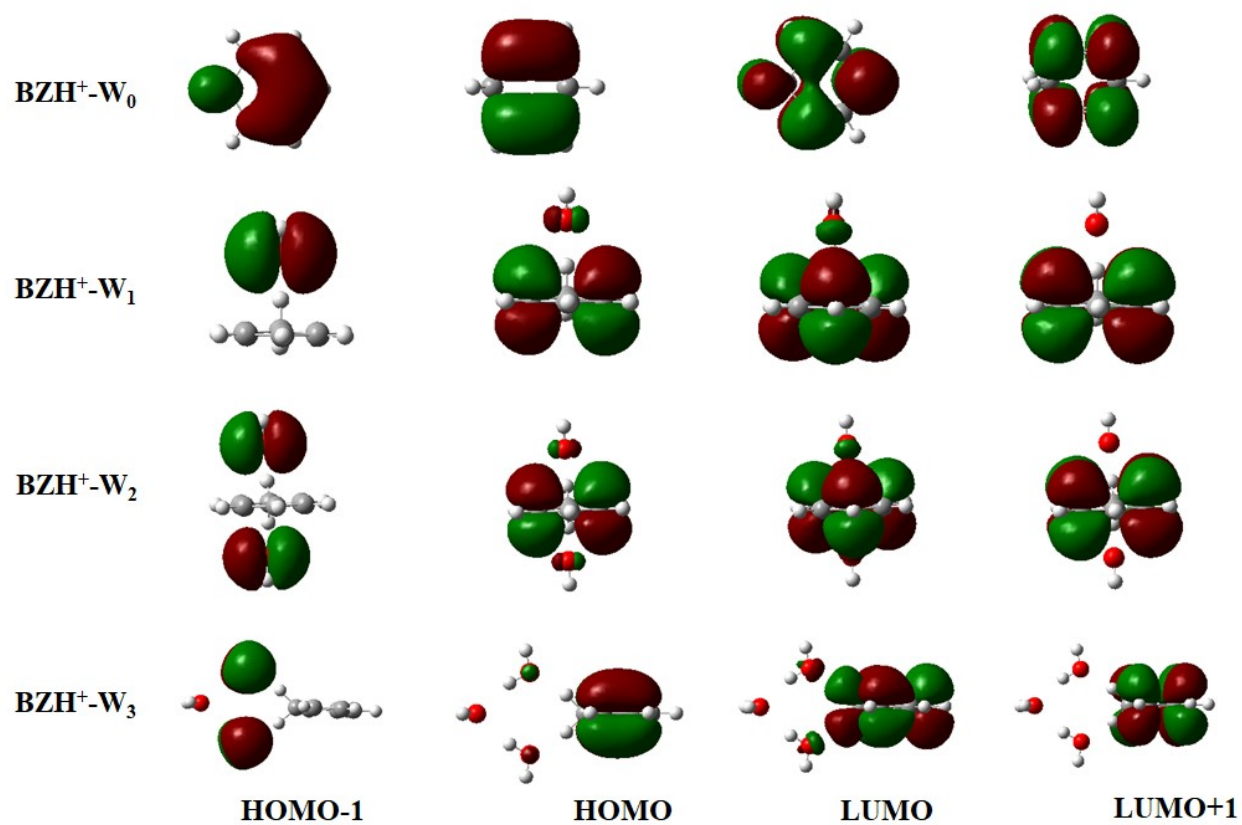


Figure S2: Molecular Orbital diagram of BzH⁺-W_n (n=0-3) clusters.

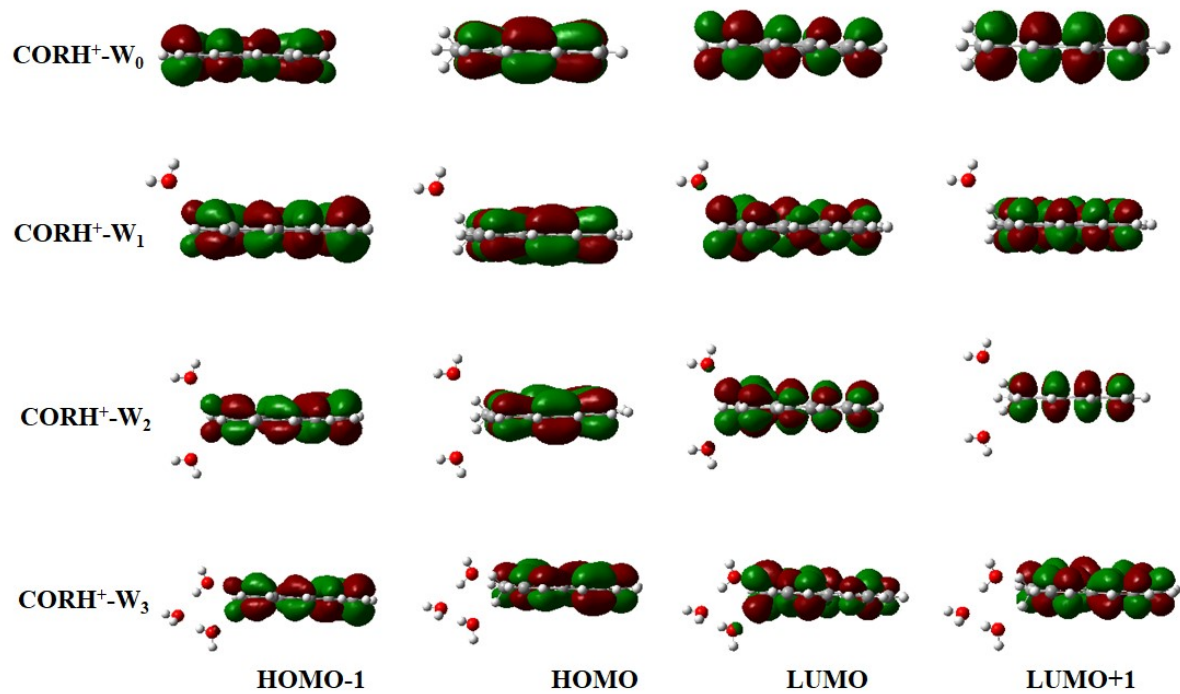


Figure S3: Molecular Orbital diagram of CorH^+-W_n ($n=0-3$) clusters.

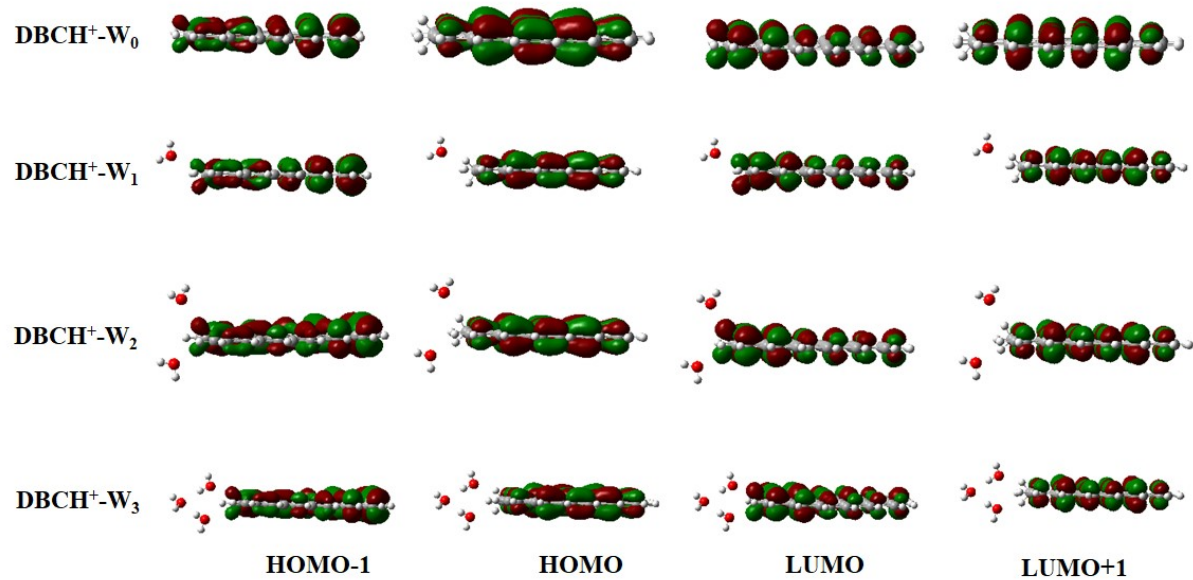
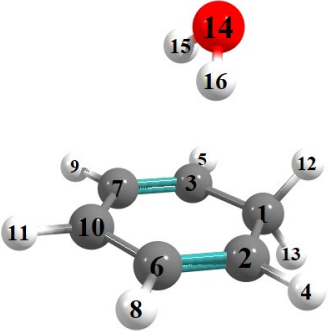
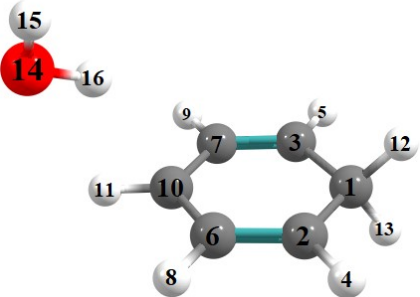
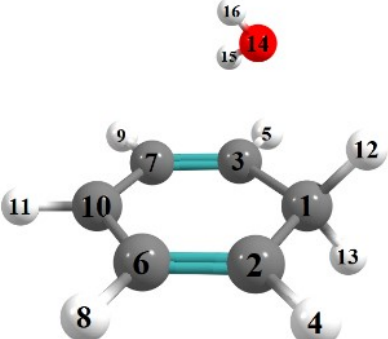
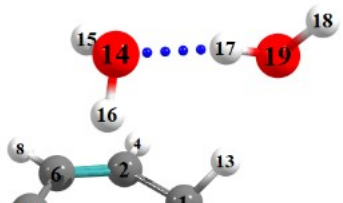
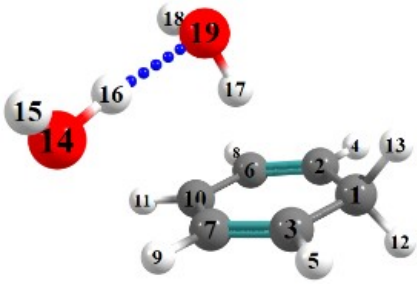
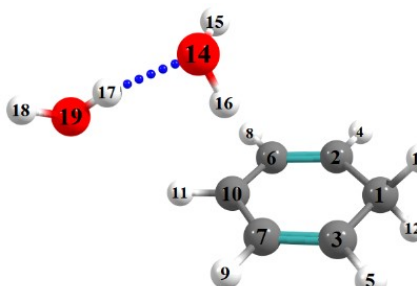
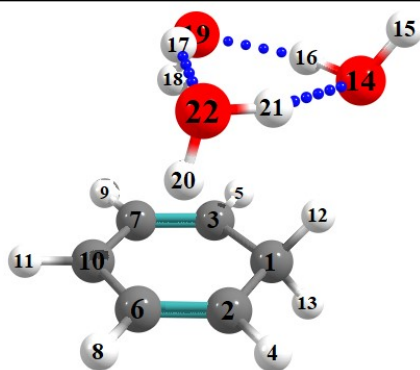


Figure S4: Molecular Orbital diagram of DbcH⁺-W_n (n=0-3) clusters.

Table S2: Optimized equilibrium structures of BzH^+-W_n , CorH^+-W_n and DbcH^+-W_n ($n = 1, 2, 3$) clusters regenerated from PBE0/6-311++G** optimized geometries using CREST approach. C1, C2 and C3 represents the different minimum energy confirmations. These conformers are generated from CREST algorithm using tight-binding semi-empirical method. The total conformational relative energies are provided in kcal/mol.

 <p style="text-align: center;">C1-BzH⁺-W₁ [-21.40866996]</p>	<table border="1"> <tbody> <tr><td>C</td><td>0.226212830</td><td>0.215386678</td><td>1.491105670</td></tr> <tr><td>C</td><td>0.409117635</td><td>-1.130449820</td><td>0.877787890</td></tr> <tr><td>C</td><td>0.427836551</td><td>1.329616984</td><td>0.522271877</td></tr> <tr><td>H</td><td>0.285969244</td><td>-1.983554975</td><td>1.528242177</td></tr> <tr><td>H</td><td>0.318849174</td><td>2.333699523</td><td>0.904372418</td></tr> <tr><td>C</td><td>0.717623548</td><td>-1.292593486</td><td>-0.433601781</td></tr> <tr><td>C</td><td>0.735851420</td><td>1.109318185</td><td>-0.780652297</td></tr> <tr><td>H</td><td>0.841637462</td><td>-2.288430397</td><td>-0.836487155</td></tr> <tr><td>H</td><td>0.873862786</td><td>1.948414963</td><td>-1.448684330</td></tr> <tr><td>C</td><td>0.885409373</td><td>-0.191468773</td><td>-1.289746133</td></tr> <tr><td>H</td><td>1.134271572</td><td>-0.343262960</td><td>-2.327061526</td></tr> <tr><td>H</td><td>-0.780072317</td><td>0.287382577</td><td>1.936328307</td></tr> <tr><td>H</td><td>0.913831844</td><td>0.333448457</td><td>2.344231227</td></tr> <tr><td>O</td><td>-2.531814986</td><td>-0.041294105</td><td>-0.361281169</td></tr> <tr><td>H</td><td>-1.980525704</td><td>0.705934835</td><td>-0.605978334</td></tr> <tr><td>H</td><td>-1.959563479</td><td>-0.812536895</td><td>-0.373779728</td></tr> </tbody> </table>	C	0.226212830	0.215386678	1.491105670	C	0.409117635	-1.130449820	0.877787890	C	0.427836551	1.329616984	0.522271877	H	0.285969244	-1.983554975	1.528242177	H	0.318849174	2.333699523	0.904372418	C	0.717623548	-1.292593486	-0.433601781	C	0.735851420	1.109318185	-0.780652297	H	0.841637462	-2.288430397	-0.836487155	H	0.873862786	1.948414963	-1.448684330	C	0.885409373	-0.191468773	-1.289746133	H	1.134271572	-0.343262960	-2.327061526	H	-0.780072317	0.287382577	1.936328307	H	0.913831844	0.333448457	2.344231227	O	-2.531814986	-0.041294105	-0.361281169	H	-1.980525704	0.705934835	-0.605978334	H	-1.959563479	-0.812536895	-0.373779728
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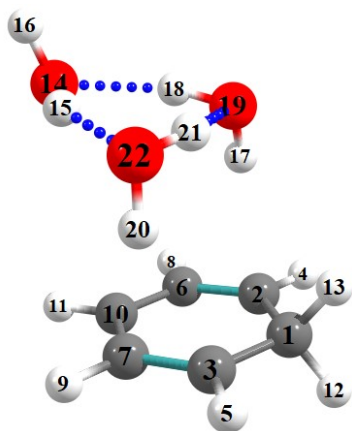
<p style="text-align: center;">C1-BzH⁺-W₂ [-26.49150944]</p>	<table border="0"> <tbody> <tr><td>C</td><td>-0.643636352</td><td>-0.874739298</td><td>-1.213643805</td></tr> <tr><td>C</td><td>-0.527586354</td><td>-0.774419371</td><td>1.264824620</td></tr> <tr><td>H</td><td>-0.366350986</td><td>-1.340425059</td><td>-2.147240407</td></tr> <tr><td>H</td><td>-0.164428192</td><td>-1.164158534</td><td>2.203660968</td></tr> <tr><td>C</td><td>-1.482062379</td><td>0.191600859</td><td>-1.190479895</td></tr> <tr><td>C</td><td>-1.367198546</td><td>0.292082368</td><td>1.232841250</td></tr> <tr><td>H</td><td>-1.881599573</td><td>0.582858846</td><td>-2.116449500</td></tr> <tr><td>H</td><td>-1.678972041</td><td>0.759754082</td><td>2.156964575</td></tr> <tr><td>C</td><td>-1.858416219</td><td>0.803247386</td><td>0.018096038</td></tr> <tr><td>H</td><td>-2.532368863</td><td>1.644357572</td><td>0.015685953</td></tr> <tr><td>H</td><td>-0.285449471</td><td>-2.532046938</td><td>0.080294854</td></tr> <tr><td>H</td><td>1.040541942</td><td>-1.412101631</td><td>-0.027067137</td></tr> <tr><td>O</td><td>1.315219387</td><td>1.789591433</td><td>-0.064765605</td></tr> <tr><td>H</td><td>0.996778699</td><td>1.851048769</td><td>-0.968475862</td></tr> <tr><td>H</td><td>0.589246631</td><td>1.421756102</td><td>0.452219138</td></tr> <tr><td>H</td><td>2.532611337</td><td>0.423780861</td><td>-0.029124834</td></tr> <tr><td>H</td><td>3.886586165</td><td>-0.242561323</td><td>0.304353535</td></tr> <tr><td>O</td><td>3.008853816</td><td>-0.424359105</td><td>-0.034099548</td></tr> </tbody> </table>	C	-0.643636352	-0.874739298	-1.213643805	C	-0.527586354	-0.774419371	1.264824620	H	-0.366350986	-1.340425059	-2.147240407	H	-0.164428192	-1.164158534	2.203660968	C	-1.482062379	0.191600859	-1.190479895	C	-1.367198546	0.292082368	1.232841250	H	-1.881599573	0.582858846	-2.116449500	H	-1.678972041	0.759754082	2.156964575	C	-1.858416219	0.803247386	0.018096038	H	-2.532368863	1.644357572	0.015685953	H	-0.285449471	-2.532046938	0.080294854	H	1.040541942	-1.412101631	-0.027067137	O	1.315219387	1.789591433	-0.064765605	H	0.996778699	1.851048769	-0.968475862	H	0.589246631	1.421756102	0.452219138	H	2.532611337	0.423780861	-0.029124834	H	3.886586165	-0.242561323	0.304353535	O	3.008853816	-0.424359105	-0.034099548				
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C1-BzH⁺-W₃

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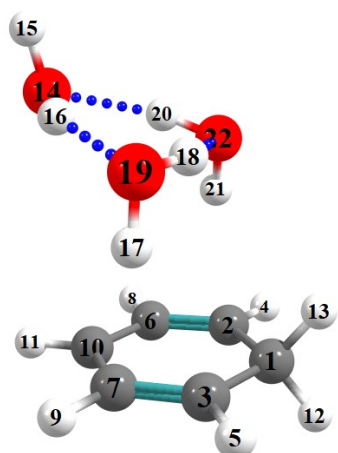
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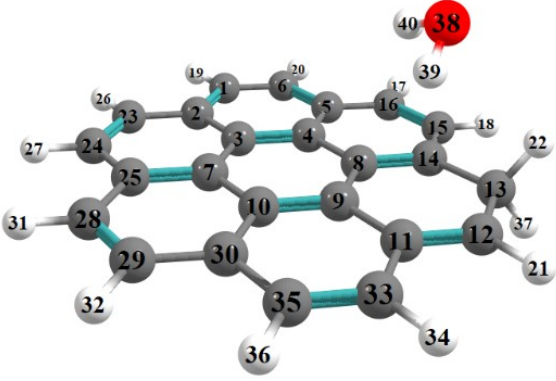
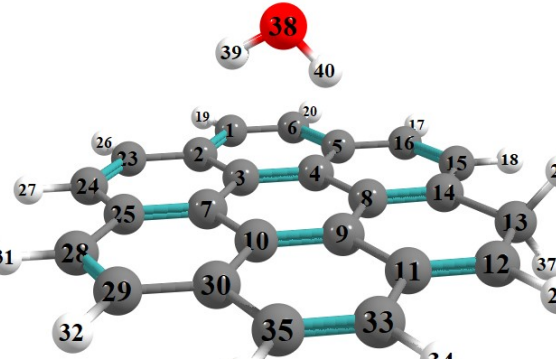
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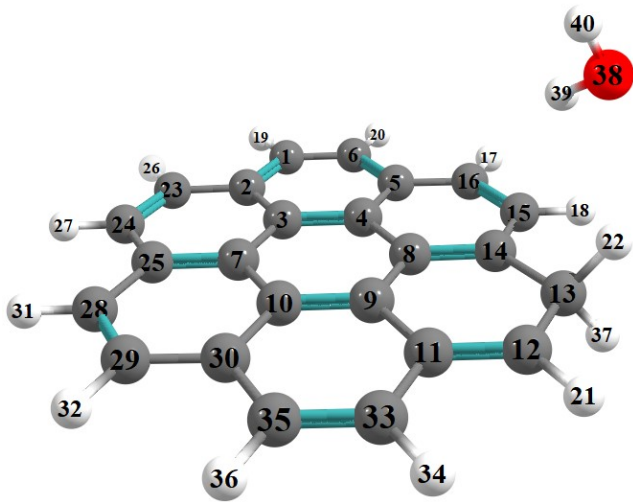
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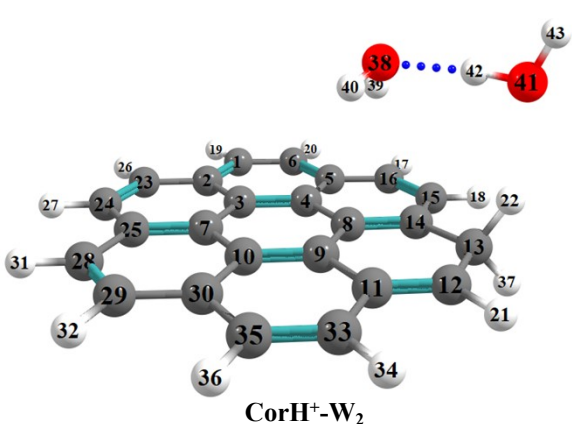
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C	-1.114128502	-1.362489043	0.324578075
H	-0.907260715	-2.416561442	0.395782093
H	-2.616510836	1.984427968	0.247957636
H	-0.930997972	2.279474769	-0.078174959
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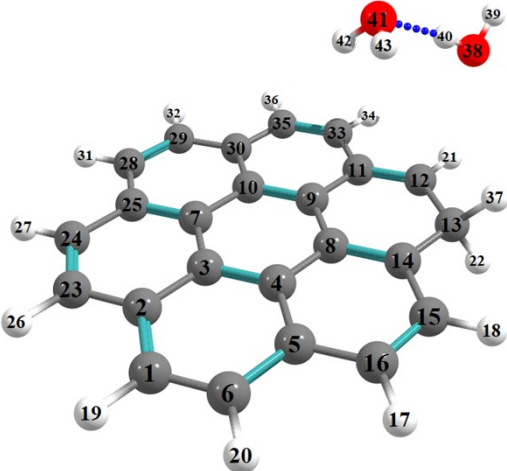
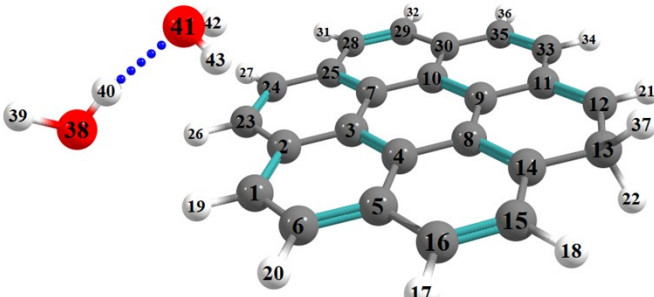


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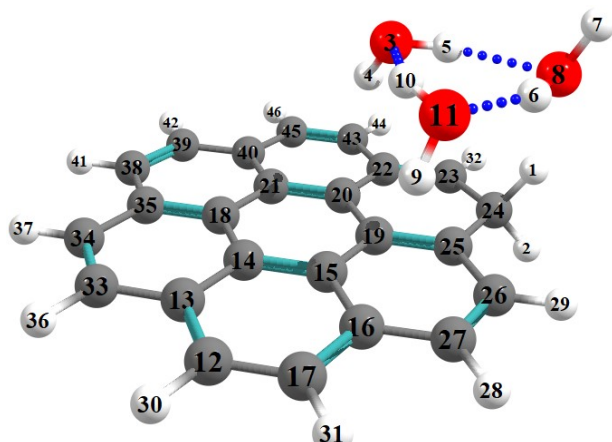
<p style="text-align: center;">C3-BzH⁺-W₃ [-31.57521202]</p>	<table border="1"> <tbody> <tr><td>H</td><td>-1.139322616</td><td>-0.042185773</td><td>-2.146577288</td></tr> <tr><td>O</td><td>3.010763380</td><td>0.454184845</td><td>1.045522007</td></tr> <tr><td>H</td><td>3.965974244</td><td>0.392895079</td><td>0.996672895</td></tr> <tr><td>H</td><td>2.666782501</td><td>-0.386529175</td><td>0.687910376</td></tr> <tr><td>H</td><td>0.891848919</td><td>-1.691806582</td><td>-0.259448559</td></tr> <tr><td>H</td><td>1.663134353</td><td>-0.610921906</td><td>-1.052471656</td></tr> <tr><td>O</td><td>1.774724795</td><td>-1.430551398</td><td>-0.536146789</td></tr> <tr><td>H</td><td>2.114002606</td><td>1.275497385</td><td>-0.384851951</td></tr> <tr><td>H</td><td>0.659102173</td><td>1.550142154</td><td>-0.820323713</td></tr> <tr><td>O</td><td>1.512458597</td><td>1.251214772</td><td>-1.149973907</td></tr> </tbody> </table>	H	-1.139322616	-0.042185773	-2.146577288	O	3.010763380	0.454184845	1.045522007	H	3.965974244	0.392895079	0.996672895	H	2.666782501	-0.386529175	0.687910376	H	0.891848919	-1.691806582	-0.259448559	H	1.663134353	-0.610921906	-1.052471656	O	1.774724795	-1.430551398	-0.536146789	H	2.114002606	1.275497385	-0.384851951	H	0.659102173	1.550142154	-0.820323713	O	1.512458597	1.251214772	-1.149973907																																																																																																																								
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 <p style="text-align: center;">C1-CorH⁺-W₁ [-63.14564738]</p>	<table border="1"> <tbody> <tr><td>C</td><td>2.294580955</td><td>-3.053210572</td><td>0.009542461</td></tr> <tr><td>C</td><td>2.457022256</td><td>-1.645636765</td><td>0.032491474</td></tr> <tr><td>C</td><td>1.311569469</td><td>-0.823582536</td><td>-0.062820658</td></tr> <tr><td>C</td><td>0.025802354</td><td>-1.407921342</td><td>-0.178320519</td></tr> <tr><td>C</td><td>-0.105997780</td><td>-2.815763572</td><td>-0.197217359</td></tr> <tr><td>C</td><td>1.063557215</td><td>-3.616783846</td><td>-0.100895235</td></tr> <tr><td>C</td><td>1.450253887</td><td>0.584254216</td><td>-0.042879231</td></tr> <tr><td>C</td><td>-1.126466291</td><td>-0.584243811</td><td>-0.270816293</td></tr> <tr><td>C</td><td>-0.977309381</td><td>0.833348298</td><td>-0.252997654</td></tr> <tr><td>C</td><td>0.298551514</td><td>1.410712747</td><td>-0.141204719</td></tr> <tr><td>C</td><td>-2.139776247</td><td>1.671976649</td><td>-0.356764239</td></tr> <tr><td>C</td><td>-3.385240537</td><td>1.119734028</td><td>-0.459312188</td></tr> <tr><td>C</td><td>-3.634041901</td><td>-0.342475149</td><td>-0.444124386</td></tr> <tr><td>C</td><td>-2.392950432</td><td>-1.179824592</td><td>-0.375277590</td></tr> <tr><td>C</td><td>-2.499401056</td><td>-2.566965765</td><td>-0.394686261</td></tr> <tr><td>C</td><td>-1.386670606</td><td>-3.374114229</td><td>-0.309233685</td></tr> <tr><td>H</td><td>-1.492074911</td><td>-4.449050239</td><td>-0.326116870</td></tr> <tr><td>H</td><td>-3.480219549</td><td>-3.014206994</td><td>-0.476155792</td></tr> <tr><td>H</td><td>3.177606426</td><td>-3.672500523</td><td>0.082151996</td></tr> <tr><td>H</td><td>0.948813539</td><td>-4.691301871</td><td>-0.117580732</td></tr> <tr><td>H</td><td>-4.251653933</td><td>1.759860857</td><td>-0.541397297</td></tr> <tr><td>H</td><td>-4.272767056</td><td>-0.584559745</td><td>0.419017146</td></tr> <tr><td>C</td><td>3.725487235</td><td>-1.038854946</td><td>0.147327630</td></tr> <tr><td>C</td><td>3.859205102</td><td>0.318518497</td><td>0.166632276</td></tr> <tr><td>C</td><td>2.731433367</td><td>1.165515548</td><td>0.071920704</td></tr> <tr><td>H</td><td>4.596578550</td><td>-1.674868940</td><td>0.220064836</td></tr> <tr><td>H</td><td>4.836870508</td><td>0.770939807</td><td>0.254691290</td></tr> <tr><td>C</td><td>2.846143756</td><td>2.573730251</td><td>0.087446329</td></tr> <tr><td>C</td><td>1.739427164</td><td>3.371195342</td><td>-0.009604151</td></tr> <tr><td>C</td><td>0.451251363</td><td>2.821454678</td><td>-0.126228349</td></tr> <tr><td>H</td><td>3.830020330</td><td>3.011628013</td><td>0.176382538</td></tr> <tr><td>H</td><td>1.841937887</td><td>4.447394966</td><td>0.001496488</td></tr> <tr><td>C</td><td>-1.943548309</td><td>3.091925678</td><td>-0.346118416</td></tr> <tr><td>H</td><td>-2.819005714</td><td>3.719853144</td><td>-0.428308871</td></tr> <tr><td>C</td><td>-0.708953700</td><td>3.635010549</td><td>-0.233444935</td></tr> <tr><td>H</td><td>-0.580979940</td><td>4.708391557</td><td>-0.224232895</td></tr> <tr><td>H</td><td>-4.222844443</td><td>-0.626251696</td><td>-1.327557226</td></tr> <tr><td>O</td><td>-2.577612215</td><td>-0.089407473</td><td>2.695579567</td></tr> <tr><td>H</td><td>-2.386960743</td><td>0.697952830</td><td>2.179840603</td></tr> <tr><td>H</td><td>-1.926726963</td><td>-0.747714485</td><td>2.442278304</td></tr> </tbody> </table>	C	2.294580955	-3.053210572	0.009542461	C	2.457022256	-1.645636765	0.032491474	C	1.311569469	-0.823582536	-0.062820658	C	0.025802354	-1.407921342	-0.178320519	C	-0.105997780	-2.815763572	-0.197217359	C	1.063557215	-3.616783846	-0.100895235	C	1.450253887	0.584254216	-0.042879231	C	-1.126466291	-0.584243811	-0.270816293	C	-0.977309381	0.833348298	-0.252997654	C	0.298551514	1.410712747	-0.141204719	C	-2.139776247	1.671976649	-0.356764239	C	-3.385240537	1.119734028	-0.459312188	C	-3.634041901	-0.342475149	-0.444124386	C	-2.392950432	-1.179824592	-0.375277590	C	-2.499401056	-2.566965765	-0.394686261	C	-1.386670606	-3.374114229	-0.309233685	H	-1.492074911	-4.449050239	-0.326116870	H	-3.480219549	-3.014206994	-0.476155792	H	3.177606426	-3.672500523	0.082151996	H	0.948813539	-4.691301871	-0.117580732	H	-4.251653933	1.759860857	-0.541397297	H	-4.272767056	-0.584559745	0.419017146	C	3.725487235	-1.038854946	0.147327630	C	3.859205102	0.318518497	0.166632276	C	2.731433367	1.165515548	0.071920704	H	4.596578550	-1.674868940	0.220064836	H	4.836870508	0.770939807	0.254691290	C	2.846143756	2.573730251	0.087446329	C	1.739427164	3.371195342	-0.009604151	C	0.451251363	2.821454678	-0.126228349	H	3.830020330	3.011628013	0.176382538	H	1.841937887	4.447394966	0.001496488	C	-1.943548309	3.091925678	-0.346118416	H	-2.819005714	3.719853144	-0.428308871	C	-0.708953700	3.635010549	-0.233444935	H	-0.580979940	4.708391557	-0.224232895	H	-4.222844443	-0.626251696	-1.327557226	O	-2.577612215	-0.089407473	2.695579567	H	-2.386960743	0.697952830	2.179840603	H	-1.926726963	-0.747714485	2.442278304
C	2.294580955	-3.053210572	0.009542461																																																																																																																																																														
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C	2.846143756	2.573730251	0.087446329																																																																																																																																																														
C	1.739427164	3.371195342	-0.009604151																																																																																																																																																														
C	0.451251363	2.821454678	-0.126228349																																																																																																																																																														
H	3.830020330	3.011628013	0.176382538																																																																																																																																																														
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H	-2.386960743	0.697952830	2.179840603																																																																																																																																																														
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	 <p style="text-align: center;">C3-CorH⁺-W₁ [-63.14534884]</p>	<p>C 1.310661090 0.576486934 0.018560632 C -1.246880499 -0.593618350 -0.370118070 C -1.101058846 0.824453993 -0.337832621 C 0.165547478 1.402929876 -0.146556550 C -2.256162056 1.662526173 -0.498783327 C -3.491536180 1.110169266 -0.680684176 C -3.735017874 -0.352957579 -0.721966602 C -2.502690116 -1.190162745 -0.555417358 C -2.606769176 -2.577249421 -0.580988250 C -1.501603371 -3.383897356 -0.425023823 H -1.605598710 -4.458835591 -0.446591345 H -3.580237358 -3.025286134 -0.725486917 H 3.028625622 -3.679749832 0.255005675 H 0.817426102 -4.699535749 -0.085182324 H -4.354041385 1.749677578 -0.801330494 H -4.462936201 -0.621158143 0.058431733 C 3.569915575 -1.045991604 0.352855092 C 3.701437376 0.311448476 0.382890720 C 2.581552265 1.158398018 0.217952960 H 4.434878585 -1.681415567 0.480400198 H 4.670951876 0.764284126 0.534095691 C 2.693001943 2.566553373 0.248811548 C 1.592831654 3.363185511 0.089835050 C 0.314907781 2.813302881 -0.109108831 H 3.668807691 3.004454853 0.401708507 H 1.692826700 4.439159550 0.116587037 C -2.064093976 3.082150764 -0.458536375 H -2.935062512 3.709791537 -0.580371777 C -0.839074812 3.626175394 -0.272229061 H -0.714011122 4.699447322 -0.242351751 H -4.226075095 -0.613406046 -1.671247791 O -0.365397499 0.059869370 2.936015434 H 0.529456987 0.142163618 2.598535606 H -0.946130347 0.045257987 2.171614111</p>
	<p>C 2.312229623 -2.997237740 0.063083500 C 2.501421482 -1.593412063 0.025213189 C 1.368864078 -0.752945562 -0.065912424 C 0.069285945 -1.315102144 -0.117583843 C -0.088678732 -2.720099450 -0.079248037 C 1.068067908 -3.540119383 0.012884666 C 1.534105883 0.651576393 -0.107180186 C -1.069317564 -0.472112773 -0.206037818 C -0.894246276 0.940753699 -0.248101816 C 0.395255637 1.496144651 -0.201387519 C -2.042910607 1.796892665 -0.347756671 C -3.300596248 1.265953713 -0.390445869 C -3.575744671 -0.188365855 -0.315669532 C -2.348741000 -1.045424145 -0.254594310 C -2.481942094 -2.431199797 -0.221037961 C -1.382058499 -3.257355664 -0.134823792 H -1.508214563 -4.330237519 -0.110798298 H -3.473319843 -2.861023595 -0.264352442 H 3.185424294 -3.630946445 0.132107957 H 0.932884039 -4.612222742 0.040843943 H -4.157544875 1.919621167 -0.468673510 H -4.190425007 -0.392047571 0.574765689</p>	

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	C	2.829276500	1.211030128	-0.057574566
	H	4.645282677	-1.658089122	0.144422022
	H	4.932090113	0.781862755	0.072616673
	C	2.971011423	2.615992454	-0.103160756
	C	1.876523139	3.430837674	-0.197095913
	C	0.575207170	2.902938039	-0.249404921
	H	3.965434965	3.037351437	-0.063990515
	H	1.999921170	4.504455585	-0.233368907
	C	-1.819965543	3.211699019	-0.401349546
	H	-2.685754541	3.853717060	-0.480063912
	C	-0.572646828	3.734578978	-0.351956492
	H	-0.424169332	4.804921523	-0.390747434
	H	-4.198323875	-0.492242060	-1.168543838
	O	-3.774502732	-1.565977786	2.665965114
	H	-3.083226930	-2.013940541	2.169679296
	H	-3.379084616	-1.257256434	3.483268982
 <p style="text-align: center;">CorH⁺-W₂ [-68.22943558]</p>	C	-1.175628439	-3.617927886	0.190991104
	C	-1.861530883	-2.389078911	0.025691285
	C	-1.137038774	-1.180931914	0.139046743
	C	0.252813811	-1.209357112	0.413605334
	C	0.911145921	-2.451810137	0.574889156
	C	0.156472005	-3.649948387	0.455102953
	C	-1.800723932	0.058428370	-0.020561064
	C	0.985434584	0.003182147	0.519077061
	C	0.308759476	1.246329323	0.357481015
	C	-1.071371490	1.272609844	0.095095127
	C	1.042310832	2.475008632	0.478492245
	C	2.385786548	2.456657517	0.725699412
	C	3.175888659	1.210712144	0.843307967
	C	2.364012781	-0.043628930	0.780326051
	C	2.990010237	-1.275959537	0.943886576
	C	2.287907222	-2.458018964	0.844524559
	H	2.792957460	-3.404118283	0.974979587
	H	4.051366901	-1.297685157	1.143115268
	H	-1.739590278	-4.535858561	0.103246106
	H	0.671358263	-4.591762133	0.581542372
	H	2.925985406	3.387451784	0.820914972
	H	3.913427656	1.180106887	0.025354558
	C	-3.244407134	-2.332462087	-0.247092092
	C	-3.885012125	-1.137835160	-0.399037086
	C	-3.186267298	0.086298312	-0.289535515
	H	-3.791450215	-3.260932091	-0.332652600
	H	-4.945498466	-1.108242140	-0.605886701
	C	-3.829973372	1.334928364	-0.438481704
	C	-3.131208091	2.505043071	-0.321809210
	C	-1.751780369	2.508875031	-0.054375878
	H	-4.890667522	1.348898030	-0.644516263
	H	-3.637583264	3.453676666	-0.434400792
	C	0.317294925	3.702705089	0.333679914
	H	0.869785337	4.626165400	0.431898998
	C	-1.011393001	3.714993627	0.076645259
	H	-1.540589409	4.651321592	-0.033889381
H	3.772892745	1.228297809	1.764249582	
O	2.175460145	-0.997989132	-2.342968274	

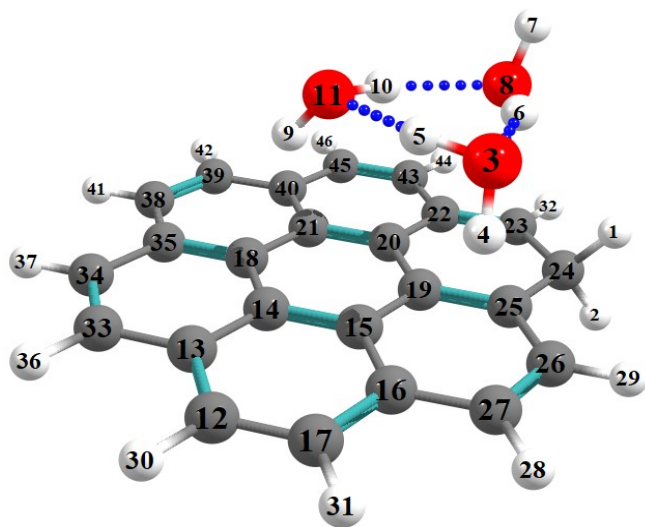
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 <p style="text-align: center;">C2-CorH⁺-W₂ [-68.22657551]</p>	C -1.615947619 -3.873908643 0.690881070 C -2.139418755 -2.578965139 0.451615559 C -1.246130619 -1.524279192 0.157156176 C 0.148618911 -1.768611477 0.104734301 C 0.642515314 -3.070580159 0.349695046 C -0.279304983 -4.111364633 0.642668274 C -1.747143534 -0.223334616 -0.084137766 C 1.047009969 -0.711506201 -0.193155283 C 0.533793477 0.594367644 -0.439401225 C -0.848948026 0.836590703 -0.381834403 C 1.439614928 1.667740614 -0.740213380 C 2.787630758 1.452703982 -0.785078596 C 3.403474945 0.123644634 -0.550977833 C 2.425206098 -0.969466786 -0.238981893 C 2.889776377 -2.257675427 0.007042090 C 2.025460177 -3.290722768 0.294999933 H 2.408123990 -4.283719982 0.481558781 H 3.954163066 -2.445377660 -0.031071945 H -2.308243465 -4.673631541 0.914296299 H 0.111112155 -5.102303779 0.826824368 H 3.456084161 2.277227443 -0.980790553 H 3.992543072 -0.159917150 -1.435597150 C -3.523358520 -2.308965621 0.498523726 C -4.006095130 -1.054259763 0.267199853 C -3.136439857 0.020128542 -0.028848625 H -4.199965327 -3.121606993 0.723460975 H -5.068814408 -0.860690043 0.306659050 C -3.613358439 1.328001931 -0.270787504 C -2.750797888 2.350490337 -0.555314543 C -1.363102057 2.138329695 -0.619109246 H -4.678125746 1.506985504 -0.226931965 H -3.129439819 3.346537206 -0.738538295 C 0.883488923 2.969898993 -0.976976416 H 1.572801605 3.768900615 -1.207058521 C -0.452166120 3.188923735 -0.916890210 H -0.855531614 4.175346658 -1.100240189 H 4.138716602 0.203069635 0.263190552 O 3.918632797 4.326310294 0.332456414 H 4.356970963 5.082375112 0.725548986 H 3.241641253 4.044516144 0.968792589 O 1.825549409 3.377167119 1.973887184 H 1.104668473 3.477086361 1.342721783 H 1.961280043 2.433443256 2.086776456
 <p style="text-align: center;">C3-CorH⁺-W₂ [-68.22638814]</p>	C 0.125615105 -3.091348693 -0.951912283 C -0.768038311 -1.993068050 -0.862921915 C -0.269262301 -0.729894847 -0.472518408 C 1.108284637 -0.569817049 -0.181559315 C 1.978268133 -1.680453052 -0.279882915 C 1.446400872 -2.940191592 -0.669489184 C -1.148675636 0.373855283 -0.371174008 C 1.611323146 0.699052667 0.205978423

	C	0.720139098	1.806207391	0.302738711
	C	-0.646041734	1.644331791	0.018331818
	C	1.224036143	3.092650612	0.694059696
	C	2.550211125	3.261191198	0.972139426
	C	3.547415838	2.164806303	0.895172781
	C	2.978148722	0.839361356	0.486797121
	C	3.817517679	-0.265472221	0.384171270
	C	3.337347441	-1.501307452	0.011108375
	H	4.007096575	-2.345834744	-0.062568400
	H	4.869762515	-0.144806523	0.603163710
	H	-0.276740519	-4.050412151	-1.243496155
	H	2.123264537	-3.779846585	-0.739021570
	H	2.919557882	4.233698577	1.265106064
	H	4.345226470	2.448568760	0.192547703
	C	-2.145350272	-2.132311339	-1.143795338
	C	-2.992522562	-1.067060778	-1.042401208
	C	-2.521595042	0.209927576	-0.656919958
	H	-2.510427970	-3.106293296	-1.435162395
	H	-4.044907935	-1.183000766	-1.259728566
	C	-3.380791140	1.326350981	-0.548305147
	C	-2.899523330	2.550789098	-0.174600302
	C	-1.537899520	2.743678241	0.115453374
	H	-4.430448696	1.194464671	-0.768801843
	H	-3.568529731	3.396606450	-0.097019058
	C	0.292880122	4.178881317	0.780231436
	H	0.675260129	5.145866519	1.074610486
	C	-1.021160600	4.008985254	0.504310717
	H	-1.708817825	4.840365007	0.574759883
	H	4.048867611	2.060491978	1.868977418
	O	-2.249806110	-5.475806027	-0.404099182
	H	-2.625498914	-6.307188722	-0.111851979
	H	-2.113204015	-4.941774249	0.395369227
	O	-1.726980270	-3.667831079	1.695032894
	H	-2.216516294	-2.904333917	1.375567441
	H	-0.797653905	-3.485275252	1.530076080
	H	3.863665019	0.980606644	-0.367154862
	H	3.670720877	0.976721875	-2.103729417
	O	1.592367408	1.106422024	2.406018682
	H	1.092534036	1.513575105	1.694305295
	H	2.529301027	1.166762345	2.155760921
	H	3.706061078	-0.492023382	1.828313437
	H	4.828722498	0.332914473	2.495371641
	O	4.226806569	0.332244835	1.749250812
	H	1.814170637	-1.962150559	1.484775707
	H	1.803428151	-0.764089549	2.467920173
	O	2.302138362	-1.558815079	2.206416056
	C	-1.401891117	-3.610868726	-0.175343630
	C	-2.026758581	-2.350327350	-0.005262355
	C	-1.261354568	-1.177012573	-0.190274477
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	C	-0.089238303	-3.705461071	-0.511922395
	C	-1.865548484	0.092098461	-0.030877078
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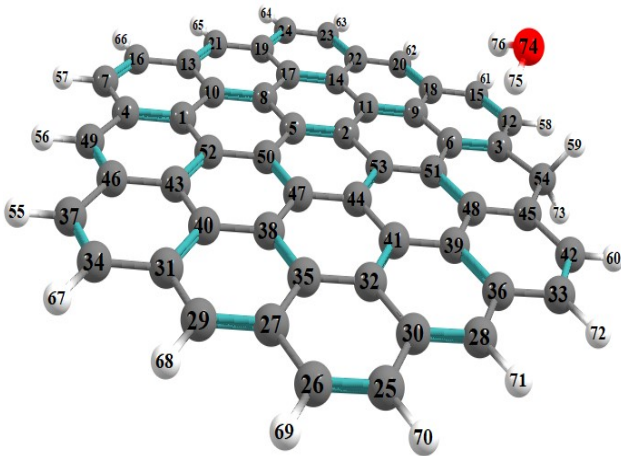
C1-CorH⁺-W₃
[-73.31607843]

	C	1.039565276	2.375246097	-0.755923795
	C	2.368303800	2.294821821	-1.064147809
	C	3.104343115	1.012951559	-1.164398949
	C	2.244635583	-0.205561199	-1.034383662
	C	2.809566675	-1.466095826	-1.202962515
	C	2.064691552	-2.614308150	-1.045409865
	H	2.522462324	-3.583256062	-1.179936653
	H	3.857448013	-1.538426651	-1.456031295
	H	-1.997027269	-4.501722383	-0.032575568
	H	0.379026110	-4.670714591	-0.641583208
	H	2.938395833	3.199042979	-1.220396642
	C	-3.389011070	-2.229204584	0.340836487
	C	-3.971816448	-1.005456687	0.493889535
	C	-3.231670867	0.184980766	0.311225913
	H	-3.967109930	-3.131550540	0.482519609
	H	-5.016949783	-0.926391354	0.757740919
	C	-3.816130012	1.463053289	0.456872240
	C	-3.079958991	2.599617350	0.265998972
	C	-1.718237073	2.538625114	-0.075964551
	H	-4.862129435	1.526563011	0.720352791
	H	-3.540936349	3.571218479	0.376584262
	C	0.370759765	3.635536314	-0.616657382
	H	0.951854086	4.532074385	-0.777474555
	C	-0.940223329	3.708961867	-0.287735208
	H	-1.425484794	4.668952038	-0.181177382
	H	4.047267874	0.966530786	-0.777412985
	H	3.615097555	0.974024271	-2.470904142
	O	2.555615621	-1.406143202	2.005855426
	H	2.352149348	-1.888260070	1.200950463
	H	1.700493141	-1.163726473	2.403766668
	H	2.888381799	0.375784022	1.852859735
	H	3.198388775	1.616303292	2.719348757
	O	2.719776668	1.334108325	1.937984280
	H	-0.426477848	0.210878192	2.109884851
	H	0.974720207	0.786193593	2.431115034
	O	0.331666985	0.101835407	2.688251242
	C	-1.245091266	-3.618762122	-0.143743731
	C	-1.857194476	-2.357521030	0.061247770
	C	-1.102736118	-1.185627051	-0.171192168
	C	0.244924381	-1.279600068	-0.598761054
	C	0.828967372	-2.553344596	-0.795342069
	C	0.045723519	-3.714547438	-0.555618881
	C	-1.693311010	0.085269255	0.029766971
	C	1.007508781	-0.103186561	-0.823358532
	C	0.405669032	1.171451640	-0.622279743
	C	-0.931593732	1.264615460	-0.200385645
	C	1.170497477	2.364092589	-0.850744591
	C	2.471431553	2.283927902	-1.254687913
	C	3.185170341	1.001264438	-1.459372158
	C	2.343055442	-0.216898207	-1.237245034
	C	2.897491614	-1.478613520	-1.429515420
	C	2.165043794	-2.626991310	-1.216160099
	H	2.614886752	-3.596662250	-1.372263847
	H	3.926634497	-1.554823997	-1.751446333
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	H	0.505379667	-4.680449969	-0.709364711



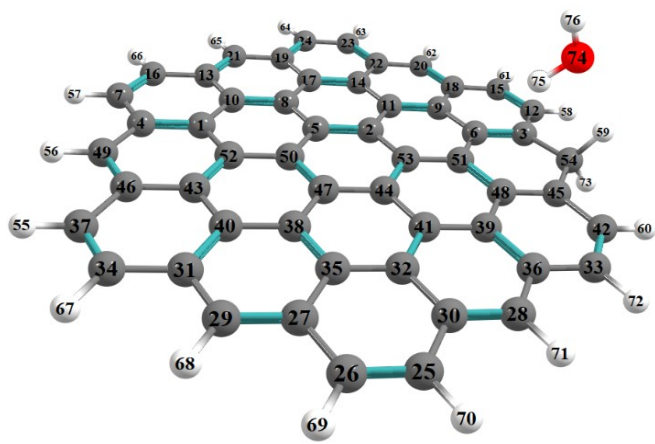
C2-CorH⁺-W₃
[-73.31470982]

	H	3.039432742	3.187708854	-1.420740443
	C	-3.195096301	-2.234274422	0.491427572
	C	-3.764588911	-1.010154178	0.685149405
	C	-3.034445800	0.179655614	0.461911086
	H	-3.765111324	-3.135661528	0.666857141
	H	-4.790383265	-0.929514241	1.015394257
	C	-3.601611565	1.458378438	0.659099758
	C	-2.871723399	2.593892784	0.437092036
	C	-1.535339466	2.532214975	0.007126662
	H	-4.628120279	1.523188853	0.989648462
	H	-3.319393173	3.565627690	0.591455406
	C	0.524232369	3.625070803	-0.638355779
	H	1.102600724	4.520920752	-0.811912811
	C	-0.762733535	3.701829133	-0.227331009
	H	-1.232742755	4.662089667	-0.067071952
<p style="text-align: center;">C3-CorH⁺-W₃ [-73.31455321]</p>	H	4.128816043	0.957068101	-1.080075058
	H	3.571547439	1.032747542	-2.734268106
	O	2.413790365	1.301065067	1.951732715
	H	3.059196256	1.438190438	2.647530785
	H	2.232755024	0.341723174	1.942804786
	H	0.862611364	-1.643545090	1.642338056
	H	0.642658553	-0.611820984	2.777327660
	O	1.310115410	-1.181861188	2.355300418
	H	-0.865149987	1.390597609	2.446813415
	H	0.668856007	1.455095356	2.641513097
	O	-0.152809092	1.086397050	3.012917412
	C	-1.074135716	-3.706274227	-0.275633642
	C	-1.681172962	-2.461393028	0.025579177
	C	-0.955403632	-1.271916782	-0.212965413
	C	0.360676294	-1.333963450	-0.738312003
	C	0.941491863	-2.591770925	-1.025563357
	C	0.185044260	-3.770041781	-0.781686465
	C	-1.540046896	-0.017766358	0.082197578
	C	1.096170235	-0.140879279	-0.963487505
	C	0.498285708	1.117193218	-0.669237614
	C	-0.806975279	1.177383428	-0.154244184
	C	1.236579025	2.326803096	-0.895382647
	C	2.509500705	2.277851309	-1.384639002
	C	3.217326903	1.012296857	-1.693328125
	C	2.402575090	-0.223891997	-1.465489492
	C	2.953453242	-1.470506585	-1.744700024
	C	2.245878784	-2.633382282	-1.535236381
	H	2.693018919	-3.591037158	-1.758099657
	H	3.961381635	-1.521777388	-2.132988008
	H	-1.639161445	-4.609262475	-0.092903873
	H	0.639349774	-4.723781688	-1.008647307
	H	3.058771419	3.193907059	-1.547559316
	C	-2.984473219	-2.371340844	0.557835791
	C	-3.547685603	-1.162466369	0.843913789
	C	-2.845896855	0.043099179	0.615725104
	H	-3.532046525	-3.285699857	0.737388218
	H	-4.546311857	-1.106876915	1.252989556
	C	-3.409406880	1.306267526	0.905601206
	C	-2.708696834	2.458910068	0.675416117
	C	-1.405871331	2.429931325	0.146792339
H	-4.409350060	1.345933193	1.312320119	

	H	-3.153118511	3.418516379	0.899525835
	C	0.596119946	3.570995349	-0.588234993
	H	1.154280278	4.479595296	-0.761285722
	C	-0.661267959	3.617118356	-0.090311431
	H	-1.127641679	4.564521089	0.141296646
 <p style="text-align: center;">C1-DbcH⁺-W₁ [-130.73921443]</p>	C	-3.637483599	1.274531572	0.037647247
	C	0.601251876	1.215480052	-0.091107774
	C	4.836178271	1.190401897	-0.212769302
	C	-5.056006205	1.289720833	0.081306614
	C	-0.807115449	1.233631615	-0.048596796
	C	3.436157562	1.185363641	-0.175710777
	C	-5.719739407	2.550448524	0.100226429
	C	-1.502126674	2.470655721	-0.031101535
	C	2.734062958	2.418693930	-0.166058914
	C	-2.913248835	2.489269344	0.012761198
	C	1.322312054	2.435112398	-0.120213636
	C	5.521461766	2.404524174	-0.250627853
	C	-3.602970334	3.729771659	0.030696787
	C	0.628854040	3.666274470	-0.104734934
	C	4.854973031	3.604804002	-0.245311930
	C	-5.025978883	3.714401143	0.075840728
	C	-0.781967049	3.684054089	-0.058886379
	C	3.448811038	3.645403778	-0.198861420
	C	-1.484340666	4.920988484	-0.041848904
	C	2.738760640	4.858118066	-0.183072651
	C	-2.872780376	4.918228451	0.003065107
	C	1.356547050	4.889974159	-0.136005818
	C	0.623347579	6.116813564	-0.117748427
	C	-0.727533219	6.131139063	-0.072483532
	C	0.442773035	-6.136066297	-0.112977138
	C	-0.907957949	-6.110551215	-0.068137043
	C	-1.628764476	-4.878594032	-0.038340160
	C	2.594413870	-4.940290424	-0.177820558
	C	-3.016526087	-4.834885273	0.006356654
	C	1.211834042	-4.931383995	-0.131557124
	C	-3.711379290	-3.625406122	0.033155104
	C	0.520525450	-3.686744738	-0.101406782
	C	4.746663904	-3.749968944	-0.239407058
	C	-5.133320200	-3.568070913	0.078144357
	C	-0.890223091	-3.662910908	-0.056003589
	C	3.339903456	-3.749047858	-0.193917710
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	C	-1.574327249	-2.428803794	-0.029195529
	C	2.661629670	-2.501818521	-0.162585565
	C	-2.985390412	-2.405787410	0.014480763
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C	5.448227832	-2.569899709	-0.245657966	
C	-3.673518287	-1.170216596	0.038485198	
C	0.565141820	-1.236220599	-0.089784367	
C	4.798994820	-1.336072769	-0.209812631	
C	-5.091872198	-1.143560965	0.082073494	
C	-0.843152960	-1.212816747	-0.047529443	
C	3.399765557	-1.289752289	-0.173302050	
C	-5.752775626	0.083095214	0.103313783	
C	-1.533040256	0.020849276	-0.025147398	
C	2.703865845	-0.041655810	-0.148745150	

	C	-2.948229495	0.041725448	0.017417197
	C	1.299946398	-0.020936792	-0.109242193
	C	5.618320041	-0.084584931	-0.183827783
	H	-6.872558548	-2.357009054	0.135622923
	H	-6.833544272	0.099038094	0.136714452
	H	-6.800145064	2.555165897	0.134226085
	H	6.601900486	2.390367855	-0.281138583
	H	6.229145820	-0.092291065	0.729487373
	H	6.528648536	-2.587613662	-0.275511097
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	H	3.293652641	5.785584906	-0.208048647
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	H	-5.679145080	-4.501047630	0.092865653
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	H	3.121720635	-5.883744049	-0.201839939
	H	5.267851384	-4.695564883	-0.266791760
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	O	4.461230252	-0.002126117	2.861808639
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	C	-5.103270411	1.301026897	0.032301995
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	C	-3.662817213	3.748356678	-0.027491434
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	C	4.798178093	3.666654987	-0.215929154
	C	-5.085988504	3.725675954	0.006765916
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	C	3.391307449	3.699748095	-0.186981532
	C	-1.549939683	4.950281023	-0.091277046
	C	2.674806768	4.908746995	-0.187337503
C	-2.938672366	4.940468049	-0.058517680	
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C	0.552063349	6.156699838	-0.154938828	
C	-0.799286278	6.164246565	-0.123794638	
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C	-0.915208320	-6.077861599	-0.024870712	
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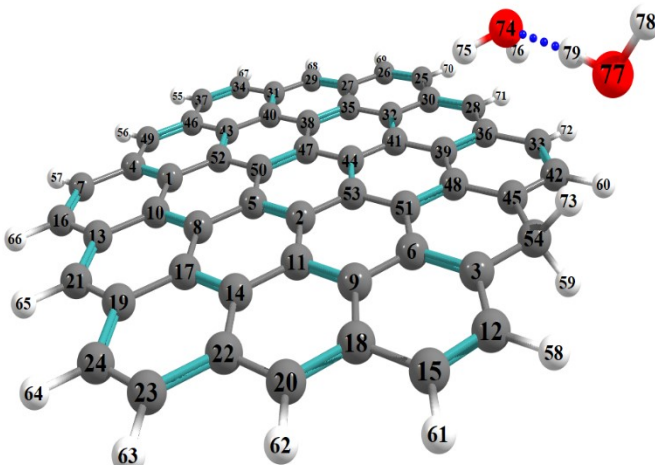
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C	-5.820341474	-2.376453683	0.079431775
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C	2.635552092	-2.450321622	-0.130315027
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C	-3.707478682	-1.151724545	0.020151956
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H	6.551725966	2.461049788	-0.225767197
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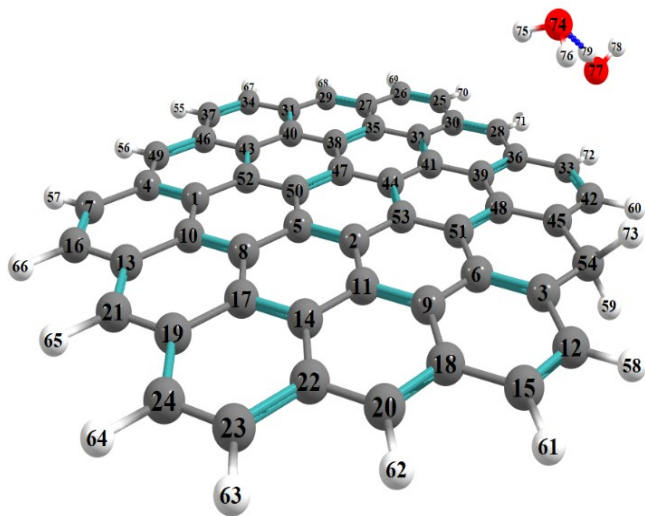
C3-DbcH⁺-W₁

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C	-5.064003526	1.290057084	0.073831372
C	-0.814711153	1.234676809	-0.046659137
C	3.429116321	1.187307755	-0.164132517
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C	-2.921280073	2.489984847	0.008736887
C	1.314773666	2.436397717	-0.120239839

C	5.513631509	2.405622962	-0.250771106
C	-3.611254183	3.730399548	0.023529234
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C	4.846803978	3.605562378	-0.258049302
C	-5.034284293	3.714747099	0.066355867
C	-0.790047602	3.685043042	-0.064012235
C	3.440787807	3.646450436	-0.209139855
C	-1.492795671	4.921856140	-0.050670037
C	2.730333590	4.859008962	-0.199478244
C	-2.881214236	4.918924400	-0.005796197
C	1.348211755	4.891009324	-0.148769536
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C	-0.736177962	6.132010404	-0.085848578
C	0.436142278	-6.134444999	-0.125981374
C	-0.914489597	-6.109369621	-0.077510237
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C	-3.023258862	-4.834219624	0.001563845
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C	3.393045576	-1.288193659	-0.162509386
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C	1.292850042	-0.019547042	-0.100388379
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H	-6.879992100	-2.357018935	0.125414360
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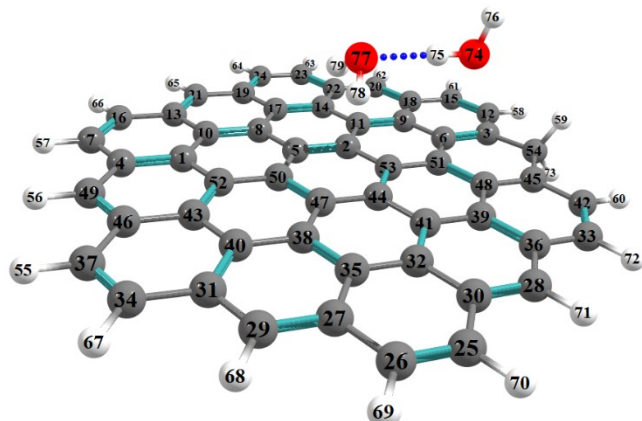
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	C	-5.389414116	-0.034797004	-0.228326209
	C	-1.280927402	1.020903866	0.055125507
	C	2.821013762	2.082761374	0.325432766
	C	-6.357158886	1.008877581	-0.294216576
	C	-2.272964892	2.033468718	-0.008961787
	C	1.822733683	3.089329284	0.273684208
	C	-3.637367097	1.682867303	-0.103972994
	C	0.458123515	2.736866255	0.180413080
	C	4.512849125	3.803224467	0.448059435
	C	-4.625072866	2.700235045	-0.168444031
	C	-0.531204207	3.744005204	0.120717022
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	C	-5.991912276	2.313714878	-0.265258180
	C	-1.895148202	3.392863275	0.024278307
	C	2.191443576	4.460021923	0.311627131
	C	-2.894355831	4.403483905	-0.038484856
	C	1.191095626	5.445212642	0.253820932
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	H	6.111695051	-3.113205336	0.656163824
	H	5.851998708	1.540199985	-0.494753579
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	H	4.833160520	-1.813790223	-1.890418077
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	C	-2.378248464	2.157288163	0.067653475
	C	1.674001394	3.377702495	0.310786597
	C	-3.728323935	1.751891524	-0.013685598
	C	0.323906875	2.970344638	0.230016313
	C	4.333074359	4.199695085	0.470783662
	C	-4.758988350	2.727787982	-0.030327437
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	C	3.337424293	5.144961878	0.452476022
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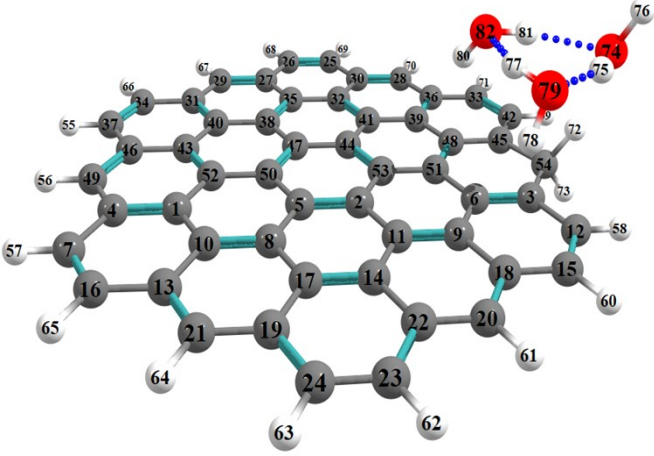
C2-DbcH⁺-W₂
[-135.82039139]

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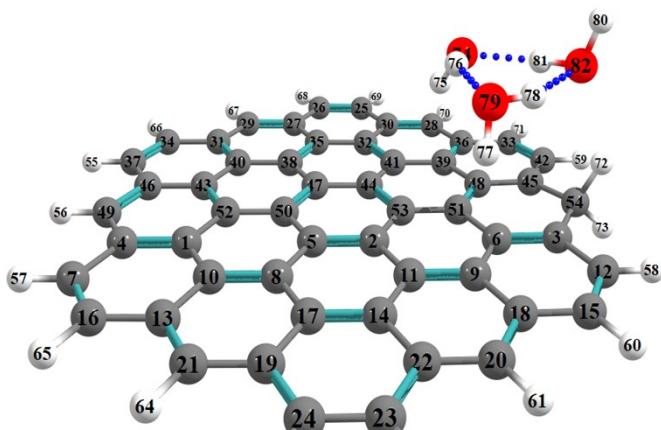


C3-DbcH⁺-W₂
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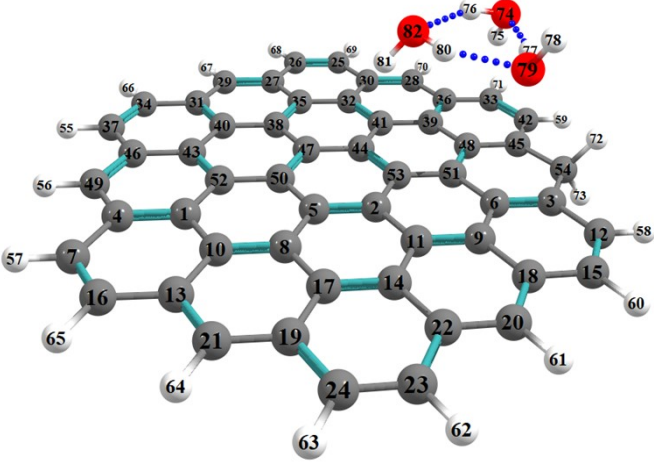
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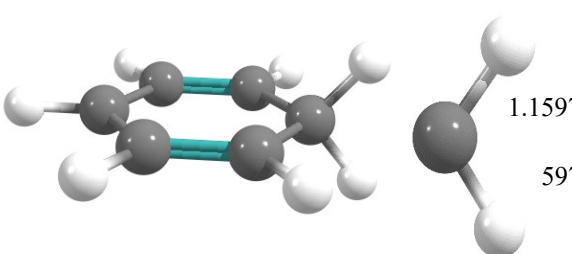
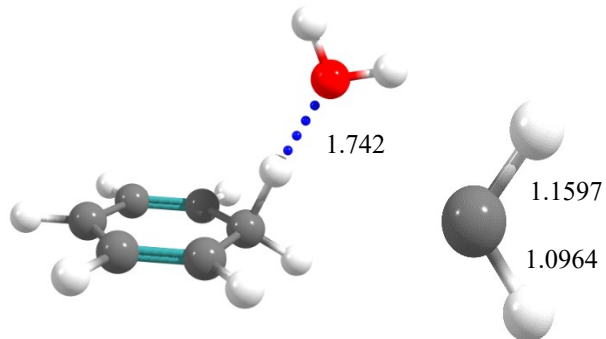
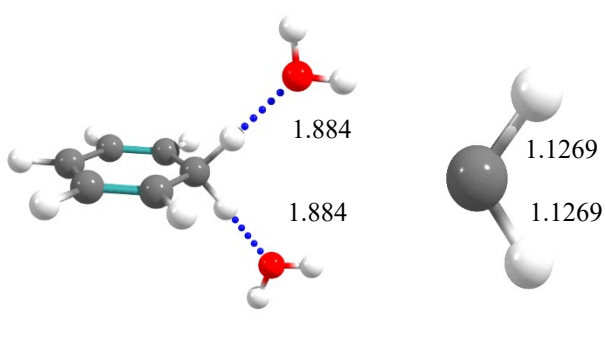


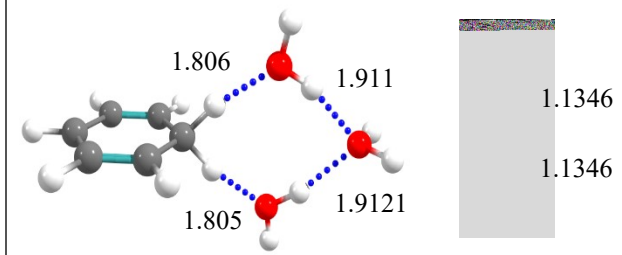
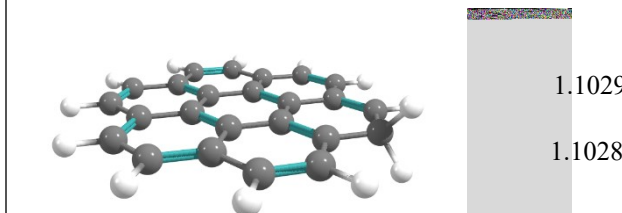
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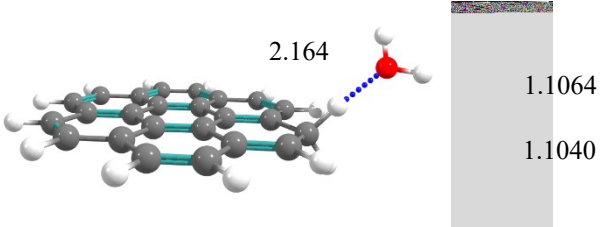
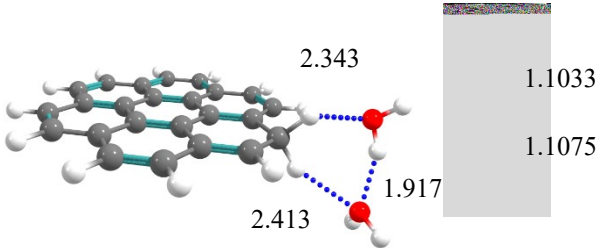
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	H	4.601775214	-5.075929071	0.301095028
	H	2.746950623	-6.664566709	0.070843063
	H	0.349049288	-7.103026648	-0.217224610
	H	-1.945542763	-6.270460538	-0.478772998
	H	-4.244140569	-5.440062931	-0.721840906
	H	-5.869134529	-1.016612724	0.346406386
	H	-6.078880434	-1.096072209	-1.394953419
	O	-2.594851530	-1.860109498	2.709811077
	H	-2.043509904	-2.130473837	1.972499514
	H	-2.483970235	-0.897864393	2.803597913
	H	-3.109194679	1.414449786	1.845700074
	H	-4.072878093	0.434898247	2.560548631
	O	-3.196211068	0.852078630	2.618339812
	H	-5.584456495	-1.227123254	3.457501168
	H	-4.385451782	-1.590638286	2.558550872
	O	-5.225450327	-1.092253225	2.578744953
 <p style="text-align: center;">C3-DbcH⁺-W₃ [-140.90819894]</p>	C	3.533445438	1.892407188	0.125462988
	C	-0.627173428	1.207179727	-0.335487364
	C	-4.786742716	0.555907093	-0.789224955
	C	4.926413835	2.117269424	0.277673794
	C	0.755162193	1.433182472	-0.180630776
	C	-3.410219615	0.757304899	-0.643527779
	C	5.396952181	3.461935004	0.301002537
	C	1.260000523	2.759057071	-0.151042711
	C	-2.898924448	2.079557575	-0.613357721
	C	2.645166279	2.986168347	0.001211134
	C	-1.513411591	2.305789515	-0.459327947
	C	-5.637463452	1.654390283	-0.908407673
	C	3.144097061	4.314712295	0.029111463
	C	-1.009120801	3.625398644	-0.428235734
	C	-5.156248130	2.939778391	-0.884855817
	C	4.545971681	4.510095426	0.182688489
	C	0.375813599	3.852025026	-0.274779588
	C	-3.778972098	3.187074799	-0.735474819
	C	0.887705147	5.178998673	-0.244341116
	C	-3.256518481	4.491318876	-0.702917186
	C	2.253686706	5.381755549	-0.093891892
	C	-1.901758445	4.727922628	-0.553128038
	C	-1.358326083	6.049472783	-0.518337000
	C	-0.031796192	6.263739714	-0.371419570
	C	0.590275882	-6.038980373	-0.023275011
	C	1.914906947	-5.813456130	0.123586508
	C	2.446121048	-4.488783071	0.151167714
	C	-1.697461673	-5.175493956	-0.310171865
	C	3.804621679	-4.240007135	0.300746619
	C	-0.339201772	-4.961894143	-0.158770553
C	4.313690094	-2.941486404	0.326692260	
C	0.161105615	-3.629008920	-0.135471305	
C	-3.986136860	-4.317464711	-0.596403160	
C	5.703962768	-2.674353744	0.478224529	
C	1.544767059	-3.396265238	0.019842175	
C	-2.601662648	-4.107795818	-0.443466388	
C	6.181428724	-1.406270785	0.501449688	
C	2.039719040	-2.074838043	0.044835636	

C	-2.115387084	-2.772827807	-0.421389016
C	3.423915893	-1.843008368	0.198432139
C	-0.730459375	-2.540797213	-0.267997456
C	-4.846149786	-3.252455922	-0.718077409
C	3.922123776	-0.519540614	0.224035013
C	-0.236321823	-1.211777721	-0.241185640
C	-4.385067520	-1.936005337	-0.693718836
C	5.313310834	-0.283281621	0.376293781
C	1.145652018	-0.980393824	-0.084490608
C	-3.015873385	-1.682774321	-0.547919497
C	5.786170534	1.027228548	0.399292208
C	1.645192754	0.341712332	-0.055298590
C	-2.513888014	-0.346502140	-0.520317394
C	3.033885744	0.571491239	0.098201293
C	-1.136157068	-0.118385338	-0.368432025
C	-5.373108857	-0.819745500	-0.809183499
H	7.239819618	-1.219526098	0.617089512
H	6.846901083	1.202904409	0.515014314
H	6.458998266	3.626492981	0.416899440
H	-6.699268794	1.481277811	-1.018862971
H	-5.906018857	-3.431169677	-0.833382843
H	-5.831246050	3.778237449	-0.977433903
H	-3.936413729	5.326789731	-0.797214882
H	-2.044051315	6.879644427	-0.613398742
H	0.364946432	7.269009179	-0.346535737
H	2.638351611	6.392343053	-0.071479865
H	4.918288909	5.524777512	0.202793183
H	6.375308298	-3.516035875	0.575256585
H	4.486239406	-5.073817349	0.399775020
H	2.606343384	-6.638143702	0.224768857
H	0.200511844	-7.046916146	-0.041865333
H	-2.080644412	-6.186138580	-0.328007141
H	-4.362402909	-5.329683794	-0.618200706
H	-6.093020714	-0.903762035	0.015253559
H	-5.956964308	-0.949310183	-1.729789605
O	-3.938617026	-2.776265821	2.561253881
H	-3.876196266	-3.326040677	1.776816127
H	-3.025667130	-2.543175143	2.805659433
H	-4.239280605	-0.986598390	2.349441103
H	-4.400649508	0.328363379	3.145610751
O	-4.019829271	-0.035138413	2.344569657
H	-2.250581536	-0.623540149	2.609404724
H	-0.915002654	-1.229331813	2.112390889
O	-1.588338453	-1.314267153	2.790612138

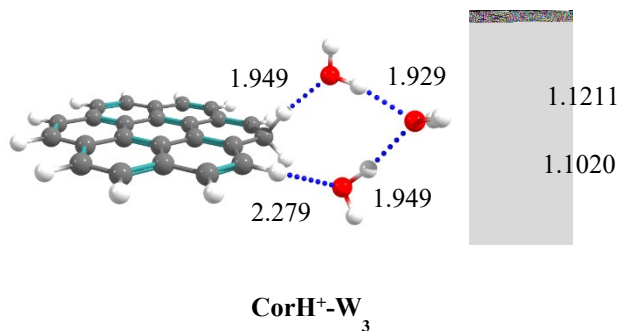
Table S3: PBE0+D3/6-311++G** optimized equilibrium structures of BzH⁺, CorH⁺ and DbcH⁺ and of the most stable forms of the BzH⁺-W_n, CorH⁺-W_n and DbcH⁺-W_n (n = 1 – 3) complexes. Close view of the sp³ C-H bond distances (before and after hydration) and the intermonomer distances (in Å) are given.

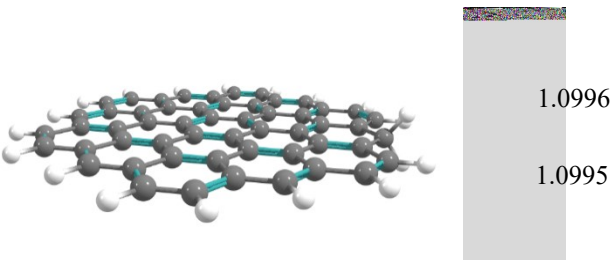
	<p>C 1.386622000 -0.000018000 0.000119000 C 0.627945000 -1.248054000 -0.000148000 C 0.627977000 1.248038000 -0.000148000 H 1.178337000 -2.184576000 -0.000223000 H 1.178395000 2.184546000 -0.000223000 C -0.738165000 -1.236247000 -0.000080000 C -0.738133000 1.236267000 -0.000080000 H -1.306871000 -2.158859000 -0.000223000 H -1.306815000 2.158894000 -0.000223000 C -1.408235000 0.000018000 0.000188000 H -2.495570000 0.000033000 0.000363000 H 2.101559000 -0.000027000 0.847298000 H 2.102891000 -0.000027000 -0.845881000</p>
 <p style="text-align: center;">BzH⁺-W₁</p>	<p>C 0.448369000 0.000991000 0.925029000 C -0.193672000 -1.238865000 0.549404000 C -0.195099000 1.239793000 0.548392000 H 0.255725000 -2.173969000 0.869609000 H 0.253161000 2.175684000 0.867895000 C -1.309492000 -1.231081000 -0.247628000 C -1.310905000 1.230610000 -0.248627000 H -1.776535000 -2.156925000 -0.562789000 H -1.779033000 2.155105000 -0.564526000 C -1.859334000 -0.000990000 -0.636992000 H -2.747399000 -0.001757000 -1.263490000 H 0.930908000 0.001664000 1.909550000 H 1.403499000 0.001111000 0.267263000 O 2.898345000 -0.000189000 -0.628516000 H 3.011761000 0.000266000 -1.582909000 H 3.781946000 0.000881000 -0.249940000</p>
 <p style="text-align: center;">BzH⁺-W₂</p>	<p>C 0.284888000 -0.000067000 -0.000026000 C -0.460796000 -0.000596000 -1.236370000 C -0.460751000 0.000438000 1.236346000 H 0.091908000 -0.000988000 -2.171036000 H 0.091987000 0.000848000 2.170992000 C -1.831994000 -0.000619000 -1.230953000 C -1.831950000 0.000415000 1.230980000 H -2.397158000 -0.001020000 -2.155739000 H -2.397080000 0.000797000 2.155787000 C -2.504346000 -0.000114000 0.000026000 H -3.591218000 -0.000134000 0.000046000 H 1.046553000 -0.830676000 0.000284000 H 1.046572000 0.830522000 -0.000371000 O 2.273508000 -2.260076000 0.000436000 H 3.233166000 -2.221842000 -0.000683000 H 2.050888000 -3.194517000 0.001570000 H 2.049912000 3.194780000 -0.001511000 H 3.232610000 2.222616000 0.000673000 O 2.272936000 2.260435000 -0.000439000</p>
	<p>C 0.511896000 -0.000067000 0.000582000 C 1.248396000 -0.018589000 -1.233104000 C 1.249369000 0.018500000 1.233689000</p>

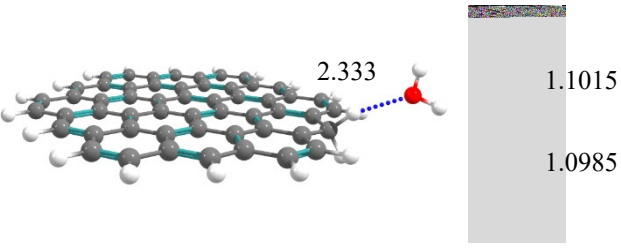
 <p style="text-align: center;">BzH⁺-W₃</p>	<table border="1"> <tbody> <tr><td>H</td><td>0.693697000</td><td>-0.032763000</td><td>-2.166280000</td></tr> <tr><td>H</td><td>0.695444000</td><td>0.032628000</td><td>2.167326000</td></tr> <tr><td>C</td><td>2.621370000</td><td>-0.018491000</td><td>-1.229261000</td></tr> <tr><td>C</td><td>2.622334000</td><td>0.018486000</td><td>1.228751000</td></tr> <tr><td>H</td><td>3.184914000</td><td>-0.032423000</td><td>-2.154903000</td></tr> <tr><td>H</td><td>3.186613000</td><td>0.032445000</td><td>2.153945000</td></tr> <tr><td>C</td><td>3.295115000</td><td>0.000020000</td><td>-0.000524000</td></tr> <tr><td>H</td><td>4.381782000</td><td>0.000053000</td><td>-0.000949000</td></tr> <tr><td>H</td><td>-0.297298000</td><td>0.795232000</td><td>-0.010863000</td></tr> <tr><td>H</td><td>-0.297257000</td><td>-0.795410000</td><td>0.012447000</td></tr> <tr><td>O</td><td>-1.833068000</td><td>1.745093000</td><td>-0.021237000</td></tr> <tr><td>H</td><td>-2.693404000</td><td>1.299295000</td><td>-0.016427000</td></tr> <tr><td>H</td><td>-1.999115000</td><td>2.689600000</td><td>-0.036330000</td></tr> <tr><td>H</td><td>-2.000067000</td><td>-2.689357000</td><td>0.037847000</td></tr> <tr><td>H</td><td>-2.692935000</td><td>-1.298345000</td><td>0.017326000</td></tr> <tr><td>O</td><td>-1.833057000</td><td>-1.745060000</td><td>0.020545000</td></tr> <tr><td>H</td><td>-4.678180000</td><td>0.010634000</td><td>0.766581000</td></tr> <tr><td>H</td><td>-4.676968000</td><td>-0.011003000</td><td>-0.766995000</td></tr> <tr><td>O</td><td>-4.096138000</td><td>-0.000001000</td><td>0.000252000</td></tr> </tbody> </table>	H	0.693697000	-0.032763000	-2.166280000	H	0.695444000	0.032628000	2.167326000	C	2.621370000	-0.018491000	-1.229261000	C	2.622334000	0.018486000	1.228751000	H	3.184914000	-0.032423000	-2.154903000	H	3.186613000	0.032445000	2.153945000	C	3.295115000	0.000020000	-0.000524000	H	4.381782000	0.000053000	-0.000949000	H	-0.297298000	0.795232000	-0.010863000	H	-0.297257000	-0.795410000	0.012447000	O	-1.833068000	1.745093000	-0.021237000	H	-2.693404000	1.299295000	-0.016427000	H	-1.999115000	2.689600000	-0.036330000	H	-2.000067000	-2.689357000	0.037847000	H	-2.692935000	-1.298345000	0.017326000	O	-1.833057000	-1.745060000	0.020545000	H	-4.678180000	0.010634000	0.766581000	H	-4.676968000	-0.011003000	-0.766995000	O	-4.096138000	-0.000001000	0.000252000																																																																								
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H	3.532910000	3.560664000	0.233738000																																																																																																																																																														
C	-0.488658000	3.661114000	-0.131208000																																																																																																																																																														
H	-1.086041000	4.565616000	-0.179244000																																																																																																																																																														
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H	-3.816867000	1.037232000	-1.364923000																																																																																																																																																														
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H	-6.635750000	0.099052000	0.954433000																																																																																																																																																														
H	-5.716081000	-0.473389000	2.024809000																																																																																																																																																														
 <p style="text-align: center;">CorH⁺-W₂</p>	<table border="1"> <tbody> <tr><td>C</td><td>-1.905908000</td><td>-3.559702000</td><td>0.086835000</td></tr> <tr><td>C</td><td>-2.474823000</td><td>-2.259180000</td><td>0.112681000</td></tr> <tr><td>C</td><td>-1.615676000</td><td>-1.134873000</td><td>0.040702000</td></tr> <tr><td>C</td><td>-0.215698000</td><td>-1.316959000</td><td>-0.069605000</td></tr> <tr><td>C</td><td>0.325927000</td><td>-2.621711000</td><td>-0.093052000</td></tr> <tr><td>C</td><td>-0.555846000</td><td>-3.735191000</td><td>-0.015266000</td></tr> <tr><td>C</td><td>-2.157822000</td><td>0.170992000</td><td>0.045706000</td></tr> <tr><td>C</td><td>0.649031000</td><td>-0.192107000</td><td>-0.133067000</td></tr> <tr><td>C</td><td>0.097959000</td><td>1.120182000</td><td>-0.132019000</td></tr> <tr><td>C</td><td>-1.296860000</td><td>1.301121000</td><td>-0.028981000</td></tr> <tr><td>C</td><td>0.952031000</td><td>2.282309000</td><td>-0.219333000</td></tr> <tr><td>C</td><td>2.304546000</td><td>2.106908000</td><td>-0.305053000</td></tr> <tr><td>C</td><td>2.941267000</td><td>0.793559000</td><td>-0.289902000</td></tr> <tr><td>C</td><td>2.042142000</td><td>-0.384199000</td><td>-0.235889000</td></tr> <tr><td>C</td><td>2.562776000</td><td>-1.680843000</td><td>-0.279345000</td></tr> <tr><td>C</td><td>1.721559000</td><td>-2.772422000</td><td>-0.207889000</td></tr> </tbody> </table>	C	-1.905908000	-3.559702000	0.086835000	C	-2.474823000	-2.259180000	0.112681000	C	-1.615676000	-1.134873000	0.040702000	C	-0.215698000	-1.316959000	-0.069605000	C	0.325927000	-2.621711000	-0.093052000	C	-0.555846000	-3.735191000	-0.015266000	C	-2.157822000	0.170992000	0.045706000	C	0.649031000	-0.192107000	-0.133067000	C	0.097959000	1.120182000	-0.132019000	C	-1.296860000	1.301121000	-0.028981000	C	0.952031000	2.282309000	-0.219333000	C	2.304546000	2.106908000	-0.305053000	C	2.941267000	0.793559000	-0.289902000	C	2.042142000	-0.384199000	-0.235889000	C	2.562776000	-1.680843000	-0.279345000	C	1.721559000	-2.772422000	-0.207889000																																																																																																
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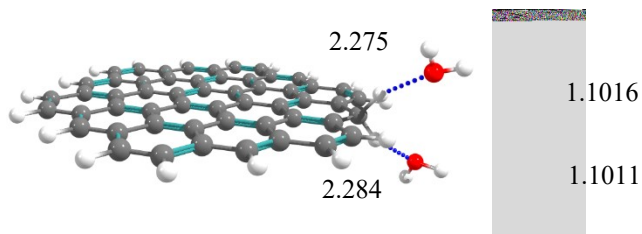
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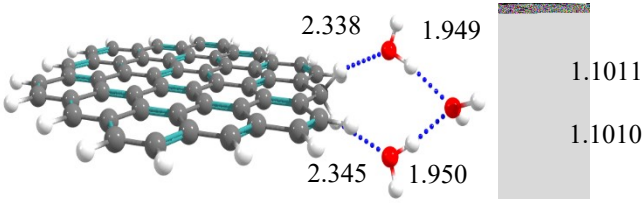
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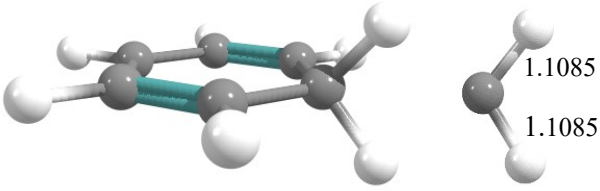
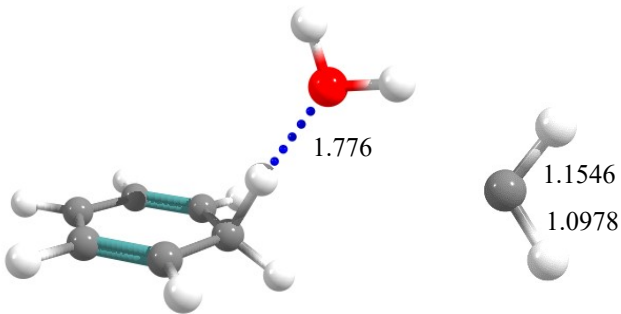
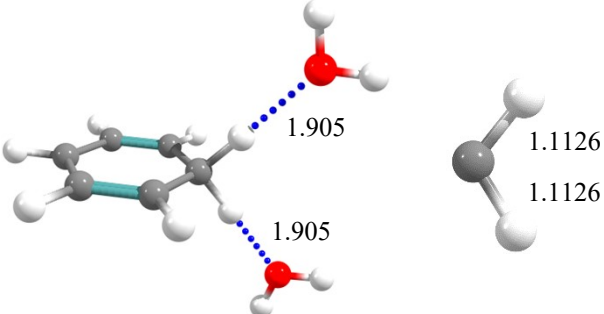
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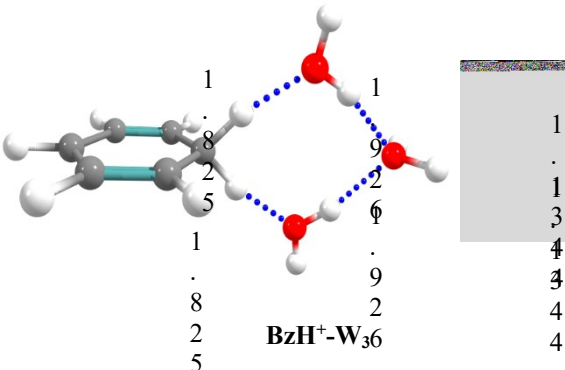
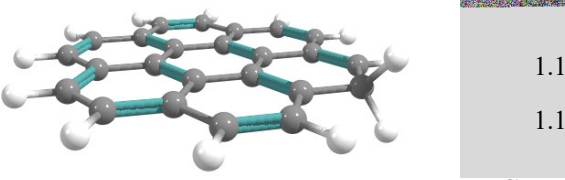
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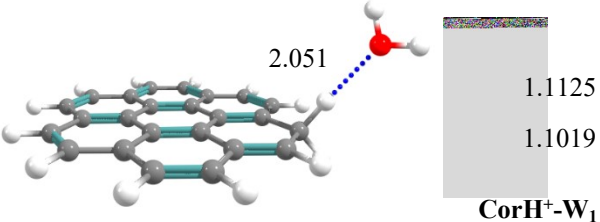
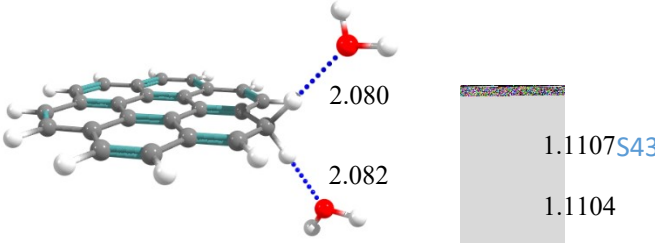
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 <p>DbcH⁺-W₃</p>				

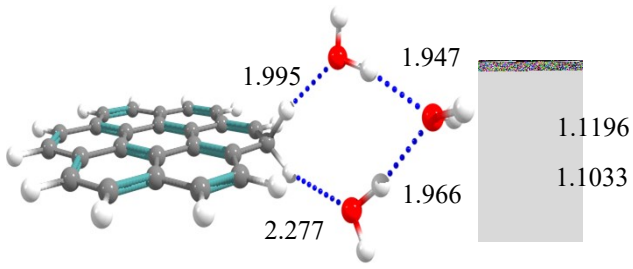
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Table S4: PBE0/6-311++G** optimized equilibrium structures of BzH⁺, CorH⁺ and DbcH⁺ and of the most stable forms of the BzH⁺-W_n, CorH⁺-W_n and DbcH⁺-W_n (n = 1 – 3) complexes. Close view of the sp³ C-H bond distances (before and after hydration) and the intermonomer distances (in Å) are given.

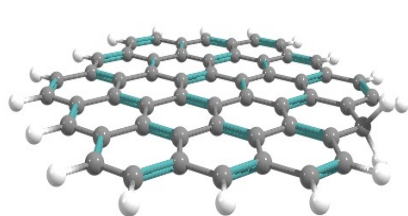
 <p style="text-align: center;">BzH⁺</p>	<table border="1"> <tbody> <tr><td>C</td><td>1.386622000</td><td>0.000000000</td><td>-0.000119000</td></tr> <tr><td>C</td><td>0.627961000</td><td>1.248046000</td><td>0.000148000</td></tr> <tr><td>C</td><td>0.627961000</td><td>-1.248046000</td><td>0.000148000</td></tr> <tr><td>H</td><td>1.178365000</td><td>2.184561000</td><td>0.000223000</td></tr> <tr><td>H</td><td>1.178366000</td><td>-2.184561000</td><td>0.000223000</td></tr> <tr><td>C</td><td>-0.738149000</td><td>1.236257000</td><td>0.000080000</td></tr> <tr><td>C</td><td>-0.738149000</td><td>-1.236257000</td><td>0.000080000</td></tr> <tr><td>H</td><td>-1.306843000</td><td>2.158876000</td><td>0.000223000</td></tr> <tr><td>H</td><td>-1.306843000</td><td>-2.158877000</td><td>0.000223000</td></tr> <tr><td>C</td><td>-1.408235000</td><td>0.000000000</td><td>-0.000188000</td></tr> <tr><td>H</td><td>-2.495570000</td><td>0.000000000</td><td>-0.000363000</td></tr> <tr><td>H</td><td>2.101559000</td><td>0.000000000</td><td>-0.847298000</td></tr> <tr><td>H</td><td>2.102891000</td><td>0.000000000</td><td>0.845881000</td></tr> </tbody> </table>	C	1.386622000	0.000000000	-0.000119000	C	0.627961000	1.248046000	0.000148000	C	0.627961000	-1.248046000	0.000148000	H	1.178365000	2.184561000	0.000223000	H	1.178366000	-2.184561000	0.000223000	C	-0.738149000	1.236257000	0.000080000	C	-0.738149000	-1.236257000	0.000080000	H	-1.306843000	2.158876000	0.000223000	H	-1.306843000	-2.158877000	0.000223000	C	-1.408235000	0.000000000	-0.000188000	H	-2.495570000	0.000000000	-0.000363000	H	2.101559000	0.000000000	-0.847298000	H	2.102891000	0.000000000	0.845881000																								
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 <p style="text-align: center;">BzH⁺-W₁</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.450725000</td><td>0.000075000</td><td>0.889358000</td></tr> <tr><td>C</td><td>0.201043000</td><td>1.239691000</td><td>0.524939000</td></tr> <tr><td>C</td><td>0.200920000</td><td>-1.239624000</td><td>0.525006000</td></tr> <tr><td>H</td><td>-0.254437000</td><td>2.175779000</td><td>0.833788000</td></tr> <tr><td>H</td><td>-0.254655000</td><td>-2.175650000</td><td>0.833902000</td></tr> <tr><td>C</td><td>1.337829000</td><td>1.230899000</td><td>-0.240861000</td></tr> <tr><td>C</td><td>1.337705000</td><td>-1.230983000</td><td>-0.240798000</td></tr> <tr><td>H</td><td>1.813979000</td><td>2.156040000</td><td>-0.544161000</td></tr> <tr><td>H</td><td>1.813758000</td><td>-2.156188000</td><td>-0.544052000</td></tr> <tr><td>C</td><td>1.897210000</td><td>-0.000080000</td><td>-0.614285000</td></tr> <tr><td>H</td><td>2.802572000</td><td>-0.000142000</td><td>-1.215594000</td></tr> <tr><td>H</td><td>-0.919460000</td><td>0.000137000</td><td>1.882038000</td></tr> <tr><td>H</td><td>-1.416099000</td><td>0.000093000</td><td>0.255982000</td></tr> <tr><td>O</td><td>-2.971055000</td><td>-0.000001000</td><td>-0.601961000</td></tr> <tr><td>H</td><td>-3.119273000</td><td>0.000159000</td><td>-1.551587000</td></tr> <tr><td>H</td><td>-3.841832000</td><td>-0.000094000</td><td>-0.194778000</td></tr> </tbody> </table>	C	-0.450725000	0.000075000	0.889358000	C	0.201043000	1.239691000	0.524939000	C	0.200920000	-1.239624000	0.525006000	H	-0.254437000	2.175779000	0.833788000	H	-0.254655000	-2.175650000	0.833902000	C	1.337829000	1.230899000	-0.240861000	C	1.337705000	-1.230983000	-0.240798000	H	1.813979000	2.156040000	-0.544161000	H	1.813758000	-2.156188000	-0.544052000	C	1.897210000	-0.000080000	-0.614285000	H	2.802572000	-0.000142000	-1.215594000	H	-0.919460000	0.000137000	1.882038000	H	-1.416099000	0.000093000	0.255982000	O	-2.971055000	-0.000001000	-0.601961000	H	-3.119273000	0.000159000	-1.551587000	H	-3.841832000	-0.000094000	-0.194778000												
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C	-2.055273000	3.138199000	0.000959000																																																																																																																																														
H	-2.296912000	4.195806000	0.003011000																																																																																																																																														

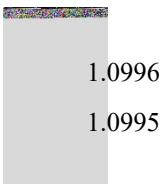
 <p style="text-align: center;">CorH⁺-W₁</p>	<table border="1"> <tbody> <tr><td>H</td><td>-3.939754000</td><td>-2.033985000</td><td>-0.865603000</td></tr> <tr><td>C</td><td>1.987738000</td><td>-3.374230000</td><td>0.081081000</td></tr> <tr><td>C</td><td>2.375522000</td><td>-2.009191000</td><td>0.139643000</td></tr> <tr><td>C</td><td>1.380648000</td><td>-1.008525000</td><td>0.010945000</td></tr> <tr><td>C</td><td>0.022325000</td><td>-1.374704000</td><td>-0.154241000</td></tr> <tr><td>C</td><td>-0.336442000</td><td>-2.740393000</td><td>-0.214375000</td></tr> <tr><td>C</td><td>0.680654000</td><td>-3.727662000</td><td>-0.089288000</td></tr> <tr><td>C</td><td>1.739345000</td><td>0.357715000</td><td>0.074943000</td></tr> <tr><td>C</td><td>-0.977165000</td><td>-0.374005000</td><td>-0.286092000</td></tr> <tr><td>C</td><td>-0.609215000</td><td>1.000890000</td><td>-0.227028000</td></tr> <tr><td>C</td><td>0.742790000</td><td>1.364185000</td><td>-0.062200000</td></tr> <tr><td>C</td><td>-1.603703000</td><td>2.040006000</td><td>-0.361326000</td></tr> <tr><td>C</td><td>-2.912085000</td><td>1.688123000</td><td>-0.539542000</td></tr> <tr><td>C</td><td>-3.368571000</td><td>0.301209000</td><td>-0.573339000</td></tr> <tr><td>C</td><td>-2.325840000</td><td>-0.747315000</td><td>-0.457699000</td></tr> <tr><td>C</td><td>-2.663316000</td><td>-2.102179000</td><td>-0.507134000</td></tr> <tr><td>C</td><td>-1.692236000</td><td>-3.075505000</td><td>-0.389275000</td></tr> <tr><td>H</td><td>-1.972783000</td><td>-4.123479000</td><td>-0.432755000</td></tr> <tr><td>H</td><td>-3.702267000</td><td>-2.387753000</td><td>-0.637041000</td></tr> <tr><td>H</td><td>2.752179000</td><td>-4.138542000</td><td>0.175497000</td></tr> <tr><td>H</td><td>0.399293000</td><td>-4.774997000</td><td>-0.133379000</td></tr> <tr><td>H</td><td>-3.663418000</td><td>2.466727000</td><td>-0.644876000</td></tr> <tr><td>H</td><td>-4.116683000</td><td>0.176886000</td><td>0.240619000</td></tr> <tr><td>C</td><td>3.726583000</td><td>-1.616431000</td><td>0.314717000</td></tr> <tr><td>C</td><td>4.074755000</td><td>-0.295692000</td><td>0.366278000</td></tr> <tr><td>C</td><td>3.094002000</td><td>0.722964000</td><td>0.244112000</td></tr> <tr><td>H</td><td>4.486490000</td><td>-2.385193000</td><td>0.409237000</td></tr> <tr><td>H</td><td>5.112955000</td><td>-0.009145000</td><td>0.500103000</td></tr> <tr><td>C</td><td>3.423956000</td><td>2.095214000</td><td>0.292548000</td></tr> <tr><td>C</td><td>2.464266000</td><td>3.073665000</td><td>0.171214000</td></tr> <tr><td>C</td><td>1.110283000</td><td>2.738803000</td><td>-0.005040000</td></tr> <tr><td>H</td><td>4.464086000</td><td>2.377016000</td><td>0.426682000</td></tr> <tr><td>H</td><td>2.747471000</td><td>4.120068000</td><td>0.211793000</td></tr> <tr><td>C</td><td>-1.196364000</td><td>3.416383000</td><td>-0.307108000</td></tr> <tr><td>H</td><td>-1.957081000</td><td>4.183544000</td><td>-0.407345000</td></tr> <tr><td>C</td><td>0.104871000</td><td>3.747710000</td><td>-0.136429000</td></tr> <tr><td>H</td><td>0.408157000</td><td>4.788535000</td><td>-0.095099000</td></tr> <tr><td>H</td><td>-3.985640000</td><td>0.143372000</td><td>-1.472618000</td></tr> <tr><td>O</td><td>-5.561923000</td><td>-0.089512000</td><td>1.672231000</td></tr> <tr><td>H</td><td>-6.515486000</td><td>-0.055935000</td><td>1.565144000</td></tr> <tr><td>H</td><td>-5.418688000</td><td>-0.271231000</td><td>2.604010000</td></tr> </tbody> </table>	H	-3.939754000	-2.033985000	-0.865603000	C	1.987738000	-3.374230000	0.081081000	C	2.375522000	-2.009191000	0.139643000	C	1.380648000	-1.008525000	0.010945000	C	0.022325000	-1.374704000	-0.154241000	C	-0.336442000	-2.740393000	-0.214375000	C	0.680654000	-3.727662000	-0.089288000	C	1.739345000	0.357715000	0.074943000	C	-0.977165000	-0.374005000	-0.286092000	C	-0.609215000	1.000890000	-0.227028000	C	0.742790000	1.364185000	-0.062200000	C	-1.603703000	2.040006000	-0.361326000	C	-2.912085000	1.688123000	-0.539542000	C	-3.368571000	0.301209000	-0.573339000	C	-2.325840000	-0.747315000	-0.457699000	C	-2.663316000	-2.102179000	-0.507134000	C	-1.692236000	-3.075505000	-0.389275000	H	-1.972783000	-4.123479000	-0.432755000	H	-3.702267000	-2.387753000	-0.637041000	H	2.752179000	-4.138542000	0.175497000	H	0.399293000	-4.774997000	-0.133379000	H	-3.663418000	2.466727000	-0.644876000	H	-4.116683000	0.176886000	0.240619000	C	3.726583000	-1.616431000	0.314717000	C	4.074755000	-0.295692000	0.366278000	C	3.094002000	0.722964000	0.244112000	H	4.486490000	-2.385193000	0.409237000	H	5.112955000	-0.009145000	0.500103000	C	3.423956000	2.095214000	0.292548000	C	2.464266000	3.073665000	0.171214000	C	1.110283000	2.738803000	-0.005040000	H	4.464086000	2.377016000	0.426682000	H	2.747471000	4.120068000	0.211793000	C	-1.196364000	3.416383000	-0.307108000	H	-1.957081000	4.183544000	-0.407345000	C	0.104871000	3.747710000	-0.136429000	H	0.408157000	4.788535000	-0.095099000	H	-3.985640000	0.143372000	-1.472618000	O	-5.561923000	-0.089512000	1.672231000	H	-6.515486000	-0.055935000	1.565144000	H	-5.418688000	-0.271231000	2.604010000
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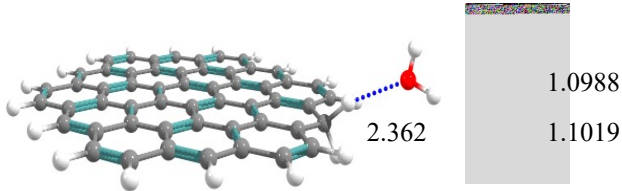
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	H	-3.017354000	-4.162041000	0.005332000
	H	-0.637857000	-4.774432000	0.004915000
	H	3.386191000	2.499755000	-0.004695000
	H	3.796761000	0.200038000	-0.857352000
	C	-4.027421000	-1.649586000	0.003924000
	C	-4.392549000	-0.332571000	0.001710000
	C	-3.414720000	0.696113000	0.000160000
	H	-4.785475000	-2.426035000	0.004386000
	H	-5.442189000	-0.056535000	0.002365000
	C	-3.761959000	2.065579000	-0.003616000
	C	-2.804856000	3.052549000	-0.006126000
	C	-1.434892000	2.730896000	-0.005888000
	H	-4.813527000	2.336635000	-0.003075000
	H	-3.100643000	4.096303000	-0.009859000
	C	0.885272000	3.428783000	-0.007079000
	H	1.645417000	4.203104000	-0.008090000
	C	-0.430933000	3.748517000	-0.007285000
H	-0.746433000	4.786564000	-0.010415000	
H	3.789997000	0.205115000	0.859931000	
O	5.041424000	-0.057310000	-2.506444000	
H	5.999752000	-0.026362000	-2.552595000	
H	4.752230000	-0.240740000	-3.403298000	
O	5.020332000	-0.012721000	2.523163000	
H	5.978310000	0.018431000	2.575940000	
H	4.724888000	-0.196728000	3.417858000	
 <p>CorH⁺-W₃</p>	H	-3.236462000	-0.707423000	0.553651000
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	O	-4.772574000	-0.940653000	1.805901000
	H	-5.626912000	-0.578394000	1.531703000
	H	-4.791395000	-0.977465000	2.764013000
	H	-5.561620000	1.048080000	-2.260445000
	H	-5.936891000	0.556710000	-0.854864000
	O	-5.184121000	0.744451000	-1.432510000
	H	-7.859009000	-0.561040000	0.410230000
	H	-7.664562000	0.851373000	0.970523000
	O	-7.189672000	0.105234000	0.592700000
	C	2.357058000	3.539211000	0.152841000
	C	2.898322000	2.226728000	0.164431000
	C	2.017016000	1.123025000	0.060947000
	C	0.622375000	1.337310000	-0.065537000
	C	0.108593000	2.653270000	-0.074849000
	C	1.012502000	3.745485000	0.034575000
	C	2.531298000	-0.195156000	0.051765000
	C	-0.265196000	0.232334000	-0.159350000
	C	0.257103000	-1.092336000	-0.173979000
C	1.647699000	-1.305146000	-0.055279000	
C	-0.618678000	-2.231119000	-0.295190000	
C	-1.969034000	-2.020840000	-0.401249000	
C	-2.570919000	-0.700712000	-0.346616000	
C	-1.652590000	0.453668000	-0.275994000	
C	-2.144690000	1.764017000	-0.304616000	
C	-1.283373000	2.835388000	-0.205275000	
H	-1.677504000	3.847051000	-0.229530000	

	H	-3.212903000	1.915701000	-0.423579000
	H	3.033758000	4.383546000	0.235594000
	H	0.614301000	4.755214000	0.023613000
	H	-2.635624000	-2.875311000	-0.487743000
	C	4.291136000	1.984908000	0.280385000
	C	4.787232000	0.711604000	0.282374000
	C	3.923273000	-0.408943000	0.169446000
	H	4.963359000	2.832596000	0.364875000
	H	5.855546000	0.541419000	0.370248000
	C	4.407663000	-1.736070000	0.159661000
	C	3.560419000	-2.812115000	0.041739000
	C	2.169636000	-2.628252000	-0.072591000
	H	5.477448000	-1.901083000	0.246872000
	H	3.960455000	-3.820528000	0.033181000
	C	-0.058237000	-3.551635000	-0.308473000
	H	-0.731812000	-4.396951000	-0.404345000
	C	1.278980000	-3.739072000	-0.199514000
	H	1.698096000	-4.739783000	-0.208586000
	C	-3.604956000	-1.041110000	-0.003513000
	C	0.633075000	-1.265402000	-0.002994000
	C	4.863660000	-1.521898000	-0.000921000
	C	-5.024217000	-0.963796000	0.000675000
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	C	3.464283000	-1.426321000	0.004154000
	C	-5.778068000	-2.178451000	-0.000754000
	C	-1.552533000	-2.380072000	-0.005466000
	C	2.680768000	-2.609978000	-0.003498000
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	C	5.473665000	-2.782772000	-0.002237000
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	C	-1.699507000	-4.833110000	-0.001291000
	C	2.523204000	-5.049728000	0.000214000
	C	-3.086462000	-4.736560000	-0.001974000
	C	1.140760000	-4.993231000	0.000887000
	C	0.327556000	-6.176345000	-0.000401000
	C	-1.024069000	-6.098952000	-0.001019000
	C	0.961275000	6.109872000	-0.000412000
	C	-0.391140000	6.171943000	-0.001013000
	C	-1.193226000	4.982307000	-0.001277000
	C	3.029369000	4.763346000	0.000185000
	C	-2.582757000	5.028958000	-0.001948000
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	C	5.101336000	3.428617000	-0.001762000
	C	-4.786682000	3.903205000	-0.001390000
	C	-0.536117000	3.715395000	0.004744000
	C	3.694428000	3.520270000	0.000056000
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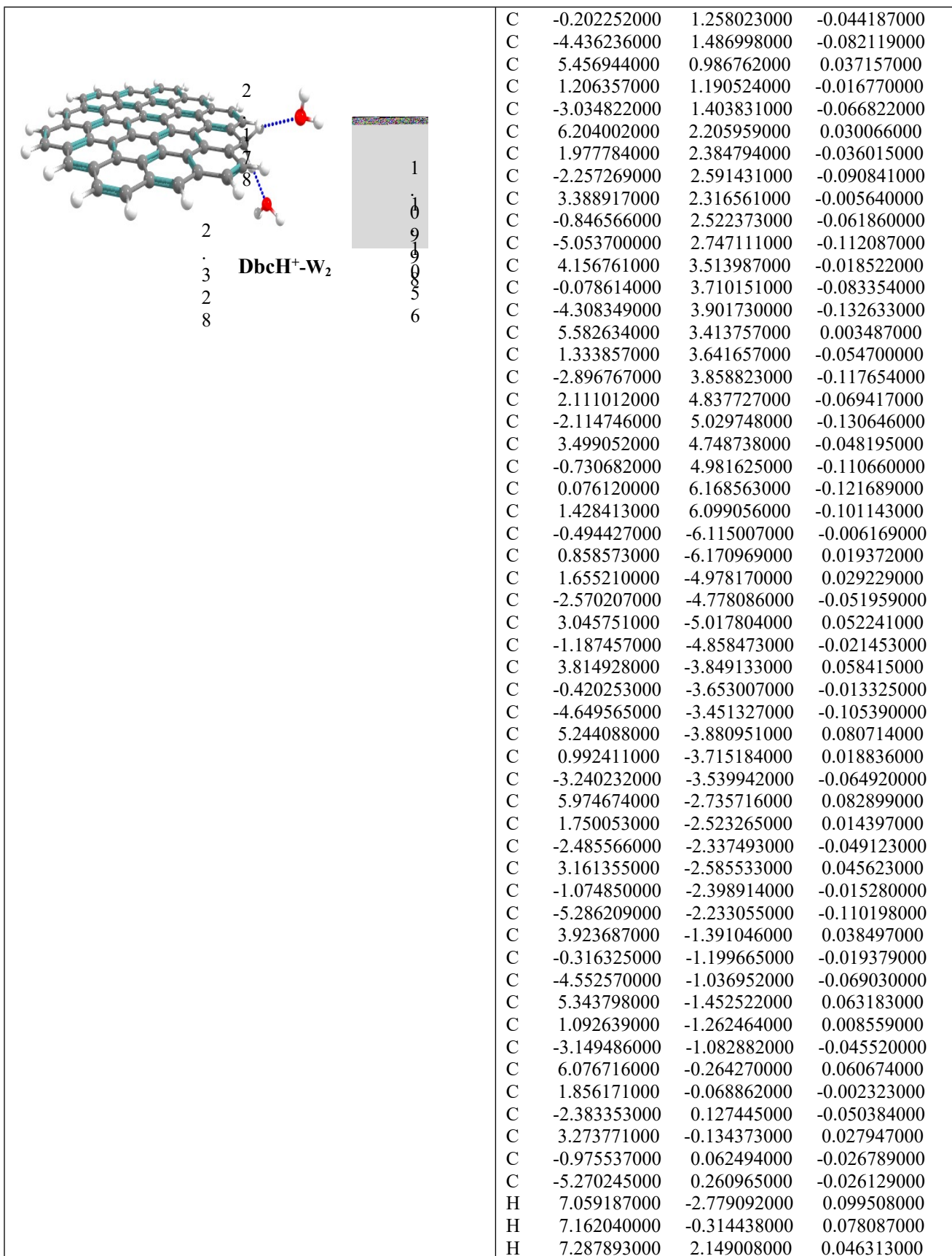


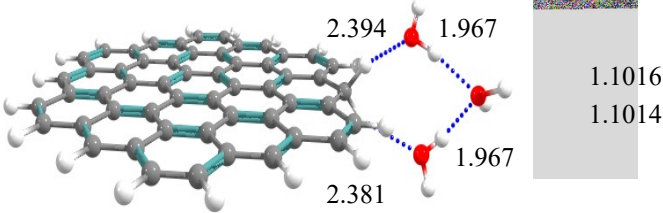
DbcH⁺



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	C	5.730928000	2.204870000	-0.002251000
	C	-3.478712000	1.406462000	-0.003504000
	C	0.759906000	1.193560000	-0.002998000
	C	4.994433000	1.013447000	-0.000925000
	C	-4.898397000	1.475569000	0.000687000
	C	-0.648415000	1.263491000	0.006438000
	C	3.592649000	1.062352000	0.004144000
	C	-5.637510000	0.290762000	0.000612000
	C	-1.418525000	0.073163000	-0.003165000
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	C	5.710214000	-0.294511000	0.000561000
	H	-6.607638000	2.810299000	-0.000622000
	H	-6.722679000	0.346723000	0.002444000
	H	-6.861710000	-2.115616000	-0.000655000
	H	6.557503000	-2.847059000	-0.004075000
	H	6.386550000	-0.329377000	-0.865550000
	H	6.815629000	2.157314000	-0.004106000
	H	5.212352000	-4.903570000	-0.002158000
	H	3.018181000	-6.016749000	0.001926000
	H	0.822735000	-7.142113000	-0.000172000
	H	-1.624577000	-7.003016000	-0.002291000
	H	-3.681381000	-5.645190000	-0.005178000
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	H	3.621200000	5.674317000	0.001885000
	H	5.689196000	4.341303000	-0.002194000
	H	6.380875000	-0.329100000	0.871274000
	C	-3.597238000	1.686938000	0.042690000
	C	0.608571000	1.126664000	-0.060958000
	C	4.812374000	0.598427000	-0.180480000
	C	-5.006348000	1.872176000	0.071679000
	C	-0.789311000	1.312088000	-0.035003000
	C	3.419297000	0.763549000	-0.146082000
	C	-5.523180000	3.205289000	0.085449000
	C	-1.333773000	2.625119000	-0.006247000
	C	2.868332000	2.070905000	-0.105733000
	C	-2.734386000	2.810333000	0.016154000
	C	1.467998000	2.255060000	-0.084566000
	C	5.648958000	1.723482000	-0.160727000
	C	-3.275175000	4.126047000	0.037496000
	C	0.925841000	3.561474000	-0.052351000
	C	5.120635000	2.993458000	-0.129704000
	C	-4.695617000	4.282653000	0.068997000
	C	-0.475653000	3.746608000	-0.030453000
	C	3.725042000	3.203155000	-0.111713000
	C	-1.025709000	5.062868000	-0.006383000
	C	3.165096000	4.495833000	-0.089280000
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 <p>DbcH⁺-W₁</p>				

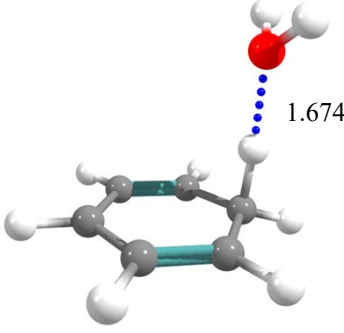
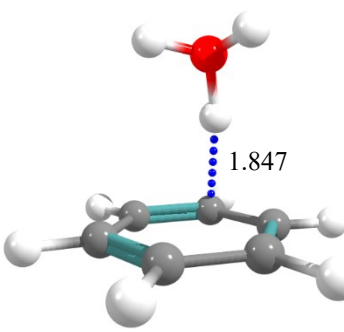
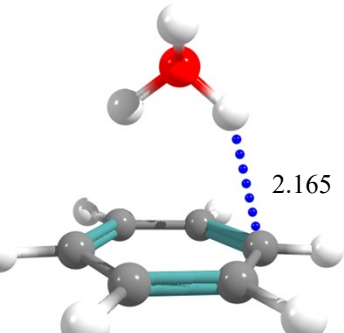
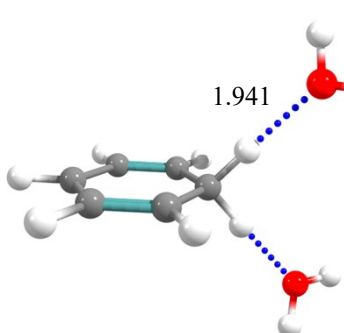
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	C	-0.423972000	-6.181608000	0.001459000
	C	-1.764532000	-5.993956000	0.031557000
	C	-2.334432000	-4.677265000	0.034876000
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	C	4.137962000	-4.306976000	-0.130950000
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	C	4.475612000	-1.912764000	-0.180011000
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	C	-1.116168000	-1.122402000	-0.024409000
	C	3.088441000	-1.705270000	-0.139026000
	C	-5.839768000	0.752183000	0.092437000
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	C	2.550472000	-0.376055000	-0.120704000
	C	-3.059656000	0.378249000	0.019164000
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	H	6.723978000	1.572830000	-0.154348000
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	H	6.055300000	-3.371060000	-0.200930000
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	H	3.829726000	5.355232000	-0.093989000
	H	1.879153000	6.866508000	-0.052264000
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	H	-2.823885000	6.226331000	0.039493000
	H	-5.105481000	5.287513000	0.080999000
	H	-6.328314000	-3.816198000	0.123323000
	H	-4.375602000	-5.324335000	0.090540000
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	H	2.270295000	-6.242925000	-0.064265000
	H	4.547989000	-5.312276000	-0.126338000
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	H	9.180678000	-0.271119000	0.778924000
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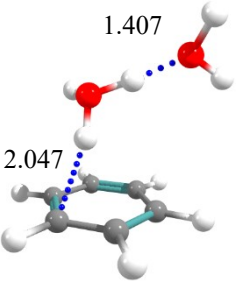
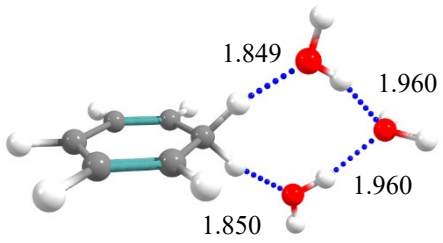


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	H	-4.803850000	4.867612000	-0.157933000
	H	-2.614414000	5.994210000	-0.153709000
	H	-0.423965000	7.131588000	-0.146130000
	H	2.023708000	7.006598000	-0.109752000
	H	4.088987000	5.660652000	-0.057580000
	H	6.165949000	4.328993000	-0.002684000
	H	5.740053000	-4.846241000	0.094550000
	H	3.548558000	-5.980499000	0.062296000
	H	1.366951000	-7.129874000	0.030808000
	H	-1.081643000	-7.027817000	-0.014722000
	H	-3.157029000	-5.692376000	-0.064283000
	H	-5.231498000	-4.367730000	-0.134747000
	H	-5.854998000	0.302100000	0.911335000
	O	-7.893845000	-0.748555000	-1.783293000
	H	-8.798922000	-0.459197000	-1.646989000
	H	-7.871902000	-1.067754000	-2.688478000
	O	-6.953699000	0.852097000	2.710052000
	H	-7.757364000	0.451981000	3.049142000
	H	-6.556012000	1.290611000	3.465480000
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	C	0.047516000	1.229479000	0.008531000
	C	-4.192436000	1.259531000	-0.005115000
	C	5.714086000	1.225711000	0.018429000
	C	1.458122000	1.228382000	0.019708000
	C	-2.788696000	1.241247000	0.009928000
	C	6.402517000	2.479056000	0.032563000
	C	2.172027000	2.458168000	0.022106000
	C	-2.068346000	2.464487000	0.012599000
	C	3.585033000	2.456443000	0.034064000
	C	-0.655981000	2.461859000	0.029330000
	C	-4.872363000	2.487952000	-0.024721000
	C	4.295152000	3.689082000	0.042945000
	C	0.054682000	3.684880000	0.031316000
	C	-4.180439000	3.675329000	-0.009054000
	C	5.724518000	3.656091000	0.044645000
	C	1.469218000	3.683021000	0.043589000
	C	-2.767977000	3.699781000	0.016700000
	C	2.188522000	4.914599000	0.051765000
	C	-2.042462000	4.906029000	0.031771000
	C	3.579646000	4.891269000	0.053948000
	C	-0.657175000	4.923707000	0.042850000
	C	0.092215000	6.147479000	0.056669000
	C	1.446579000	6.142200000	0.061729000
	C	0.104104000	-6.148546000	-0.060492000
	C	1.458453000	-6.140651000	-0.064453000
	C	2.198018000	-4.911615000	-0.053729000
	C	-2.032989000	-4.911218000	-0.037963000
	C	3.589087000	-4.885608000	-0.054878000
	C	-0.647656000	-4.926234000	-0.045607000
	C	4.302275000	-3.682058000	-0.041504000
	C	0.061776000	-3.685961000	-0.041436000
	C	-4.173437000	-3.684596000	-0.004692000
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C	1.460492000	-1.226968000	-0.008059000
C	-2.786262000	-1.247872000	-0.010984000
C	6.392422000	0.005495000	0.004544000
C	2.166663000	0.001495000	-0.003130000
C	-2.078017000	-0.002551000	-0.007864000
C	3.586269000	0.002727000	0.009005000
C	-0.668160000	-0.001326000	0.004173000
C	-4.968223000	-0.005371000	-0.007221000
H	7.492793000	-2.460166000	-0.025282000
H	7.479052000	0.006508000	0.007345000
H	7.488027000	2.473277000	0.033951000
H	-5.956598000	2.477608000	-0.074443000
H	-5.952033000	-2.490449000	0.052855000
H	-4.719993000	4.617739000	-0.021184000
H	-2.587407000	5.845975000	0.035228000
H	-0.453235000	7.085888000	0.063378000
H	1.998001000	7.077055000	0.071807000
H	4.125576000	5.830230000	0.061751000
H	6.263756000	4.597964000	0.054809000
H	6.272634000	-4.587138000	-0.052456000
H	4.136831000	-5.823454000	-0.067861000
H	2.011686000	-7.074419000	-0.075961000
H	-0.439531000	-7.088003000	-0.067658000
H	-2.576098000	-5.852231000	-0.038821000
H	-4.711237000	-4.628017000	0.006348000
H	-5.664750000	-0.025243000	0.845933000
H	-5.665817000	0.012831000	-0.859303000
O	-7.646677000	-1.221909000	1.404628000
H	-8.453142000	-0.834120000	1.039095000
H	-7.893882000	-1.565601000	2.265101000
H	-7.923533000	1.559383000	-2.249151000
H	-8.466594000	0.832096000	-1.013411000
O	-7.665030000	1.218700000	-1.390800000
H	-10.501655000	-0.620387000	-0.421329000
H	-10.495094000	0.621401000	0.476282000
O	-9.917416000	0.000355000	0.023442000

Table S5: MP2/6-311++G** optimized equilibrium structures of $\text{BzH}^+ \cdot \text{W}_n$ ($n = 1 - 3$) complexes. the intermonomer distances (in Å) are given.

 <p style="text-align: center;">BzH⁺-W_{1a} [-308.1677143147]</p>	<table border="1"> <tbody> <tr><td>C</td><td>0.388089000</td><td>0.000506000</td><td>1.160202000</td></tr> <tr><td>C</td><td>-0.183829000</td><td>-1.241067000</td><td>0.700215000</td></tr> <tr><td>C</td><td>-0.185145000</td><td>1.241398000</td><td>0.699987000</td></tr> <tr><td>H</td><td>0.200059000</td><td>-2.178851000</td><td>1.093901000</td></tr> <tr><td>H</td><td>0.197698000</td><td>2.179655000</td><td>1.093573000</td></tr> <tr><td>C</td><td>-1.126728000</td><td>-1.230027000</td><td>-0.318454000</td></tr> <tr><td>C</td><td>-1.127987000</td><td>1.229136000</td><td>-0.318716000</td></tr> <tr><td>H</td><td>-1.528073000</td><td>-2.160542000</td><td>-0.706825000</td></tr> <tr><td>H</td><td>-1.530345000</td><td>2.159142000</td><td>-0.707270000</td></tr> <tr><td>C</td><td>-1.607355000</td><td>-0.000756000</td><td>-0.802244000</td></tr> <tr><td>H</td><td>-2.358587000</td><td>-0.001226000</td><td>-1.588710000</td></tr> <tr><td>H</td><td>0.902771000</td><td>0.000883000</td><td>2.121126000</td></tr> <tr><td>H</td><td>1.284650000</td><td>0.000928000</td><td>0.373779000</td></tr> <tr><td>O</td><td>2.478219000</td><td>0.000075000</td><td>-0.800658000</td></tr> <tr><td>H</td><td>3.027586000</td><td>0.765663000</td><td>-1.004208000</td></tr> <tr><td>H</td><td>3.036216000</td><td>-0.761393000</td><td>-0.996043000</td></tr> </tbody> </table>	C	0.388089000	0.000506000	1.160202000	C	-0.183829000	-1.241067000	0.700215000	C	-0.185145000	1.241398000	0.699987000	H	0.200059000	-2.178851000	1.093901000	H	0.197698000	2.179655000	1.093573000	C	-1.126728000	-1.230027000	-0.318454000	C	-1.127987000	1.229136000	-0.318716000	H	-1.528073000	-2.160542000	-0.706825000	H	-1.530345000	2.159142000	-0.707270000	C	-1.607355000	-0.000756000	-0.802244000	H	-2.358587000	-0.001226000	-1.588710000	H	0.902771000	0.000883000	2.121126000	H	1.284650000	0.000928000	0.373779000	O	2.478219000	0.000075000	-0.800658000	H	3.027586000	0.765663000	-1.004208000	H	3.036216000	-0.761393000	-0.996043000
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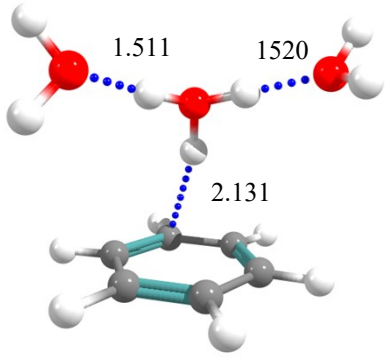
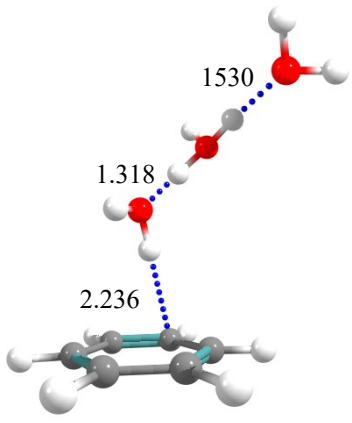
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 <p style="text-align: center;">BzH⁺-W_{3c} [-460.7999350202]</p>	<table border="0"> <tbody> <tr><td>C</td><td>-1.791681000</td><td>-0.557001000</td><td>1.295853000</td></tr> <tr><td>C</td><td>-2.461113000</td><td>-1.056602000</td><td>0.166714000</td></tr> <tr><td>C</td><td>-1.299439000</td><td>0.758843000</td><td>1.295328000</td></tr> <tr><td>H</td><td>-2.863468000</td><td>-2.065762000</td><td>0.176542000</td></tr> <tr><td>H</td><td>-0.810644000</td><td>1.154842000</td><td>2.181544000</td></tr> <tr><td>C</td><td>-2.627102000</td><td>-0.244786000</td><td>-0.964967000</td></tr> <tr><td>C</td><td>-1.467473000</td><td>1.569425000</td><td>0.163560000</td></tr> <tr><td>H</td><td>-3.163769000</td><td>-0.624170000</td><td>-1.830130000</td></tr> <tr><td>H</td><td>-1.111195000</td><td>2.595914000</td><td>0.172833000</td></tr> <tr><td>C</td><td>-2.130959000</td><td>1.067274000</td><td>-0.965720000</td></tr> <tr><td>H</td><td>-2.286968000</td><td>1.705196000</td><td>-1.831785000</td></tr> <tr><td>H</td><td>-1.688948000</td><td>-1.175648000</td><td>2.183685000</td></tr> <tr><td>H</td><td>-0.091786000</td><td>-0.829023000</td><td>-0.131363000</td></tr> <tr><td>O</td><td>0.650206000</td><td>-0.947757000</td><td>-0.754341000</td></tr> <tr><td>H</td><td>0.425799000</td><td>-0.412112000</td><td>-1.524393000</td></tr> <tr><td>H</td><td>1.873628000</td><td>-0.961632000</td><td>-0.263597000</td></tr> <tr><td>H</td><td>3.280490000</td><td>-1.911204000</td><td>-0.003212000</td></tr> <tr><td>H</td><td>3.514297000</td><td>-0.300862000</td><td>0.054618000</td></tr> <tr><td>O</td><td>2.863357000</td><td>-1.062652000</td><td>0.190047000</td></tr> <tr><td>H</td><td>4.833863000</td><td>1.342569000</td><td>0.703513000</td></tr> <tr><td>H</td><td>5.023553000</td><td>1.121436000</td><td>-0.807727000</td></tr> <tr><td>O</td><td>4.452906000</td><td>0.902601000</td><td>-0.063847000</td></tr> </tbody> </table>	C	-1.791681000	-0.557001000	1.295853000	C	-2.461113000	-1.056602000	0.166714000	C	-1.299439000	0.758843000	1.295328000	H	-2.863468000	-2.065762000	0.176542000	H	-0.810644000	1.154842000	2.181544000	C	-2.627102000	-0.244786000	-0.964967000	C	-1.467473000	1.569425000	0.163560000	H	-3.163769000	-0.624170000	-1.830130000	H	-1.111195000	2.595914000	0.172833000	C	-2.130959000	1.067274000	-0.965720000	H	-2.286968000	1.705196000	-1.831785000	H	-1.688948000	-1.175648000	2.183685000	H	-0.091786000	-0.829023000	-0.131363000	O	0.650206000	-0.947757000	-0.754341000	H	0.425799000	-0.412112000	-1.524393000	H	1.873628000	-0.961632000	-0.263597000	H	3.280490000	-1.911204000	-0.003212000	H	3.514297000	-0.300862000	0.054618000	O	2.863357000	-1.062652000	0.190047000	H	4.833863000	1.342569000	0.703513000	H	5.023553000	1.121436000	-0.807727000	O	4.452906000	0.902601000	-0.063847000
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Table S6: Calculated total energy (TE), relative energies (RE) and thermal corrected energies. All values are in a.u. (bare protonated surface (CorH⁺). we have computed at PBE0/6-311++G** level. Case (i): A σ complex where the proton is attached to an external carbon of the aromatic compound (i.e. aliphatic sp³ C-H⁺). Case (ii) A π complex where the proton interacts with the π orbital of these aromatics. Case3 (iii) A σ complex where the proton is attached to an internal carbon of PAHs possessing more than one aromatic ring.

Energies in	Case (i)	Case (ii)	Case (iii)
Total Energy (TE)	-921.3588	-921.3286	-921.3286
Relative Energy (RE)	0	0.0302 a.u. (18 kcal/mol)	0.0302 a.u. (18 kcal/mol)
Zero Point Energy (ZPE) Corrected TE	-921.067	-921.0372	-921.0372
G corrected TE	-921.1076	-921.0774	-921.0218
H Corrected TE	-921.0514	-921.0774	-921.0218

Table S7: Calculated total energy (TE), relative energies (RE) and thermal corrected energies (a.u) of CorH⁺-W₁ cluster. we have computed at PBE0/6-311++G** level. Case (i): A σ complex where the proton is attached to an external carbon of the aromatic compound (i.e. aliphatic sp³ C-H⁺). Case (ii) A π complex where the proton interacts with the π orbital of these aromatics. Case3 (iii) A σ complex where the proton is attached to an internal carbon of PAHs possessing more than one aromatic ring.

Energies in (a.u)	Case (i)	Case (ii)	Case (iii)
Total Energy (TE)	-997.7430	-997.7189	-997.7189
Relative Energy (RE)	0	0.0242 a.u. (15 kcal/mol)	0.0242 a.u. (15 kcal/mol)
Zero Point Energy (ZPE) Corrected TE	-997.4277	-997.4048	-997.0372
G corrected TE	-997.4748	-997.4519	-997.4519
H Corrected TE	-997.4081	-997.3854	-997.3854

Table S8: Singlet electronic states of BzH⁺-W_n, CorH⁺-W_n and DbcH⁺-W_n (n=0-3) clusters with excitation energies (E, in eV), transition wavelength (λ , in nm) and oscillator strength (f). We give also the corresponding electron promotion. These computations are done using the TD-DFT method at the PBE0/6-311++G** level.

Compound	State	E	λ	Electron promotion	f
BZH ⁺	S1	4.24	292	HOMO to LUMO	0.12
	S2	5.13	241	HOMO-2 to LUMO	0.00
	S3	5.45	227	HOMO-3 to LUMO	0.0047
	S4	5.78	214	HOMO-1 to LUMO	0.075
BZH ⁺ -W ₁	S1	4.40	281	HOMO to LUMO	0.1085
	S2	4.83	257	HOMO-1 to LUMO	0.0041
	S3	5.43	228	HOMO-3 to LUMO	0.0039
	S4	5.53	223	HOMO to LUMO+1	0.074
	S5	5.77	214	HOMO to LUMO+1	0.0596
BZH ⁺ -W ₂	S1	4.38	282	HOMO to LUMO	0.1069
	S2	4.67	265	HOMO-2 to LUMO	0.0
	S3	4.68	264	HOMO-1 to LUMO	0.0061
	S4	5.37	230	HOMO-5 to LUMO	0.0
	S5	5.48	226	HOMO-4 to LUMO	0.023
	S6	5.65	219	HOMO to LUMO+1	0.1588
BZH ⁺ -W ₃	S1	4.45	278	HOMO to LUMO	0.1028
	S2	4.68	264	HOMO-1 to LUMO	0.006
	S3	4.73	262	HOMO-2 to LUMO	0.0
	S4	5.51	225	HOMO-6 to LUMO	0.0
	S5	5.52	225	HOMO-5 to LUMO	0.021
	S6	5.55	223	HOMO to LUMO+1	0.2276
CORH ⁺	S1	2.08	595	HOMO to LUMO	0.0788
	S2	2.49	496	HOMO-1 to LUMO	0.1377
	S3	3.09	400	HOMO to LUMO+1	0.0367
	S4	3.38	366	HOMO to LUMO+1	0.0229
	S5	3.83	323	HOMO to LUMO+1	0.0086
	S6	3.95	313	HOMO-1 to LUMO+1	0.0378
	S7	4.06	305	HOMO-1 to LUMO+1	0.215
	S8	4.44	279	HOMO to LUMO+1	0.1165
	S9	4.46	277	HOMO-1 to LUMO+1	0.1014
	S10	4.57	271	HOMO-6 to LUMO+1	0.0002
	S11	4.59	270	HOMO-1 to LUMO+1	0.1373
	S12	4.17	263	HOMO-7 to LUMO+1	0.0002

	S13	4.81	257	HOMO-1 to LUMO+2	0.2727
	S14	4.88	253	HOMO-1 to LUMO+2	0.0143
	S15	4.95	250	HOMO-2 to LUMO+1	0.0809
	S16	5.09	243	HOMO-1 to LUMO+2	0.1568
	S17	5.11	242	HOMO-1 to LUMO+2	0.043
	S18	5.26	235	HOMO-3 to LUMO+1	0.0231
	S19	5.30	234	HOMO-2 to LUMO+1	0.1196
	S20	5.48	226	HOMO-4 to LUMO+1	0.0036
	S21	5.52	224	HOMO-3 to LUMO+1	0.0295
	S22	5.59	222	HOMO-3 to LUMO+1	0.0464
	S23	5.71	217	HOMO-3 to LUMO+1	0.0368
	S24	5.73	216	HOMO-10 to LUMO+1	0.0003
	S25	5.75	215	HOMO-10 to LUMO+1	0.0001
	S26	5.76	215	HOMO-3 to LUMO+2	0.0193
	S27	5.92	209	HOMO-7 to LUMO+1	0.0003
	S28	5.93	208	HOMO-4 to LUMO+1	0.0328
	S29	5.96	207	HOMO-4 to LUMO+1	0.0298
	S30	6.02	205	HOMO to HOMO+6	0
CORH ⁺ -W ₁	S1	2.16	573	HOMO to LUMO	0.0826
	S2	2.53	488	HOMO-1 to LUMO	0.139
	S3	3.16	391	HOMO to LUMO+1	0.0341
	S4	3.45	358	HOMO to LUMO+1	0.0173
	S5	3.87	320	HOMO to LUMO+1	0.0246
	S6	3.94	314	HOMO-1 to LUMO+1	0.0313
	S7	4.08	303	HOMO to LUMO+1	0.229
	S8	4.45	278	HOMO-1 to LUMO+1	0.1581
	S9	4.46	278	HOMO-1 to LUMO+1	0.0657
	S10	4.58	270	HOMO-1 to LUMO+1	0.1283
	S11	4.65	266	HOMO-7 to LUMO	0.0001
	S12	4.76	260	HOMO-6 to LUMO	0.002
	S13	4.72	259	HOMO-6 to LUMO	0.0001
	S14	4.81	258	HOMO-1 to LUMO+2	0.3063
	S15	4.86	254	HOMO-1 to LUMO+2	0.008
	S16	4.95	250	HOMO-2 to LUMO+1	0.1005
	S17	5.08	243	HOMO-2 to LUMO+1	0.1064
	S18	5.16	240	HOMO-2 to LUMO+1	0.104
	S19	5.25	236	HOMO-4 to LUMO+1	0.0036
	S20	5.30	233	HOMO-1 to LUMO+2	0.0974
	S21	5.49	225	HOMO-2 to LUMO+2	0.0153
	S22	5.55	223	HOMO-3 to LUMO+2	0.0243

	S23	5.59	221	HOMO-2 to LUMO+2	0.0421
	S24	5.72	217	HOMO-3 to LUMO+2	0.0277
	S25	5.76	215	HOMO-3 to LUMO+2	0.0266
	S26	5.79	214	HOMO-11 to LUMO	0.002
	S27	5.80	213	HOMO-12 to LUMO	0.0003
	S28	5.86	211	HOMO to HOMO+6	0.0001
	S29	5.93	208	HOMO-4 to LUMO+1	0.0292
	S30	5.96	208	HOMO-3 to LUMO+2	0.0293
CORH ⁺ -W ₂	S1	2.23	555	HOMO to LUMO	0.086
	S2	2.57	481	HOMO-1 to LUMO	0.1393
	S3	3.23	384	HOMO to LUMO+1	0.0309
	S4	3.52	352	HOMO to LUMO+1	0.0127
	S5	3.91	317	HOMO to LUMO+1	0.048
	S6	3.94	314	HOMO-1 to LUMO+1	0.0372
	S7	4.10	302	HOMO-1 to LUMO	0.2252
	S8	4.45	278	HOMO-5 to LUMO	0.1926
	S9	4.46	278	HOMO-1 to LUMO+1	0.0434
	S10	4.59	270	HOMO-5 to LUMO	0.1065
	S11	4.71	263	HOMO-8 to LUMO	0.0002
	S12	4.80	258	HOMO-6 to LUMO	0.0711
	S13	4.81	258	HOMO-1 to LUMO+2	0.2698
	S14	4.85	255	HOMO-1 to LUMO+3	0.0037
	S15	4.88	254	HOMO-6 to LUMO	0.0003
	S16	4.89	253	HOMO-6 to LUMO	0.0001
	S17	4.95	250	HOMO-2 to LUMO+1	0.1155
	S18	5.08	244	HOMO-3 to LUMO+1	0.0884
	S19	5.19	239	HOMO-2 to LUMO+2	0.1233
	S20	5.25	236	HOMO-1 to LUMO+4	0.0183
	S21	5.33	232	HOMO-3 to LUMO+1	0.0528
	S22	5.49	225	HOMO-4 to LUMO+1	0.0185
	S23	5.59	222	HOMO-4 to LUMO+1	0.0617
	S24	5.60	221	HOMO-3 to LUMO+2	0.0066
	S25	5.72	216	HOMO-3 to LUMO+2	0.0058
	S26	5.73	216	HOMO-3 to LUMO+2	0.0107
	S27	5.77	214	HOMO-3 to LUMO+2	0.0348
	S28	5.81	213	HOMO-12 to LUMO	0.0037
	S29	5.84	211	HOMO-12 to LUMO	0
	S30	5.93	208	HOMO-2 to LUMO+2	0.0251
CORH ⁺ -W ₃	S1	2.25	549	HOMO to LUMO	0.0851

	S2	2.57	481	HOMO-1 to LUMO	0.1406
	S3	3.24	382	HOMO to LUMO+1	0.0315
	S4	3.54	354	HOMO to LUMO+1	0
	S5	3.91	316	HOMO to LUMO+1	0.0498
	S6	3.93	314	HOMO-1 to LUMO+1	0.0528
	S7	4.11	301	HOMO-1 to LUMO	0.2247
	S8	4.43	287	HOMO-1 to LUMO+1	0.191
	S9	4.46	277	HOMO-1 to LUMO+2	0.0084
	S10	4.57	271	HOMO-1 to LUMO+1	0.1703
	S11	4.62	268	HOMO-6 to LUMO	0.0024
	S12	4.70	264	HOMO-1 to LUMO+2	0.0343
	S13	4.73	262	HOMO-8 to LUMO	0.0041
	S14	4.80	258	HOMO-3 to LUMO	0.2436
	S15	4.83	256	HOMO-2 to LUMO+1	0.0442
	S16	4.84	256	HOMO-2 to LUMO+1	0.002
	S17	4.94	251	HOMO-2 to LUMO+1	0.1356
	S18	5.07	244	HOMO-2 to LUMO+1	0.0726
	S19	5.19	239	HOMO-2 to LUMO+1	0.126
	S20	5.25	236	HOMO-2 to LUMO+1	0.0367
	S21	5.33	232	HOMO-3 to LUMO+1	0.0396
	S22	5.43	228	HOMO to LUMO+4	0.0001
	S23	5.48	226	HOMO-2 to LUMO+2	0.018
	S24	5.58	222	HOMO-2 to LUMO+2	0.0681
	S25	5.61	220	HOMO-3 to LUMO+2	0.0013
	S26	5.72	216	HOMO-2 to LUMO+2	0.012
	S27	5.75	215	HOMO-1 to LUMO+4	0.0004
	S28	5.77	214	HOMO-3 to LUMO+2	0.0452
	S29	5.79	213	HOMO-12 to LUMO	0.0019
	S30	5.87	211	HOMO-14 to LUMO	0.0007
DBCH ⁺	S1	1.48	836	HOMO to LUMO	0.1379
	S2	1.96	360	HOMO-1 to LUMO	0.2152
	S3	2.24	553	HOMO to LUMO	0.131
	S4	2.30	539	HOMO-3 to LUMO	0.0047
	S5	2.86	432	HOMO to LUMO+1	0.508
	S6	2.92	423	HOMO-1 to LUMO+1	0.0014
	S7	3.02	410	HOMO to LUMO+1	0.0665
	S8	3.04	407	HOMO-1 to LUMO+1	0.0003
	S9	3.21	386	HOMO-2 to LUMO+1	0.0567
	S10	3.23	383	HOMO-1 to LUMO+1	0.1114
	S11	3.26	379	HOMO-2 to LUMO+1	0.0014

	S12	3.31	374	HOMO-1 to LUMO+1	0.133
	S13	3.35	369	HOMO-3 to LUMO+1	0.0284
	S14	3.49	354	HOMO-1 to LUMO+1	0.1311
	S15	3.53	351	HOMO-2 to LUMO+1	0.0096
	S16	3.56	347	HOMO-2 to LUMO+1	0.0627
	S17	3.62	342	HOMO-1 to LUMO+1	0.0132
	S18	3.65	339	HOMO-2 to LUMO+2	0.2008
	S19	3.67	337	HOMO-2 to LUMO+1	0.0612
	S20	3.78	327	HOMO-1 to LUMO+3	0.0046
	S21	3.84	322	HOMO-3 to LUMO+2	0
	S22	3.89	318	HOMO-2 to LUMO+2	0.0412
	S23	3.90	318	HOMO-1 to LUMO+2	0.0271
	S24	4.03	307	HOMO-2 to LUMO+2	0.0492
	S25	4.10	302	HOMO-2 to LUMO+1	0.0206
	S26	4.11	301	HOMO-2 to LUMO+2	0.0211
	S27	4.15	298	HOMO-3 to LUMO+2	0.015
	S28	4.21	294	HOMO-4 to LUMO+1	0.0002
	S29	4.22	294	HOMO-2 to LUMO+2	0.0719
	S30	4.28	289	HOMO-3 to LUMO+3	0.0346
DBCH ⁺ -W ₁	S1	1.51	816	HOMO to LUMO	0.1436
	S2	1.98	624	HOMO to LUMO+1	0.2116
	S3	2.26	547	HOMO to LUMO	0.1273
	S4	2.33	530	HOMO-3 to LUMO+2	0.0054
	S5	2.87	432	HOMO to LUMO+1	0.5419
	S6	2.92	424	HOMO-1 to LUMO+1	0.0046
	S7	3.03	408	HOMO-4 to LUMO	0.0525
	S8	3.07	403	HOMO-3 to LUMO	0.0011
	S9	3.22	384	HOMO-2 to LUMO+1	0.0468
	S10	3.25	380	HOMO-4 to LUMO	0.1733
	S11	3.28	377	HOMO-2 to LUMO+1	0.0068
	S12	3.32	373	HOMO-3 to LUMO+1	0.0779
	S13	3.38	366	HOMO-3 to LUMO+1	0.0303
	S14	3.51	353	HOMO-1 to LUMO+1	0.1303
	S15	3.53	350	HOMO-2 to LUMO+1	0.0002
	S16	3.58	346	HOMO-2 to LUMO+1	0.0746
	S17	3.63	341	HOMO-1 to LUMO+1	0.0159
	S18	3.65	339	HOMO-3 to LUMO+1	0.1847
	S19	3.68	336	HOMO-1 to LUMO+2	0.0565
	S20	3.79	327	HOMO-1 to LUMO+3	0.0023
	S21	3.84	322	HOMO-3 to LUMO+2	0.0001

	S22	3.88	319	HOMO-2 to LUMO+2	0.0389
	S23	3.89	318	HOMO-1 to LUMO+2	0.0284
	S24	4.04	306	HOMO-2 to LUMO+2	0.0582
	S25	4.11	301	HOMO-2 to LUMO+1	0.0227
	S26	4.13	300	HOMO-2 to LUMO+2	0.0201
	S27	4.15	298	HOMO-3 to LUMO+2	0.0125
	S28	4.22	294	HOMO-3 to LUMO+2	0.0031
	S29	4.23	293	HOMO-2 to LUMO+2	0.0597
	S30	4.28	289	HOMO-2 to LUMO+2	0.0591
DBCH ⁺ -W ₂	S1	1.56	791	HOMO to LUMO	0.1509
	S2	2.00	617	HOMO to LUMO+1	0.2061
	S3	2.30	538	HOMO to LUMO	0.1211
	S4	2.38	519	HOMO-3 to LUMO	0.0061
	S5	2.87	432	HOMO to LUMO+1	0.5795
	S6	2.92	424	HOMO-1 to LUMO+1	0.012
	S7	3.05	405	HOMO-4 to LUMO	0.0342
	S8	3.11	399	HOMO-5 to LUMO	0.0003
	S9	3.23	383	HOMO-4 to LUMO	0.0353
	S10	3.27	378	HOMO-1 to LUMO+1	0.2536
	S11	3.31	373	HOMO-2 to LUMO+1	0.0141
	S12	3.34	371	HOMO-1 to LUMO+1	0.0111
	S13	3.41	363	HOMO-3 to LUMO+1	0.0261
	S14	3.52	352	HOMO-1 to LUMO+1	0.1286
	S15	3.53	351	HOMO-2 to LUMO+1	0.0023
	S16	3.60	344	HOMO-1 to LUMO+2	0.077
	S17	3.63	341	HOMO-1 to LUMO+1	0.0178
	S18	3.64	340	HOMO-2 to LUMO+2	0.1742
	S19	3.68	337	HOMO-2 to LUMO+1	0.0486
	S20	3.79	326	HOMO-1 to LUMO+3	0.0008
	S21	3.84	323	HOMO-3 to LUMO+2	0
	S22	3.88	319	HOMO-2 to LUMO+2	0.0349
	S23	3.89	318	HOMO-1 to LUMO+2	0.0303
	S24	4.05	306	HOMO-2 to LUMO+2	0.0634
	S25	4.12	301	HOMO-3 to LUMO+2	0.0266
	S26	4.16	298	HOMO-3 to LUMO+2	0.0092
	S27	4.17	298	HOMO-3 to LUMO+2	0.0166
	S28	4.21	293	HOMO-3 to LUMO+2	0.0069
	S29	4.23	293	HOMO-2 to LUMO+2	0.0426
	S30	4.27	290	HOMO-4 to LUMO+1	0.0802

DBCH ⁺ -W ₃	S1	1.57	785	HOMO to LUMO	0.1528
	S2	2.01	614	HOMO to LUMO+1	0.2061
	S3	2.30	537	HOMO to LUMO	0.1201
	S4	2.40	516	HOMO-3 to LUMO	0.0063
	S5	2.87	431	HOMO to LUMO+1	0.588
	S6	2.92	424	HOMO-1 to LUMO+1	0.0128
	S7	3.05	406	HOMO-4 to LUMO	0.0388
	S8	3.11	398	HOMO-5 to LUMO	0
	S9	3.24	382	HOMO-2 to LUMO	0.031
	S10	3.27	378	HOMO-1 to LUMO+1	0.2647
	S11	3.32	373	HOMO-2 to LUMO+1	0.0144
	S12	3.34	370	HOMO-1 to LUMO+1	0.006
	S13	3.42	362	HOMO-2 to LUMO+1	0.0269
	S14	3.52	351	HOMO-1 to LUMO+1	0.1345
	S15	3.53	351	HOMO-2 to LUMO+1	0.0028
	S16	3.61	343	HOMO-1 to LUMO+2	0.0798
	S17	3.63	341	HOMO-3 to LUMO+1	0.0215
	S18	3.65	339	HOMO-3 to LUMO+1	0.1519
	S19	3.68	336	HOMO-2 to LUMO+1	0.0481
	S20	3.81	325	HOMO-1 to LUMO+3	0.0002
	S21	3.84	323	HOMO-3 to LUMO+2	0.0001
	S22	3.88	319	HOMO-2 to LUMO+2	0.0354
	S23	3.89	318	HOMO-1 to LUMO+2	0.0301
	S24	4.04	306	HOMO-2 to LUMO+2	0.0706
	S25	4.13	300	HOMO-2 to LUMO+1	0.0222
	S26	4.16	297	HOMO-3 to LUMO+2	0.0089
	S27	4.17	297	HOMO-2 to LUMO+2	0.0197
	S28	4.22	293	HOMO-3 to LUMO+2	0.0098
	S29	4.24	292	HOMO-2 to LUMO+2	0.0441
	S30	4.27	290	HOMO-4 to LUMO+1	0.0642

Table S9: Triplet electronic states of BzH⁺-W_n, CorH⁺-W_n and DbcH⁺-W_n (n=0-3) clusters with excitation energies (E, in eV), transition wavelength (λ, in nm) and oscillator strength (f). We give also the corresponding electron promotion. These computations are done using the TD-DFT method at the PBE0/6-311++G** level.

Compound	State	E	λ	Electron promotion
BZH ⁺	T1	2.21	560	HOMO to LUMO
	T2	3.82	324	HOMO-1 to LUMO
	T3	4.48	276	HOMO to LUMO+1
	T4	4.82	257	HOMO-2 to LUMO
	T5	4.95	250	HOMO-3 to LUMO
BZH ⁺ -W ₁	T1	2.51	493	HOMO to LUMO
	T2	3.84	322	HOMO-2 to LUMO
	T3	4.35	285	HOMO to LUMO+1
	T4	4.77	260	HOMO-1 to LUMO
	T5	5.11	242	HOMO-3 to LUMO
	T6	5.16	240	HOMO-4 to LUMO
BZH ⁺ -W ₂	T1	2.52	492	HOMO to LUMO
	T2	3.85	322	HOMO-3 to LUMO
	T3	4.36	284	HOMO to LUMO+1
	T4	4.64	267	HOMO-1 to LUMO
	T5	4.65	266	HOMO-2 to LUMO
	T6	4.96	249	HOMO-4 to LUMO
	T7	5.07	244	HOMO-5 to LUMO
BZH ⁺ -W ₃	T1	2.65	467	HOMO to LUMO
	T2	3.78	328	HOMO to LUMO+1
	T3	4.35	284	HOMO to LUMO+1
	T4	4.63	267	HOMO-1 to LUMO
	T5	4.70	264	HOMO-2 to LUMO
	T6	5.00	248	HOMO-5 to LUMO
	T7	5.21	238	HOMO-6 to LUMO
	T8	5.86	211	HOMO-3 to LUMO
CORH ⁺	T1	1.20	1031	HOMO to LUMO
	T2	1.75	704	HOMO to LUMO
	T3	2.59	477	HOMO to LUMO+1
	T4	2.65	467	HOMO-2 to LUMO
	T5	2.87	430	HOMO to LUMO+1
	T6	2.97	416	HOMO-1 to LUMO+1
	T7	3.50	353	HOMO to LUMO+1

	T8	3.66	338	HOMO to LUMO+1
	T9	3.75	330	HOMO-3 to LUMO+1
	T10	3.84	322	HOMO-1 to LUMO+1
	T11	3.96	312	HOMO to LUMO+1
	T12	4.04	306	HOMO-1 to LUMO+1
	T13	4.30	288	HOMO-2 to LUMO+2
	T14	4.40	281	HOMO-1 to LUMO+3
	T15	4.46	278	HOMO-6 to LUMO
	T16	4.50	275	HOMO-1 to LUMO+3
	T17	4.57	271	HOMO-2 to LUMO+1
	T18	4.58	271	HOMO-2 to LUMO+1
	T19	4.68	264	HOMO-2 to LUMO+1
	T20	4.73	262	HOMO-2 to LUMO+2
	T21	4.83	256	HOMO-2 to LUMO+2
	T22	4.94	250	HOMO-2 to LUMO+1
	T23	5.05	245	HOMO-2 to LUMO+2
	T24	5.13	242	HOMO-3 to LUMO+1
	T25	5.15	241	HOMO-2 to LUMO+2
	T26	5.26	235	HOMO-2 to LUMO+2
	T27	5.36	231	HOMO-3 to LUMO+1
	T28	5.56	223	HOMO-10 to LUMO
	T29	5.57	222	HOMO-4 to LUMO+1
	T30	5.60	221	HOMO-6 to LUMO+1
CORH ⁺ -W ₁	T1	1.28	961	HOMO to LUMO
	T2	1.82	678	HOMO-1 to LUMO
	T3	2.61	473	HOMO to LUMO+1
	T4	2.73	453	HOMO-1 to LUMO
	T5	2.92	423	HOMO to LUMO+1
	T6	3.03	407	HOMO-1 to LUMO
	T7	3.50	353	HOMO to LUMO+1
	T8	3.66	338	HOMO-1 to LUMO+1
	T9	3.77	328	HOMO-1 to LUMO+1
	T10	3.84	322	HOMO-1 to LUMO+1
	T11	3.97	312	HOMO-1 to LUMO+2
	T12	4.04	306	HOMO-1 to LUMO+1
	T13	4.31	288	HOMO to LUMO+3
	T14	4.43	280	HOMO-2 to LUMO+1
	T15	4.49	275	HOMO-2 to LUMO+1
	T16	4.53	273	HOMO-7 to LUMO
	T17	4.57	271	HOMO-2 to LUMO+1

	T18	4.61	268	HOMO-8 to LUMO
	T19	4.69	264	HOMO-2 to LUMO+2
	T20	4.76	260	HOMO-2 to LUMO+3
	T21	4.77	259	HOMO-2 to LUMO+3
	T22	4.84	256	HOMO-2 to LUMO+3
	T23	4.95	250	HOMO-3 to LUMO+1
	T24	5.05	245	HOMO-3 to LUMO+1
	T25	5.11	242	HOMO-3 to LUMO+2
	T26	5.16	240	HOMO-2 to LUMO+2
	T27	5.27	235	HOMO-3 to LUMO+2
	T28	5.36	231	HOMO-3 to LUMO+2
	T29	5.57	222	HOMO-3 to LUMO+2
	T30	5.60	221	HOMO-3 to LUMO+2
CORH ⁺ -W ₂	T1	1.36	905	HOMO to LUMO
	T2	1.88	657	HOMO-1 to LUMO
	T3	2.62	472	HOMO to LUMO+1
	T4	2.80	442	HOMO-2 to LUMO
	T5	2.98	415	HOMO to LUMO+1
	T6	3.09	401	HOMO-1 to LUMO+1
	T7	3.50	354	HOMO to LUMO+1
	T8	3.66	338	HOMO to LUMO+1
	T9	3.78	327	HOMO-1 to LUMO+1
	T10	3.84	322	HOMO-1 to LUMO+1
	T11	3.99	310	HOMO to LUMO+1
	T12	4.04	306	HOMO-1 to LUMO+1
	T13	4.31	287	HOMO-3 to LUMO+1
	T14	4.45	278	HOMO-4 to LUMO+2
	T15	4.49	275	HOMO-1 to LUMO+2
	T16	4.57	271	HOMO-2 to LUMO+1
	T17	4.59	270	HOMO-9 to LUMO
	T18	4.65	266	HOMO-7 to LUMO
	T19	4.69	264	HOMO-4 to LUMO+1
	T20	4.78	259	HOMO to LUMO+1
	T21	4.86	255	HOMO-2 to LUMO+2
	T22	4.87	254	HOMO-6 to LUMO
	T23	4.88	254	HOMO-6 to LUMO
	T24	4.95	250	HOMO-2 to LUMO+1
	T25	5.06	245	HOMO-3 to LUMO+1
	T26	5.10	243	HOMO-3 to LUMO+1
	T27	5.18	239	HOMO-2 to LUMO+2

	T28	5.28	235	HOMO-3 to LUMO+2
	T29	5.36	231	HOMO-3 to LUMO+2
	T30	5.59	222	HOMO-2 to LUMO+2
CORH ⁺ -W ₃	T1	1.39	889	HOMO to LUMO
	T2	1.89	653	HOMO-1 to LUMO
	T3	2.63	471	HOMO to LUMO+1
	T4	2.81	441	HOMO-2 to LUMO
	T5	3.00	413	HOMO to LUMO+1
	T6	3.10	399	HOMO-1 to LUMO+1
	T7	3.49	354	HOMO-1 to LUMO+2
	T8	3.64	340	HOMO-1 to LUMO+1
	T9	3.78	327	HOMO-1 to LUMO+1
	T10	3.84	323	HOMO-1 to LUMO+1
	T11	3.99	311	HOMO-2 to LUMO+1
	T12	4.04	306	HOMO-1 to LUMO+1
	T13	4.31	287	HOMO-3 to LUMO+1
	T14	4.45	278	HOMO-2 to LUMO+1
	T15	4.47	277	HOMO-2 to LUMO+1
	T16	4.54	273	HOMO-2 to LUMO+1
	T17	4.58	271	HOMO-1 to LUMO+1
	T18	4.58	270	HOMO-6 to LUMO
	T19	4.60	269	HOMO-6 to LUMO
	T20	4.62	267	HOMO-6 to LUMO
	T21	4.68	265	HOMO-2 to LUMO
	T22	4.73	262	HOMO-2 to LUMO+1
	T23	4.79	259	HOMO-1 to LUMO+2
	T24	4.88	254	HOMO-2 to LUMO+2
	T25	4.95	250	HOMO-2 to LUMO+1
	T26	5.06	245	HOMO-2 to LUMO+2
	T27	5.09	243	HOMO-1 to LUMO+2
	T28	5.17	239	HOMO-2 to LUMO+1
	T29	5.27	235	HOMO-3 to LUMO+2
	T30	5.35	231	HOMO-3 to LUMO+2
	T31	5.42	228	HOMO to LUMO+4
DBCH ⁺	T1	0.87	1411	HOMO to LUMO
	T2	1.32	935	HOMO-1 to LUMO
	T3	1.76	703	HOMO to LUMO+1
	T4	1.93	640	HOMO to LUMO
	T5	2.10	589	HOMO to LUMO+1

	T6	2.43	509	HOMO-1 to LUMO+1
	T7	2.48	499	HOMO-2 to LUMO
	T8	2.56	483	HOMO-4 to LUMO
	T9	2.79	444	HOMO to LUMO+1
	T10	2.81	440	HOMO-1 to LUMO+1
	T11	2.88	429	HOMO-1 to LUMO
	T12	2.89	429	HOMO-1 to LUMO+1
	T13	2.96	418	HOMO-4 to LUMO
	T14	3.04	406	HOMO-1 to LUMO+2
	T15	3.12	396	HOMO-2 to LUMO+2
	T16	3.19	388	HOMO-2 to LUMO+1
	T17	3.28	378	HOMO-2 to LUMO+1
	T18	3.31	374	HOMO-1 to LUMO+1
	T19	3.38	366	HOMO-1 to LUMO+3
	T20	3.39	366	HOMO to LUMO+1
	T21	3.50	354	HOMO-2 to LUMO+1
	T22	3.51	353	HOMO-3 to LUMO+1
	T23	3.56	348	HOMO-1 to LUMO+2
	T24	3.58	346	HOMO-1 to LUMO+3
	T25	3.61	343	HOMO-2 to LUMO+3
	T26	3.62	342	HOMO-1 to LUMO+3
	T27	3.71	334	HOMO-2 to LUMO+1
	T28	3.75	330	HOMO-2 to LUMO+1
	T29	3.81	324	HOMO-2 to LUMO+2
	T30	3.85	322	HOMO-2 to LUMO+2
DBCH ⁺ -W ₁	T1	0.91	1356	HOMO to LUMO
	T2	1.35	912	HOMO-1 to LUMO
	T3	1.77	700	HOMO to LUMO+1
	T4	1.95	633	HOMO to LUMO
	T5	2.13	158	HOMO to LUMO+1
	T6	2.43	508	HOMO-1 to LUMO+1
	T7	2.48	499	HOMO-2 to LUMO+1
	T8	2.57	480	HOMO to LUMO+2
	T9	2.80	441	HOMO to LUMO+1
	T10	2.83	438	HOMO-1 to LUMO+1
	T11	2.89	429	HOMO-1 to LUMO+1
	T12	2.90	427	HOMO-1 to LUMO
	T13	2.99	414	HOMO to LUMO+2
	T14	3.06	405	HOMO to LUMO+1
	T15	3.14	394	HOMO-1 to LUMO+3

	T16	3.20	386	HOMO-2 to LUMO+1
	T17	3.28	377	HOMO-2 to LUMO+1
	T18	3.32	373	HOMO-1 to LUMO+3
	T19	3.39	366	HOMO to LUMO+1
	T20	3.40	364	HOMO-1 to LUMO+3
	T21	3.50	354	HOMO-1 to LUMO+4
	T22	3.51	353	HOMO-3 to LUMO+1
	T23	3.56	348	HOMO-2 to LUMO+3
	T24	3.59	345	HOMO-3 to LUMO+1
	T25	3.62	342	HOMO-2 to LUMO+3
	T26	3.63	341	HOMO-1 to LUMO+3
	T27	3.72	333	HOMO-2 to LUMO+1
	T28	3.75	330	HOMO-1 to LUMO+4
	T29	3.82	324	HOMO-1 to LUMO+3
	T30	3.86	321	HOMO-2 to LUMO+2
DBCH ⁺ -W ₂	T1	0.96	1287	HOMO to LUMO+1
	T2	1.39	886	HOMO-1 to LUMO
	T3	1.77	697	HOMO to LUMO+1
	T4	1.99	621	HOMO to LUMO
	T5	2.17	571	HOMO to LUMO+1
	T6	2.44	508	HOMO-1 to LUMO+1
	T7	2.48	498	HOMO-1 to LUMO+1
	T8	2.59	477	HOMO-1 to LUMO+1
	T9	2.83	438	HOMO to LUMO+1
	T10	2.84	435	HOMO-1 to LUMO+1
	T11	2.89	429	HOMO-1 to LUMO+1
	T12	2.91	425	HOMO to LUMO+1
	T13	3.02	410	HOMO to LUMO+2
	T14	3.07	402	HOMO to LUMO+1
	T15	3.17	391	HOMO-2 to LUMO+2
	T16	3.21	385	HOMO-2 to LUMO+1
	T17	3.29	377	HOMO-2 to LUMO+1
	T18	3.33	372	HOMO-1 to LUMO+1
	T19	3.38	366	HOMO to LUMO+1
	T20	3.40	346	HOMO-2 to LUMO+2
	T21	3.49	354	HOMO-2 to LUMO+1
	T22	3.51	352	HOMO-3 to LUMO+1
	T23	3.56	348	HOMO-1 to LUMO+2
	T24	3.59	354	HOMO-3 to LUMO+1
	T25	3.63	341	HOMO-1 to LUMO+2

	T26	3.64	340	HOMO-2 to LUMO+2
	T27	3.72	332	HOMO-2 to LUMO+1
	T28	3.75	330	HOMO-1 to LUMO+2
	T29	3.82	324	HOMO-2 to LUMO+2
	T30	3.87	320	HOMO-2 to LUMO+2
DBCH ⁺ -W ₃	T1	0.97	1273	HOMO to LUMO
	T2	1.41	879	HOMO-1 to LUMO
	T3	1.78	696	HOMO to LUMO+1
	T4	1.99	621	HOMO to LUMO
	T5	2.18	568	HOMO to LUMO+1
	T6	2.44	507	HOMO-1 to LUMO+1
	T7	2.47	500	HOMO-1 to LUMO+2
	T8	2.59	477	HOMO-1 to LUMO+1
	T9	2.83	438	HOMO to LUMO+1
	T10	2.84	435	HOMO-1 to LUMO+1
	T11	2.89	429	HOMO-1 to LUMO+1
	T12	2.92	424	HOMO-1 to LUMO+1
	T13	3.03	409	HOMO to LUMO+2
	T14	3.08	402	HOMO to LUMO+1
	T15	3.17	390	HOMO-2 to LUMO+2
	T16	3.22	384	HOMO-2 to LUMO+1
	T17	3.29	376	HOMO-2 to LUMO+1
	T18	3.34	371	HOMO-1 to LUMO+1
	T19	3.38	366	HOMO to LUMO+1
	T20	3.41	363	HOMO-2 to LUMO+2
	T21	3.49	354	HOMO-2 to LUMO+1
	T22	3.52	352	HOMO to LUMO+4
	T23	3.59	345	HOMO-3 to LUMO+1
	T24	3.63	341	HOMO-1 to LUMO+2
	T25	3.65	340	HOMO-2 to LUMO+2
	T26	3.72	333	HOMO-2 to LUMO+1
	T27	3.76	329	HOMO-1 to LUMO+2
	T28	3.82	324	HOMO-1 to LUMO+3
	T39	3.87	320	HOMO-2 to LUMO+2