Supplementary Materials

Quantum-Chemical Search for Keto Tautomers of Azulenols in *Vacuo* and Aqueous Solution

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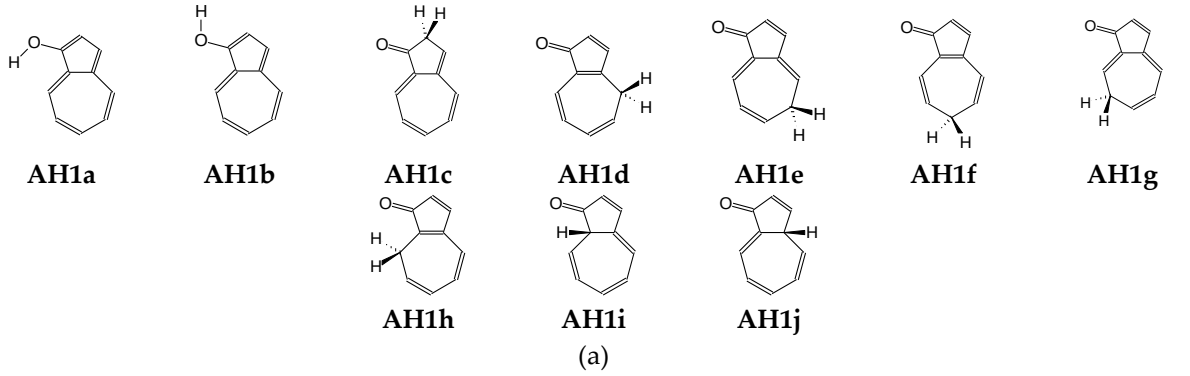
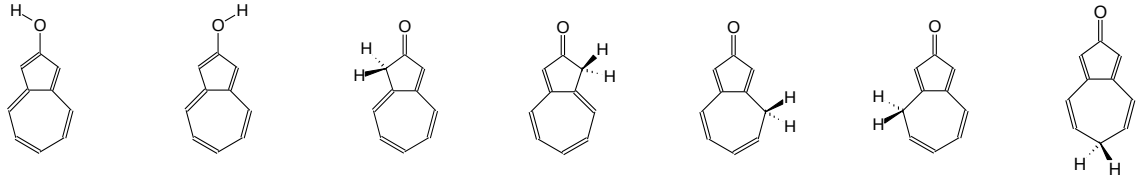


AH1a **AH1b** **AH1c** **AH1d** **AH1e** **AH1f** **AH1g**

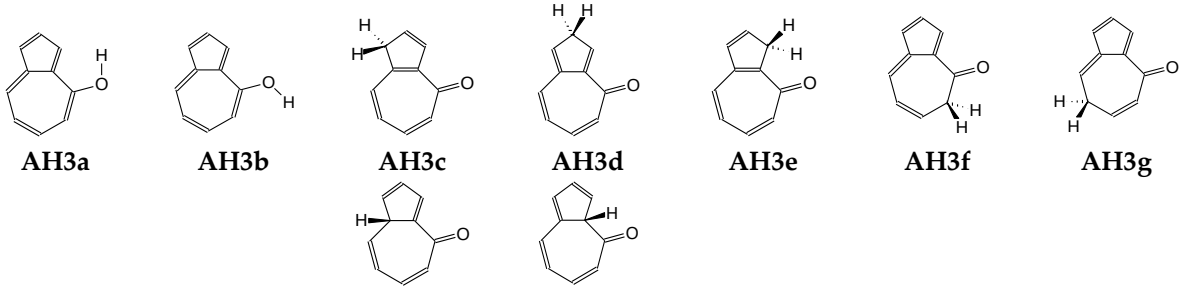
AH1h **AH1i** **AH1j**

(a)



AH2a **AH2b** **AH2c** **AH2d** **AH2e** **AH2f** **AH2g**

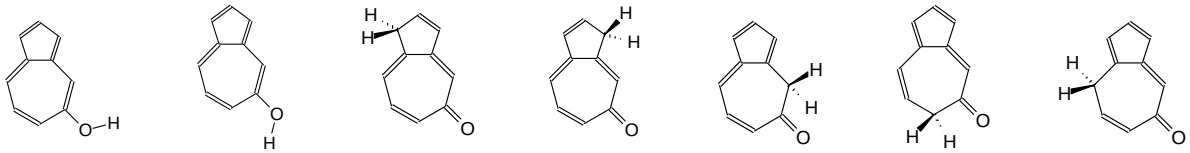
(**b**)



AH3a **AH3b** **AH3c** **AH3d** **AH3e** **AH3f** **AH3g**

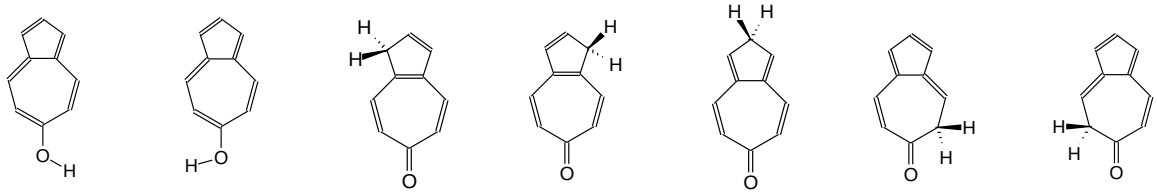
AH3h **AH3i**

(**c**)



AH4a **AH4b** **AH4c** **AH4d** **AH4e** **AH4f** **AH4g**

(**d**)



AH5a **AH5b** **AH5c** **AH5d** **AH5e** **AH5f** **AH5g**

AH5h **AH5i**

(**e**)

Figure S1. The Lewis structures of all possible neutral isomers of investigated azulenols: **AH1** (**a**), AH2 (**b**), **AH3** (c), **AH4** (**d**), and **AH5** (**e**).

PCM parameters

Polarizable Continuum Model (PCM)

Model:	PCM
Atomic radii:	UA0 (Simple United Atom Topological Model)
Polarization charges:	Total charges
Charge compensation:	None
Solution method:	Matrix inversion
Cavity:	GePol (RMin=0.200 OFac=0.890)
	Default sphere list used, NSphG= 9
	Tesserae with average area of 0.200 Ang**2
1st derivatives:	Analytical V*U(x)*V algorithm (CHGder, D1EAlg=0)
	Cavity 1st derivative terms included
Solvent:	Water
	Eps = 78.390000
	Eps(inf)= 1.776000
	RSolv = 1.385000 Ang

Table S1 The atom coordinates for all possible isolated and hydrated structures of neutral isomers of investigated azulenols optimized in *vacuo* {DFT(B3LYP)/6-311+G(d,p)} and aqueous solution {PCM(water)//DFT(B3LYP)/6-311+G(d,p)}.

(**a**) Enol isomers

DFT(B3LYP)/6-311+G(d,p)				**PCM(water)//DFT(B3LYP)/6-311+G(d,p)**			
		AH1a				**AH1a**	
C	0.288578	-0.461780	0.000000	C	0.285626	-0.463968	0.000000
C	0.293784	1.042679	0.000000	C	0.291165	1.040622	0.000000
C	1.643410	1.442095	0.000000	C	1.641169	1.443651	0.000000
C	2.454110	0.303581	0.000000	C	2.453025	0.303564	0.000000
C	1.640623	-0.843036	0.000000	C	1.640674	-0.846378	0.000000
C	-0.819358	-1.301120	0.000000	C	-0.825118	-1.302827	0.000000
C	-2.173422	-0.973823	0.000000	C	-2.179604	-0.969894	0.000000
C	-2.759871	0.299698	0.000000	C	-2.765933	0.304994	0.000000
C	-2.168665	1.557800	0.000000	C	-2.172102	1.564590	0.000000
C	-0.802091	1.883460	0.000000	C	-0.804660	1.886747	0.000000
H	1.987215	2.466683	0.000000	H	1.983527	2.472407	0.000000
H	3.535222	0.282947	0.000000	H	3.538490	0.287314	0.000000
O	2.167093	-2.102180	0.000000	O	2.183126	-2.098956	0.000000
H	-0.613614	-2.371936	0.000000	H	-0.616536	-2.375723	0.000000
H	-2.863669	-1.810981	0.000000	H	-2.872578	-1.808456	0.000000
H	-3.846858	0.301601	0.000000	H	-3.855983	0.308007	0.000000
H	-2.851883	2.401078	0.000000	H	-2.854819	2.411963	0.000000
H	-0.570728	2.946541	0.000000	H	-0.570098	2.952518	0.000000
H	1.461772	-2.756847	0.000000	H	1.502276	-2.803714	0.000000
		AH1b				**AH1b**	
C	0.310503	-0.441588	0.000000	C	0.310720	-0.445578	0.000000
C	0.307575	1.058777	0.000000	C	0.305874	1.056391	0.000000
C	1.651108	1.467007	0.000000	C	1.651110	1.466839	0.000000
C	2.471417	0.327444	0.000000	C	2.473639	0.328051	0.000000
C	1.663511	-0.820229	0.000000	C	1.666994	-0.823648	0.000000
C	-0.776138	-1.302412	0.000000	C	-0.780797	-1.304713	0.000000
C	-2.137326	-0.987866	0.000000	C	-2.142232	-0.987802	0.000000
C	-2.735241	0.275445	0.000000	C	-2.740570	0.278371	0.000000
C	-2.158457	1.546007	0.000000	C	-2.161774	1.548762	0.000000
C	-0.801490	1.889581	0.000000	C	-0.801940	1.890841	0.000000
H	1.992047	2.492581	0.000000	H	1.989612	2.496755	0.000000
H	3.554750	0.330110	0.000000	H	3.559880	0.324967	0.000000
O	2.060904	-2.128767	0.000000	O	2.072138	-2.126583	0.000000
H	-0.528169	-2.360914	0.000000	H	-0.542535	-2.368533	0.000000
H	-2.818269	-1.832811	0.000000	H	-2.825806	-1.834092	0.000000
H	-3.822412	0.267119	0.000000	H	-3.830524	0.270525	0.000000
H	-2.854533	2.378790	0.000000	H	-2.857752	2.385146	0.000000
H	-0.583572	2.955686	0.000000	H	-0.581702	2.959536	0.000000
H	3.021741	-2.175111	0.000000	H	3.053614	-2.176386	0.000000
		AH2a/AH2b				**AH2a/AH2b**	
C	0.294012	-0.480525	0.012677	C	0.292232	-0.481323	0.012830
C	0.291764	1.019133	0.017364	C	0.291972	1.018608	0.017559
C	1.634318	1.425057	0.031580	C	1.635324	1.426512	0.031721

C	2.431971	0.267360	0.035577	C	2.434901	0.267888	0.035697
C	1.632405	-0.887655	0.024227	C	1.632803	-0.889358	0.024468
C	-0.817245	-1.322130	-0.000655	C	-0.818823	-1.325670	-0.000645
C	-2.171047	-0.992345	-0.012640	C	-2.174334	-0.994752	-0.012785
C	-2.769162	0.270133	-0.014425	C	-2.772235	0.269345	-0.014581
C	-2.172621	1.530249	-0.004728	C	-2.174517	1.531471	-0.004724
C	-0.815990	1.860265	0.009356	C	-0.817009	1.862583	0.009537
H	1.986860	2.447831	0.038215	H	1.993173	2.450333	0.038326
O	3.784832	0.208423	0.048402	O	3.784790	0.207687	0.048262
H	1.997803	-1.903844	0.024519	H	1.993134	-1.911437	0.024697
H	-0.590953	-2.385991	-0.001834	H	-0.592284	-2.392591	-0.001816
H	-2.856418	-1.834646	-0.021883	H	-2.861547	-1.839061	-0.022158
H	-3.855559	0.269685	-0.024874	H	-3.861471	0.269236	-0.025203
H	-2.857405	2.373082	-0.008660	H	-2.861024	2.376391	-0.008730
H	-0.590793	2.924493	0.014881	H	-0.591193	2.929627	0.015099
H	4.149840	1.099656	0.054741	H	4.172721	1.112743	0.054287
		AH3a				**AH3a**	
C	-1.501091	-0.452080	0.105371	C	-1.507903	-0.452011	0.106719
C	-1.482179	1.028375	0.210293	C	-1.481562	1.030674	0.210600
C	-2.782927	1.420941	0.585948	C	-2.781832	1.429826	0.587531
C	-3.577361	0.278583	0.712497	C	-3.582967	0.288576	0.713065
C	-2.808598	-0.862505	0.422980	C	-2.817921	-0.856553	0.425568
C	0.888598	-0.910079	-0.564998	C	0.882740	-0.907239	-0.563307
C	1.452398	0.354675	-0.621188	C	1.449615	0.357318	-0.620946
C	0.889068	1.613033	-0.377703	C	0.889618	1.619019	-0.377799
C	-0.417903	1.902829	-0.008149	C	-0.417334	1.909218	-0.007571
H	-4.622938	0.266667	0.990011	H	-4.632076	0.280555	0.991091
H	1.535351	-1.748709	-0.799525	H	1.536986	-1.743836	-0.799532
H	2.502557	0.367068	-0.899913	H	2.502567	0.365988	-0.901120
H	-0.651668	2.955725	0.132347	H	-0.652305	2.964937	0.133957
H	-3.097686	2.442665	0.745751	H	-3.089695	2.457174	0.747060
H	-3.191237	-1.875175	0.449577	H	-3.193137	-1.875115	0.449837
H	1.556310	2.460873	-0.492385	H	1.560063	2.467720	-0.493402
C	-0.426845	-1.281208	-0.242270	C	-0.434009	-1.286169	-0.240405
O	-0.616119	-2.627843	-0.291975	O	-0.602271	-2.632435	-0.294507
H	-1.528451	-2.838294	-0.064680	H	-1.509298	-2.922108	-0.074851
		AH3b				**AH3b**	
C	-1.501738	-0.436788	0.087321	C	-1.501454	-0.436202	0.087526
C	-1.479939	1.046245	0.213781	C	-1.479830	1.042720	0.213607
C	-2.783052	1.427694	0.598424	C	-2.783974	1.429889	0.598734
C	-3.571557	0.279866	0.708102	C	-3.576140	0.281540	0.709668
C	-2.800199	-0.857247	0.399085	C	-2.804375	-0.856892	0.400585
C	0.879618	-0.888693	-0.593646	C	0.883844	-0.887889	-0.594129
C	1.448978	0.380252	-0.633598	C	1.449443	0.381286	-0.633309
C	0.891422	1.632336	-0.371874	C	0.890003	1.637165	-0.371150
C	-0.419438	1.920183	0.006466	C	-0.418601	1.924130	0.006452
H	-4.616719	0.262635	0.987737	H	-4.624642	0.265111	0.990313
H	1.548816	-1.708613	-0.846844	H	1.550557	-1.713307	-0.846908
H	2.498332	0.392144	-0.914847	H	2.501898	0.394489	-0.915107
H	-0.648790	2.971897	0.162027	H	-0.651715	2.978150	0.162842
H	-3.100633	2.445833	0.774737	H	-3.097221	2.452977	0.774028

H	-3.139240	-1.881518	0.398871	H	-3.150431	-1.882220	0.402369
H	1.559768	2.480235	-0.476014	H	1.560511	2.487143	-0.476004
C	-0.434288	-1.266113	-0.273843	C	-0.430973	-1.270894	-0.274974
O	-0.741589	-2.593526	-0.309636	O	-0.736465	-2.590895	-0.311142
H	0.034656	-3.104492	-0.564068	H	0.043971	-3.133971	-0.571220
		AH4a				**AH4a**	
C	0.331541	-0.500928	0.000000	C	0.332201	-0.503257	0.000000
C	0.325380	1.001302	0.000000	C	0.323663	0.996557	0.000000
C	1.670233	1.406995	0.000000	C	1.670851	1.407098	0.000000
C	2.478662	0.259227	0.000000	C	2.482178	0.259828	0.000000
C	1.680470	-0.894224	0.000000	C	1.683955	-0.896984	0.000000
C	-0.775524	-1.337959	0.000000	C	-0.775495	-1.343738	0.000000
C	-2.130206	-0.993783	0.000000	C	-2.130047	-0.996728	0.000000
C	-2.726673	0.262109	0.000000	C	-2.726867	0.261653	0.000000
C	-2.136470	1.529846	0.000000	C	-2.138959	1.532921	0.000000
C	-0.776418	1.846463	0.000000	C	-0.775811	1.846364	0.000000
H	2.014047	2.431828	0.000000	H	2.009176	2.436949	0.000000
H	3.561256	0.264362	0.000000	H	3.568207	0.267028	0.000000
H	2.031906	-1.916260	0.000000	H	2.035446	-1.922382	0.000000
H	-0.559117	-2.403674	0.000000	H	-0.559714	-2.412676	0.000000
H	-2.823653	-1.828887	0.000000	H	-2.826379	-1.833135	0.000000
H	-3.812074	0.284233	0.000000	H	-3.815992	0.274957	0.000000
H	-0.540028	2.911134	0.000000	H	-0.544526	2.914822	0.000000
O	-3.057136	2.556489	0.000000	O	-3.054290	2.560231	0.000000
H	-2.604407	3.405717	0.000000	H	-2.605810	3.434482	0.000000
		AH4b				**AH4b**	
C	0.319353	-0.500449	0.000000	C	0.321070	-0.500203	0.000000
C	0.302825	1.002607	0.000000	C	0.304063	1.000116	0.000000
C	1.651015	1.417650	0.000000	C	1.653757	1.418079	0.000000
C	2.461635	0.279175	0.000000	C	2.467162	0.277800	0.000000
C	1.665516	-0.883353	0.000000	C	1.670994	-0.885753	0.000000
C	-0.786491	-1.347261	0.000000	C	-0.785198	-1.348881	0.000000
C	-2.136812	-1.010588	0.000000	C	-2.137176	-1.009778	0.000000
C	-2.738889	0.250810	0.000000	C	-2.741301	0.250557	0.000000
C	-2.157677	1.516969	0.000000	C	-2.159762	1.520028	0.000000
C	-0.793861	1.843099	0.000000	C	-0.794437	1.843507	0.000000
H	1.985259	2.445341	0.000000	H	1.985636	2.449960	0.000000
H	3.544215	0.287692	0.000000	H	3.553174	0.287325	0.000000
H	2.025064	-1.902701	0.000000	H	2.028862	-1.909029	0.000000
H	-0.563571	-2.411512	0.000000	H	-0.562678	-2.416362	0.000000
H	-2.829537	-1.846196	0.000000	H	-2.831847	-1.847525	0.000000
H	-3.828003	0.240409	0.000000	H	-3.832884	0.246055	0.000000
H	-0.591175	2.910862	0.000000	H	-0.583297	2.913524	0.000000
O	-2.972159	2.629521	0.000000	O	-2.974036	2.627208	0.000000
H	-3.896637	2.361645	0.000000	H	-3.922032	2.367094	0.000000
		AH6a/AH6b				**AH6a/AH6b**	
C	0.336219	-0.475495	0.000000	C	0.338626	-0.472764	0.000000
C	0.332973	1.011194	0.000000	C	0.335839	1.010630	0.000000
C	1.677912	1.416848	0.000000	C	1.683226	1.419594	0.000000
C	2.490683	0.270531	0.000000	C	2.497122	0.271694	0.000000
C	1.686029	-0.877046	0.000000	C	1.690009	-0.877593	0.000000

C	-0.771273	-1.315194	0.000000	C	-0.771771	-1.316066	0.000000
C	-2.126795	-0.998371	0.000000	C	-2.126683	-1.002259	0.000000
C	-2.732448	0.265565	0.000000	C	-2.736346	0.262868	0.000000
C	-2.132215	1.532670	0.000000	C	-2.131096	1.532728	0.000000
C	-0.780659	1.848927	0.000000	C	-0.780328	1.850810	0.000000
H	2.020047	2.442691	0.000000	H	2.023105	2.449553	0.000000
H	3.572802	0.273769	0.000000	H	3.582633	0.274603	0.000000
H	2.032173	-1.901502	0.000000	H	2.033110	-1.906404	0.000000
H	-0.548098	-2.379864	0.000000	H	-0.547846	-2.383823	0.000000
H	-2.809701	-1.845505	0.000000	H	-2.815513	-1.847541	0.000000
O	-4.098963	0.325815	0.000000	O	-4.095613	0.325227	0.000000
H	-2.835680	2.357880	0.000000	H	-2.831756	2.364803	0.000000
H	-0.557972	2.913666	0.000000	H	-0.558715	2.919023	0.000000
H	-4.468624	-0.563719	0.000000	H	-4.501596	-0.572221	0.000000

(**b**) Keto isomers

AH1c				**AH1c**			
C	0.286874	-0.469963	0.016246	C	0.291257	-0.473298	0.016376
C	0.367316	0.997355	-0.019107	C	0.368637	0.998094	-0.019219
C	1.662812	1.401282	-0.032564	C	1.663382	1.404398	-0.033091
C	2.618780	0.243030	-0.007674	C	2.614303	0.242198	-0.008097
C	1.698494	-0.980893	0.024580	C	1.697008	-0.975607	0.025198
C	-0.771735	-1.309618	0.039305	C	-0.771792	-1.312181	0.038983
C	-2.176653	-0.975164	0.035214	C	-2.176156	-0.978158	0.034567
C	-2.737503	0.259071	0.007304	C	-2.735408	0.259275	0.007111
C	-2.098694	1.562988	-0.025589	C	-2.098551	1.564572	-0.025136
C	-0.784558	1.883079	-0.036961	C	-0.782943	1.885173	-0.036604
H	1.979407	2.436108	-0.058295	H	1.984456	2.440754	-0.059009
H	3.278235	0.231084	0.868506	H	3.275994	0.231616	0.868478
O	2.044698	-2.141312	0.051062	O	2.055360	-2.142974	0.054121
H	-0.523466	-2.368012	0.063965	H	-0.537131	-2.376576	0.063774
H	-2.856840	-1.820833	0.057298	H	-2.857337	-1.826579	0.056198
H	-3.823163	0.292298	0.009523	H	-3.824277	0.293147	0.009245
H	-2.791817	2.398761	-0.043557	H	-2.795128	2.401101	-0.042604
H	-0.541007	2.942491	-0.062939	H	-0.537034	2.947274	-0.062222
H	3.272830	0.188927	-0.886319	H	3.269370	0.188450	-0.888069
AH1d				**AH1d**			
C	-0.161715	-0.433950	-0.300535	C	-0.160642	-0.437371	-0.306822
C	-0.166952	0.927279	-0.289520	C	-0.162955	0.925562	-0.293263
C	-1.573880	1.415118	-0.208690	C	-1.571053	1.418111	-0.202367
C	-2.430951	0.383533	-0.236257	C	-2.428573	0.385610	-0.230602
C	-1.612073	-0.877323	-0.322379	C	-1.610126	-0.869442	-0.321992
C	0.956195	-1.318222	-0.251184	C	0.959158	-1.321379	-0.257942
C	2.169890	-1.002781	0.292036	C	2.171211	-1.002479	0.292005
C	2.500087	0.232729	0.963352	C	2.493460	0.232827	0.968319
C	1.967124	1.454003	0.741208	C	1.957013	1.454173	0.743042
C	1.064166	1.766585	-0.430600	C	1.065749	1.764116	-0.439665
H	-1.831401	2.466378	-0.165663	H	-1.825186	2.473771	-0.154053
H	-3.510468	0.397032	-0.223930	H	-3.512197	0.400494	-0.214120
O	-2.022630	-2.010937	-0.412022	O	-2.028268	-2.008602	-0.408301
H	0.779586	-2.343419	-0.563106	H	0.794653	-2.349815	-0.576852

H	2.902445	-1.801002	0.367342	H	2.908102	-1.800630	0.368013
H	2.210835	2.264920	1.420750	H	2.189908	2.269485	1.425813
H	1.570552	1.520876	-1.373706	H	1.576909	1.508860	-1.378301
H	3.234569	0.147649	1.761020	H	3.227925	0.148253	1.770238
H	0.816680	2.829651	-0.457267	H	0.816971	2.826575	-0.472300
		AH1e				**AH1e**	
C	-0.212384	-0.452907	0.132961	C	-0.226789	-0.466078	0.112599
C	-0.232309	0.997283	-0.050771	C	-0.238598	0.991571	-0.043433
C	-1.649241	1.378666	-0.162754	C	-1.650364	1.382634	-0.134243
C	-2.461664	0.325102	0.056339	C	-2.467342	0.321768	0.060234
C	-1.643451	-0.892955	0.294579	C	-1.654182	-0.892746	0.263506
C	0.802230	-1.317022	-0.098387	C	0.790635	-1.328466	-0.119046
C	2.124215	-0.963172	-0.572626	C	2.127277	-0.976968	-0.554653
C	2.729310	0.234365	-0.457792	C	2.735645	0.220107	-0.436419
C	2.213040	1.397970	0.357625	C	2.220515	1.420601	0.324174
C	0.820815	1.835534	-0.033478	C	0.810789	1.834520	-0.022694
H	-1.966689	2.397199	-0.352209	H	-1.966443	2.410477	-0.295221
H	-3.542366	0.322367	0.080045	H	-3.552010	0.326335	0.088509
O	-2.040561	-2.016627	0.534732	O	-2.064169	-2.030307	0.485949
H	0.556739	-2.374919	-0.042570	H	0.553664	-2.392302	-0.083479
H	2.654837	-1.746828	-1.106767	H	2.678475	-1.773990	-1.052711
H	3.687499	0.370979	-0.950597	H	3.721596	0.330135	-0.886494
H	2.902358	2.239201	0.268719	H	2.895528	2.263069	0.161665
H	0.659175	2.890937	-0.235691	H	0.629956	2.896250	-0.190071
H	2.206479	1.113877	1.420491	H	2.263848	1.202439	1.403678
		AH1f				**AH1f**	
C	0.257027	-0.452459	-0.037421	C	0.258373	-0.456799	-0.034544
C	0.284681	0.923443	-0.044501	C	0.283880	0.921311	-0.046475
C	1.709767	1.371923	0.065571	C	1.711102	1.373638	0.057619
C	2.534221	0.319825	0.143264	C	2.534644	0.319745	0.141223
C	1.692891	-0.921546	0.048953	C	1.690972	-0.915019	0.057814
C	-0.849804	-1.313000	-0.314857	C	-0.850621	-1.315464	-0.316926
C	-2.141348	-0.977137	-0.092105	C	-2.143137	-0.974817	-0.095899
C	-2.517784	0.256806	0.691801	C	-2.516459	0.254287	0.697638
C	-2.114479	1.470382	-0.104666	C	-2.114976	1.464909	-0.103861
C	-0.818431	1.792682	-0.328133	C	-0.816687	1.790546	-0.327436
H	1.992972	2.417237	0.086010	H	1.993207	2.423200	0.069228
H	3.609095	0.307178	0.245111	H	3.613655	0.307744	0.243095
O	2.080466	-2.068078	0.017767	O	2.085185	-2.068848	0.046450
H	-0.614773	-2.280331	-0.750147	H	-0.625423	-2.282126	-0.767171
H	-2.935380	-1.620480	-0.457624	H	-2.942014	-1.609973	-0.473838
H	-1.987755	0.255717	1.653089	H	-1.981151	0.251470	1.656575
H	-2.895605	2.117744	-0.491909	H	-2.900154	2.113239	-0.490010
H	-0.588430	2.748199	-0.793644	H	-0.584464	2.753503	-0.783494
H	-3.588091	0.271745	0.900960	H	-3.586692	0.269306	0.907530
		AH1g				**AH1g**	
C	-0.163436	-0.488643	0.028520	C	-0.215393	-0.479628	-0.094423
C	-0.210516	0.947637	-0.249071	C	-0.235825	0.996822	-0.063521
C	-1.624940	1.327287	-0.211426	C	-1.624786	1.381780	0.110675
C	-2.409382	0.290304	0.156320	C	-2.440184	0.296559	0.187368
C	-1.567813	-0.909104	0.389289	C	-1.639249	-0.927021	0.067238

C	0.856044	-1.344161	-0.118860	C	0.803830	-1.335966	-0.232563
C	2.187822	-0.990714	-0.731923	C	2.267517	-1.067500	-0.402141
C	2.813870	0.274801	-0.190025	C	2.808215	0.336461	-0.442013
C	2.224118	1.481234	-0.092601	C	2.204634	1.537257	-0.347243
C	0.831842	1.814327	-0.318034	C	0.799672	1.861245	-0.171684
H	-1.964669	2.334781	-0.421042	H	-1.942756	2.420020	0.169005
H	-3.482200	0.292904	0.288408	H	-3.517524	0.297986	0.316634
O	-1.927395	-2.006794	0.767179	O	-2.046022	-2.089500	0.092844
H	0.678805	-2.381272	0.156597	H	0.544902	-2.396888	-0.222006
H	2.047781	-0.888057	-1.819459	H	2.597109	-1.586488	-1.317362
H	3.856853	0.200779	0.103291	H	3.890871	0.357675	-0.572403
H	2.849467	2.311521	0.225569	H	2.859802	2.404933	-0.410501
H	0.599858	2.870758	-0.427663	H	0.563499	2.924200	-0.123125
H	2.882782	-1.822086	-0.598625	H	2.800578	-1.616445	0.391665
		AH1h				**AH1h**	
C	-0.143120	-0.368260	0.376913	C	-0.145319	-0.373528	0.371638
C	-0.190682	0.990345	0.401088	C	-0.190322	0.987669	0.401907
C	-1.634615	1.420907	0.413797	C	-1.635482	1.423892	0.420930
C	-2.436770	0.352946	0.355322	C	-2.437138	0.354711	0.357672
C	-1.557208	-0.872257	0.318347	C	-1.555895	-0.865198	0.313287
C	1.086152	-1.207573	0.496516	C	1.087044	-1.210271	0.496046
C	1.989629	-0.867359	-0.664730	C	1.993126	-0.871331	-0.664204
C	2.491698	0.367187	-0.884266	C	2.492943	0.366008	-0.884274
C	2.133831	1.590259	-0.203339	C	2.131711	1.589179	-0.205691
C	0.923115	1.888866	0.355383	C	0.919093	1.888271	0.355806
H	-1.937481	2.460238	0.444583	H	-1.934908	2.467728	0.460335
H	-3.515295	0.315163	0.319194	H	-3.519898	0.317331	0.322430
O	-1.913524	-2.029634	0.267439	O	-1.923917	-2.027835	0.256680
H	0.815275	-2.264737	0.485965	H	0.827126	-2.270858	0.487137
H	2.263053	-1.668338	-1.345469	H	2.274931	-1.677257	-1.340658
H	2.854986	2.400066	-0.272087	H	2.850588	2.404336	-0.282159
H	3.227629	0.476494	-1.677206	H	3.236596	0.476169	-1.674071
H	0.755590	2.911061	0.684236	H	0.745253	2.914694	0.677158
H	1.597848	-1.002956	1.446453	H	1.594578	-1.001290	1.448168
		AH1i				**AH1i**	
C	0.183640	-0.586138	0.429513	C	0.186410	-0.586483	0.421688
C	0.208306	0.926595	0.363623	C	0.210838	0.926036	0.353092
C	1.591479	1.349248	0.463851	C	1.591023	1.348924	0.451113
C	2.440758	0.297201	0.536655	C	2.439784	0.291155	0.533094
C	1.681128	-0.962127	0.439619	C	1.677870	-0.955679	0.454538
C	-0.595871	-1.225872	-0.685204	C	-0.590785	-1.221382	-0.699687
C	-1.865918	-0.909923	-0.999434	C	-1.865640	-0.908535	-1.003438
C	-2.672882	0.150893	-0.431615	C	-2.673910	0.145427	-0.421497
C	-2.241562	1.312001	0.132530	C	-2.241555	1.308065	0.143073
C	-0.874368	1.737253	0.295098	C	-0.873659	1.737632	0.292221
H	1.883269	2.393456	0.477493	H	1.886242	2.396148	0.464107
H	3.519896	0.331221	0.595796	H	3.522471	0.328067	0.599690
O	2.121287	-2.089044	0.347860	O	2.119923	-2.097609	0.402514
H	-0.096522	-2.027159	-1.222099	H	-0.092389	-2.012623	-1.258362
H	-3.746039	0.043769	-0.564035	H	-3.750119	0.035000	-0.550084
H	-3.000229	2.042330	0.398804	H	-3.001295	2.039228	0.415430

H	-0.706463	2.810171	0.359954	H	-0.705087	2.813433	0.357298
H	-2.354981	-1.510454	-1.762297	H	-2.358295	-1.504347	-1.771991
H	-0.227028	-0.909033	1.399177	H	-0.233927	-0.908070	1.392491
		AH1j				**AH1j**	
C	0.213933	-0.461576	0.234982	C	0.217476	-0.464111	0.233563
C	0.192398	1.043204	0.349370	C	0.196815	1.041936	0.343669
C	1.663738	1.387658	0.451676	C	1.664344	1.386744	0.443199
C	2.453129	0.306391	0.408635	C	2.452832	0.300161	0.408997
C	1.632189	-0.927105	0.275486	C	1.629658	-0.920442	0.280514
C	-0.871211	-1.260633	0.186150	C	-0.871486	-1.263596	0.189509
C	-2.233108	-0.805506	0.072808	C	-2.233276	-0.809690	0.072657
C	-2.642283	0.359221	-0.505840	C	-2.640915	0.354736	-0.511749
C	-1.806008	1.357198	-1.137246	C	-1.807018	1.359284	-1.137704
C	-0.519838	1.633747	-0.843998	C	-0.520830	1.640211	-0.842973
H	2.004328	2.412909	0.544807	H	2.007585	2.415456	0.528218
H	3.533282	0.283951	0.464876	H	3.536866	0.278645	0.468333
O	2.029759	-2.076779	0.239094	O	2.034732	-2.082187	0.249837
H	-0.698515	-2.333942	0.220666	H	-0.711493	-2.341946	0.231865
H	-3.004630	-1.511004	0.367366	H	-3.005969	-1.519855	0.363012
H	-3.713489	0.495514	-0.627185	H	-3.714845	0.486856	-0.640784
H	-2.268991	1.910173	-1.950773	H	-2.276953	1.922286	-1.944293
H	0.029781	2.325523	-1.476330	H	0.022998	2.351715	-1.463648
H	-0.329713	1.356215	1.266746	H	-0.315768	1.358956	1.269068
		AH2c/AH2d				**AH2c/AH2d**	
C	0.311626	-0.444140	0.013860	C	0.307058	-0.441192	0.014067
C	0.280880	1.020553	0.013881	C	0.278427	1.015669	0.014158
C	1.713492	1.494480	0.013898	C	1.711107	1.487048	0.014291
C	2.552253	0.207849	0.013917	C	2.538809	0.203583	0.013533
C	1.609043	-0.897227	0.013856	C	1.618042	-0.895243	0.013732
C	-0.846844	-1.306075	0.013834	C	-0.840681	-1.304936	0.014233
C	-2.164728	-0.974783	0.013821	C	-2.164077	-0.971137	0.014041
C	-2.787442	0.320201	0.013825	C	-2.784118	0.318541	0.013581
C	-2.188958	1.541954	0.013846	C	-2.185390	1.546408	0.013507
C	-0.787770	1.858486	0.013872	C	-0.789567	1.860972	0.013889
H	1.950380	2.100000	0.894282	H	1.943286	2.096335	0.895733
O	3.770856	0.166087	0.013841	O	3.778271	0.170043	0.012482
H	1.915080	-1.934722	0.013823	H	1.915727	-1.938888	0.013468
H	-0.617135	-2.367904	0.013824	H	-0.611053	-2.370155	0.014482
H	-2.858785	-1.810416	0.013802	H	-2.859428	-1.809844	0.014173
H	-3.872721	0.310460	0.013807	H	-3.872630	0.308708	0.013271
H	-2.851280	2.402516	0.013844	H	-2.850226	2.408884	0.013119
H	-0.560421	2.921362	0.013885	H	-0.558775	2.926419	0.013859
H	1.950404	2.100017	-0.866468	H	1.943148	2.097485	-0.866369
		AH2e/AH2f				**AH2e/AH2f**	
C	0.024655	-0.479830	-0.170112	C	0.019652	-0.491002	-0.149417
C	0.032989	1.039191	-0.115403	C	0.028031	1.033534	-0.093599
C	-1.227904	1.485537	-0.198696	C	-1.233474	1.473707	-0.225694
C	-2.142001	0.302513	-0.327758	C	-2.129891	0.291567	-0.393207
C	-1.254386	-0.896792	-0.320375	C	-1.258560	-0.903707	-0.351144
C	1.174639	-1.336934	-0.038022	C	1.147828	-1.357035	0.030237
C	2.392864	-1.026041	0.471193	C	2.381714	-1.041906	0.510289

C	2.895151	0.239453	0.978865	C	2.936274	0.231727	0.924815
C	2.421128	1.478769	0.764462	C	2.461357	1.475491	0.718457
C	1.277387	1.873856	-0.129958	C	1.247028	1.899335	-0.052224
H	-1.573415	2.509415	-0.213550	H	-1.578554	2.501930	-0.248039
O	-3.352376	0.320874	-0.416287	O	-3.348253	0.314270	-0.531632
H	-1.616923	-1.912756	-0.381483	H	-1.616295	-1.924599	-0.426121
H	1.002778	-2.376311	-0.302776	H	0.953387	-2.409542	-0.172663
H	3.090821	-1.853605	0.565232	H	3.061535	-1.883664	0.639848
H	3.789886	0.156981	1.589782	H	3.888887	0.156478	1.447363
H	2.959473	2.305316	1.218518	H	3.068775	2.304195	1.080306
H	1.658964	1.849667	-1.165794	H	1.578608	2.017861	-1.101869
H	1.005800	2.915447	0.055721	H	0.951479	2.906109	0.257855
		AH2g				**AH2g**	
C	0.395880	-0.474825	0.048427	C	0.392712	-0.477584	0.048827
C	0.395992	1.047406	0.048141	C	0.392833	1.050167	0.048603
C	1.674917	1.472389	-0.051146	C	1.676535	1.471588	-0.050932
C	2.574617	0.286099	-0.120699	C	2.561893	0.286096	-0.119625
C	1.674743	-0.900032	-0.050701	C	1.676335	-0.899235	-0.050767
C	-0.751402	-1.343261	0.137548	C	-0.748768	-1.347978	0.137574
C	-2.055696	-1.030802	0.238346	C	-2.055347	-1.030176	0.238283
C	-2.759226	0.286568	0.292332	C	-2.751528	0.286569	0.291268
C	-2.055503	1.603815	0.237853	C	-2.055157	1.603192	0.237710
C	-0.751163	1.916044	0.136937	C	-0.748528	1.920762	0.136913
H	2.027399	2.493645	-0.078618	H	2.028167	2.497242	-0.078252
O	3.786953	0.285993	-0.214734	O	3.787539	0.285986	-0.214831
H	2.027075	-1.921350	-0.077791	H	2.027806	-1.924952	-0.077788
H	-0.506705	-2.402106	0.118906	H	-0.503425	-2.409759	0.119207
H	-2.744139	-1.871115	0.291791	H	-2.748736	-1.870032	0.292236
H	-3.380526	0.286784	1.202885	H	-3.379974	0.286766	1.198859
H	-2.743822	2.444249	0.290982	H	-2.748436	2.443170	0.291161
H	-0.506310	2.974846	0.117899	H	-0.503038	2.982500	0.118036
H	-3.512765	0.286473	-0.512247	H	-3.510563	0.286497	-0.510373
		AH3c				**AH3c**	
C	-0.348066	-0.232043	0.074600	C	-0.349895	-0.242539	0.075150
C	-0.397670	1.149159	-0.018739	C	-0.400399	1.145686	-0.018819
C	1.025019	1.667712	-0.005135	C	1.019361	1.664344	-0.005272
C	1.854013	0.426092	0.105959	C	1.850908	0.428131	0.105179
C	1.048412	-0.652737	0.150018	C	1.049478	-0.656103	0.150317
C	-2.833188	-0.825266	0.029352	C	-2.826178	-0.824235	0.029361
C	-3.413455	0.404384	-0.071409	C	-3.410759	0.409880	-0.071953
C	-2.830887	1.705059	-0.137940	C	-2.831765	1.705847	-0.138073
C	-1.503668	2.031086	-0.114774	C	-1.499443	2.029431	-0.114532
H	2.935089	0.424212	0.143003	H	2.935555	0.430990	0.141683
H	-3.497114	-1.684077	0.063658	H	-3.502356	-1.677737	0.062988
H	-4.499895	0.398885	-0.107610	H	-4.500010	0.399588	-0.108099
H	-1.259433	3.088434	-0.176755	H	-1.251153	3.088786	-0.176251
H	1.190265	2.356627	0.834025	H	1.182893	2.356818	0.833038
H	1.338193	-1.690336	0.228602	H	1.360302	-1.690636	0.229707
H	-3.534106	2.528065	-0.216183	H	-3.535427	2.532203	-0.216420
C	-1.429115	-1.231457	0.103820	C	-1.432716	-1.225430	0.103215
O	-1.147308	-2.429877	0.192769	O	-1.153970	-2.443143	0.194675

H	1.249244	2.238089	-0.916571	H	1.241905	2.240130	-0.915203
		AH3d				**AH3d**	
C	-0.324360	-0.312938	-0.033917	C	-0.326860	-0.319636	-0.033684
C	-0.340255	1.173587	-0.033943	C	-0.345328	1.168471	-0.034068
C	0.949179	1.611546	-0.033935	C	0.945581	1.608550	-0.034168
C	1.882543	0.444830	-0.033929	C	1.877321	0.444652	-0.033764
C	0.961929	-0.732713	-0.033918	C	0.964970	-0.735815	-0.033392
C	-2.865204	-0.831732	-0.033961	C	-2.859700	-0.831909	-0.034138
C	-3.399849	0.412172	-0.033993	C	-3.395961	0.416641	-0.033812
C	-2.792041	1.725508	-0.033989	C	-2.795232	1.729417	-0.033842
C	-1.480437	2.056636	-0.033967	C	-1.479965	2.056426	-0.034037
H	2.548884	0.443968	0.840656	H	2.548356	0.446474	0.839630
H	-3.548640	-1.674705	-0.033983	H	-3.555320	-1.669601	-0.034210
H	-4.486871	0.440259	-0.034025	H	-4.486531	0.440633	-0.033611
H	-1.236975	3.115475	-0.033977	H	-1.229717	3.117299	-0.034125
H	1.262817	2.647115	-0.033945	H	1.258841	2.647981	-0.034451
H	1.272650	-1.767499	-0.033905	H	1.296503	-1.767664	-0.033234
H	-3.500087	2.548089	-0.034015	H	-3.506671	2.552855	-0.033696
C	-1.462062	-1.275866	-0.033885	C	-1.464554	-1.273008	-0.034155
O	-1.231084	-2.481236	-0.034014	O	-1.234788	-2.490997	-0.035013
H	2.548896	0.443953	-0.908504	H	2.548090	0.445677	-0.907380
		AH3e				**AH3e**	
C	-0.380168	-0.290724	-0.026780	C	-0.382486	-0.301177	-0.027203
C	-0.397488	1.093447	-0.026784	C	-0.400539	1.089802	-0.027331
C	0.995130	1.567936	-0.026767	C	0.988858	1.567665	-0.026755
C	1.835995	0.518965	-0.026742	C	1.832079	0.518781	-0.025818
C	1.048515	-0.754468	-0.026751	C	1.050004	-0.757362	-0.026095
C	-2.865042	-0.849846	-0.026761	C	-2.859051	-0.848994	-0.025998
C	-3.431947	0.386926	-0.026761	C	-3.429555	0.391089	-0.025395
C	-2.829935	1.685456	-0.026789	C	-2.830818	1.686414	-0.027029
C	-1.504951	1.998023	-0.026799	C	-1.501832	1.996794	-0.027997
H	2.916846	0.563224	-0.026724	H	2.916591	0.561985	-0.024964
H	-3.536180	-1.703876	-0.026726	H	-3.542303	-1.697726	-0.024770
H	-4.518798	0.398540	-0.026739	H	-4.519371	0.398794	-0.023703
H	-1.248226	3.053523	-0.026807	H	-1.240188	3.054269	-0.028940
H	1.269088	2.615740	-0.026770	H	1.255865	2.620396	-0.026925
H	1.257949	-1.390126	0.843031	H	1.270779	-1.387204	0.846994
H	-3.526601	2.518017	-0.026791	H	-3.528648	2.521890	-0.027228
C	-1.459219	-1.272778	-0.026820	C	-1.461661	-1.266686	-0.028923
O	-1.194652	-2.480938	-0.026657	O	-1.201541	-2.494087	-0.031948
H	1.257985	-1.390140	-0.896514	H	1.272119	-1.387741	-0.898421
		AH3f				**AH3f**	
C	-1.529257	-0.352290	0.020938	C	-1.532860	-0.354349	0.008690
C	-1.500265	1.113844	-0.071564	C	-1.506093	1.113454	-0.051338
C	-2.888579	1.539130	-0.239374	C	-2.890027	1.541006	-0.203985
C	-3.685193	0.434629	-0.211586	C	-3.691855	0.432769	-0.209525
C	-2.845614	-0.735117	-0.042110	C	-2.856956	-0.735976	-0.068981
C	0.991144	-0.773474	-0.298410	C	0.996096	-0.788383	-0.252848
C	1.529054	0.480315	0.321992	C	1.531479	0.495631	0.305053
C	0.901299	1.663067	0.477019	C	0.903437	1.680412	0.454742
C	-0.469783	1.975830	0.147136	C	-0.476251	1.982035	0.164072

H	-4.762520	0.415908	-0.299776	H	-4.772191	0.416356	-0.302772
H	1.683225	-1.601785	-0.145800	H	1.681238	-1.605926	-0.020436
H	2.569307	0.431675	0.630467	H	2.591138	0.465375	0.556375
H	-0.713310	3.035461	0.122842	H	-0.730255	3.042776	0.154959
H	-3.202564	2.570512	-0.323613	H	-3.201184	2.578792	-0.263038
H	-3.188356	-1.759561	0.006408	H	-3.211758	-1.761078	-0.051207
C	-0.399962	-1.281443	0.108327	C	-0.410934	-1.277502	0.087523
O	-0.540090	-2.459185	0.391038	O	-0.565522	-2.477014	0.324933
H	1.484207	2.487408	0.876739	H	1.500996	2.519797	0.805743
H	0.925077	-0.611934	-1.387222	H	0.999322	-0.695185	-1.354511
		AH3g				**AH3g**	
C	-1.602963	-0.333870	-0.097919	C	-1.600259	-0.338597	-0.098696
C	-1.546010	1.131971	0.060992	C	-1.543303	1.128083	0.060322
C	-2.936689	1.582048	0.183804	C	-2.928544	1.578286	0.183711
C	-3.748205	0.495792	0.106416	C	-3.747363	0.490819	0.107301
C	-2.924417	-0.687257	-0.067790	C	-2.929536	-0.689427	-0.066644
C	0.910495	-0.900825	-0.292733	C	0.906327	-0.900642	-0.292069
C	1.499394	0.298037	-0.191446	C	1.495655	0.301837	-0.190549
C	0.962365	1.683630	-0.009726	C	0.959257	1.682920	-0.011120
C	-0.495065	1.972066	0.098358	C	-0.492474	1.973594	0.097769
H	-4.828056	0.494475	0.163043	H	-4.830519	0.491187	0.165088
H	1.556070	-1.764464	-0.422386	H	1.561808	-1.760904	-0.420752
H	2.586484	0.292425	-0.249508	H	2.585482	0.294727	-0.247972
H	-0.720462	3.029309	0.226691	H	-0.719528	3.033505	0.226662
H	-3.230666	2.614620	0.313397	H	-3.217999	2.615841	0.313647
H	-3.284392	-1.702250	-0.161196	H	-3.306592	-1.701998	-0.158407
H	1.361668	2.304010	-0.828535	H	1.362393	2.305846	-0.828244
C	-0.517050	-1.308913	-0.262987	C	-0.515394	-1.302243	-0.263042
O	-0.765935	-2.506035	-0.382069	O	-0.764713	-2.513509	-0.385429
H	1.450874	2.114271	0.879436	H	1.452740	2.119718	0.874263
		AH3h				**AH3h**	
C	-0.424094	-0.313368	0.269605	C	-0.427686	-0.317273	0.266783
C	-0.466199	1.201279	0.318630	C	-0.464182	1.197308	0.306667
C	0.992705	1.569729	0.382345	C	0.992512	1.563120	0.369129
C	1.743852	0.449480	0.406225	C	1.745722	0.441212	0.406070
C	0.869694	-0.713752	0.346057	C	0.870998	-0.717804	0.353029
C	-2.953906	-0.673161	0.053816	C	-2.947597	-0.676668	0.050742
C	-3.330202	0.471443	-0.556116	C	-3.325272	0.468923	-0.565006
C	-2.522825	1.556130	-1.100218	C	-2.528490	1.562849	-1.099362
C	-1.270905	1.889798	-0.754144	C	-1.274912	1.896749	-0.752319
H	2.823213	0.404548	0.468732	H	2.827833	0.392980	0.473936
H	-3.725686	-1.384085	0.331250	H	-3.727978	-1.386997	0.318416
H	-4.399378	0.592150	-0.715613	H	-4.397398	0.578616	-0.732919
H	-0.808036	2.741759	-1.241769	H	-0.819442	2.767751	-1.220271
H	1.348243	2.591452	0.415469	H	1.345839	2.589538	0.393300
H	1.190891	-1.746314	0.380277	H	1.204367	-1.749836	0.401932
H	-3.019772	2.172755	-1.843738	H	-3.037166	2.192702	-1.827557
C	-1.589249	-1.214447	0.261594	C	-1.589347	-1.208114	0.266306
O	-1.454953	-2.424955	0.421870	O	-1.456739	-2.431684	0.439095
H	-0.915834	1.479278	1.291946	H	-0.903503	1.486346	1.288247
		AH3i				**AH3i**	

C	-0.476884	-0.442813	0.469610	C	-0.475597	-0.447411	0.452792
C	-0.507294	1.073594	0.497781	C	-0.507344	1.070189	0.480564
C	0.785371	1.509369	0.613529	C	0.785451	1.508938	0.608996
C	1.695829	0.384560	0.587517	C	1.696383	0.385291	0.594895
C	0.987061	-0.762994	0.480221	C	0.988672	-0.764725	0.478602
C	-2.712693	-0.826516	-0.788531	C	-2.712369	-0.828448	-0.784070
C	-3.382849	0.297451	-0.419895	C	-3.385988	0.295967	-0.404307
C	-2.940544	1.529247	0.183157	C	-2.943512	1.528769	0.187980
C	-1.672865	1.896476	0.516033	C	-1.667613	1.897465	0.500522
H	2.773705	0.464474	0.636965	H	2.776271	0.466561	0.668696
H	-3.254377	-1.574952	-1.358208	H	-3.266402	-1.573259	-1.353039
H	-4.435227	0.306302	-0.694377	H	-4.444262	0.297408	-0.667940
H	-1.515063	2.931530	0.808550	H	-1.500391	2.938398	0.778238
H	1.082434	2.546018	0.716409	H	1.078749	2.548679	0.726498
H	1.371294	-1.768915	0.404732	H	1.383719	-1.772293	0.432948
H	-3.712144	2.284676	0.289733	H	-3.716536	2.285860	0.298501
C	-1.318398	-1.210282	-0.557783	C	-1.322067	-1.202052	-0.568221
O	-0.852634	-2.204072	-1.092867	O	-0.851394	-2.195196	-1.127888
H	-0.891002	-0.780685	1.438502	H	-0.892049	-0.787672	1.427313
		AH4c				**AH4c**	
C	0.167143	-0.483373	0.058164	C	0.168863	-0.483764	0.058444
C	0.147878	0.971227	0.058141	C	0.148351	0.966454	0.059786
C	1.549915	1.408985	0.058146	C	1.545728	1.411756	0.060077
C	2.382838	0.358010	0.058168	C	2.379775	0.357730	0.058105
C	1.618041	-0.936235	0.058185	C	1.616275	-0.933645	0.056717
C	-0.890894	-1.332721	0.058173	C	-0.891365	-1.336567	0.058955
C	-2.284020	-0.997037	0.058166	C	-2.277952	-0.995770	0.059959
C	-2.896021	0.215683	0.058138	C	-2.889613	0.223116	0.058778
C	-2.347402	1.580945	0.058084	C	-2.338376	1.574480	0.056163
C	-0.907087	1.835967	0.058116	C	-0.913255	1.834440	0.059638
H	3.464085	0.408025	0.058178	H	3.465037	0.405993	0.057334
H	1.850508	-1.551196	0.936427	H	1.849044	-1.552801	0.933342
H	-0.669620	-2.396964	0.058196	H	-0.672057	-2.404259	0.058533
H	-2.950555	-1.855626	0.058185	H	-2.951017	-1.853325	0.061176
H	-3.982091	0.225143	0.058148	H	-3.979427	0.220366	0.058936
O	-3.129957	2.536056	0.058202	O	-3.135029	2.544532	0.050244
H	-0.682044	2.899098	0.058111	H	-0.673610	2.898225	0.060041
H	1.838726	2.452179	0.058132	H	1.831020	2.459854	0.061185
H	1.850526	-1.551236	-0.820023	H	1.847579	-1.549884	-0.822378
		AH4d				**AH4d**	
C	0.167143	-0.483373	0.058164	C	0.170344	-0.479960	0.062418
C	0.147878	0.971227	0.058141	C	0.157763	0.970315	0.062782
C	1.549915	1.408985	0.058146	C	1.603814	1.438503	0.063103
C	2.382838	0.358010	0.058168	C	2.387509	0.159186	0.062362
C	1.618041	-0.936235	0.058185	C	1.567239	-0.907245	0.062039
C	-0.890894	-1.332721	0.058173	C	-0.906812	-1.331958	0.062592
C	-2.284020	-0.997037	0.058166	C	-2.280497	-0.977771	0.063062
C	-2.896021	0.215683	0.058138	C	-2.886117	0.250571	0.062705
C	-2.347402	1.580945	0.058084	C	-2.324456	1.590440	0.061314
C	-0.907087	1.835967	0.058116	C	-0.887897	1.838647	0.062541
H	3.464085	0.408025	0.058178	H	1.823389	2.059959	0.941212

H	1.850508	-1.551196	0.936427	H	3.472801	0.126669	0.062185
H	-0.669620	-2.396964	0.058196	H	1.867096	-1.951008	0.061560
H	-2.950555	-1.855626	0.058185	H	-0.689926	-2.399145	0.062509
H	-3.982091	0.225143	0.058148	H	-2.964134	-1.826689	0.063600
O	-3.129957	2.536056	0.058202	H	-3.975267	0.254984	0.063078
H	-0.682044	2.899098	0.058111	O	-3.101003	2.576168	0.060962
H	1.838726	2.452179	0.058132	H	-0.647475	2.902524	0.062773
H	1.850526	-1.551236	-0.820023	H	1.823441	2.061068	-0.814196
		AH4e				**AH4e**	
C	-1.322369	-0.419073	-0.379475	C	-1.323643	-0.421066	-0.377173
C	-1.317617	1.054709	-0.345446	C	-1.319095	1.052235	-0.336378
C	-2.605800	1.459735	-0.479373	C	-2.606796	1.461428	-0.474968
C	-3.478896	0.282701	-0.616032	C	-3.480792	0.283615	-0.618186
C	-2.716820	-0.834590	-0.581501	C	-2.718408	-0.836061	-0.584506
C	-0.281686	-1.266456	-0.184773	C	-0.282263	-1.269902	-0.186433
C	1.078716	-0.957778	0.213785	C	1.075936	-0.955635	0.216157
C	1.639086	0.217570	0.576962	C	1.636787	0.221045	0.582912
C	1.027426	1.568998	0.618404	C	1.030881	1.566883	0.611934
C	-0.097693	1.924170	-0.343008	C	-0.098930	1.922939	-0.336039
H	-2.947263	2.486420	-0.506526	H	-2.947856	2.491759	-0.503358
H	-4.555321	0.325391	-0.711740	H	-4.560313	0.329477	-0.716803
H	-3.047603	-1.862359	-0.626092	H	-3.046818	-1.867968	-0.633259
H	-0.494274	-2.328342	-0.277717	H	-0.488948	-2.335428	-0.285864
H	1.719131	-1.831359	0.304290	H	1.719867	-1.830150	0.308490
H	2.653950	0.205233	0.962242	H	2.654711	0.200122	0.969912
H	0.363935	1.883187	-1.343601	H	0.361201	1.880508	-1.339024
O	1.505217	2.409572	1.358717	O	1.522286	2.424301	1.340093
H	-0.367268	2.964932	-0.157235	H	-0.372956	2.964559	-0.155627
		AH4f				**AH4f**	
C	-1.452443	-0.515496	0.124506	C	-1.452783	-0.519545	0.128759
C	-1.414592	0.972760	0.181417	C	-1.414155	0.970760	0.178376
C	-2.786424	1.413010	0.473462	C	-2.785340	1.415138	0.471687
C	-3.567121	0.313177	0.581345	C	-3.566259	0.314906	0.589360
C	-2.742630	-0.879205	0.379844	C	-2.742548	-0.882042	0.390099
C	-0.353143	-1.423499	-0.108524	C	-0.356180	-1.428850	-0.115006
C	0.892527	-1.133028	-0.516417	C	0.889945	-1.134666	-0.521984
C	1.467250	0.206618	-0.891582	C	1.472893	0.207758	-0.876776
C	1.064676	1.457608	-0.124867	C	1.057514	1.457970	-0.126832
C	-0.360955	1.808693	0.084396	C	-0.362996	1.811205	0.076980
H	-4.628348	0.297430	0.789787	H	-4.630247	0.298482	0.802696
H	-0.588735	-2.471773	0.056216	H	-0.596045	-2.481479	0.034491
H	1.577026	-1.964006	-0.655495	H	1.574554	-1.965393	-0.682539
H	1.204446	0.414759	-1.942688	H	1.231343	0.420621	-1.934078
O	1.915375	2.243076	0.253224	O	1.911809	2.254404	0.248182
H	-0.515409	2.870457	0.256313	H	-0.528228	2.876916	0.239073
H	-3.081389	2.446995	0.578453	H	-3.076429	2.454502	0.572017
H	-3.106611	-1.896935	0.433229	H	-3.109146	-1.902274	0.447662
H	2.557510	0.171460	-0.854418	H	2.563308	0.163690	-0.823968
		AH4g				**AH4g**	
C	-1.386876	-0.586537	0.327031	C	-1.390136	-0.589663	0.322677
C	-1.386912	0.894026	0.369922	C	-1.387054	0.893156	0.362153

C	-2.777958	1.306638	0.623159	C	-2.774121	1.312178	0.630408
C	-3.538976	0.192366	0.672480	C	-3.536761	0.197927	0.693644
C	-2.671749	-0.983464	0.495584	C	-2.674029	-0.983335	0.508131
C	-0.195760	-1.494703	0.258321	C	-0.205515	-1.502523	0.227973
C	1.049145	-1.042486	-0.444779	C	1.058925	-1.038479	-0.419342
C	1.541367	0.185391	-0.657249	C	1.553131	0.192774	-0.631718
C	1.013310	1.516398	-0.283635	C	1.003233	1.517569	-0.304359
C	-0.382161	1.766278	0.149199	C	-0.386396	1.769051	0.130160
H	-4.611477	0.149076	0.805535	H	-4.610912	0.154868	0.842486
H	-0.509015	-2.449821	-0.175709	H	-0.513171	-2.436569	-0.256045
H	1.681658	-1.866247	-0.769257	H	1.714058	-1.862213	-0.707464
O	1.757429	2.487260	-0.382323	O	1.739340	2.504790	-0.435745
H	-0.589752	2.828824	0.240098	H	-0.606973	2.833054	0.217614
H	-3.101321	2.335178	0.690786	H	-3.091124	2.346316	0.700514
H	-3.017998	-2.009148	0.517753	H	-3.024442	-2.010845	0.535680
H	2.514146	0.270195	-1.131976	H	2.546309	0.266559	-1.072409
H	0.117351	-1.750503	1.285010	H	0.090089	-1.815895	1.245592
		AH5c/AH5d				**AH5c/AH5d**	
C	0.251549	-0.298325	0.098534	C	0.252423	-0.301575	0.098536
C	0.252292	1.084995	0.098514	C	0.253771	1.088375	0.098496
C	1.642999	1.548750	0.098510	C	1.641611	1.553330	0.098438
C	2.480622	0.495322	0.098524	C	2.476387	0.494285	0.098554
C	1.684757	-0.775610	0.098543	C	1.683690	-0.776321	0.098592
C	-0.859194	-1.184247	0.098541	C	-0.855338	-1.179980	0.098470
C	-2.192117	-0.903515	0.098538	C	-2.194717	-0.895181	0.098613
C	-2.905544	0.378976	0.098541	C	-2.896049	0.378094	0.099307
C	-2.199904	1.671199	0.098504	C	-2.201698	1.662990	0.098740
C	-0.875458	1.967434	0.098498	C	-0.872701	1.964071	0.098476
H	1.926807	2.593643	0.098495	H	1.923354	2.602154	0.098328
H	1.902862	-1.398891	0.975978	H	1.902194	-1.403029	0.975316
H	-0.603374	-2.241818	0.098550	H	-0.604864	-2.241805	0.098344
H	-2.880088	-1.743502	0.098540	H	-2.873463	-1.746842	0.098389
O	-4.139822	0.378380	0.098478	O	-4.150875	0.379026	0.097951
H	-2.897893	2.503173	0.098485	H	-2.891894	2.505780	0.098569
H	-0.626672	3.026028	0.098478	H	-0.629028	3.027028	0.098293
H	3.561354	0.531559	0.098525	H	3.560915	0.527333	0.098548
H	1.902866	-1.398923	-0.778867	H	1.902327	-1.403104	-0.778050
		AH5e				**AH5e**	
C	0.198082	-0.351135	0.337258	C	0.197000	-0.350706	0.336917
C	0.274331	1.085510	-0.025660	C	0.273207	1.085060	-0.025826
C	1.559038	1.499374	0.123840	C	1.559889	1.501080	0.123594
C	2.411187	0.362585	0.594545	C	2.407099	0.362596	0.593728
C	1.438574	-0.770329	0.697202	C	1.439242	-0.772017	0.697859
C	-0.976066	-1.195290	0.323295	C	-0.974613	-1.193168	0.322960
C	-2.246641	-0.896557	-0.011250	C	-2.248974	-0.892988	-0.012725
C	-2.853671	0.373584	-0.468067	C	-2.847450	0.373572	-0.466825
C	-2.111961	1.641006	-0.652276	C	-2.114701	1.637452	-0.651857
C	-0.809957	1.934434	-0.467319	C	-0.808732	1.932260	-0.466599
H	1.927622	2.498867	-0.065153	H	1.930270	2.503914	-0.065920
H	2.896094	0.579988	1.557033	H	2.896522	0.579749	1.555913
H	1.700993	-1.771148	1.013518	H	1.703101	-1.776174	1.015384

H	-0.787362	-2.221019	0.631506	H	-0.788205	-2.222908	0.631721
H	-2.988341	-1.686585	0.047505	H	-2.986390	-1.691686	0.049165
O	-4.058486	0.376036	-0.711494	O	-4.065609	0.376099	-0.712733
H	-2.769644	2.433973	-0.993409	H	-2.767191	2.439086	-0.994160
H	-0.512423	2.959222	-0.677099	H	-0.513060	2.961045	-0.677842
H	3.230340	0.142405	-0.104955	H	3.230304	0.142654	-0.103735
AH5f/AH5g				**AH5f/AH5g**			
C	-1.608225	-0.450736	0.137830	C	-1.614716	-0.452388	0.116002
C	-1.591023	1.025202	0.166063	C	-1.594760	1.021147	0.177092
C	-2.990279	1.452937	0.213565	C	-2.991436	1.448761	0.249342
C	-3.776631	0.343527	0.238589	C	-3.782483	0.337308	0.250149
C	-2.927197	-0.831542	0.191882	C	-2.937340	-0.836028	0.168992
C	-0.498764	-1.348030	0.003320	C	-0.511501	-1.346959	-0.027217
C	0.818193	-1.085480	-0.181983	C	0.816542	-1.086840	-0.179537
C	1.503279	0.207356	-0.283527	C	1.513872	0.189454	-0.227736
C	0.923229	1.509933	0.284199	C	0.922943	1.518843	0.240883
C	-0.528753	1.850752	0.211607	C	-0.531835	1.847631	0.217179
H	-3.312144	2.484447	0.246129	H	-3.309890	2.484082	0.308567
H	-4.856484	0.323388	0.287798	H	-4.865565	0.317152	0.305322
H	-3.282386	-1.854104	0.185698	H	-3.292367	-1.862233	0.144338
H	-0.778696	-2.399317	-0.000421	H	-0.792830	-2.400890	-0.056925
H	1.487315	-1.920367	-0.361774	H	1.478119	-1.933781	-0.350765
O	2.629762	0.259826	-0.754014	O	2.693831	0.218516	-0.595226
H	1.517215	2.316182	-0.153094	H	1.476371	2.304341	-0.284232
H	-0.738319	2.917738	0.253447	H	-0.738198	2.917115	0.289439
H	1.201168	1.500580	1.351907	H	1.252503	1.617061	1.291554
AH5h/AH5i				**AH5h/AH5i**			
C	0.089811	-0.369212	0.467734	C	0.088695	-0.365797	0.463992
C	0.099256	1.146196	0.461803	C	0.103994	1.147524	0.448343
C	1.570884	1.475651	0.447072	C	1.574502	1.472347	0.436579
C	2.287517	0.335436	0.522658	C	2.289774	0.328664	0.530303
C	1.379134	-0.800970	0.548137	C	1.379329	-0.803252	0.559528
C	-1.083834	-1.197683	0.453348	C	-1.077674	-1.194259	0.441266
C	-2.353529	-0.855695	0.136243	C	-2.355975	-0.851315	0.133546
C	-2.878725	0.399506	-0.435642	C	-2.875287	0.396653	-0.429929
C	-2.015010	1.515989	-0.910038	C	-2.024704	1.515983	-0.900164
C	-0.768362	1.842661	-0.553948	C	-0.771774	1.843065	-0.554649
H	1.956082	2.486430	0.425248	H	1.960359	2.486642	0.408672
H	3.365957	0.260768	0.568333	H	3.370774	0.250449	0.588239
H	1.687262	-1.836766	0.620908	H	1.681952	-1.843027	0.651542
H	-0.914450	-2.235134	0.733671	H	-0.905291	-2.239208	0.704284
H	-3.129147	-1.608571	0.230690	H	-3.123911	-1.616347	0.230526
O	-4.089984	0.504427	-0.610613	O	-4.100922	0.500377	-0.611599
H	-2.543228	2.164613	-1.602063	H	-2.554389	2.175622	-1.586068
H	-0.343047	2.742266	-0.990633	H	-0.354735	2.749801	-0.993045
H	-0.266005	1.461367	1.457691	H	-0.254135	1.477355	1.449235

Table S2. The electronic energies (*E* at 0 K in Hartree, 1 Hartree = 2625.499748 kJ mol^{-1}) for all possible isolated and hydrated structures of neutral isomers of azulenols calculated in *vacuo* {DFT(B3LYP)/6-311+G(d,p)} and aqueous solution {PCM(water)//DFT(B3LYP)/6-311+G(d,p)}.

Structure	*E*(gas)	*E*(water)	Structure	*E*(gas)	*E*(water)
AH1a	-461.176758	-461.195322	**AH3e**	-461.181960	-461.199606
AH1b	-461.178316	-461.197033	**AH3f**	-461.166882	-461.182575
AH1c	-461.173214	-461.186677	**AH3g**	-461.162305	-461.180254
AH1d	-461.155959	-461.168799	**AH3h**	-461.152946	-461.170272
AH1e	-461.167265	-461.182785	**AH3i**	-461.162917	-461.178920
AH1f	-461.157840	-461.171113	**AH4a**	-461.180261	-461.199728
AH1g	-461.167893	-461.183832	**AH4b**	-461.180295	-461.199921
AH1h	-461.155853	-461.168799	**AH4c**	-461.179062	-461.199064
AH1i	-461.170449	-461.186425	**AH4d**	-461.180326	-461.199773
AH1j	-461.164672	-461.181461	**AH4e**	-461.160508	-461.175059
AH2a/AH2b	-461.185795	-461.205316	**AH4f**	-461.161960	-461.175554
AH2c/AH2d	-461.184928	-461.204711	**AH4g**	-461.154643	-461.169575
AH2e/AH2f	-461.153840	-461.168887	**AH5a/AH5b**	-461.185719	-461.205765
AH2g	-461.158051	-461.174458	**AH5c/AH5d**	-461.179480	-461.199254
AH3a	-461.187550	-461.203661	**AH5e**	-461.169478	-461.186265
AH3b	-461.185671	-461.205884	**AH5f/AH5g**	-461.167673	-461.183954
AH3c	-461.182289	-461.200186	**AH5h/AH5i**	-461.154753	-461.172961
AH3d	-461.166843	-461.182328			

Table S3. The atom coordinates for five anion structures of azulenols (given in Figure 4) optimized in *vacuo* {DFT(B3LYP)/6-311+G(d,p)} and their DFT-calculated electronic energies (*E* at 0 K in Hartree).

Anion structure				**Anion structure**			
A$^-$1				**A$^-$2**			
E: -460.625029				*E*: -460.643016			
C	0.300731	-0.459956	0.000000	C	0.311458	-0.491790	0.012791
C	0.296743	1.052012	0.000000	C	0.313106	1.024600	0.017584
C	1.655266	1.439772	0.000000	C	1.633106	1.425280	0.031545
C	2.477873	0.317665	0.000000	C	2.520075	0.263938	0.036383
C	1.694783	-0.908169	0.000000	C	1.630583	-0.895420	0.024208
C	-0.777925	-1.296744	0.000000	C	-0.823281	-1.326040	-0.000748
C	-2.164672	-0.985744	0.000000	C	-2.175446	-0.989900	-0.012686
C	-2.750360	0.281078	0.000000	C	-2.788400	0.269870	-0.014606
C	-2.173367	1.555848	0.000000	C	-2.172709	1.528266	-0.004720
C	-0.794760	1.886945	0.000000	C	-0.819816	1.861383	0.009332
H	1.988000	2.472868	0.000000	H	1.985835	2.449750	0.038178
H	3.562157	0.323368	0.000000	O	3.769545	0.262542	0.048436
O	2.122591	-2.091585	0.000000	H	1.981085	-1.920676	0.024361
H	-0.516134	-2.355175	0.000000	H	-0.603318	-2.392767	-0.001997
H	-2.846563	-1.832058	0.000000	H	-2.859735	-1.837257	-0.021935
H	-3.841092	0.279132	0.000000	H	-3.875948	0.271085	-0.025054
H	-2.864673	2.394634	0.000000	H	-2.855155	2.377150	-0.008602
H	-0.567578	2.954529	0.000000	H	-0.597535	2.927616	0.014831

A¯3			
E: -460.649234			
C	-1.507416	-0.450393	0.107224
C	-1.478133	1.008700	0.207800
C	-2.787488	1.421819	0.587174
C	-3.590276	0.286418	0.716456
C	-2.809680	-0.856988	0.423650
C	0.904630	-0.906744	-0.569078
C	1.451478	0.349102	-0.621404
C	0.886918	1.629757	-0.375836
C	-0.414529	1.902834	-0.008959
H	-4.638330	0.279858	0.994982
H	1.565246	-1.737476	-0.806820
H	2.505566	0.372064	-0.900472
H	-0.662594	2.954823	0.135291
H	-3.087844	2.451596	0.743710
H	-3.134988	-1.887569	0.433662
H	1.558094	2.476949	-0.491606
C	-0.444408	-1.379760	-0.244777
O	-0.650924	-2.614541	-0.281887

A¯4			
E: -460.634377			
C	0.327838	-0.510582	0.000000
C	0.296015	0.985634	0.000000
C	1.664544	1.415542	0.000000
C	2.475006	0.285502	0.000000
C	1.684268	-0.888459	0.000000
C	-0.786136	-1.352073	0.000000
C	-2.138212	-0.990719	0.000000
C	-2.757510	0.252407	0.000000
C	-2.226062	1.592562	0.000000
C	-0.791742	1.829047	0.000000
H	1.985905	2.448403	0.000000
H	3.560352	0.298168	0.000000
H	2.049604	-1.907453	0.000000
H	-0.575616	-2.420568	0.000000
H	-2.828536	-1.834343	0.000000
H	-3.845498	0.246011	0.000000
H	-0.564144	2.894642	0.000000
O	-3.006816	2.588268	0.000000

A¯5			
E: -460.652178			
C	0.342249	-0.455220	0.000000
C	0.342540	0.996375	0.000000
C	1.694024	1.413618	0.000000
C	2.514149	0.270050	0.000000
C	1.693458	-0.873138	0.000000
C	-0.793690	-1.300568	0.000000
C	-2.133076	-1.008134	0.000000
C	-2.835684	0.271115	0.000000
C	-2.132810	1.550306	0.000000
C	-0.793277	1.842267	0.000000
H	2.028539	2.444365	0.000000
H	3.598152	0.269731	0.000000
H	2.027505	-1.904073	0.000000
H	-0.556551	-2.365852	0.000000
H	-2.824419	-1.847241	0.000000
O	-4.091087	0.271150	0.000000
H	-2.823960	2.389556	0.000000
H	-0.555833	2.907531	0.000000

Table S4. The enthalpies and Gibbs energies (*H* and *G*, respectively, at 298 K in Hartree) calculated in *vacuo* {DFT(B3LYP)/6-311+G(d,p)} for selected neutral isomers of azulenols and for their anions.

Structure	*H*	*G*	Structure	*H*	*G*
AH1a	-461.019092	-461.060806	**AH4b**	-461.021886	-461.064505
AH1b	-461.019556	-461.062869	**AH4c**	-461.020268	-461.063424
AH1c	-461.014523	-461.057460	**AH4d**	-461.021531	-461.064641
AH2a/AH2b	-461.026712	-461.069026	**AH5a/AH5b**	-461.026979	-461.069279
AH2c/AH2d	-461.025978	-461.068921	**AH5c/AH5d**	-461.020998	-461.064213
AH3a	-461.028537	-461.071148	**A¯1**	-460.480896	-460.522966
AH3b	-461.026717	-461.069029	**A¯2**	-460.498175	-460.540072
AH3c	-461.023595	-461.066523	**A¯3**	-460.504116	-460.546076
AH3e	-461.023359	-461.066228	**A¯4**	-460.490024	-460.532346
AH4a	-461.021829	-461.064485	**A¯5**	-460.507154	-460.549162

Table S5. The relative *G*ibbs energies (Δ*G* at 298 K in kJ mol^{-1}) calculated for selected neutral isomers of azulenols in *vacuo* {DFT(B3LYP)/6-311+G(d,p)} and aqueous solution {PCM(water)//DFT(B3LYP)/6-311+G(d,p)}.

	Δ*G*			Δ*G*	
Structure	**Gas**	**Water**	**Structure**	**Gas**	**Water**
AH1a	5.4	4.8	**AH3e**	12.9	18.4
AH1b	0.0	0.0	**AH4a**	0.4	0.5
AH1c	14.2	29.4	**AH4b**	0.4	0.0
AH2a/AH2b	0.0	0.0	**AH4c**	3.2	4.2
AH2c/AH2d	0.3	3.5	**AH4d**	0.0	2.3
AH3a	0.0	6.2	**AH5a/AH5b**	0.0	0.0
AH3b	5.6	0.0	**AH5c/AH5d**	13.3	19.2
AH3c	12.1	17.1			