

Table S1. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for **1**. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.274	1.514	-0.24	-230.7682	-230.7316	-230.5205
1.294	1.494	-0.20	-230.7812	-230.7380	-230.5621
1.314	1.474	-0.16	-230.7909	-230.7397	-230.5990
1.334	1.454	-0.12	-230.7978	-230.7370	-230.6314
1.354	1.434	-0.08	-230.8023	-230.7299	-230.6596
1.374	1.414	-0.04	-230.8048	-230.7186	-230.6834
1.394	1.394	0.00	-230.8056	-230.7031	-230.7031
1.414	1.374	0.04	-230.8048	-230.6834	-230.7186
1.434	1.354	0.08	-230.8023	-230.6596	-230.7299
1.454	1.334	0.12	-230.7978	-230.6314	-230.7370
1.474	1.314	0.16	-230.7909	-230.5990	-230.7397
1.494	1.294	0.20	-230.7812	-230.5621	-230.7380
1.514	1.274	0.24	-230.7682	-230.5205	-230.7316

Table S2. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for **2**. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.223	1.517	-0.294	-343.9780	-343.9438	-343.7003
1.243	1.497	-0.254	-343.9945	-343.9538	-343.7499
1.263	1.477	-0.214	-344.0071	-343.9584	-343.7942
1.283	1.457	-0.174	-344.0163	-343.9581	-343.8334
1.303	1.437	-0.134	-344.0230	-343.9530	-343.8678
1.323	1.417	-0.094	-344.0278	-343.9434	-343.8977
1.343	1.397	-0.054	-344.0311	-343.9295	-343.9233
1.363	1.377	-0.014	-344.0334	-343.9114	-343.9446
1.370	1.370	0.000	-344.0340	-343.9040	-343.9511
1.383	1.357	0.026	-344.0351	-343.8892	-343.9618
1.403	1.337	0.066	-344.0348	-343.8630	-343.9751
1.423	1.317	0.106	-344.0338	-343.8331	-343.9845
1.443	1.297	0.146	-344.0308	-343.7993	-343.9901
1.463	1.277	0.186	-344.0256	-343.7619	-343.9920
1.483	1.257	0.226	-344.0183	-343.7212	-343.9904

Table S3. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for **3**. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.287	1.503	-0.216	-461.3337	-461.2930	-461.1012
1.307	1.483	-0.176	-461.3453	-461.2968	-461.1418
1.327	1.463	-0.136	-461.3542	-461.2963	-461.1779
1.347	1.443	-0.096	-461.3606	-461.2913	-461.2096
1.367	1.423	-0.056	-461.3651	-461.2821	-461.2370
1.387	1.403	-0.016	-461.3680	-461.2687	-461.2603
1.395	1.395	0.000	-461.3688	-461.2622	-461.2684
1.407	1.383	0.024	-461.3698	-461.2512	-461.2794
1.427	1.363	0.064	-461.3697	-461.2296	-461.2944
1.447	1.343	0.104	-461.3683	-461.2038	-461.3052
1.467	1.323	0.144	-461.3648	-461.1739	-461.3119
1.487	1.303	0.184	-461.3587	-461.1397	-461.3142
1.507	1.283	0.224	-461.3497	-461.1011	-461.3122

Table S4. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for **4**. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.295	1.554	-0.259	-457.5750	-457.5289	-457.4100
1.315	1.534	-0.219	-457.5871	-457.5303	-457.4525
1.335	1.514	-0.179	-457.5974	-457.5280	-457.4935
1.355	1.494	-0.139	-457.6061	-457.5198	-457.5251
1.375	1.474	-0.099	-457.6154	-457.5084	-457.5526
1.395	1.454	-0.059	-457.6256	-457.4947	-457.5769
1.415	1.434	-0.019	-457.6364	-457.4791	-457.5982
1.425	1.425	0.000	-457.6413	-457.4708	-457.6073
1.435	1.414	0.021	-457.6470	-457.4615	-457.6167
1.455	1.394	0.061	-457.6566	-457.4420	-457.6325
1.475	1.374	0.101	-457.6644	-457.4198	-457.6450
1.495	1.354	0.141	-457.6700	-457.3949	-457.6544
1.515	1.334	0.181	-457.6733	-457.3672	-457.6604
1.535	1.314	0.221	-457.6731	-457.3364	-457.6631
1.555	1.294	0.261	-457.6697	-457.2966	-457.6614

Table S5. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for 5. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.365	1.505	-0.140	-230.5252	-230.4799	-230.3468
1.385	1.485	-0.100	-230.5381	-230.4840	-230.3843
1.405	1.465	-0.060	-230.5492	-230.4844	-230.4180
1.425	1.445	-0.020	-230.5588	-230.4811	-230.4479
1.435	1.435	0.000	-230.5631	-230.4780	-230.4615
1.445	1.425	0.020	-230.5672	-230.4741	-230.4742
1.465	1.405	0.060	-230.5746	-230.4635	-230.4969
1.485	1.385	0.100	-230.5809	-230.4494	-230.5160
1.505	1.365	0.140	-230.5857	-230.4316	-230.5314
1.525	1.345	0.180	-230.5896	-230.4101	-230.5432
1.545	1.325	0.220	-230.5888	-230.3848	-230.5512
1.565	1.305	0.260	-230.5878	-230.3558	-230.5554
1.585	1.285	0.300	-230.5831	-230.3227	-230.5556
1.605	1.265	0.340	-230.5750	-230.2854	-230.5517
1.625	1.245	0.380	-230.5633	-230.2439	-230.5434

Table S6. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for 6. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.554	1.246	0.308	-1097.2927	-1097.0452	-1097.2582
1.534	1.266	0.268	-1097.3060	-1097.0870	-1097.2654
1.514	1.286	0.228	-1097.3166	-1097.1248	-1097.2686
1.494	1.306	0.188	-1097.3248	-1097.1587	-1097.2679
1.474	1.326	0.148	-1097.3310	-1097.1888	-1097.2635
1.454	1.346	0.108	-1097.3359	-1097.2152	-1097.2556
1.434	1.366	0.068	-1097.3394	-1097.2379	-1097.2439
1.414	1.386	0.028	-1097.3418	-1097.2570	-1097.2287
1.400	1.400	0.000	-1097.3430	-1097.2679	-1097.2159
1.394	1.406	-0.012	-1097.3434	-1097.2722	-1097.2098
1.374	1.426	-0.052	-1097.3432	-1097.2840	-1097.1875
1.354	1.446	-0.092	-1097.3419	-1097.2922	-1097.1616
1.334	1.466	-0.132	-1097.3384	-1097.2966	-1097.1319
1.314	1.486	-0.172	-1097.3323	-1097.2972	-1097.0985
1.294	1.506	-0.212	-1097.3234	-1097.2938	-1097.0611

Table S7. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for 7. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.267	1.507	-0.240	-457.4840	-457.4474	-457.2471
1.287	1.487	-0.200	-457.4936	-457.4499	-457.2879
1.307	1.467	-0.160	-457.5006	-457.4481	-457.3243
1.327	1.447	-0.120	-457.5053	-457.4420	-457.3564
1.347	1.427	-0.080	-457.5084	-457.4318	-457.3843
1.367	1.407	-0.040	-457.5104	-457.4177	-457.4082
1.387	1.387	0.000	-457.5119	-457.3997	-457.4283
1.407	1.367	0.040	-457.5131	-457.3780	-457.4446
1.427	1.347	0.080	-457.5128	-457.3528	-457.4573
1.447	1.327	0.120	-457.5122	-457.3240	-457.4666
1.467	1.307	0.160	-457.5099	-457.2919	-457.4724
1.487	1.287	0.200	-457.5058	-457.2565	-457.4749
1.507	1.267	0.240	-457.5002	-457.2186	-457.4746

Table S8. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for **8**. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.539	1.263	0.276	-565.0620	-564.8127	-565.0290
1.519	1.283	0.236	-565.0714	-564.8520	-565.0322
1.499	1.303	0.196	-565.0788	-564.8880	-565.0320
1.479	1.323	0.156	-565.0850	-564.9211	-565.0290
1.459	1.343	0.116	-565.0897	-564.9506	-565.0223
1.439	1.363	0.076	-565.0935	-564.9768	-565.0123
1.419	1.383	0.036	-565.0966	-564.9995	-564.9988
1.401	1.401	0.000	-565.0989	-565.0168	-564.9836
1.399	1.403	-0.004	-565.0991	-565.0186	-564.9818
1.379	1.423	-0.044	-565.1013	-565.0341	-564.9612
1.359	1.443	-0.084	-565.1008	-565.0459	-564.9368
1.339	1.463	-0.124	-565.1000	-565.0539	-564.9086
1.319	1.483	-0.164	-565.0965	-565.0579	-564.8765
1.299	1.503	-0.204	-565.0901	-565.0578	-564.8403
1.279	1.523	-0.244	-565.0806	-565.0533	-564.7998

Table S9. The energies (Hartree) of ground state (GS), the endo-Kelulé structure (K_{endo}) and the exo-Kelulé structure (K_{exo}) for **9**. The bond lengths are given in Å.

R_{endo}	R_{exo}	ΔR	GS	K_{endo}	K_{exo}
1.268	1.546	-0.278	-691.7207	-691.6811	-691.4777
1.288	1.526	-0.238	-691.7393	-691.6927	-691.5249
1.308	1.506	-0.198	-691.7548	-691.6998	-691.5673
1.328	1.486	-0.158	-691.7675	-691.7025	-691.6051
1.348	1.466	-0.118	-691.7781	-691.7011	-691.6387
1.368	1.446	-0.078	-691.7867	-691.6956	-691.6680
1.388	1.426	-0.038	-691.7937	-691.6862	-691.6933
1.407	1.407	0.000	-691.7991	-691.6737	-691.7137
1.428	1.386	0.042	-691.8034	-691.6558	-691.7321
1.448	1.366	0.082	-691.8058	-691.6347	-691.7455
1.468	1.346	0.122	-691.8056	-691.6097	-691.7551
1.488	1.326	0.162	-691.8035	-691.5807	-691.7606
1.508	1.306	0.202	-691.7985	-691.5475	-691.7620
1.528	1.286	0.242	-691.7904	-691.5101	-691.7593