SUPPORTING INFORMATION

Revisiting Aromaticity Tests to include Lowest-Lying Triplet States and Charged and Heterocyclic Rings

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Table S1. B3LYP/6-311++G(d,p) optimized cartesian XYZ coordinates of all analyzed species.

Table S2-S25. PDI (electrons), $FLU^{1/2}$, MCI (electrons), I_{NB}, I_{ring} (electrons), I_{NG}, $EDDB_P$ (electrons), NICS(0) (ppm), NICS(1) (ppm), and $NICS(1)_{zz}$ (ppm) results for the twenty-seven tests analyzed.

Table S26. Test T10 for HF, B3LYP, MP2, and CCSD results for MCI, I_{NB}, I_{ring}, I_{NG} indicators of aromaticity.

Table S1. B3LYP/6-311++G(d,p) optimized cartesian XYZ coordinates of all analyzed species.

Benzene Distortions

T1-T5. The optimized geometries can be found at the supporting information of the reference F. Feixas et al. J. Phys. Chem. A 2007, 111, 4513-4521, https://doi.org/10.1021/jp0703206.

Substitution and complexation in benzene.

T6

X=H

6	0.000000	1.394663	0.000000
6	1.207814	0.697332	0.000000
6	1.207814	-0.697332	0.000000
6	0.000000	-1.394663	0.000000
6	-1.207814	-0.697332	0.000000
6	-1.207814	0.697332	0.000000
1	0.000000	2.479089	0.000000
1	2.146954	1.239544	0.000000
1	2.146954	-1.239544	0.000000
1	0.000000	-2.479089	0.000000
1	-2.146954	-1.239544	0.000000
1	-2.146954	1.239544	0.000000

X=F

6	-1.215806	0.259980	0.000000
6	-1.206760	-1.134311	0.000000
6	0.000000	-1.833153	0.000000
6	1.206760	-1.134311	0.000000
6	1.215806	0.259980	0.000000
6	0.000000	0.925809	0.000000
9	0.000000	2.282918	0.000000
1	0.000000	-2.916547	0.000000
1	-2.138829	0.826056	0.000000
1	2.138829	0.826056	0.000000
1	-2.147289	-1.672892	0.000000
1	2.147289	-1.672892	0.000000

X=CCH

6	0.000609	-2.209655	0.000000
6	-1.206111	-1.510255	0.000000
6	-1.210765	-0.119555	0.000000
6	0.000000	0.593807	0.000000
6	1.211014	-0.118967	0.000000
6	1.206971	-1.509699	0.000000
6	-0.000485	2.021987	0.000000
1	2.146431	0.427389	0.000000
1	2.147733	-2.048484	0.000000
1	0.000861	-3.293691	0.000000
1	-2.146617	-2.049491	0.000000
1	-2.146381	0.426446	0.000000
6	-0.001594	3.227049	0.000000
1	0.000141	4.289554	0.000000

X=CHO

6	1.614935	-1.230301	0.000000
6	1.327875	0.132276	0.000000
6	0.000000	0.572246	0.000000
6	-1.044507	-0.362437	0.000000
6	-0.757154	-1.720847	0.000000
6	0.571914	-2.155168	0.000000
6	-0.284706	2.025369	0.000000
1	-2.066389	-0.001933	0.000000
1	-1.562659	-2.446195	0.000000
1	0.792117	-3.216826	0.000000
1	2.643889	-1.570591	0.000000
1	2.132755	0.860849	0.000000
8	-1.391038	2.516976	0.000000
1	0.618450	2.672059	0.000000

X=$COCH_3$

6	-1.981668	1.103537	0.000149
6	-2.550565	-0.172256	0.000049
6	-1.724241	-1.291841	-0.000114
6	-0.337883	-1.142807	-0.000176
6	0.242220	0.131713	-0.000088
6	-0.602114	1.256368	0.000082
6	1.701868	0.301454	-0.000181
6	2.482930	1.346000	0.000214
6	2.685616	-0.884590	0.000026
1	-0.169244	2.250318	0.000158
1	-2.617779	1.981391	0.000276
1	-3.628125	-0.288664	0.000095
1	-2.155202	-2.286572	-0.000190
1	0.289830	-2.025627	-0.000296
1	3.725558	-0.545900	-0.000539
1	2.529342	-1.484793	0.898980
1	2.528647	-1.485635	-0.898248

X=COCl

6	2.594516	1.266902	0.000000
6	1.503343	2.137280	0.000000
6	0.210882	1.630118	0.000000
6	0.000000	0.241608	0.000000
6	1.097026	-0.627421	0.000000
6	2.389263	-0.111751	0.000000
1	0.938262	-1.696660	0.000000
1	3.236054	-0.787720	0.000000
1	3.603378	1.663658	0.000000
1	1.661540	3.209273	0.000000
1	-0.645890	2.291773	0.000000
6	-1.412284	-0.212076	0.000000
17	-1.652515	-2.028579	0.000000
8	-2.374633	0.482195	0.000000

X=COOH

6	-0.964164	-1.993456	0.000000
6	-1.125353	-0.611100	0.000000
6	0.000000	0.221743	0.000000
6	1.282596	-0.338849	0.000000
6	1.438244	-1.720196	0.000000
6	0.315205	-2.548529	0.000000
6	-0.114929	1.703806	0.000000
1	2.140468	0.321996	0.000000
1	2.432251	-2.152078	0.000000
1	0.437278	-3.625873	0.000000
1	-1.835668	-2.637806	0.000000
1	-2.115081	-0.173997	0.000000
8	0.817434	2.473119	0.000000
8	-1.402420	2.137166	0.000000
1	-1.368949	3.104962	0.000000

X=$COOCH_3$

6	2.212600	1.234959	0.000000
6	1.391589	0.110944	0.000000
6	0.000000	0.262493	0.000000
6	-0.558993	1.545477	0.000000
6	0.264918	2.665692	0.000000
6	1.651568	2.511784	0.000000
6	-0.928811	-0.903650	0.000000
1	-1.637450	1.643544	0.000000
1	-0.171787	3.657705	0.000000
1	2.293835	3.385379	0.000000
1	3.289940	1.115423	0.000000
1	1.820124	-0.882344	0.000000
8	-2.135733	-0.820041	0.000000
8	-0.274499	-2.086246	0.000000
6	-1.103944	-3.261436	0.000000
1	-0.414342	-4.102650	0.000000
1	-1.736017	-3.282166	0.888720
1	-1.736017	-3.282166	-0.888720

X=$CONH_2$

6	1.851353	1.226452	-0.139939
6	0.458778	1.191721	-0.157092
6	-0.219649	-0.024785	-0.016842
6	0.516469	-1.205618	0.127165
6	1.906512	-1.168583	0.154592
6	2.576961	0.047675	0.022338
6	-1.718716	-0.136805	-0.037537
1	-0.021349	-2.141548	0.213656
1	2.468339	-2.087769	0.275026
1	3.660611	0.075871	0.038132
1	2.368628	2.171268	-0.261619
1	-0.090656	2.112739	-0.315911
8	-2.285185	-1.181193	-0.314109
7	-2.418507	1.008154	0.252455
1	-3.419148	0.909874	0.335093
1	-1.985654	1.771688	0.745201

X=CN

6	1.209094	-1.480487	0.000000
6	1.215157	-0.090122	0.000000
6	0.000000	0.610344	0.000000
6	-1.214876	-0.090665	0.000000
6	-1.208191	-1.481008	0.000000
6	0.000613	-2.176651	0.000000
6	-0.000450	2.042515	0.000000
1	-2.148770	0.457518	0.000000
1	-2.147125	-2.021842	0.000000
1	0.000834	-3.260477	0.000000
1	2.148279	-2.020884	0.000000
1	2.148829	0.458443	0.000000
7	-0.001446	3.197669	0.000000

X=NH_2

6	1.170643	1.200836	0.003313
6	-0.220576	1.206375	-0.004820
6	-0.936894	0.000140	-0.007529
6	-0.220602	-1.206208	-0.004761
6	1.170605	-1.200952	0.003338
6	1.879603	-0.000076	0.007653
7	-2.333441	-0.000002	-0.072364
1	-0.760023	-2.148285	-0.013819
1	1.703683	-2.145555	0.006840
1	2.962912	0.000039	0.014557
1	1.703933	2.145321	0.006657
1	-0.759799	2.148559	-0.013725
1	-2.786400	-0.838067	0.260834
1	-2.786907	0.837318	0.262043

X=NO

8	-1.333915	2.406766	0.000000
7	-0.181762	2.024943	0.000000
1	0.778755	-3.176570	0.000000
6	0.000000	0.596317	0.000000
6	-1.057331	-0.322437	0.000000
1	-2.075718	0.046461	0.000000
6	-0.768658	-1.678675	0.000000
1	-1.572955	-2.405395	0.000000
6	0.562749	-2.114048	0.000000
6	1.610808	-1.194595	0.000000
1	2.637846	-1.539869	0.000000
6	1.329223	0.168655	0.000000
1	2.114977	0.915343	0.000000

X=NO_2

6	-0.429918	1.218633	0.000000
6	0.241737	0.000003	0.000000
6	-0.429918	-1.218629	0.000000
6	-1.821248	-1.210116	0.000000
6	-2.515605	0.000000	0.000000
6	-1.821248	1.210115	0.000000
7	1.722363	0.000000	0.000000
8	2.290932	-1.084330	0.000000
8	2.290937	1.084324	0.000000
1	0.135010	-2.140423	0.000000
1	-2.362415	-2.148633	0.000000
1	-3.599475	0.000003	0.000000
1	-2.362419	2.148630	0.000000
1	0.135002	2.140433	0.000000

X=NN^+

6	1.221019	-1.480463	0.000000
6	1.243137	-0.096667	0.000000
6	0.000000	0.562626	0.000000
6	-1.243049	-0.096888	0.000000
6	-1.220685	-1.480660	0.000000
6	0.000235	-2.165545	0.000000
7	-0.000172	1.941555	0.000000
1	-2.170562	0.461738	0.000000
1	-2.154272	-2.028914	0.000000
1	0.000301	-3.249204	0.000000
1	2.154721	-2.028519	0.000000
1	2.170572	0.462089	0.000000
7	-0.000500	3.048215	0.000000

X=OH

6	-1.203937	0.231932	0.000000
6	-1.187890	-1.162126	0.000000
6	0.020269	-1.855253	0.000000
6	1.218336	-1.138884	0.000000
6	1.215468	0.252074	0.000000
6	0.000000	0.938451	0.000000
1	0.029635	-2.938553	0.000000
1	2.165288	-1.667106	0.000000
1	2.138563	0.819051	0.000000
1	-2.148683	0.768176	0.000000
1	-2.127082	-1.703895	0.000000
8	0.051348	2.307369	0.000000
1	-0.841975	2.666215	0.000000

X=OCH_3

6	-0.891747	-2.126216	0.000000
6	0.468599	-1.840275	0.000000
6	0.925254	-0.519450	0.000000
6	0.000000	0.527751	0.000000
6	-1.371931	0.245310	0.000000
6	-1.809324	-1.071731	0.000000
8	0.332320	1.852754	0.000000
6	1.707650	2.208356	0.000000
1	-2.071031	1.072903	0.000000
1	-2.873785	-1.278387	0.000000
1	-1.236608	-3.153266	0.000000
1	1.193111	-2.647148	0.000000
1	1.989151	-0.324512	0.000000
1	1.733203	3.296808	0.000000
1	2.218193	1.834549	0.894252
1	2.218193	1.834549	-0.894252

T7

6	0.702453	-1.227729	-1.612897
6	-0.702453	-1.227729	-1.612897
1	2.497560	0.003464	-1.580046
6	1.414471	0.005522	-1.612897
6	-1.414471	0.005522	-1.612897
6	-0.712018	1.222207	-1.612897
6	0.712018	1.222207	-1.612897
1	-2.497560	0.003464	-1.580046
1	-1.251780	2.161218	-1.580046
1	1.251780	2.161218	-1.580046
24	0.000000	0.000000	0.107268
6	0.000000	1.510267	1.178287
8	0.000000	2.475062	1.823373
6	1.307930	-0.755134	1.178287
8	2.143466	-1.237531	1.823373
6	-1.307930	-0.755134	1.178287
8	-2.143466	-1.237531	1.823373
1	1.245780	-2.164682	-1.580046
1	-1.245780	-2.164682	-1.580046

Ring size and atom size dependence

T8

$C_7H_7^+$

6	1.002967	1.257706	0.000000
6	1.608629	0.000009	0.000000
6	-0.357961	1.568321	0.000000
6	-1.449327	0.697953	0.000000
6	-1.449327	-0.697982	0.000000
6	-0.357948	-1.568315	0.000000
6	1.002968	-1.257689	0.000000
1	-2.427386	-1.169011	0.000000
1	-0.599502	-2.626661	0.000000
1	1.679808	-2.106424	0.000000
1	2.694203	-0.000002	0.000000
1	1.679797	2.106447	0.000000
1	-0.599523	2.626674	0.000000
1	-2.427400	1.168957	0.000000

$C_8H_8^{2+}$

6	0.704042	1.699710	0.000000
6	-0.704041	1.699714	0.000000
6	-1.699710	0.704040	0.000000
6	-1.699715	-0.704042	0.000000
6	-0.704041	-1.699711	0.000000
6	0.704041	-1.699715	0.000000
6	1.699707	-0.704039	0.000000
6	1.699718	0.704044	0.000000
1	1.120629	2.705415	0.000000
1	-1.120624	2.705420	0.000000
1	-2.705418	1.120622	0.000000
1	-2.705418	-1.120632	0.000000
1	-1.120627	-2.705417	0.000000
1	1.120623	-2.705421	0.000000
1	2.705413	-1.120625	0.000000
1	2.705422	1.120629	0.000000

T9

7	1.132320	0.637643	0.182396
7	1.132315	-0.637649	-0.182399
7	-0.000002	-1.279604	0.000093
7	-1.132322	-0.637612	0.182493
7	-1.132318	0.637618	-0.182490
7	0.000006	1.279604	-0.000094

Heteroaromatic species

T10

Pyridine

6	-1.219557	-0.580364	0.000000
6	-0.071127	-1.370527	0.000000
6	1.169232	-0.738454	0.000000
6	1.207016	0.653164	0.000000
6	0.000000	1.350595	0.000000
7	-1.197773	0.756463	0.000000
1	2.085999	-1.317527	0.000000
1	-2.203481	-1.041047	0.000000
1	-0.152413	-2.451047	0.000000
1	2.147749	1.190899	0.000000
1	-0.006828	2.436999	0.000000

Pyridazine

7	0.000000	0.665698	-1.228545
6	0.000000	1.322178	-0.067807
6	0.000000	0.690789	1.177694
6	0.000000	-0.690789	1.177694
6	0.000000	-1.322178	-0.067807
7	0.000000	-0.665698	-1.228545
1	0.000000	1.269052	2.094181
1	0.000000	2.403771	-0.153681
1	0.000000	-1.269052	2.094181
1	0.000000	-2.403771	-0.153681

Pyrimidine

6	0.000000	0.000000	-1.309860
7	0.000000	1.194934	-0.714173
6	0.000000	1.183265	0.622042
6	0.000000	0.000000	1.353474
6	0.000000	-1.183265	0.622042
7	0.000000	-1.194934	-0.714173
1	0.000000	2.151072	1.115810
1	0.000000	0.000000	-2.395805
1	0.000000	0.000000	2.436410
1	0.000000	-2.151072	1.115810

Pyrazine

6	0.000000	1.132301	0.697482
6	0.000000	1.132301	-0.697482
7	0.000000	0.000000	-1.404299
6	0.000000	-1.132301	-0.697482
6	0.000000	-1.132301	0.697482
7	0.000000	0.000000	1.404299
1	0.000000	2.064259	1.254860
1	0.000000	2.064259	-1.254860

1	0.000000	-2.064259	-1.254860
1	0.000000	-2.064259	1.254860

Triazine

6	0.000000	0.000000	-1.294350
7	0.000000	1.187239	-0.685473
6	0.000000	1.120921	0.647174
6	0.000000	-1.120921	0.647174
7	0.000000	-1.187239	-0.685473
1	0.000000	2.061628	1.190259
1	0.000000	0.000000	-2.380573
1	0.000000	-2.061628	1.190259
7	0.000000	0.000000	1.370956

T11

X=CH^-

6	0.372001	1.144849	0.000000
1	0.707445	2.177331	0.000000
6	-0.973909	0.707543	0.000000
1	-1.852134	1.345710	0.000000
6	0.372001	-1.144849	0.000000
1	0.707445	-2.177331	0.000000
6	-0.973909	-0.707543	0.000000
1	-1.852134	-1.345710	0.000000
6	1.203812	0.000000	0.000000
1	2.289401	0.000000	0.000000

X=NH

6	0.000000	1.124886	0.331177
6	0.000000	0.712382	-0.982359
6	0.000000	-0.712382	-0.982359
6	0.000000	-1.124886	0.331177
7	0.000000	0.000000	1.121570
1	0.000000	0.000000	2.127602
1	0.000000	2.112170	0.763257
1	0.000000	1.359416	-1.845462
1	0.000000	-1.359416	-1.845462
1	0.000000	-2.112170	0.763257

X=O

6	0.000000	0.717679	-0.957756
6	0.000000	-0.717679	-0.957756
6	0.000000	-1.095144	0.346923
8	0.000000	0.000000	1.158526
6	0.000000	1.095144	0.346923
1	0.000000	1.373404	-1.813697
1	0.000000	-1.373404	-1.813697
1	0.000000	-2.049761	0.844593
1	0.000000	2.049761	0.844593

X=CH_2

6	0.000000	0.734115	-0.990161
6	0.000000	-0.734115	-0.990161
6	0.000000	-1.179318	0.281653
6	0.000000	0.000000	1.216052
6	0.000000	1.179318	0.281653
1	0.000000	1.347888	-1.881848
1	0.000000	-1.347888	-1.881848
1	0.000000	-2.210462	0.607439
1	-0.877146	0.000000	1.877297
1	0.877146	0.000000	1.877297
1	0.000000	2.210462	0.607439

X=BH

6	0.049984	1.252498	0.000000
1	0.275144	2.311270	0.000000
6	-1.198962	0.759131	0.000000
1	-2.121676	1.332029	0.000000
6	0.049983	-1.252498	0.000000
1	0.275143	-2.311270	0.000000
6	-1.198962	-0.759130	0.000000
1	-2.121677	-1.332027	0.000000
5	1.017294	0.000000	0.000000
1	2.206448	-0.000001	0.000000

X=CH^+

6	-1.199545	0.348803	0.000000
1	-2.209841	0.728029	0.000000
6	-0.787183	-0.932269	0.000000
1	-1.390093	-1.831539	0.000000
6	1.199544	0.348812	0.000000
1	2.209840	0.728037	0.000000
6	0.787184	-0.932265	0.000000
1	1.390101	-1.831530	0.000000
6	0.000000	1.160087	0.000000
1	-0.000004	2.247993	0.000000

Clar's systems

T12

Phenanthrene

6	1.907313	-3.017175	0.000000
6	2.685629	-1.846679	0.000000
6	2.080243	-0.605325	0.000000
6	0.673458	-0.470416	0.000000
6	-0.110005	-1.660320	0.000000
6	0.532164	-2.919243	0.000000
6	-1.541303	-1.568725	0.000000
6	-2.168682	-0.365155	0.000000
6	-1.424136	0.860572	0.000000
6	0.000000	0.821402	0.000000
6	0.694915	2.051932	0.000000
1	1.777163	2.061414	0.000000
1	2.707622	0.276555	0.000000
6	0.023855	3.259080	0.000000
6	-1.381438	3.291335	0.000000
6	-2.088558	2.107921	0.000000
1	2.387079	-3.989357	0.000000
1	3.767637	-1.916957	0.000000
1	-0.080180	-3.815163	0.000000
1	-2.116109	-2.489029	0.000000
1	-3.252311	-0.309323	0.000000
1	0.585819	4.186369	0.000000
1	-1.903732	4.241343	0.000000
1	-3.173718	2.118929	0.000000

Pyrene

6	0.000127	-3.518966	0.000000
6	-1.208869	-2.829282	0.000000
6	-1.234523	-1.427212	0.000000
6	-0.000003	-0.712453	0.000000
6	1.234397	-1.427026	0.000000
6	1.208893	-2.829318	0.000000
6	2.460928	-0.679538	0.000000
6	2.460928	0.679539	0.000000
6	1.234398	1.427027	0.000000
6	-0.000003	0.712453	0.000000
6	-1.234523	1.427211	0.000000
6	-2.460958	0.679507	0.000000
6	-2.460958	-0.679508	0.000000
6	-1.208869	2.829282	0.000000
6	0.000126	3.518966	0.000000
6	1.208893	2.829319	0.000000
1	-3.397792	-1.226925	0.000000
1	-3.397791	1.226924	0.000000
1	-0.000033	-4.603162	0.000000
1	-2.146110	-3.375683	0.000000
1	2.146302	-3.375426	0.000000
1	3.397679	-1.227069	0.000000
1	3.397679	1.227069	0.000000
1	-2.146110	3.375681	0.000000
1	-0.000032	4.603162	0.000000
1	2.146301	3.375428	0.000000

Triphenylene

6	-2.431423	2.879416	0.000000
6	-2.434607	1.496230	0.000000
6	-1.237320	0.745059	0.000000
6	0.000000	1.444316	0.000000
6	-0.025222	2.857357	0.000000
6	-1.211696	3.568628	0.000000
6	2.512737	1.360197	0.000000
6	1.263931	0.699212	0.000000
6	1.250869	-0.722429	0.000000
6	-0.026624	-1.444243	0.000000
6	-1.250945	-0.722123	0.000000
6	2.487097	-1.406697	0.000000
6	3.696492	-0.734754	0.000000
6	3.709438	0.665761	0.000000
6	-2.461986	-1.450582	0.000000
6	-2.484447	-2.833657	0.000000
6	-1.277925	-3.545288	0.000000
6	-0.078343	-2.856523	0.000000
1	-3.371741	3.423819	0.000000
1	-3.391753	0.988623	0.000000
1	-1.193214	4.654994	0.000000
1	2.505547	-2.489939	0.000000
1	4.627616	-1.294671	0.000000
1	4.650723	1.208458	0.000000
1	-3.409177	-0.924765	0.000000
1	-3.434681	-3.360561	0.000000
1	-1.279275	-4.631832	0.000000
1	0.840006	-3.431249	0.000000
1	2.551976	2.442946	0.000000
1	0.903806	3.414903	0.000000

1,2-Benzo-pyrene

6	-0.918645	-3.524067	0.000000
6	0.297569	-2.843503	0.000000
6	0.356047	-1.444797	0.000000
6	-0.867842	-0.717353	0.000000
6	-2.110651	-1.420619	0.000000
6	-2.113133	-2.823732	0.000000
6	-3.337736	-0.678098	0.000000
6	-3.337735	0.678096	0.000000
6	-2.110654	1.420620	0.000000
6	-0.867842	0.717353	0.000000
6	0.356046	1.444797	0.000000
6	1.624608	0.709685	0.000000
6	1.624606	-0.709685	0.000000
6	0.297566	2.843503	0.000000
6	-0.918646	3.524069	0.000000
6	-2.113134	2.823731	0.000000
6	2.864569	-1.382586	0.000000
6	4.065085	-0.699619	0.000000
6	4.065085	0.699620	0.000000
6	2.864569	1.382587	0.000000
1	-0.923552	-4.608188	0.000000
1	1.207566	-3.427479	0.000000
1	-3.060941	-3.351185	0.000000
1	-4.272087	-1.229433	0.000000
1	-4.272090	1.229426	0.000000
1	1.207563	3.427480	0.000000
1	-0.923555	4.608189	0.000000
1	-3.060943	3.351182	0.000000
1	2.889844	-2.463617	0.000000
1	4.999975	-1.248289	0.000000
1	4.999977	1.248286	0.000000
1	2.889844	2.463618	0.000000

1,2-5,6-Dibenzo-anthrancene

6	2.501838	-1.454140	0.000000
6	1.225895	-0.742886	0.000000
6	1.225895	0.689244	0.000000
6	2.477150	1.396160	0.000000
6	3.659312	0.733187	0.000000
6	3.711133	-0.703904	0.000000
6	0.012636	1.386960	0.000000
6	-1.225895	0.742886	0.000000
6	-1.225895	-0.689244	0.000000
6	-0.012636	-1.386960	0.000000
6	-2.477150	-1.396161	0.000000
6	-3.659313	-0.733187	0.000000
6	-3.711133	0.703904	0.000000
6	-2.501838	1.454140	0.000000
6	-2.596215	2.861840	0.000000
6	-3.821352	3.503043	0.000000
6	-5.011256	2.758063	0.000000
6	-4.950532	1.379052	0.000000
6	2.596216	-2.861840	0.000000
6	3.821352	-3.503043	0.000000
6	5.011256	-2.758063	0.000000
6	4.950532	-1.379052	0.000000
1	2.454897	2.480962	0.000000
1	4.596202	1.280419	0.000000
1	0.062850	2.468952	0.000000
1	-0.062850	-2.468952	0.000000
1	-2.454898	-2.480962	0.000000
1	-4.596202	-1.280419	0.000000
1	-1.696759	3.464064	0.000000
1	-3.860955	4.586524	0.000000
1	-5.970211	3.263613	0.000000
1	-5.863105	0.791827	0.000000
1	1.696760	-3.464065	0.000000
1	3.860955	-4.586523	0.000000
1	5.970212	-3.263612	0.000000
1	5.863105	-0.791827	0.000000

Pentafulvenes and Heptafulvenes 1 S_0

T13

Pentafulvenes 1 – S_0

X=NH_2^+

6	0.000000	0.695878	0.000000
6	1.202665	-0.156428	0.000000
1	2.220793	0.202950	0.000000
6	0.757738	-1.420960	0.000000
1	1.361452	-2.318039	0.000000
6	-1.202625	-0.156686	0.000000
1	-2.220751	0.202702	0.000000
6	-0.757497	-1.421104	0.000000
1	-1.360976	-2.318335	0.000000
7	-0.000224	1.991154	0.000000
1	0.864800	2.524373	0.000000
1	-0.865435	2.524071	0.000000

X=O

6	0.000000	0.000000	0.823052
6	0.000000	1.204646	-0.088504
1	0.000000	2.223506	0.268126
6	0.000000	0.751566	-1.346802
1	0.000000	1.346186	-2.250654
6	0.000000	-1.204646	-0.088504
1	0.000000	-2.223506	0.268126
6	0.000000	-0.751566	-1.346802
1	0.000000	-1.346186	-2.250654
8	0.000000	0.000000	2.031302

X=NH

6	0.000000	0.793915	0.000000
6	-1.181577	-0.117759	0.000000
1	-2.210238	0.214166	0.000000
6	-0.718416	-1.379562	0.000000
1	-1.312983	-2.283572	0.000000
6	1.198611	-0.088275	0.000000
1	2.211627	0.284532	0.000000
6	0.770496	-1.361757	0.000000
1	1.385413	-2.251489	0.000000
7	0.056508	2.069109	0.000000
1	-0.884059	2.473230	0.000000

X=CH_2

6	0.000000	0.759956	0.000000
6	-1.178320	-0.125629	0.000000
1	-2.202957	0.217754	0.000000
6	-0.737261	-1.403679	0.000000
1	-1.350344	-2.294931	0.000000
6	1.178321	-0.125625	0.000000
1	2.202956	0.217760	0.000000
6	0.737265	-1.403677	0.000000
1	1.350353	-2.294927	0.000000
6	-0.000005	2.101827	0.000000
1	-0.925181	2.667650	0.000000
1	0.925166	2.667658	0.000000

X=BH_2^-

6	-0.794095	0.000005	0.000000
6	0.087739	1.148802	0.000000
1	-0.250384	2.179551	0.000000
6	1.404805	0.720193	0.000000
1	2.289224	1.349735	0.000000
6	0.087739	-1.148798	0.000000
1	-0.250384	-2.179547	0.000000
6	1.404805	-0.720191	0.000000
1	2.289223	-1.349734	0.000000
5	-2.278570	-0.000008	0.000000
1	-2.915409	1.029267	0.000000
1	-2.915380	-1.029303	0.000000

Heptafulvenes 1 – S_0

X=NH_2^+

6	0.686049	-1.911788	0.000000
6	1.552632	-0.790742	0.000000
6	-0.685871	-1.911851	0.000000
6	-1.552553	-0.790867	0.000000
6	-1.266904	0.549956	0.000000
6	0.000000	1.206614	0.000000
6	1.266909	0.550104	0.000000
1	-2.126866	1.213671	0.000000
1	2.126886	1.213799	0.000000
1	2.611223	-1.031326	0.000000
1	1.174737	-2.880184	0.000000
1	-1.174461	-2.880297	0.000000
1	-2.611128	-1.031515	0.000000
7	-0.000206	2.547614	0.000000
1	-0.859586	3.076913	0.000000
1	0.859064	3.077078	0.000000

X=O

6	0.680562	-1.846819	0.000000
6	1.562598	-0.718338	0.000000
6	-0.680532	-1.846844	0.000000
6	-1.562607	-0.718398	0.000000
6	-1.284295	0.611249	0.000000
6	0.000000	1.327143	0.000000
6	1.284302	0.611299	0.000000
1	-2.125603	1.297971	0.000000
1	2.125631	1.297991	0.000000
1	2.618869	-0.974154	0.000000
1	1.168314	-2.816619	0.000000
1	-1.168248	-2.816668	0.000000
1	-2.618873	-0.974232	0.000000
8	-0.000031	2.558744	0.000000

X=NH

6	0.693060	-1.861329	0.000000
6	1.571649	-0.720618	0.000000
6	-0.663122	-1.870968	0.000000
6	-1.552205	-0.739001	0.000000
6	-1.279660	0.587909	0.000000
6	0.000000	1.310197	0.000000
6	1.285199	0.602816	0.000000
1	-2.142883	1.250040	0.000000
1	2.123236	1.292580	0.000000
1	2.629386	-0.968425	0.000000
1	1.189120	-2.827162	0.000000
1	-1.148829	-2.841707	0.000000
1	-2.607779	-0.997335	0.000000
7	0.070144	2.602784	0.000000
1	-0.862791	3.018479	0.000000

X=CH_2

6	0.676294	-1.889034	0.000000
6	1.564903	-0.746685	0.000000
6	-0.675913	-1.889272	0.000000
6	-1.564793	-0.747065	0.000000
6	-1.281978	0.574934	0.000000
6	0.000000	1.284964	0.000000
6	1.281919	0.575328	0.000000
1	-2.141778	1.240127	0.000000
1	2.141798	1.240404	0.000000
1	2.621465	-0.999615	0.000000
1	1.169078	-2.856600	0.000000
1	-1.168393	-2.856985	0.000000
1	-2.621317	-1.000132	0.000000
6	-0.000382	2.640357	0.000000
1	0.923143	3.206099	0.000000
1	-0.924302	3.205544	0.000000

X=BH_2^-

6	0.674071	-1.873641	0.000000
6	1.580627	-0.718739	0.000000
6	-0.674082	-1.873542	0.000000
6	-1.580593	-0.718697	0.000000
6	-1.267649	0.605334	0.000000
6	0.000000	1.331685	0.000000
6	1.267734	0.605251	0.000000
1	-2.130883	1.271808	0.000000
1	2.130962	1.271749	0.000000
1	2.639591	-0.970998	0.000000
1	1.164683	-2.846540	0.000000
1	-1.164756	-2.846430	0.000000
1	-2.639558	-0.970915	0.000000
5	-0.000009	2.811642	0.000000
1	-1.034012	3.443412	0.000000
1	1.033375	3.443796	0.000000

Chemical Reactivity

T14

Diels-Alder TS

6	-0.426946	1.432986	0.496319
6	-0.427164	-1.433129	0.496368
6	-1.323801	0.701175	-0.262393
6	-1.323835	-0.701151	-0.262354
6	1.556444	0.694313	-0.257168
6	1.556966	-0.694220	-0.257321
1	-0.374636	2.509940	0.377999
1	-0.094413	1.068759	1.458987
1	-0.374996	-2.510113	0.378071
1	-0.094247	-1.068877	1.458896
1	-1.891630	1.211696	-1.035200
1	-1.891764	-1.211594	-1.035148
1	2.078276	1.230638	0.526642
1	1.444038	1.233732	-1.188035
1	2.078743	-1.230482	0.526531
1	1.444506	-1.233676	-1.188135

T15

Acetylene trimerization TS

6	-1.151754	1.366558	0.000000
6	0.000000	1.787096	0.000000
6	1.759490	0.314231	0.000000
6	-1.547911	-0.893513	0.000000
6	1.548345	-0.893519	0.000000
6	-0.608105	-1.680949	0.000000
1	0.729765	2.561162	0.000000
1	-2.208608	1.488055	0.000000
1	-2.583048	-0.648206	0.000000
1	2.392812	1.168973	0.000000
1	-0.184259	-2.656652	0.000000
1	1.852950	-1.912756	0.000000

Triplet-Excited State Species

T16

Five-Member Rings (5-MRs)

X=CH^+

6	-0.028953000	-1.210720000	0.000003000
6	-1.160680000	-0.346686000	-0.000052000
6	0.735140000	0.962580000	0.000036000
6	1.142772000	-0.401768000	0.000033000
1	-0.054808000	-2.292278000	-0.000007000
1	-2.197165000	-0.656553000	-0.000100000
1	1.391508000	1.822564000	0.000061000
1	2.163252000	-0.760857000	0.000060000
1	-1.302798000	1.886989000	-0.000035000
6	-0.688277000	0.996617000	-0.000016000

X=BH

6	0.696304000	0.956450000	0.000020000
6	1.203460000	-0.391913000	-0.000026000
6	-1.204095000	-0.389774000	0.000025000
6	-0.694644000	0.957556000	-0.000010000
1	1.305589000	1.853161000	0.000417000
1	2.270008000	-0.589569000	-0.000347000
1	-2.270950000	-0.585722000	-0.000002000
1	-1.302388000	1.855328000	-0.000364000
5	-0.001226000	-1.356593000	0.000042000
1	-0.002275000	-2.544147000	0.000031000

X=CH_2

6	-1.276696000	0.000005000	0.000327000
6	-0.316165000	-1.166966000	-0.000361000
6	1.059248000	0.679228000	0.000048000
6	-0.316149000	1.166983000	-0.000827000
1	-0.610122000	-2.207684000	-0.001073000
1	1.934025000	1.315226000	0.000016000
1	-0.610089000	2.207700000	0.001085000
1	1.934015000	-1.315245000	0.000625000
6	1.059240000	-0.679248000	0.000279000
1	-1.951251000	0.000135000	0.876029000
1	-1.953447000	-0.000140000	-0.873477000

X=O

6	-0.965211000	0.725189000	0.022526000
6	0.417664000	1.077261000	0.029396000
6	0.339747000	-1.155137000	-0.003736000
6	-1.059470000	-0.625018000	-0.052538000
1	-1.773351000	1.441749000	0.055211000
1	0.921474000	1.992782000	0.297458000
1	0.671064000	-1.903173000	0.718659000
1	-1.947935000	-1.234025000	-0.108557000
8	1.216546000	-0.053888000	-0.117082000

X=NH

6	-0.997514000	0.705402000	0.035409000
6	0.368788000	1.102629000	0.061249000
7	1.185038000	-0.029029000	-0.221780000
6	0.346313000	-1.173229000	0.027449000
6	-1.061534000	-0.652205000	-0.069190000
1	-1.829733000	1.395363000	0.059837000
1	0.802380000	2.065458000	0.284924000
1	0.634789000	-1.841608000	0.846537000
1	-1.941298000	-1.268407000	-0.171960000
1	2.102278000	-0.043186000	0.203621000

X=CH^-

6	0.026276000	1.187004000	-0.000189000
6	1.175503000	0.330797000	-0.000006000
6	-0.760327000	-0.932304000	0.000032000
6	-1.161154000	0.375938000	0.000081000
1	0.047716000	2.273078000	0.000126000
1	2.206417000	0.659064000	0.000050000
1	-1.396450000	-1.810416000	0.000137000
1	-2.177188000	0.747989000	0.000230000
1	1.319898000	-1.865395000	0.000071000
6	0.719636000	-0.962154000	-0.000021000

T17

Pentafulvenes I – T_1

X=NH_2^+

6	1.491467000	-0.694232000	-0.000198000
6	1.491784000	0.693669000	-0.000232000
6	0.133524000	1.153664000	0.000562000
6	-0.719427000	0.000226000	0.000219000
6	0.132945000	-1.153224000	0.000505000
1	2.361060000	-1.335613000	-0.000785000
1	2.361777000	1.334577000	-0.000421000
1	-0.192879000	2.185252000	-0.000373000
1	-0.193805000	-2.184670000	-0.000365000
1	-2.580953000	0.861890000	-0.000504000
7	-2.050951000	0.000013000	-0.000433000
1	-2.580299000	-0.862144000	0.000336000

X=O

6	-1.418195000	0.688628000	-0.000041000
6	-1.418246000	-0.688538000	-0.000102000
6	-0.053348000	-1.154575000	0.000166000
6	0.839963000	-0.000003000	0.000061000
6	-0.053388000	1.154503000	0.000112000
1	-2.294253000	1.322001000	-0.000212000
1	-2.294329000	-1.321868000	-0.000326000
1	0.277868000	-2.183977000	0.000382000
1	0.278362000	2.183738000	0.000367000
8	2.081455000	0.000001000	-0.000173000

X=NH

6	1.458982000	-0.661198000	-0.000212000
6	1.433085000	0.707133000	0.000147000
6	0.046700000	1.138176000	-0.000153000
6	-0.809108000	-0.025013000	0.000147000
6	0.091436000	-1.148597000	0.000072000
1	2.341494000	-1.285052000	-0.000461000
1	2.289730000	1.366149000	0.000300000
1	-0.295895000	2.165091000	0.000331000
1	-0.224020000	-2.182666000	0.000703000
1	-2.551589000	0.797683000	-0.000221000
7	-2.126613000	-0.132029000	-0.000094000

$X=CH_2$

6	-1.482000000	-0.680820000	-0.000003000
6	-1.482015000	0.680813000	0.000003000
6	-0.093937000	1.135502000	-0.000003000
6	0.777447000	0.000009000	0.000000000
6	-0.093958000	-1.135491000	0.000003000
1	-2.347596000	-1.327809000	-0.000005000
1	-2.347608000	1.327802000	0.000006000
1	0.227259000	2.168892000	-0.000002000
1	0.227258000	-2.168874000	-0.000004000
6	2.171022000	-0.000009000	0.000001000
1	2.730654000	-0.926497000	0.000003000
1	2.730679000	0.926464000	-0.000004000

$X=BH_2^-$

6	-1.474693000	-0.679544000	0.000231000
6	-1.474595000	0.679492000	0.000069000
6	-0.065970000	1.120320000	-0.000004000
6	0.825835000	0.000036000	-0.000704000
6	-0.066015000	-1.120275000	-0.000180000
1	-2.341324000	-1.330236000	0.000308000
1	-2.341138000	1.330310000	-0.000217000
1	0.247804000	2.158821000	0.000877000
1	0.247967000	-2.158731000	0.000525000
1	2.970242000	1.042489000	0.000640000
5	2.355723000	-0.000058000	0.000040000
1	2.970466000	-1.042537000	0.001200000

T18

Heptafulvenes I – T_1

$X=NH_2^+$

6	0.568296000	-1.297568000	0.000025000
6	1.186832000	0.000008000	-0.000009000
6	0.568239000	1.297575000	0.000011000
6	-0.813548000	-1.594192000	-0.000091000
6	-0.813614000	1.594179000	0.000055000
6	-1.881957000	-0.740420000	0.000045000
6	-1.882000000	0.740380000	-0.000014000
1	-2.867031000	-1.192900000	0.000183000
1	1.249029000	-2.141629000	0.000219000
1	1.248957000	2.141649000	-0.000189000
1	-1.048696000	-2.653451000	-0.000118000
1	-1.048779000	2.653436000	0.000018000
1	-2.867094000	1.192811000	-0.000202000
7	2.519919000	0.000036000	-0.000008000
1	3.050357000	0.864330000	-0.000019000
1	3.050341000	-0.864276000	0.000036000

X=O

6	-0.634859000	-1.295946000	-0.000151000
6	-1.297603000	-0.000013000	0.000017000
6	-0.634905000	1.295942000	0.000001000
6	0.751932000	-1.587725000	-0.000046000
6	0.751875000	1.587729000	-0.000073000
6	1.820078000	-0.734944000	0.000137000
6	1.820050000	0.734983000	-0.000009000
1	2.805347000	-1.189225000	0.000327000
1	-1.330981000	-2.126172000	-0.000268000
1	-1.331033000	2.126160000	0.000045000
1	0.994695000	-2.646817000	0.000050000
1	0.994616000	2.646827000	-0.000100000
1	2.805301000	1.189305000	-0.000135000
8	-2.549669000	-0.000029000	0.000102000

X=NH

6	0.649528000	-1.260528000	0.000427000
6	1.274220000	0.035245000	0.000064000
6	0.592549000	1.302083000	0.000201000
6	-0.733550000	-1.586415000	0.000035000
6	-0.800795000	1.565064000	0.000178000
6	-1.823632000	-0.763221000	-0.000279000
6	-1.857160000	0.696713000	-0.000144000
1	-2.795573000	-1.246040000	-0.000534000
1	1.338042000	-2.099903000	0.000760000
1	1.262794000	2.152703000	0.000179000
1	-0.946786000	-2.652007000	0.000208000
1	-1.059925000	2.620478000	0.000470000
1	-2.849628000	1.135133000	-0.000360000
7	2.603365000	0.136369000	-0.000454000
1	3.020561000	-0.798588000	-0.000431000

X=CH_2

6	0.601092000	-1.275207000	-0.000287000
6	1.251764000	-0.000011000	-0.000025000
6	0.601141000	1.275192000	-0.000170000
6	-0.787003000	-1.569459000	-0.000032000
6	-0.786948000	1.569462000	-0.000051000
6	-1.865389000	-0.726126000	0.000270000
6	-1.865363000	0.726162000	-0.000017000
1	-2.845937000	-1.191384000	-0.000194000
1	1.265143000	-2.132824000	-0.000410000
1	1.265213000	2.132791000	-0.000253000
1	-1.021506000	-2.630991000	0.000372000
1	-1.021435000	2.631003000	0.000056000
1	-2.845893000	1.191453000	0.000288000
6	2.648317000	-0.000041000	0.000184000
1	3.209220000	0.926414000	0.000697000
1	3.209530000	-0.926302000	0.000204000

X=BH_2^-

6	0.627416000	-1.266505000	-0.000196000
6	1.307635000	-0.000185000	-0.000377000
6	0.627264000	1.266287000	-0.000119000
6	-0.751526000	-1.564288000	0.000155000
6	-0.751527000	1.564256000	0.000138000
6	-1.856120000	-0.715112000	0.000007000
6	-1.856176000	0.715237000	-0.000098000
1	-2.834238000	-1.192938000	0.000327000
1	1.284825000	-2.133030000	-0.000319000
1	1.284772000	2.132711000	0.000417000
1	-0.988609000	-2.629080000	0.000559000
1	-0.988469000	2.629073000	-0.000061000
1	-2.834283000	1.193040000	0.000091000
5	2.820371000	0.000232000	0.000202000
1	3.445659000	1.033085000	0.000638000
1	3.446681000	-1.032159000	0.000276000

T19

Pentafulvenes II – S_0

X=NH_2^+

6	0.000000000	0.720082000	-2.232607000
6	0.000000000	-0.720082000	-2.232607000
6	0.000000000	-1.160405000	-0.930001000
6	0.000000000	0.000000000	-0.069077000
6	0.000000000	1.160405000	-0.930001000
1	0.000000000	1.347194000	-3.113835000
1	0.000000000	-1.347194000	-3.113835000
1	0.000000000	-2.197248000	-0.618378000
1	0.000000000	2.197248000	-0.618378000
6	0.000000000	0.000000000	1.319074000
7	0.000000000	-1.152247000	2.047615000
1	0.000000000	-1.153036000	3.051364000
1	0.000000000	-2.036913000	1.573201000
7	0.000000000	1.152247000	2.047615000
1	0.000000000	1.153036000	3.051364000
1	0.000000000	2.036913000	1.573201000

X=H

6	1.403817000	0.737282000	-0.000109000
6	1.403808000	-0.737298000	0.000051000
6	0.125639000	-1.178370000	-0.000048000
6	-0.759765000	0.000012000	0.000163000
6	0.125654000	1.178376000	0.000038000
1	2.295364000	1.350079000	-0.000133000
1	2.295349000	-1.350103000	0.000100000
1	-0.218151000	-2.202918000	-0.000047000
1	-0.218115000	2.202931000	0.000106000
6	-2.102025000	0.000002000	-0.000074000
1	-2.668592000	-0.924849000	-0.000114000
1	-2.668625000	0.924831000	-0.000032000

X=CN

6	2.574396000	-0.742878000	-0.000049000
6	2.574390000	0.742886000	0.000096000
6	1.300727000	1.185779000	-0.000055000
6	0.428957000	-0.000011000	-0.000034000
6	1.300737000	-1.185784000	-0.000005000
1	3.465798000	-1.354803000	-0.000064000
1	3.465789000	1.354813000	0.000135000
1	0.950067000	2.206538000	-0.000106000
1	0.950090000	-2.206547000	-0.000020000
6	-0.933361000	0.000000000	0.000015000
6	-1.684837000	-1.216406000	0.000082000
7	-2.292063000	-2.199005000	-0.000028000
6	-1.684826000	1.216411000	0.000015000
7	-2.292057000	2.199007000	-0.000020000

T20

Heptafulvenes II – S_0

$X=NH_2^+$

6	0.001355000	-2.689124000	0.672931000
6	0.001924000	-1.534420000	1.566459000
6	0.001355000	-0.214111000	1.274836000
6	0.000095000	0.501391000	0.000000000
6	0.001355000	-0.214111000	-1.274836000
6	0.001924000	-1.534420000	-1.566459000
6	0.001355000	-2.689124000	-0.672931000
1	0.001106000	-3.655165000	1.169846000
1	0.002889000	-1.782601000	2.623663000
1	0.002165000	0.409712000	2.163819000
1	0.002165000	0.409712000	-2.163819000
1	0.002889000	-1.782601000	-2.623663000
1	0.001106000	-3.655165000	-1.169846000
6	-0.001876000	1.884258000	0.000000000
7	-0.003008000	2.656240000	1.146917000
1	-0.002967000	2.245310000	2.059295000
1	-0.004589000	3.658040000	1.095063000
7	-0.003008000	2.656240000	-1.146917000
1	-0.004589000	3.658040000	-1.095063000
1	-0.002967000	2.245310000	-2.059295000

X=H

6	1.889111000	0.676427000	0.000042000
6	0.746859000	1.564868000	-0.000182000
6	-0.575326000	1.281595000	-0.000014000
6	-1.284996000	-0.000174000	0.000177000
6	-0.574976000	-1.281755000	-0.000137000
6	0.747257000	-1.564817000	-0.000053000
6	1.889344000	-0.676103000	0.000127000
1	2.856864000	1.169117000	0.000190000
1	0.999449000	2.621612000	-0.000361000
1	-1.240497000	2.141552000	-0.000115000
1	-1.239995000	-2.141842000	-0.000408000
1	1.000075000	-2.621505000	-0.000096000
1	2.857234000	-1.168504000	0.000364000
6	-2.640733000	-0.000167000	0.000101000
1	-3.206679000	-0.923633000	-0.000446000
1	-3.205693000	0.923955000	0.000509000

X=CN

6	3.022934000	-0.680754000	0.001878000
6	1.889663000	-1.552789000	-0.000316000
6	0.556819000	-1.270029000	-0.001928000
6	-0.132273000	-0.000068000	-0.001069000
6	0.556914000	1.269950000	-0.001958000
6	1.889702000	1.552773000	-0.000837000
6	3.022999000	0.680702000	0.001537000
1	3.990174000	-1.173020000	0.003681000
1	2.132597000	-2.611223000	-0.000669000
1	-0.097974000	-2.135241000	-0.003591000
1	-0.097990000	2.135082000	-0.003685000
1	2.132687000	2.611197000	-0.001716000
1	3.990250000	1.172926000	0.002931000
6	-1.531409000	0.000013000	-0.000651000
6	-2.281507000	-1.206977000	0.000159000
7	-2.880390000	-2.198173000	0.001143000
6	-2.281679000	1.206906000	0.000353000
7	-2.880000000	2.198446000	0.001720000

T21

Pentafulvenes II – T_1

X=NH_2^+

6	0.000000000	0.676592000	-2.319440000
6	0.000000000	-0.676592000	-2.319440000
6	0.000000000	-1.138765000	-0.921669000
6	0.000000000	0.000000000	-0.049380000
6	0.000000000	1.138765000	-0.921669000
1	0.000000000	1.327367000	-3.182200000
1	0.000000000	-1.327367000	-3.182200000
1	0.000000000	-2.179813000	-0.626464000
1	0.000000000	2.179813000	-0.626464000
6	0.000000000	0.000000000	1.346517000
7	0.000000000	1.173775000	2.090600000
1	0.000000000	2.066667000	1.636417000
1	0.000000000	1.162695000	3.093285000
7	0.000000000	-1.173775000	2.090600000
1	0.000000000	-1.162695000	3.093285000
1	0.000000000	-2.066667000	1.636417000

X=H

6	1.481883000	0.680987000	0.000027000
6	1.481881000	-0.680987000	0.000029000
6	0.094011000	-1.135301000	-0.000059000
6	-0.777329000	0.000002000	-0.000030000
6	0.094003000	1.135304000	-0.000062000
1	2.346971000	1.328611000	0.000229000
1	2.346970000	-1.328610000	0.000232000
1	-0.226710000	-2.168940000	-0.000311000
1	-0.226717000	2.168944000	-0.000317000
6	-2.171036000	-0.000004000	0.000068000
1	-2.730493000	-0.926564000	0.000146000
1	-2.730501000	0.926552000	0.000187000

X=CN

6	-2.652381000	0.684365000	-0.000006000
6	-2.652381000	-0.684363000	-0.000006000
6	-1.274904000	-1.139145000	0.000003000
6	-0.420603000	0.000000000	0.000009000
6	-1.274904000	1.139146000	0.000003000
1	-3.516529000	1.332338000	-0.000011000
1	-3.516529000	-1.332337000	-0.000011000
1	-0.946294000	-2.169506000	0.000005000
1	-0.946294000	2.169507000	0.000004000
6	0.996278000	0.000001000	0.000018000
6	1.720077000	-1.214380000	0.000003000
7	2.282719000	-2.228206000	-0.000011000
6	1.720078000	1.214379000	0.000003000
7	2.282722000	2.228205000	-0.000011000

T22

Heptafulvenes II – T_1

$X=NH_2^+$

6	0.000000000	0.716103000	-2.666799000
6	0.000000000	1.555893000	-1.570851000
6	0.000000000	1.267192000	-0.189585000
6	0.000000000	0.000000000	0.480899000
6	0.000000000	-1.267192000	-0.189585000
6	0.000000000	-1.555893000	-1.570851000
6	0.000000000	-0.716103000	-2.666799000
1	0.000000000	1.194117000	-3.641451000
1	0.000000000	2.618748000	-1.800534000
1	0.000000000	2.159665000	0.424298000
1	0.000000000	-2.159665000	0.424298000
1	0.000000000	-2.618748000	-1.800534000
1	0.000000000	-1.194117000	-3.641451000
6	0.000000000	0.000000000	1.902089000
7	0.000000000	1.145577000	2.651498000
1	0.000000000	2.047684000	2.216751000
1	0.000000000	1.113172000	3.654894000
7	0.000000000	-1.145577000	2.651498000
1	0.000000000	-1.113172000	3.654894000
1	0.000000000	-2.047684000	2.216751000

X=H

6	1.865373000	0.726269000	-0.001121000
6	0.786907000	1.569456000	-0.000473000
6	-0.601019000	1.275124000	0.001569000
6	-1.251895000	-0.000091000	-0.000008000
6	-0.601046000	-1.275184000	-0.000992000
6	0.787045000	-1.569420000	0.000577000
6	1.865422000	-0.726189000	0.000847000
1	2.845954000	1.191441000	-0.003108000
1	1.021288000	2.631020000	-0.001643000
1	-1.265144000	2.132711000	0.003239000
1	-1.264968000	-2.132934000	-0.002156000
1	1.021463000	-2.630982000	0.001624000
1	2.846040000	-1.191276000	0.002414000
6	-2.648412000	0.000012000	-0.000278000
1	-3.209546000	-0.926287000	-0.001924000
1	-3.209335000	0.926445000	0.000824000

X=CN

6	3.014136000	-0.728387000	0.000501000
6	1.939174000	-1.566232000	0.000579000
6	0.544339000	-1.269582000	-0.000193000
6	-0.087347000	0.000024000	0.000090000
6	0.544314000	1.269595000	0.000395000
6	1.939191000	1.566230000	-0.000552000
6	3.014142000	0.728382000	-0.000703000
1	3.994352000	-1.193294000	0.001286000
1	2.166603000	-2.628432000	0.001317000
1	-0.110483000	-2.131790000	-0.000616000
1	-0.110506000	2.131807000	0.000958000
1	2.166632000	2.628427000	-0.001254000
1	3.994367000	1.193267000	-0.001645000
6	-1.529599000	-0.000001000	0.000120000
6	-2.288030000	-1.194701000	-0.000171000
7	-2.922468000	-2.165084000	-0.000672000
6	-2.288040000	1.194693000	0.000397000
7	-2.922481000	2.165069000	0.000268000

Redox Species

T23

Borole

X=C_4H_5B

6	-0.759335000	-0.899275000	-0.000042000
6	-1.252634000	0.349827000	0.000012000
6	1.252702000	0.349504000	0.000102000
6	0.759070000	-0.899473000	-0.000037000
1	-1.331922000	-1.822277000	-0.000012000
1	-2.311501000	0.574983000	0.000369000
1	2.311618000	0.574443000	0.000156000
1	1.331416000	-1.822619000	-0.000166000
1	0.000348000	2.506095000	-0.000459000
5	0.000243000	1.317175000	-0.000021000

X=$C_4H_5B^{2-}$

6	-0.725604000	-0.931197000	-0.003135000
6	-1.223658000	0.373762000	0.004315000
6	1.223557000	0.373927000	0.004755000
6	0.725851000	-0.931117000	-0.003130000
1	-1.318697000	-1.845600000	-0.007121000
1	-2.295760000	0.579787000	0.008974000
1	2.295583000	0.580419000	0.007973000
1	1.318979000	-1.845511000	-0.007813000

1	0.000337000	2.547779000	-0.055696000
5	-0.000264000	1.334175000	0.007370000

T24

Tetrathiafulvalene (TTF)

$X=C_6H_4S_4$

6	-3.175487000	0.667235000	0.225242000
6	-3.175624000	-0.667005000	0.225094000
16	-1.652059000	-1.493527000	-0.092135000
6	-0.673659000	-0.000350000	-0.087741000
1	-4.047840000	1.286779000	0.380965000
1	-4.047943000	-1.286560000	0.380948000
16	-1.651953000	1.493392000	-0.092331000
6	0.673785000	-0.000147000	-0.087123000
16	1.652045000	-1.493346000	-0.090740000
16	1.651553000	1.493394000	-0.090614000
6	3.176021000	-0.666984000	0.223599000
6	3.175819000	0.667343000	0.223560000
1	4.048799000	-1.286292000	0.377825000
1	4.048460000	1.286912000	0.377597000

$X=C_6H_4S_4^+$

6	-3.190948000	0.671140000	-0.000608000
6	-3.190644000	-0.671365000	0.000033000
16	-1.643326000	-1.466929000	0.001091000
6	-0.698047000	0.000643000	0.000032000
1	-4.072172000	1.298574000	-0.001401000
1	-4.071921000	-1.298759000	0.000208000
16	-1.643246000	1.467071000	-0.000843000
6	0.697791000	0.000204000	0.000250000
16	1.643764000	1.467054000	0.001089000
16	1.643128000	-1.467167000	-0.000828000
6	3.190660000	0.670992000	-0.000032000
6	3.190387000	-0.671513000	-0.000732000
1	4.072154000	1.298071000	0.000547000
1	4.071632000	-1.298952000	-0.001165000

$X=C_6H_4S_4^{2+}$

6	-3.185911000	0.646218000	0.208803000
6	-3.185581000	-0.646639000	-0.209119000
16	-1.646787000	-1.366776000	-0.461344000
6	-0.728781000	0.000274000	0.000470000
1	-4.067528000	1.247062000	0.406004000
1	-4.067121000	-1.247522000	-0.406598000
16	-1.647137000	1.366787000	0.461198000
6	0.728667000	0.000198000	0.000403000
16	1.647068000	1.366856000	-0.461108000
16	1.646921000	-1.366716000	0.461334000
6	3.185796000	0.646225000	-0.209428000
6	3.185644000	-0.646527000	0.208865000
1	4.067421000	1.246936000	-0.406990000
1	4.067194000	-1.247391000	0.406339000

T25

Pentalene

$X=C_8H_6^{2-}$

6	-0.725604000	-0.931197000	-0.003135000
6	-1.223658000	0.373762000	0.004315000
6	1.223557000	0.373927000	0.004755000
6	0.725851000	-0.931117000	-0.003130000
1	-1.318697000	-1.845600000	-0.007121000
1	-2.295760000	0.579787000	0.008974000
1	2.295583000	0.580419000	0.007973000
1	1.318979000	-1.845511000	-0.007813000
1	0.000337000	2.547779000	-0.055696000
5	-0.000264000	1.334175000	0.007370000

$X=C_8H_6$

6	-0.759335000	-0.899275000	-0.000042000
6	-1.252634000	0.349827000	0.000012000
6	1.252702000	0.349504000	0.000102000
6	0.759070000	-0.899473000	-0.000037000
1	-1.331922000	-1.822277000	-0.000012000
1	-2.311501000	0.574983000	0.000369000
1	2.311618000	0.574443000	0.000156000
1	1.331416000	-1.822619000	-0.000166000
1	0.000348000	2.506095000	-0.000459000
5	0.000243000	1.317175000	-0.000021000

X=$C_8H_6^{2+}$

6	0.000000000	1.190570000	1.321789000
6	0.000000000	0.000000000	2.129860000
6	0.000000000	-1.190570000	1.321789000
6	0.000000000	-0.768813000	0.000000000
6	0.000000000	0.768813000	0.000000000
6	0.000000000	-1.190570000	-1.321789000
6	0.000000000	0.000000000	-2.129860000
6	0.000000000	1.190570000	-1.321789000
1	0.000000000	2.205250000	1.708469000
1	0.000000000	0.000000000	3.217800000
1	0.000000000	-2.205250000	1.708469000
1	0.000000000	-2.205250000	-1.708469000
1	0.000000000	0.000000000	-3.217800000
1	0.000000000	2.205250000	-1.708469000

T26

Anthracene

X=$C_{14}H_{10}$

6	-3.655933000	-0.712500000	-0.000336000
6	-2.477047000	-1.405366000	-0.000067000
6	-3.655973000	0.712429000	-0.000297000
1	-2.476487000	-2.490463000	0.000042000
1	-4.600551000	1.244668000	-0.000453000
6	-1.222068000	-0.721467000	0.000073000
6	-2.477127000	1.405355000	0.000005000
1	-2.476624000	2.490452000	0.000173000
6	-1.222100000	0.721519000	0.000119000
1	-4.600481000	-1.244790000	-0.000518000
6	0.000022000	1.402107000	0.000307000
6	-0.000068000	-1.401939000	0.000267000
6	1.222052000	-0.721457000	0.000492000
6	1.222134000	0.721540000	0.000523000
6	2.477018000	-1.405339000	0.000028000
6	2.477174000	1.405313000	0.000077000
6	3.655916000	-0.712527000	-0.000300000
6	3.656003000	0.712372000	-0.000575000
1	-0.000104000	-2.487859000	0.000412000
1	0.000017000	2.488030000	0.000019000
1	2.476446000	-2.490444000	-0.000051000
1	2.476709000	2.490421000	0.000040000
1	4.600458000	-1.244833000	-0.000639000
1	4.600607000	1.244573000	-0.000912000

X=$C_{14}H_{10}^{2+}$

6	-3.677917000	-0.693309000	0.000081000
6	-2.457140000	-1.406467000	-0.000017000
6	-3.677922000	0.693290000	0.000102000
1	-2.471515000	-2.491635000	0.000046000
1	-4.614533000	1.239243000	0.000092000
6	-1.233320000	-0.719256000	-0.000100000
6	-2.457152000	1.406466000	0.000030000
1	-2.471530000	2.491632000	0.000124000
6	-1.233329000	0.719269000	-0.000054000
1	-4.614521000	-1.239275000	0.000055000
6	-0.000023000	1.409063000	0.000008000
6	0.000012000	-1.409042000	-0.000140000
6	1.233331000	-0.719259000	-0.000013000
6	1.233319000	0.719269000	0.000001000
6	2.457101000	-1.406450000	-0.000096000
6	2.457147000	1.406468000	-0.000083000
6	3.677927000	-0.693297000	-0.000155000
6	3.677962000	0.693268000	0.000077000
1	0.000011000	-2.495856000	-0.000172000
1	-0.000040000	2.495878000	-0.000087000
1	2.471474000	-2.491617000	0.001021000
1	2.471553000	2.491635000	-0.000541000
1	4.614532000	-1.239255000	0.000662000
1	4.614595000	1.239178000	0.000956000

T27

Quinones

Quinone A (2,3-naphtoquinone)

6	-3.031831000	0.724328000	-0.000493000
6	-3.031839000	-0.724357000	-0.000139000
6	-1.872397000	1.419577000	-0.000364000
1	-3.981405000	-1.246934000	-0.000323000
1	-1.872923000	2.503586000	-0.000568000
6	-1.872391000	-1.419585000	0.000378000
6	-0.589305000	0.743774000	0.000109000
1	-1.872896000	-2.503596000	0.000683000
6	-0.589299000	-0.743763000	0.000524000
1	-3.981393000	1.246920000	-0.000815000
6	0.579106000	-1.445208000	0.000747000
6	1.881634000	-0.782015000	-0.000044000
6	1.881647000	0.782059000	0.000195000
6	0.579074000	1.445265000	0.000081000
8	2.933293000	-1.390197000	-0.001253000
1	0.584350000	2.530076000	0.000577000
1	0.584507000	-2.529930000	0.000907000
8	2.933377000	1.390126000	0.000449000

Quinone B (1,2-naphtoquinone)

6	-3.029711000	0.363079000	0.000046000
6	-2.731209000	-0.999154000	0.000098000
6	-2.003789000	1.306394000	-0.000041000
1	-3.530345000	-1.731091000	0.000085000
1	-2.240608000	2.364880000	-0.000066000
6	-1.402380000	-1.417301000	0.000042000
6	-0.664819000	0.900829000	0.000012000
1	-1.145498000	-2.469868000	0.000106000
6	-0.369149000	-0.480040000	-0.000035000
1	-4.062552000	0.692154000	0.000001000
6	1.047965000	-0.937799000	-0.000043000
6	2.159851000	0.161384000	0.000123000
6	1.719849000	1.561993000	0.000117000
6	0.413077000	1.886856000	-0.000151000
8	1.363641000	-2.105552000	-0.000183000
8	3.326670000	-0.167165000	0.000090000
1	0.119352000	2.932620000	-0.000411000
1	2.499063000	2.315594000	0.000027000

T28

Purines

1H-purine

6	0.000000000	-0.794023000	0.000000000
6	0.593457000	0.543460000	0.000000000
6	-0.242129000	1.621615000	0.000000000
6	-2.076769000	0.065031000	0.000000000
6	2.099039000	-0.908747000	0.000000000
7	1.950232000	0.417576000	0.000000000
1	0.059819000	2.660467000	0.000000000
1	-3.157946000	-0.016233000	0.000000000
1	3.082219000	-1.362441000	0.000000000
7	0.975177000	-1.693141000	0.000000000
7	-1.339117000	-1.006493000	0.000000000
7	-1.583705000	1.345479000	0.000000000
1	-2.243787000	2.110235000	0.000000000

9H-purine

6	0.000000000	0.700301000	0.000000000
6	0.449449000	-0.636483000	0.000000000
6	-0.548031000	-1.607346000	0.000000000
6	-2.122168000	0.070002000	0.000000000
6	2.202441000	0.567426000	0.000000000
7	1.834814000	-0.685098000	0.000000000
1	-0.322630000	-2.669576000	0.000000000
1	-3.176323000	0.326247000	0.000000000
1	3.226528000	0.912252000	0.000000000
7	1.146931000	1.458899000	0.000000000
7	-1.265225000	1.096581000	0.000000000
7	-1.832614000	-1.241640000	0.000000000
1	1.194939000	2.466478000	0.000000000

Table S2. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T1.

T1	ΔR	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
	0	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.923	0.989	-8.05	-10.22	-29.25
	0.05	0.102	0.045	0.070	0.0409	0.0467	0.0411	0.805	0.827	-7.91	-10.07	-28.79
	0.1	0.099	0.088	0.064	0.0403	0.0435	0.0406	0.598	0.344	-7.54	-9.65	-27.47
	0.15	0.094	0.130	0.056	0.0393	0.0389	0.0399	0.380	-0.461	-7.00	-9.02	-25.48
	0.2	0.088	0.168	0.046	0.0381	0.0333	0.0389	0.225	-1.588	-6.37	-8.26	-23.08
	0.25	0.082	0.204	0.037	0.0367	0.0280	0.0378	0.131	-3.038	-5.78	-7.45	-20.52

Table S3. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T2.

T2	α	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
	0	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.923	0.989	-8.05	-10.22	-29.25
	5	0.103	0.014	0.072	0.0410	0.0478	0.0413	0.914	0.970	-8.06	-10.21	-29.19
	10	0.103	0.029	0.071	0.0410	0.0478	0.0413	0.902	0.905	-8.08	-10.18	-28.99
	15	0.104	0.047	0.071	0.0410	0.0473	0.0412	0.887	0.761	-8.09	-10.10	-28.57
	20	0.104	0.071	0.069	0.0408	0.0465	0.0411	0.870	0.457	-8.04	-9.92	-27.76
	25	0.104	0.103	0.065	0.0404	0.0453	0.0408	0.839	-0.193	-7.85	-9.57	-26.26

Table S4. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T3.

T3	α	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
	0	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.912	0.989	-8.05	-10.22	-29.25
	5	0.103	0.000	0.072	0.0410	0.0477	0.0413	0.899	0.987	-8.00	-10.13	-29.25
	10	0.103	0.000	0.071	0.0410	0.0475	0.0412	0.881	0.986	-7.91	-10.02	-29.29
	15	0.104	0.001	0.070	0.0409	0.0470	0.0412	0.861	0.982	-7.78	-9.90	-29.31
	20	0.104	0.003	0.070	0.0408	0.0465	0.0411	0.833	0.976	-7.60	-9.74	-29.30
	25	0.105	0.004	0.069	0.0407	0.0458	0.0410	0.802	0.965	-7.31	-9.55	-29.24

Table S5. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T4.

T4	α	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
	0	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.912	0.989	-8.05	-10.22	-29.25
	5	0.103	0.000	0.072	0.0410	0.0477	0.0413	0.907	0.988	-7.88	-10.15	-29.16
	10	0.103	0.001	0.071	0.0410	0.0475	0.0412	0.887	0.984	-7.59	-10.02	-28.90
	15	0.103	0.003	0.070	0.0409	0.0469	0.0412	0.860	0.967	-7.14	-9.83	-28.48
	20	0.103	0.005	0.069	0.0409	0.0461	0.0411	0.829	0.955	-6.53	-9.59	-27.89
	25	0.104	0.007	0.068	0.0407	0.0456	0.0410	0.790	0.951	-5.77	-9.06	-26.83

Table S6. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T5.

T5	α	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
	0	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.923	0.989	-8.05	-10.22	-29.25
	5	0.103	0.000	0.072	0.0410	0.0477	0.0413	0.912	0.988	-7.98	-9.36	-26.91
	10	0.103	0.000	0.071	0.0410	0.0477	0.0413	0.912	0.986	-7.81	-8.38	-24.28
	15	0.103	0.001	0.071	0.0410	0.0475	0.0412	0.911	0.983	-7.56	-7.31	-21.42
	20	0.104	0.002	0.071	0.0410	0.0472	0.0412	0.909	0.977	-7.26	-6.17	-18.37
	25	0.104	0.003	0.071	0.0409	0.0468	0.0411	0.907	0.969	-6.92	-4.96	-15.17

Table S7. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T6.

T6	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	ASE(1)[a]	ASE(2)[a]	ASE(3)[a]	ASE(4)[a]	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
H	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.912	33.2	24.7	30.7	32.7	0.989	-8.05	-10.22	-29.25
F	0.098	0.030	0.067	0.0406	0.0445	0.0408	0.820	33.1	22.6	29.3	32.2	0.993	-9.97	-10.38	-28.24
CH_3	0.100	0.015	0.068	0.0407	0.0456	0.0410	0.829	32.6	23.7	30.4	32.1	0.984	-7.95	-9.79	-27.86
CCH	0.095	0.033	0.063	0.0402	0.0424	0.0405	0.777	33.4	24.8	31.6	32.1	0.970	-8.07	-9.90	-27.09
CHO	0.095	0.028	0.063	0.0402	0.0427	0.0405	0.764	32.3	26.4	28.9	33.0	0.980	-7.76	-10.21	-27.39
$COCH_3$	0.096	0.029	0.063	0.0402	0.0429	0.0405	0.771	34.1	27.9	31.5	31.3	0.973	-7.59	-9.42	-26.83
COCl	0.095	0.030	0.063	0.0401	0.0427	0.0405	0.765	34.2	28.0	32.2	30.9	0.978	-8.11	-10.23	-27.11
COOH	0.097	0.025	0.065	0.0403	0.0437	0.0407	0.793	33.7	27.9	33.1	31.7	0.983	-8.01	-10.28	-27.55
$COOCH_3$	0.097	0.023	0.065	0.0404	0.0437	0.0407	0.800	33.5	28.0	32.2	32.0	0.983	-7.95	-10.06	-27.40
$CONH_2$	0.098	0.021	0.066	0.0405	0.0445	0.0408	0.811	33.4	26.4	31.1	31.6	0.984	-8.18	-10.12	-27.19
CN	0.096	0.031	0.063	0.0402	0.0429	0.0405	0.810	33.5	24.9	31.9	31.6	0.977	-8.48	-10.30	-27.80
NH_2	0.093	0.040	0.060	0.0398	0.0405	0.0402	0.682	33.2	24.6	29.6	33.3	0.976	-7.83	-9.07	-25.02
NO	0.090	0.043	0.059	0.0397	0.0403	0.0401	0.697	31.3	26.9	30.3	33.1	0.981	-7.84	-9.75	-25.89
NO_2	0.095	0.029	0.064	0.0403	0.0432	0.0406	0.806	33.4	28.5	31.7	31.3	0.994	-9.04	-10.33	-27.51
NN^+	0.080	0.078	0.047	0.0382	0.0339	0.0390	0.641	35.8	31.0	36.2	28.8	0.955	-8.52	-9.64	-24.84
OCH_3	0.094	0.044	0.061	0.0400	0.0413	0.0403	0.715	35.0	21.8	28.2	31.1	0.981	-9.01	-9.95	-27.13
OH	0.095	0.039	0.063	0.0401	0.0421	0.0404	0.733	34.1	22.5	29.2	32.1	0.989	-9.08	-9.81	-26.76

[a] From ref. T. M. Krygowski, B. T. Stepień, *Chem. Rev.*, 2005, **105**, 3482, in kcal/mol.

Table S8. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T7.

T7	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
C_6H_6	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.912	0.989	-8.05	-10.22	-29.25
Cr-C_6H_6	0.040	0.091	0.020	0.0332	0.0163	0.0345	0.549	0.832	-27.32	-14.22	-24.95

Table S9. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T8.

T8	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
C_6H_6	0.000	0.072	0.0411	0.0478	0.0413	0.912	0.989	-8.05	-10.22	-29.25
$C_7H_7^+$	0.023	0.057	0.0350	0.0278	0.0352	0.737	0.984	-6.27	-9.54	-26.50
$C_8H_8^{2+}$	0.048	0.041	0.0300	0.0118	0.0295	0.577	0.896	-6.84	-9.09	-25.33

Table S10. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T9.

T9	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
C_6H_6	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.912	0.989	-8.05	-10.22	-29.25
N_6	0.131	0.081	0.071	0.0410	0.0445	0.0408	0.741	0.984	-7.29	-12.85	-33.41

Table S11. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T10.

T10	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$	RE[a]
Benzene	0.103	0.000	0.072	0.0411	0.0478	0.0413	0.912	0.989	-8.05	-10.22	-29.25	48.7
Pyridine	0.103	0.022	0.068	0.0407	0.0456	0.0410	0.845	0.995	-6.82	-10.12	-28.59	44.1
Pyradizine	0.105	0.041	0.069	0.0408	0.0469	0.0412	0.773	0.981	-5.35	-10.52	-28.28	43.9
Pyrimidine	0.101	0.032	0.065	0.0404	0.0440	0.0407	0.787	0.999	-5.53	-10.00	-27.36	40.1
Pyrazine	0.108	0.042	0.065	0.0404	0.0435	0.0406	0.845	0.996	-5.36	-10.24	-28.37	38.8
Triazine	0.096	0.043	0.063	0.0402	0.0427	0.0405	0.752	1.000	-4.07	-9.66	-25.54	44.9

[a] From ref. M. K. Cyrański, *Chem. Rev.*, 2005, **105**, 3773, in kcal/mol.

Table S12. FLU$^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, EDDB$_P$, HOMA, NICS(0), NICS(1), and NICS(1)$_{zz}$ results for T11.

T11	FLU$^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	EDDB$_P$	HOMA	ASE[a]	NICS(0)	NICS(1)	NICS(1)$_{zz}$
CH^-	0.021	0.068	0.0467	0.0475	0.0447	1.018	0.810	22.1	-12.61	-9.63	-33.68
NH	0.071	0.043	0.0426	0.0306	0.0410	0.597	0.854	20.6	-13.64	-10.12	-30.99
O	0.091	0.028	0.0392	0.0224	0.0385	0.330	0.198	14.8	-11.91	-9.42	-27.14
CH_2	0.237	0.003	0.0251	0.0079	0.0312	0.068	-0.903	0.0	-3.12	-4.95	-12.64
BH	N/A[b]	-0.003	-0.0379	0.0043	0.0416	0.005	N/A[b]	-22.5	19.99	11.29	37.30
CH^+	0.218	-0.038	-0.0625	0.0001	0.0211	0.084	-1.346	-56.7	86.04	64.91	199.70

[a] From ref. M. K. Cyrański, T. M. Krygowski, A. R. Katritzky, P. v. R. Schleyer, *J. Org. Chem*., 2002, **67**, 1333, in kcal/mol.
[b] There are no parameters available for the B–C bond.

Table S13. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T12.

T12		Molecule				
Measure	**RING**	**Phenanthrene**	**Pyrene**	**Triphenylene**	**1,2-Benzo-pyrene**	**1,2,5,6-Dibenzo-anthracene**
PDI	A	0.081	0.069	0.086	0.085	0.082
	B	0.046	0.043	0.027	0.026	0.041
	C				0.044	0.068
	D				0.072	
$FLU^{1/2}$	A	0.073	0.081	0.059	0.060	0.068
	B	0.143	0.140	0.160	0.155	0.153
	C				0.142	0.087
	D				0.076	
MCI	A	0.046	0.036	0.055	0.051	0.048
	B	0.018	0.019	0.009	0.009	0.015
	C				0.018	0.033
	D				0.039	
I_{NB}	A	0.0382	0.0366	0.0392	0.0388	0.0384
	B	0.0326	0.0328	0.0288	0.0290	0.0315
	C				0.0326	0.0360
	D				0.0371	
I_{ring}	A	0.0323	0.0256	0.0373	0.0355	0.0333
	B	0.0139	0.0147	0.0072	0.0077	0.0117
	C				0.0141	0.0237
	D				0.0277	
I_{NG}	A	0.0386	0.0372	0.0396	0.0393	0.0388
	B	0.0336	0.0339	0.0301	0.0304	0.0327
	C				0.0337	0.0367
	D				0.0377	

$EDDB_P$	A	0.532	0.442	0.612	0.575	0.555
	B	0.299	0.315	0.181	0.196	0.264
	C				0.313	0.527
	D				0.482	
HOMA	A	0.868	0.854	0.650	0.904	0.887
	B	0.457	0.579	-0.276	0.229	0.379
	C				0.542	0.816
	D				0.859	
NICS(0)	A	-8.44	-11.29	-9.07	-7.16	-8.36
	B	-5.59	-3.89	-4.90	-0.29	-4.17
	C				-4.29	-9.62
	D				-10.16	
NICS(1)	A	-10.59	-12.95	-10.81	-9.44	-10.48
	B	-8.17	-7.01	-7.36	-4.06	-7.04
	C				-7.24	-11.28
	D				-12.01	
$NICS(1)_{zz}$	A	-28.78	-35.57	-29.58	-24.85	-28.14
	B	-20.63	-16.76	-15.91	-6.90	-16.74
	C				-17.09	-30.73
	D				-32.27	

Table S14. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T13.

Pentafulvenes	**$FLU^{1/2}$**	**MCI**	**I_{NB}**	**I_{ring}**	**I_{NG}**	**$EDDB_P$**	**HOMA**	**NICS(0)**	**NICS(1)**	**$NICS(1)_{zz}$**
NH_2^+	0.260	-0.008	-0.0304	0.0104	0.0330	0.0532	-0.831	16.36	8.95	32.07
O	0.299	-0.002	-0.0231	0.0094	0.0324	0.0387	-1.498	10.84	3.84	13.05
NH	0.258	0.003	0.0258	0.0123	0.0341	0.0540	-0.807	5.62	0.64	4.63
CH_2	0.214	0.012	0.0330	0.0176	0.0367	0.0859	-0.282	0.94	-2.43	-4.17
BH_2^-	0.095	0.051	0.0441	0.0398	0.0432	0.3677	0.483	-7.57	-8.05	-25.40
Heptafulvenes	**$FLU^{1/2}$**	**MCI**	**I_{NB}**	**I_{ring}**	**I_{NG}**	**$EDDB_P$**	**HOMA**	**NICS(0)**	**NICS(1)**	**$NICS(1)_{zz}$**
NH_2^+	0.108	0.036	0.0327	0.0187	0.0333	0.3021	0.796	-2.88	-5.94	-15.01
O	0.186	0.018	0.0297	0.0110	0.0308	0.1389	0.265	1.46	-2.31	-5.96
NH	0.187	0.014	0.0286	0.0091	0.0300	0.1187	0.209	5.17	1.13	5.00
CH_2	0.185	0.011	0.0275	0.0078	0.0294	0.1143	0.158	10.57	5.83	19.23
BH_2^-	0.180	0.003	0.0224	0.0055	0.0279	0.0668	0.020	44.02	34.01	101.59

Table S15. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T14.

IRP	Energy	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
-3.597	-234.68973	0.036	0.301	0.003	0.0237	0.0027	0.0256	-9.187	-4.99	-4.24	-3.09
-3.397	-234.68520	0.037	0.302	0.003	0.0245	0.0032	0.0263	-10.583	-5.52	-4.50	-3.82
-3.097	-234.67769	0.041	0.303	0.004	0.0259	0.0043	0.0276	-12.959	-6.44	-4.95	-5.17
-2.497	-234.66127	0.050	0.307	0.009	0.0289	0.0075	0.0303	-18.747	-8.79	-6.15	-8.91
-1.897	-234.64492	0.061	0.314	0.017	0.0322	0.0131	0.0333	-25.958	-11.94	-7.78	-14.17
-1.297	-234.63083	0.075	0.328	0.030	0.0355	0.0216	0.0362	-34.614	-15.59	-9.65	-20.43
-0.697	-234.62090	0.087	0.356	0.045	0.0379	0.0304	0.0383	-44.733	-18.64	-11.15	-25.81
-0.397	-234.61789	0.092	0.377	0.050	0.0386	0.0333	0.0389	-50.351	-19.46	-11.49	-27.34
-0.099	-234.61621	0.092	0.400	0.052	0.0389	0.0347	0.0391	-56.309	-19.64	-11.48	-27.78
0.000	-234.61572	0.092	0.423	0.051	0.0388	0.0341	0.0390	-62.395	-19.21	-11.13	-27.19
0.098	-234.61614	0.089	0.445	0.047	0.0383	0.0320	0.0386	-68.818	-18.31	-10.53	-25.77
0.296	-234.61685	0.087	0.460	0.044	0.0378	0.0301	0.0382	-73.443	-17.51	-10.01	-24.48
0.496	-234.61783	0.085	0.475	0.040	0.0372	0.0277	0.0377	-78.268	-16.60	-9.43	-22.97
1.095	-234.62174	0.076	0.510	0.028	0.0352	0.0211	0.0360	-93.613	-13.75	-7.66	-18.17
1.694	-234.62614	0.068	0.535	0.020	0.0331	0.0155	0.0342	-109.998	-11.29	-6.13	-13.94
2.294	-234.63033	0.062	0.553	0.014	0.0312	0.0115	0.0325	-127.291	-9.37	-4.91	-10.58
2.893	-234.63402	0.057	0.566	0.010	0.0295	0.0085	0.0310	-145.358	-7.91	-3.97	-8.00

Table S16. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T15.

IRP	Energy	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
-3.292	-232.02508	0.024	0.900	0.002	0.0224	0.0027	0.0254	-215.125	2.79	-1.33	-1.56
-2.892	-232.02090	0.027	0.884	0.002	0.0237	0.0027	0.0265	-201.005	3.44	-1.71	-2.82
-2.293	-232.01421	0.034	0.856	0.004	0.0259	0.0053	0.0284	-180.627	4.78	-2.51	-5.40
-1.693	-232.00722	0.042	0.817	0.008	0.0282	0.0080	0.0306	-161.197	6.79	-3.71	-9.17
-1.093	-232.00043	0.053	0.763	0.014	0.0312	0.0133	0.0330	-142.739	9.76	-5.47	-14.62
-0.494	-231.99487	0.066	0.688	0.025	0.0338	0.0187	0.0356	-125.277	13.91	-7.91	-22.00
0.000	-231.99236	0.080	0.584	0.042	0.0371	0.0293	0.0380	-108.299	18.86	-10.82	-30.50
0.097	-231.99278	0.084	0.541	0.047	0.0383	0.0320	0.0386	-102.463	20.46	-11.77	-33.13
0.495	-231.99598	0.089	0.459	0.054	0.0394	0.0347	0.0393	-92.322	22.44	-12.95	-36.19
1.095	-232.00790	0.086	0.341	0.050	0.0389	0.0320	0.0388	-77.780	21.98	-12.79	-34.74
1.695	-232.02834	0.075	0.251	0.034	0.0361	0.0240	0.0367	-64.306	17.88	-10.61	-27.31
2.295	-232.05515	0.063	0.192	0.020	0.0333	0.0160	0.0341	-52.010	12.92	-8.01	-19.00
2.895	-232.08575	0.056	0.153	0.012	0.0307	0.0107	0.0324	-40.987	9.05	-6.13	-13.20
3.295	-232.10731	0.054	0.133	0.011	0.0302	0.0107	0.0320	-34.374	7.28	-5.40	-11.06
3.895	-232.14052	0.056	0.108	0.012	0.0298	0.0107	0.0325	-25.571	5.70	-4.99	-10.09
4.495	-232.17409	0.061	0.085	0.017	0.0323	0.0160	0.0340	-18.088	5.08	-5.24	-11.24
5.095	-232.20724	0.069	0.063	0.025	0.0337	0.0213	0.0359	-11.888	5.19	-5.99	-13.98
5.695	-232.23898	0.079	0.042	0.037	0.0374	0.0293	0.0378	-6.934	5.81	-7.10	-17.81
6.295	-232.26787	0.089	0.023	0.052	0.0390	0.0373	0.0395	-3.202	6.70	-8.33	-22.08
6.895	-232.29174	0.097	0.008	0.065	0.0403	0.0453	0.0407	-0.679	7.53	-9.42	-25.87
7.495	-232.30739	0.102	0.001	0.071	0.0419	0.0480	0.0413	0.667	8.00	-10.06	-28.33

Table S17. $EDDB_P$ results for T14.

IRP	$EDDB_P$
-3.716	0.0102
-3.144	0.0130
-2.572	0.0211
-2.000	0.0417
-1.429	0.0931
-0.857	0.2287
-0.286	0.5593
0.000	0.7504
0.286	0.8444
0.572	0.7539
0.857	0.5350
1.143	0.3272
1.715	0.0995
2.286	0.0166
2.858	0.0104
cyclohexene	0.0316

Table S18. $EDDB_P$ results for T15.

IRP	$EDDB_P$
-3.314	0.0091
-2.872	0.0090
-2.209	0.0105
-1.767	0.0152
-1.104	0.0378
-0.442	0.1254
0.000	0.2998
0.221	0.4439
0.663	0.7648
1.105	0.7311
1.767	0.2620
2.430	0.0751
3.093	0.0289
3.756	0.0185
4.419	0.0219
5.082	0.0424
5.745	0.1034
6.408	0.2653
7.513	0.8004
benzene	0.9115

Table S19. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, HOMER, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T16.

T16	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	HOMER	NICS(0)	NICS(1)	$NICS(1)_{zz}$
CH^-	0.140	0.024	0.038	0.028	0.040	0.424	0.293	-1.086	16.96	11.36	38.43
NH	0.172	-0.002	-0.022	0.005	0.028	0.069	-0.156	-1.307	3.76	2.73	10.31
O	0.175	0.001	0.020	0.006	0.030	0.055	-0.928	-1.008	2.88	2.44	9.08
CH_2	0.232	0.010	0.032	0.006	0.030	0.077	-1.140	-2.469	3.22	0.09	2.33
BH	N/A[a]	0.029	0.039	0.011	0.033	0.243	0.186	N/A[a]	0.24	-7.70	-20.31
CH^+	0.099	0.098	0.050	0.034	0.042	0.589	0.668	0.836	-2.53	-10.26	-25.06

[a] There are no parameters available for the B–C bond.

Table S20. FLU$^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, EDDB$_P$, HOMA, HOMER, NICS(0), NICS(1), and NICS(1)$_{zz}$ results for T17 and T18.

Pentafulvenes I	**FLU$^{1/2}$**	**MCI**	**I_{NB}**	**I_{ring}**	**I_{NG}**	**EDDB$_P$**	**HOMA**	**HOMER**	**NICS(0)**	**NICS(1)**	**NICS(1)$_{zz}$**
NH_2^+	0.137	0.059	0.045	0.026	0.040	0.393	0.560	0.536	-1.84	-7.00	-15.22
O	0.171	0.037	0.041	0.019	0.037	0.303	0.160	0.111	3.51	-3.69	-9.53
NH	0.167	0.031	0.040	0.020	0.037	0.299	0.259	0.015	3.61	-1.52	-1.42
CH_2	0.161	0.024	0.038	0.020	0.037	0.255	0.227	-0.305	5.83	1.35	7.26
BH_2^-	0.158	0.011	0.032	0.015	0.036	0.284	-0.040	-0.744	17.13	12.26	37.98
Heptafulvenes I	**FLU$^{1/2}$**	**MCI**	**I_{NB}**	**I_{ring}**	**I_{NG}**	**EDDB$_P$**	**HOMA**	**HOMER**	**NICS(0)**	**NICS(1)**	**NICS(1)$_{zz}$**
NH_2^+	0.144	0.001	0.019	0.003	0.026	0.165	0.425	-0.720	23.37	16.18	51.25
O	0.162	0.003	0.023	0.004	0.026	0.193	0.321	-0.686	15.83	9.91	29.12
NH	0.140	0.007	0.026	0.006	0.028	0.264	0.513	-0.501	12.08	7.27	23.06
CH_2	0.121	0.013	0.028	0.008	0.030	0.316	0.611	-0.385	9.45	5.14	16.82
BH_2^-	0.063	0.026	0.031	0.012	0.031	0.454	0.713	0.286	-3.39	-4.94	-15.77

Table S21. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, HOMER, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T19-22.

Pentafulvenes II S_0	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	HOMER	NICS(0)	NICS(1)	$NICS(1)_{zz}$
NH_2	0.132	0.038	0.042	0.033	0.041	0.2225	0.509	⊢	-6.69	-6.81	-17.62
H	0.214	0.012	0.033	0.018	0.037	0.0860	-0.280	⊢	0.94	-2.43	-4.17
CN	0.224	0.006	0.029	0.016	0.036	0.0708	-0.377	⊢	7.17	2.42	12.03
Heptafulvenes II S_0	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	HOMER	NICS(0)	NICS(1)	$NICS(1)_{zz}$
NH_2	0.195	0.005	0.025	0.006	0.028	0.0718	0.056	⊢	25.34	18.48	57.66
H	0.185	0.011	0.028	0.008	0.029	0.1145	0.164	⊢	10.59	5.84	19.26
CN	0.140	0.022	0.031	0.013	0.032	0.1818	0.558	⊢	4.10	-0.09	2.51
Pentafulvenes II T_1	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	HOMER	NICS(0)	NICS(1)	$NICS(1)_{zz}$
NH_2	0.179	0.011	0.032	0.014	0.035	0.2099	-0.016	-0.810	11.52	7.60	26.01
H	0.161	0.024	0.038	0.020	0.037	0.2562	0.234	-0.291	5.84	1.37	7.30
CN	0.142	0.037	0.041	0.025	0.039	0.3490	0.444	-0.022	4.29	-0.61	2.75
Heptafulvenes II T_1	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	HOMER	NICS(0)	NICS(1)	$NICS(1)_{zz}$
NH_2	0.092	0.0213	0.0304	0.0105	0.0307	0.4374	0.731	-0.049	0.27	-1.88	-4.15
H	0.121	0.0126	0.0282	0.0081	0.0295	0.3163	0.610	-0.388	9.45	5.13	16.82
CN	0.125	0.0118	0.0279	0.0085	0.0297	0.2419	0.606	-0.675	21.00	14.20	45.00

Table S22. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T23.

T23	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
C_4H_5B	N/A[a]	-0.003	-0.025	0.004	0.028	0.005	-1.082	19.99	11.30	37.29
$C_4H_5B^{2-}$	N/A[a]	0.018	0.036	0.018	0.037	0.223	0.127	0.76	-2.35	-3.96

[a] There are no parameters available for the B–C bond.

Table S23. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T24.

T24	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
$C_6H_4S_4$	0.169	0.008	0.031	0.006	0.029	0.126	0.126	-7.46	-2.90	-1.94
$C_6H_4S_4^{+}$	0.095	0.028	0.039	0.020	0.038	0.266	0.559	-9.25	-6.09	-11.01
$C_6H_4S_4^{2+}$	0.081	0.055	0.045	0.037	0.042	0.479	0.846	-12.04	-10.30	-21.81

Table S24. $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T25.

T25	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
$C_8H_6^{2-}$	0.094	0.033	0.040	0.028	0.040	0.526	0.554	9.50	6.93	19.61
C_8H_6	0.218	0.009	0.031	0.015	0.036	0.063	-0.358	24.83	17.96	58.17
$C_8H_6^{2+}$	0.174	0.006	0.028	0.005	0.028	0.189	-0.421	-3.67	-11.62	-27.01

Table S25. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T26.

T26	Ring	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
$C_{14}H_{10}$	Inner	0.065	0.102	0.027	0.035	0.020	0.036	0.454	0.720	-11.05	-12.68	-34.88
	Outer	0.065	0.126	0.029	0.035	0.022	0.036	0.309	0.629	-7.28	-9.44	-25.98
$C_{14}H_{10}^{2+}$	Inner	0.026	0.131	0.013	0.031	0.012	0.033	0.291	0.672	16.73	9.80	34.34
	Outer	0.050	0.096	0.028	0.035	0.022	0.036	0.398	0.812	11.10	4.69	18.23

Table S26. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T27.

T27	Ring	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
1,2-Naphtoquinone	A	0.046	0.190	0.011	0.030	0.010	0.032	0.105	-0.028	7.12	2.85	11.39
	B	0.044	0.257	0.002	0.023	0.003	0.026	0.045	-1.278	14.92	6.83	19.67
2,3-Naphtoquinone	A	0.087	0.043	0.055	0.039	0.038	0.040	0.674	0.963	-6.33	-8.70	-22.17
	B	0.020	0.272	0.002	0.023	0.003	0.025	0.049	-1.365	11.23	3.30	11.03

Table S27. PDI, $FLU^{1/2}$, MCI, I_{NB}, I_{ring}, I_{NG}, $EDDB_P$, HOMA, NICS(0), NICS(1), and $NICS(1)_{zz}$ results for T28.

T28	Ring	PDI	$FLU^{1/2}$	MCI	I_{NB}	I_{ring}	I_{NG}	$EDDB_P$	HOMA	NICS(0)	NICS(1)	$NICS(1)_{zz}$
1H-purine	6-MR	0.044	0.165	0.014	0.031	0.012	0.033	0.177	0.665	-7.20	-8.98	-24.13
	5-MR	–	0.159	0.027	0.039	0.028	0.040	0.197	0.666	-9.97	-12.66	-33.08
9H-purine	6-MR	0.079	0.116	0.041	0.037	0.029	0.038	0.531	0.975	-8.08	-10.84	-28.90
	5-MR	–	0.170	0.026	0.039	0.021	0.038	0.332	0.833	-11.39	-10.13	-27.16

Table S28. HF, B3LYP, MP2, and CCSD results for MCI, I_{ring}, I_{NG}, I_{NB} indicators of aromaticity for test T10.

	MCI				I_{ring}			
	HF	***B3LYP***	***MP2***	***CCSD***	***HF***	***B3LYP***	***MP2***	***CCSD***
benzene	0.0677	0.072	0.049	0.048	0.0451	0.0477	0.0339	0.0325
pyridine	0.058	0.068	0.046	0.044	0.0392	0.0456	0.0317	0.0304
pyridazine	0.056	0.069	0.045	0.044	0.0384	0.0469	0.0315	0.0304
pyrimidine	0.049	0.065	0.046	0.042	0.0333	0.0440	0.0315	0.0291
pyrazine	0.054	0.065	0.043	0.042	0.0349	0.0435	0.0291	0.0285
1,3,5-triazine	0.040	0.063	0.046	0.040	0.0275	0.0427	0.0315	0.0275

	I_{NB}				I_{NG}			
	HF	***B3LYP***	***MP2***	***CCSD***	***HF***	***B3LYP***	***MP2***	***CCSD***
benzene	0.0407	0.0411	0.0454	0.0384	0.0409	0.0413	0.0457	0.0387
pyridine	0.0396	0.0407	0.0381	0.0379	0.0399	0.0410	0.0386	0.0383
pyridazine	0.0394	0.0408	0.0380	0.0378	0.0400	0.0412	0.0385	0.0383
pyrimidine	0.0386	0.0404	0.0381	0.0376	0.0389	0.0407	0.0385	0.0380
pyrazine	0.0391	0.0404	0.0376	0.0375	0.0392	0.0406	0.0380	0.0379
1,3,5-triazine	0.0373	0.0402	0.0381	0.0372	0.0377	0.0405	0.0385	0.0377