Electronic Supplementary Information

The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity

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CONTENTS

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Ring	FLU $\times 10^1$	SA $\times 10^2$	EL $\times 10^2$	H_{RCP} $\times 10^0$	KMCI $\times 10^2$	$\mathrm{KMCI}^{1/n}$ $\times 10^0$	EDDB^k $\times 10^{-1}$	ATI $\times 10^0$	HOMA $\times 10^0$	$\mathrm{NICS}(1)_{zz}$ $\times 10^{-2}$	I_{R} $\times 10^2$	MCI $\times 10^2$	PDI $\times 10^0$
1	0.579	0.947	-0.157	0.528	0.055	0.223	0.034	–	-0.878	-0.130	0.055	0.063	–
2	0.001	0.000	0.570	0.602	0.350	0.323	0.435	–	0.753	-0.348	0.392	0.499	–
3	0.026	0.066	-0.044	0.607	0.303	0.314	0.370	–	0.787	-0.284	0.344	0.433	–
4	0.326	0.473	0.301	0.560	0.157	0.275	0.105	–	0.174	-0.196	0.201	0.198	–
5	0.291	0.302	0.496	0.583	0.180	0.283	0.132	–	0.394	-0.192	0.233	0.229	–
6	0.492	0.666	0.002	0.557	0.091	0.246	0.047	–	-0.363	-0.055	0.132	0.093	–
7	0.362	0.485	0.177	0.565	0.131	0.265	0.074	–	-0.044	-0.124	0.178	0.153	–
8	0.301	0.391	0.280	0.571	0.152	0.273	0.093	–	0.174	-0.149	0.206	0.184	–
9	0.524	0.722	-0.044	0.552	0.082	0.241	0.042	–	-0.423	0.014	0.126	0.073	–
10	0.558	0.814	-0.091	0.548	0.075	0.237	0.038	–	-0.553	0.048	0.116	0.063	–
11	0.451	0.613	0.046	0.558	0.103	0.253	0.054	–	-0.189	-0.078	0.145	0.112	–
12	0.078	0.078	0.715	0.581	0.267	0.306	0.275	–	0.627	-0.275	0.328	0.364	–
13	0.045	0.040	0.700	0.585	0.288	0.310	0.335	–	0.669	-0.286	0.348	0.398	–
14	0.424	0.577	0.099	0.561	0.113	0.257	0.061	–	-0.078	-0.096	0.155	0.128	–
15	0.252	0.334	0.367	0.575	0.173	0.280	0.117	–	0.143	-0.176	0.227	0.219	–
16	0.000	0.000	1.000	0.466	0.163	0.343	0.554	0.115	0.961	-0.306	0.240	0.243	0.103
17	0.096	0.088	0.612	0.440	0.093	0.312	0.329	0.081	0.743	–	0.135	0.132	0.076
18	0.175	0.181	0.444	0.431	0.069	0.297	0.230	0.067	0.557	–	0.101	0.094	0.065
19	0.080	0.053	0.825	0.425	0.072	0.299	0.368	0.073	0.714	–	0.101	0.100	0.069
20	0.048	0.044	0.767	0.447	0.113	0.323	0.422	0.091	0.841	–	0.142	0.163	0.084
21	0.210	0.194	0.489	0.409	0.044	0.276	0.183	0.045	0.369	–	0.057	0.057	0.047
22	0.222	0.239	0.361	0.426	0.058	0.289	0.191	0.060	0.438	–	0.062	0.077	0.060
23	0.112	0.088	0.663	0.420	0.060	0.290	0.307	0.067	0.619	–	0.073	0.082	0.064
24	0.062	0.058	0.717	0.445	0.107	0.320	0.390	0.087	0.813	–	0.134	0.153	0.081
25	0.161	0.152	0.568	0.417	0.057	0.288	0.226	0.055	0.499	–	0.073	0.076	0.055
26	0.030	0.032	0.847	0.450	0.124	0.328	0.458	0.096	0.878	–	0.157	0.180	0.088
27	0.247	0.145	0.575	0.380	0.021	0.244	0.109	0.022	-0.041	–	0.028	0.025	0.028
28	0.049	0.022	0.859	0.438	0.093	0.312	0.440	0.078	0.830	–	0.117	0.132	0.074
29	0.212	0.152	0.459	0.413	0.044	0.276	0.224	0.039	0.460	–	0.058	0.056	0.043
30	0.248	0.276	0.315	0.423	0.052	0.284	0.172	0.057	0.364	–	0.056	0.068	0.057
31	0.141	0.125	0.571	0.416	0.053	0.284	0.262	0.063	0.535	–	0.065	0.071	0.061
32	0.116	0.085	0.761	0.417	0.055	0.286	0.309	0.066	0.591	–	0.069	0.074	0.063
33	0.091	0.091	0.638	0.440	0.095	0.314	0.337	0.081	0.743	–	0.119	0.133	0.076
34	0.127	0.082	0.666	0.413	0.053	0.284	0.289	0.054	0.568	–	0.069	0.072	0.054
35	0.268	0.205	0.368	0.405	0.033	0.263	0.196	0.028	0.301	–	0.045	0.041	0.034
36	0.158	0.116	0.580	0.420	0.057	0.288	0.256	0.051	0.576	–	0.076	0.076	0.052
37	0.055	0.030	0.805	0.438	0.092	0.312	0.424	0.077	0.819	–	0.116	0.130	0.073
38	0.002	0.000	0.553	0.252	0.049	0.337	0.604	–	0.955	-0.274	0.075	0.097	–
39	0.065	0.024	0.760	0.254	0.039	0.326	0.480	–	0.925	-0.225	0.059	0.075	–
40	0.224	0.201	0.419	0.250	0.022	0.300	0.219	–	0.572	-0.075	0.033	0.038	–
41	0.417	0.385	0.265	0.242	0.016	0.287	0.131	–	0.157	-0.056	0.026	0.026	–
42	0.517	0.757	-0.051	0.240	0.008	0.260	0.057	–	-0.224	0.396	0.010	0.005	–
43	0.517	0.639	0.060	0.242	0.009	0.264	0.063	–	-0.080	0.445	0.011	0.006	–
44	0.407	0.533	0.035	0.242	0.012	0.275	0.078	–	0.026	0.164	0.016	0.014	–
45	0.581	0.921	-0.197	0.234	0.004	0.235	0.040	–	-0.482	0.190	0.006	0.004	–

Table S1. The values of aromaticity indices calculated for the T1 test set of molecular rings from Figure 2. Method: CAM-B3LYP/def2-TZVPP, equilibrium geometries.

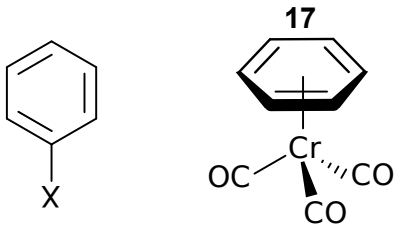
a) *All rings*	FLU	SA	EL	H_{RCP}	KMCI	$\mathrm{KMCI}^{1/n}$	EDDB^{k}	HOMA	$\mathrm{NICS}(1)_{zz}$
FLU	**1.000**	–	–	0.019	0.243	0.817	0.955	–	–
SA	0.946	**1.000**	–	0.005	0.167	0.747	0.930	–	–
EL	0.911	0.908	**1.000**	0.026	0.204	0.709	0.886	–	–
H_{RCP}	0.006	0.000	0.006	**1.000**	0.763	0.005	0.006	0.000	0.320
KMCI	0.159	0.087	0.102	0.572	**1.000**	0.168	0.128	0.144	0.667
$\mathrm{KMCI}^{1/n}$	0.811	0.728	0.701	0.005	0.142	**1.000**	0.859	0.915	0.347
EDDB^{k}	0.834	0.724	0.750	0.008	0.080	0.849	**1.000**	0.963	0.448
HOMA	0.925	0.913	0.856	0.005	0.087	0.898	0.819	**1.000**	–
$\mathrm{NICS}(1)_{zz}$	0.574	0.511	0.503	0.315	0.495	0.361	0.396	0.381	**1.000**

b) *5-MRs*	FLU	SA	EL	H_{RCP}	KMCI	$\mathrm{KMCI}^{1/n}$	EDDB^{k}	HOMA	$\mathrm{NICS}(1)_{zz}$
FLU	**1.000**	0.618	0.443	0.630	0.975	0.975	0.990	0.565	0.637
SA	0.973	**1.000**	–	0.904	0.990	0.990	0.960	–	–
EL	0.929	0.949	**1.000**	0.799	0.934	0.934	0.930	–	–
H_{RCP}	0.863	0.901	0.801	**1.000**	0.906	0.906	0.863	0.915	0.611
KMCI	0.971	0.929	0.857	0.856	**1.000**	0.997	0.986	0.983	0.794
$\mathrm{KMCI}^{1/n}$	0.985	0.987	0.931	0.902	0.964	**1.000**	0.984	0.983	0.794
EDDB^{k}	0.886	0.807	0.716	0.762	0.961	0.859	**1.000**	0.938	0.860
HOMA	0.938	0.976	0.938	0.911	0.893	0.973	0.760	**1.000**	–
$\mathrm{NICS}(1)_{zz}$	0.851	0.780	0.771	0.620	0.832	0.813	0.772	0.748	**1.000**

c) *6-MRs*	FLU	SA	EL	H_{RCP}	KMCI	$\mathrm{KMCI}^{1/n}$	EDDB^{k}	HOMA	ATI
FLU	**1.000**	–	0.826	0.648	0.784	0.784	0.911	–	0.748
SA	0.860	**1.000**	0.951	0.326	0.457	0.457	0.738	–	0.385
EL	0.844	0.924	**1.000**	0.331	0.458	0.458	0.715	0.517	0.457
H_{RCP}	0.655	0.337	0.344	**1.000**	0.971	0.971	0.742	0.858	0.905
KMCI	0.759	0.505	0.540	0.912	**1.000**	0.997	0.815	0.926	0.948
$\mathrm{KMCI}^{1/n}$	0.792	0.475	0.480	0.972	0.942	**1.000**	0.826	0.926	0.948
EDDB^{k}	0.922	0.784	0.795	0.743	0.842	0.831	**1.000**	0.959	0.792
HOMA	0.866	0.605	0.561	0.851	0.790	0.912	0.883	**1.000**	0.854
ATI	0.811	0.482	0.529	0.911	0.915	0.954	0.814	0.871	**1.000**

d) *7-MRs*	FLU	SA	EL	H_{RCP}	KMCI	$\mathrm{KMCI}^{1/n}$	EDDB^{k}	HOMA	$\mathrm{NICS}(1)_{zz}$
FLU	**1.000**	0.573	0.562	0.897	0.931	0.931	0.975	0.638	0.528
SA	0.927	**1.000**	–	0.930	0.980	0.980	0.963	–	–
EL	0.862	0.978	**1.000**	0.905	0.944	0.944	0.943	–	–
H_{RCP}	0.902	0.930	0.907	**1.000**	0.922	0.879	0.901	0.958	0.565
KMCI	0.955	0.858	0.791	0.805	**1.000**	0.997	0.952	0.973	0.701
$\mathrm{KMCI}^{1/n}$	0.951	0.977	0.939	0.874	0.925	**1.000**	0.976	0.973	0.701
EDDB^{k}	0.925	0.789	0.709	0.752	0.988	0.863	**1.000**	0.982	0.803
HOMA	0.970	0.982	0.960	0.960	0.910	0.979	0.860	**1.000**	–
$\mathrm{NICS}(1)_{zz}$	0.772	0.759	0.672	0.571	0.734	0.724	0.710	0.735	**1.000**

Tables S2a-d. Arrays of the R^2-values for linear (below the diagonal) and exponential (if available - above the diagonal) correlations between selected aromaticity indices taken from Table S1.

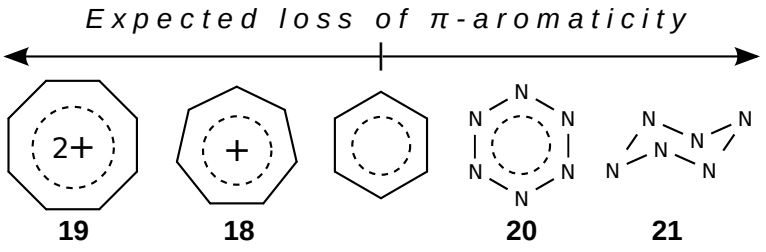


EDDB^k 3.485

KMCI 3.335

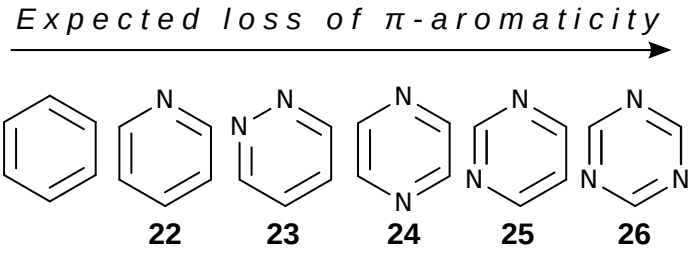
		EDDB^k	KMCI
X =	H	**5.525**	**8.689**
1	F	5.438	8.130
2	CH_3	5.376	8.326
3	CCH	5.172	7.735
4	CHO	5.045	7.689
5	$COCH_3$	5.095	7.791
6	COCl	5.038	7.645
7	COOH	5.162	7.867
8	$COOCH_3$	5.186	7.905
9	$CONH_2$	5.245	8.023
10	CN	5.177	7.798
11	NH_2	5.142	7.262
12	NO	4.693	5.824
13	NO_2	5.190	7.864
14	NN^+	4.428	6.359
15	OH	5.290	7.741
16	OCH_3	5.173	7.656

Figure S1: *Substitution and complexation in benzene.* The test is passed if the unsubstituted benzene is found to be the most aromatic 6-MR in the series. KMCI values have been multiplied by 10^3. Method: B3LYP/6-311++G**, equilibrium geometries.
Comment: Both indices pass the test with 100%.

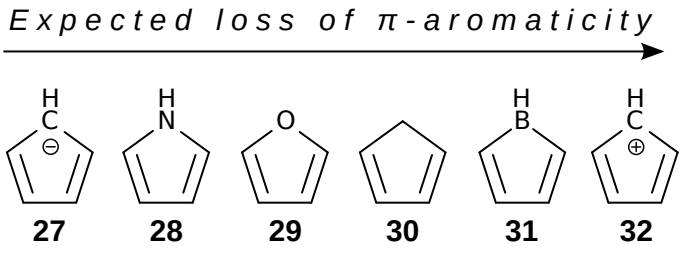


	19	**18**		**20**	**21**
$EDDB^k$	4.747	5.238	**5.525**	5.911	1.225
$EDDB^k(\pi)$	4.365	4.934	**5.305**	**5.318**	–
$EDDB^k(\sigma)$	0.382	0.304	**0.220**	0.593	–
KMCI	4.806 [a]	6.956 [b]	**8.689**	8.879	1.827
KMCI(π)	4.803 [a]	6.949 [b]	**8.661**	**8.705**	–
KMCI(σ)	0.003 [a]	0.007 [b]	**0.028**	0.174	–

Figure S2. *Ring-size and atom size dependence.* The test is passed if particular ring is no more π-aromatic than benzene; red numbers indicate the results that are in conflict with expectations. For **18** and **19** the corresponding KMCI values have been raised to the powers of 6/7 (b) and 6/8 (a) to make them comparable with 6-MR, and then multiplied by 10^3. Method: B3LYP/6-311++G**, equilibrium geometries.
Comment: Although both indices predict the cyclic delocalization of π-electrons in planar N_6 ring to be slightly more effective than in the case of benzene, the difference is only about 0.2% i.e. much below accuracy of the natural population analysis (about 0.5%). Thus we can say that both indices actually pass the test with 100%.



	22	**23**	**24**	**25**	**26**
EDDB^k	**5.525**	5.571	5.027	5.589	5.629	5.788
EDDB^k(π)	**5.305**	5.249	**4.765**	5.204	5.181	5.146
EDDB^k(σ)	**0.220**	0.322	0.262	0.385	0.448	0.642
KMCI	**0.869**	0.847	0.831	0.835	0.821	0.796
KMCI(π)	**0.866**	0.843	**0.826**	0.830	0.815	0.785
KMCI(σ)	**0.003**	0.004	0.005	0.005	0.006	0.011

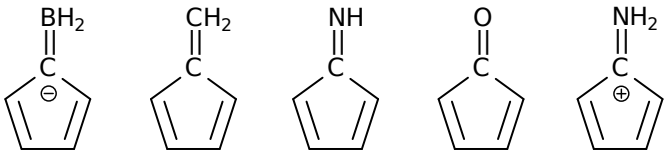


	27	**28**	**29**	**30**	**31**	**32**
EDDB^k	5.125	3.063	1.773	0.407	0.131	0.839
EDDB^k(π)	4.927	2.863	1.615	–	0.068	**0.721**
EDDB^k(σ)	0.198	0.200	0.158	–	0.063	0.118
KMCI	1.109	0.851	0.656	0.192	0.092	0.113
KMCI(π)	1.098	0.839	0.642	–	0.082	**0.100**
KMCI(σ)	0.011	0.012	0.014	–	0.010	0.013

Figure S3. *Trends of π-aromaticity changes in heteroaromatics*; red numbers indicate the results that are in conflict with expectations. KMCI values have been multiplied by 10^3. Method: B3LYP/6-311++G**, equilibrium geometry.

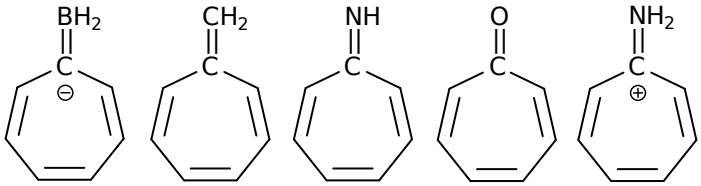
Comment: In the case of azabenzenes **22**-**26** the expected loss of π-aromaticity is reproduced by both indices only when excluding **23**, which is the only system in the series that contain the N−N bond. As regards the series of 5-MR aromatics, both EDDB^k and KMCI correctly predict loss of π-aromaticity from **27** to **31**, but incorrectly assess π-aromaticity of **32**. Thus, both indices pass this test with 82%.

Expected loss of π-aromaticity →



	38	**39**	**40**	**41**	**42**
EDDB^k	2.522	0.558	0.390	0.326	0.362
EDDB^k(π)	2.348	0.431	0.245	0.156	**0.239**
EDDB^k(σ)	0.174	0.127	0.145	0.170	0.123
KMCI	7.879	3.302	2.255	1.612	1.740
KMCI(π)	7.759	3.186	2.129	1.457	**1.622**
KMCI(σ)	0.120	0.116	0.126	0.155	0.118

Expected increase of π-aromaticity →



	43	**44**	**45**	**46**	**47**
EDDB^k	0.986	1.021	1.257	1.660	3.222
EDDB^k(π)	0.774	0.803	0.999	1.348	2.946
EDDB^k(σ)	0.212	0.218	0.258	0.312	0.276
KMCI	1.168	1.376	1.542	1.818	3.112
KMCI(π)	1.163	1.371	1.537	1.814	3.108
KMCI(σ)	0.005	0.005	0.005	0.004	0.004

Figure S4. *Trends of π-aromaticity changes in penta- and heptafulvenes*; red numbers indicate the results that are in conflict with expectations. KMCI values have been multiplied by 10^3. Method: B3LYP/6-311++G**, equilibrium geometry.

Comment: In the case of pentafulvenes **38**-**42** the expected loss of π-aromaticity is reproduced by both indices only when excluding **42**, while in the case of heptafulvenes **43**-**47**, EDDB^k and KMCI correctly predict increase of π-aromaticity in the entire series. Hence, both indices pass the test with 90%.

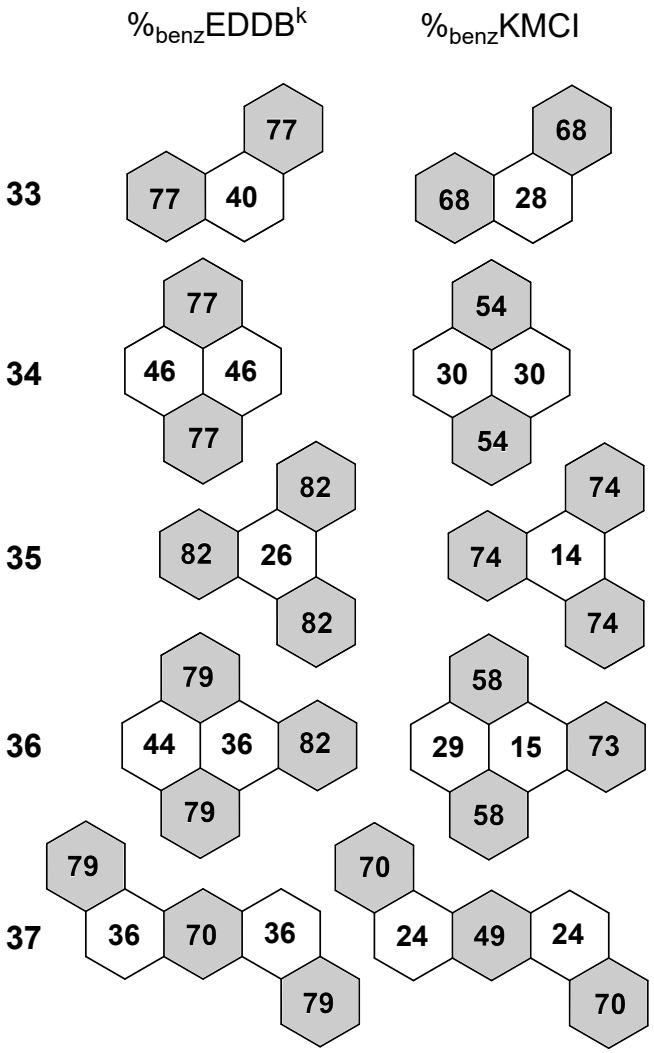


Figure S5. *Local aromaticity in claromatic systems.* Numbers inside benzenoid units refer to the percentage of the aromaticity of benzene. The test is passed if the highest values predicted by the index coincide with the positions of Clar's sextets (grey cycles). Method: B3LYP/6-311++G**, equilibrium geometries.
Comment: Both indices pass the test with 100%.

Equilibrium geometries of molecular systems from the T1 test set (CAM-B3LYP/def2-TZVPP):

Optimized geometries for the T2 test molecules were taken from the ESI of Ref. 29.

Ring 1

C	0.749455	0.969942	-0.000023
C	1.166180	-0.300269	-0.000187
C	-0.021969	-1.209664	-0.000499
C	-1.176331	-0.257822	0.000018
C	-0.714012	0.996241	-0.002590
H	-0.031426	-1.864791	0.876903
H	-0.035581	-1.865416	-0.875568
H	-2.211114	-0.562872	0.008539
H	-1.311020	1.896198	0.002909
H	1.379399	1.847128	0.006973
H	2.189804	-0.640820	-0.000068

Ring 2

C	-0.868050	0.822073	0.000000
C	-1.050582	-0.571021	0.000000
C	0.218558	-1.175120	0.000000
C	1.185606	-0.155026	0.000000
C	0.514120	1.079272	0.000000
H	0.419726	-2.239326	0.000000
H	2.259547	-0.295215	0.000000
H	0.978772	2.057669	0.000000
H	-1.655055	1.566339	0.000000
H	-2.000905	-1.090538	0.000000

Ring 3

C	0.713570	1.220464	0.000000
C	1.102883	-0.105994	0.000000
C	-0.000279	-0.968072	0.000000
C	-1.103149	-0.105522	0.000000
C	-0.712997	1.220910	0.000000
F	2.409111	-0.538178	0.000000
F	-2.409244	-0.538093	0.000000
H	0.000273	-2.045488	0.000000
H	1.365672	2.080333	0.000000
H	-1.364918	2.080877	0.000000

Ring 4

C	0.540701	-1.173227	0.000000
C	-0.317434	-0.002116	0.000000
C	0.536465	1.171917	0.000000
C	1.813604	0.723104	0.000000
C	1.816375	-0.719424	0.000000
C	-1.639155	-0.001907	0.000000
O	-2.784983	0.000648	0.000000
H	2.698332	-1.339940	0.000000
H	0.195464	-2.192845	0.000000
H	0.189566	2.190956	0.000000
H	2.693161	1.346564	0.000000

Ring 5

C	0.498442	-1.174451	0.000000
C	-0.336266	-0.003605	0.000000
C	0.490770	1.172045	0.000000
C	1.773496	0.722757	0.000000
C	1.778268	-0.716580	0.000000
N	-1.644136	-0.003191	0.000000
N	-2.760339	0.001511	0.000000
H	2.663006	-1.332836	0.000000
H	0.149147	-2.193104	0.000000
H	0.138751	2.189204	0.000000
H	2.652159	1.347510	0.000000

Ring 6

C	0.126282	-1.172669	0.000000
C	-0.756958	0.000030	0.000000
C	0.126134	1.172671	0.000000
C	1.393095	0.734876	0.000000
C	1.393346	-0.734888	0.000000
C	-2.086496	-0.000071	0.000000
H	-0.216266	-2.194518	0.000000
H	-0.215862	2.194716	0.000000
H	2.280250	1.349253	0.000000
H	2.280732	-1.348889	0.000000
H	-2.650525	-0.922906	0.000000
H	-2.650745	0.922648	0.000000

Ring 7

C	-0.860899	-1.175626	0.000000
C	0.243642	-0.225427	0.000000
C	-0.353562	1.101776	0.000000
C	-1.694411	0.945044	0.000000
C	-2.012077	-0.473931	0.000000
C	1.540163	-0.565727	0.000000
O	2.586071	0.266278	0.000000
H	-0.747299	-2.248211	0.000000
H	0.171950	2.044758	0.000000
H	-2.424543	1.739803	0.000000
H	-3.009608	-0.884309	0.000000
H	1.858816	-1.599855	0.000000
H	2.284973	1.180931	0.000000

Ring 8

C	0.871220	-1.169429	0.000000
C	-0.217694	-0.209839	0.000000
C	0.392076	1.104378	0.000000
C	1.736253	0.934310	0.000000
C	2.036503	-0.482632	0.000000
C	-1.526752	-0.549162	0.000000
N	-2.585818	0.286213	0.000000
H	0.746924	-2.241358	0.000000
H	-0.126616	2.050382	0.000000
H	2.473415	1.722726	0.000000
H	3.028481	-0.906561	0.000000
H	-1.791304	-1.599319	0.000000
H	-3.516731	-0.072235	0.000000
H	-2.463074	1.277114	0.000000

Ring 9

C	-1.376762	-1.118249	0.000000
C	-0.122830	-0.353341	0.000000
C	-0.499549	1.065796	0.000000
C	-1.836389	1.127434	0.000000
C	-2.386809	-0.241325	0.000000
C	1.105744	-0.878963	0.000000
C	2.290820	-0.091463	0.000000
N	3.259307	0.522550	0.000000
H	-1.437463	-2.194087	0.000000
H	0.200706	1.884647	0.000000
H	-2.432398	2.026138	0.000000
H	-3.438168	-0.482509	0.000000
H	1.246827	-1.951381	0.000000

Ring 10

C	1.657404	-1.208788	0.000000
C	0.484376	-0.310750	0.000000
C	1.011487	1.062550	0.000000
C	2.346226	0.973854	0.000000
C	2.751845	-0.445936	0.000000
C	-0.758750	-0.781270	0.000000
N	-1.962146	0.031574	0.000000
O	-1.876498	1.239336	0.000000
O	-3.002370	-0.589684	0.000000
H	1.600151	-2.284245	0.000000
H	0.404823	1.948077	0.000000
H	3.033828	1.804532	0.000000
H	3.773156	-0.793682	0.000000
H	-1.001530	-1.830877	0.000000

Ring 11

C	0.858031	1.181294	0.000000
C	-0.252223	0.226084	0.000000
C	0.341619	-1.108369	0.000000
C	1.676505	-0.952384	0.000000
C	1.999552	0.474954	0.000000
C	-1.536109	0.557930	0.000000
F	-2.504411	-0.355662	0.000000
H	0.746983	2.253568	0.000000
H	-0.214576	-2.030098	0.000000
H	2.405516	-1.747841	0.000000
H	2.999008	0.879965	0.000000
H	-1.921485	1.568306	0.000000

Ring 12

C	-0.729739	1.158103	0.000000
C	0.284720	0.156788	0.000000
C	-0.372001	-1.105272	0.000000
C	-1.733662	-0.876871	0.000000
C	-1.959381	0.530033	0.000000
C	1.675171	0.432795	0.000000
O	2.619745	-0.355287	0.000000
H	-0.549543	2.224823	0.000000
H	0.128066	-2.061459	0.000000
H	-2.504886	-1.636168	0.000000
H	-2.925536	1.016255	0.000000
H	1.903298	1.525389	0.000000

Ring 13

C	0.760473	-1.156706	0.000000
C	-0.272935	-0.184081	0.000000
C	0.354403	1.088958	0.000000
C	1.728009	0.892889	0.000000
C	1.983223	-0.501219	0.000000
C	-1.669703	-0.493655	0.000000
N	-2.701424	0.274695	0.000000
H	0.600810	-2.227235	0.000000
H	-0.150660	2.044705	0.000000
H	2.478078	1.673131	0.000000
H	2.957984	-0.969624	0.000000
H	-1.889175	-1.567592	0.000000
H	-2.387897	1.246643	0.000000

Ring 14

C	2.173867	-0.730083	0.000000
C	0.904276	-1.174736	0.000000
C	0.039002	-0.000573	0.000000
C	0.903099	1.174232	0.000000
C	2.173093	0.730691	0.000000
C	-1.286923	-0.000183	0.000000
F	-2.038279	-1.071950	0.000000
F	-2.037249	1.072250	0.000000
H	0.562104	-2.195510	0.000000
H	0.561269	2.195179	0.000000
H	3.058224	1.347273	0.000000
H	3.059666	-1.345724	0.000000

Ring 15

C	-2.218675	-0.720224	0.000000
C	-0.934559	-1.159672	0.000000
C	-0.072644	-0.000359	0.000000
C	-0.934248	1.159127	0.000000
C	-2.218396	0.720324	0.000000
C	1.286527	-0.000185	0.000000
O	2.052706	-1.079635	0.000000
O	2.050868	1.080378	0.000000
H	-0.624460	-2.194900	0.000000
H	-0.623507	2.194201	0.000000
H	-3.099833	1.341730	0.000000
H	-3.100306	-1.341344	0.000000
H	1.494363	1.865632	0.000000
H	1.495842	-1.865299	0.000000

Ring 16

C	-1.207773	0.678838	0.000000
C	-1.191798	-0.706502	0.000000
C	0.015971	-1.385299	0.000000
C	1.207773	-0.678840	0.000000
C	1.191797	0.706504	0.000000
C	-0.015970	1.385299	0.000000
H	-2.122102	-1.258025	0.000000
H	0.028427	-2.466733	0.000000
H	2.150530	-1.208788	0.000000
H	2.122104	1.258024	0.000000
H	-0.028430	2.466733	0.000000
H	-2.150531	1.208788	0.000000

Ring 17

C	-2.414599	-0.704321	0.000000
C	-1.237287	-1.391227	0.000000
C	0.000012	-0.708456	0.000000
C	-0.000012	0.708456	0.000000
C	-1.237317	1.391223	0.000000
C	-2.414620	0.704310	0.000000
C	1.237317	-1.391223	0.000000
C	2.414620	-0.704310	0.000000
C	2.414599	0.704321	0.000000
C	1.237287	1.391227	0.000000
H	-3.354426	-1.239046	0.000000
H	-1.234863	-2.473512	0.000000
H	-1.234827	2.473507	0.000000
H	-3.354464	1.239002	0.000000
H	1.234827	-2.473507	0.000000
H	1.234863	2.473512	0.000000
H	3.354464	-1.239002	0.000000
H	3.354426	1.239046	0.000000

Rings 18, 19

C	3.631975	0.710468	0.000000
C	2.464115	1.396751	0.000000
C	1.213094	0.714549	0.000000
C	1.213094	-0.714549	0.000000
C	2.464115	-1.396751	0.000000
C	3.631975	-0.710468	0.000000
C	0.000000	1.391599	0.000000
C	-1.213094	0.714549	0.000000
C	-1.213094	-0.714549	0.000000
C	0.000000	-1.391599	0.000000
C	-2.464115	-1.396751	0.000000
C	-3.631975	-0.710468	0.000000
C	-3.631975	0.710468	0.000000
C	-2.464115	1.396751	0.000000
H	4.574219	1.240914	0.000000
H	2.461539	2.478997	0.000000
H	2.461539	-2.478997	0.000000
H	4.574219	-1.240914	0.000000
H	0.000000	2.474785	0.000000
H	-2.461539	2.478997	0.000000
H	-4.574219	-1.240914	0.000000
H	-4.574219	1.240914	0.000000
H	-2.461539	-2.478997	0.000000
H	0.000000	-2.474785	0.000000

Rings 20, 21

C	-1.412118	0.856985	0.000000
C	-0.725945	-0.374608	0.000000
C	0.725943	-0.374609	0.000000
C	1.412117	0.856983	0.000000
C	0.672348	2.081640	0.000000
C	-0.672347	2.081639	0.000000
C	1.488936	-1.554681	0.000000
C	2.859212	-1.519298	0.000000
C	3.534146	-0.295112	0.000000
C	2.816892	0.870353	0.000000
C	-2.816892	0.870353	0.000000
C	-1.488934	-1.554680	0.000000
C	-2.859211	-1.519300	0.000000
C	-3.534145	-0.295113	0.000000
H	1.222870	3.013337	0.000000
H	-1.222867	3.013339	0.000000
H	0.996162	-2.514958	0.000000
H	3.326086	1.825428	0.000000
H	3.419639	-2.444059	0.000000
H	4.615072	-0.271402	0.000000
H	-3.326091	1.825425	0.000000
H	-4.615071	-0.271405	0.000000
H	-0.996151	-2.514952	0.000000
H	-3.419645	-2.444056	0.000000

Rings 22, 23

C	4.850890	0.713459	0.000000
C	3.687349	1.399837	0.000000
C	2.429487	0.718796	0.000000
C	2.429488	-0.718794	0.000000
C	3.687349	-1.399838	0.000000
C	4.850891	-0.713460	0.000000
C	1.227730	1.394796	0.000000
C	0.000000	0.717731	0.000000
C	0.000000	-0.717731	0.000000
C	1.227729	-1.394796	0.000000
C	-1.227730	-1.394796	0.000000
C	-2.429487	-0.718796	0.000000
C	-2.429488	0.718794	0.000000
C	-1.227729	1.394796	0.000000
C	-3.687349	-1.399837	0.000000
C	-4.850890	-0.713459	0.000000
C	-4.850891	0.713460	0.000000
C	-3.687349	1.399838	0.000000
H	5.794083	1.242225	0.000000
H	3.685884	2.482038	0.000000
H	3.685875	-2.482039	0.000000
H	5.794082	-1.242228	0.000000
H	1.228172	2.477844	0.000000
H	1.228174	-2.477843	0.000000
H	-1.228172	-2.477844	0.000000
H	-1.228174	2.477843	0.000000
H	-3.685884	-2.482038	0.000000
H	-3.685875	2.482039	0.000000
H	-5.794083	-1.242225	0.000000
H	-5.794082	1.242228	0.000000

Rings 24, 25

C	2.384079	0.938013	0.000000
C	1.857795	-0.370857	0.000000
C	0.424209	-0.556387	0.000000
C	-0.424209	0.556387	0.000000
C	0.152869	1.859831	0.000000
C	1.489918	2.042545	0.000000
C	-0.152869	-1.859831	0.000000
C	-1.489918	-2.042545	0.000000
C	-2.384079	-0.938013	0.000000
C	-1.857795	0.370857	0.000000
C	3.777657	1.134884	0.000000
C	2.772042	-1.443867	0.000000
C	4.123520	-1.229690	0.000000
C	4.637304	0.073534	0.000000
C	-3.777657	-1.134884	0.000000
C	-2.772042	1.443867	0.000000
C	-4.123520	1.229690	0.000000
C	-4.637304	-0.073534	0.000000
H	-0.488002	2.727143	0.000000
H	1.903049	3.042752	0.000000
H	0.488002	-2.727143	0.000000
H	-1.903049	-3.042752	0.000000
H	4.157047	2.148496	0.000000
H	5.706397	0.234659	0.000000
H	2.413598	-2.461174	0.000000
H	4.799190	-2.073965	0.000000
H	-4.157047	-2.148496	0.000000
H	-5.706397	-0.234659	0.000000
H	-2.413598	2.461174	0.000000
H	-4.799190	2.073965	0.000000

Rings 26, 27

C	-0.775103	-1.206355	0.000000
C	-1.433448	0.034553	0.000000
C	-0.657147	1.274168	0.000000
C	0.746658	1.223769	0.000000
C	1.432248	-0.068137	0.000000
C	0.686711	-1.258787	0.000000
C	-1.283141	2.529501	0.000000
C	-0.563302	3.697026	0.000000
C	0.826733	3.647096	0.000000
C	1.460990	2.430998	0.000000
C	-1.549639	-2.375997	0.000000
C	-2.836161	0.049721	0.000000
C	-3.572413	-1.107457	0.000000
C	-2.920648	-2.336186	0.000000
C	2.832457	-0.153466	0.000000
C	1.375464	-2.480814	0.000000
C	2.745801	-2.539343	0.000000
C	3.483898	-1.360422	0.000000
H	-2.359166	2.594799	0.000000
H	2.538908	2.419031	0.000000
H	-1.076920	4.648413	0.000000
H	1.407339	4.559144	0.000000
H	-1.068591	-3.340755	0.000000
H	-3.487851	-3.256627	0.000000
H	-3.364575	0.989338	0.000000
H	-4.652580	-1.060639	0.000000
H	0.826485	-3.408574	0.000000
H	3.245534	-3.498096	0.000000
H	3.427018	0.745833	0.000000
H	4.564643	-1.391065	0.000000

Rings 28, 29

C	-1.419039	-1.224018	0.000000
C	-0.710919	0.000001	0.000000
C	0.710919	-0.000001	0.000000
C	1.419038	-1.224014	0.000000
C	0.672942	-2.448953	0.000000
C	-0.672940	-2.448954	0.000000
C	1.419039	1.224018	0.000000
C	2.810878	1.200924	0.000000
C	3.497076	-0.000001	0.000000
C	2.810881	-1.200923	0.000000
C	-2.810878	-1.200924	0.000000
C	-1.419038	1.224014	0.000000
C	-2.810881	1.200923	0.000000
C	-3.497076	0.000001	0.000000
C	0.672940	2.448954	0.000000
C	-0.672942	2.448953	0.000000
H	1.220591	-3.382412	0.000000
H	-1.220586	-3.382415	0.000000
H	3.354265	-2.136739	0.000000
H	3.354268	2.136737	0.000000
H	4.578448	0.000004	0.000000
H	-3.354268	-2.136737	0.000000
H	-4.578448	-0.000004	0.000000
H	-3.354265	2.136740	0.000000
H	-1.220591	3.382412	0.000000
H	1.220586	3.382415	0.000000

Rings 30, 31, 32

C	-6.070348	-0.715186	0.000000
C	-4.909187	-1.401609	0.000000
C	-3.647520	-0.721339	0.000000
C	-3.647522	0.721342	0.000000
C	-4.909189	1.401610	0.000000
C	-6.070349	0.715182	0.000000
C	-2.451825	-1.396900	0.000000
C	-1.215814	-0.720464	0.000000
C	-1.215814	0.720467	0.000000
C	-2.451824	1.396904	0.000000
C	0.000002	1.396672	0.000000
C	1.215814	0.720464	0.000000
C	1.215814	-0.720468	0.000000
C	-0.000002	-1.396672	0.000000
C	2.451825	1.396900	0.000000
C	3.647520	0.721339	0.000000
C	3.647522	-0.721342	0.000000
C	2.451824	-1.396904	0.000000
C	4.909187	1.401610	0.000000
C	6.070347	0.715186	0.000000
C	6.070349	-0.715182	0.000000
C	4.909189	-1.401610	0.000000
H	-7.014138	-1.242866	0.000000
H	-4.908129	-2.483790	0.000000
H	-4.908129	2.483790	0.000000
H	-7.014137	1.242864	0.000000
H	-2.452720	-2.479906	0.000000
H	-2.452717	2.479909	0.000000
H	0.000004	2.479592	0.000000
H	-0.000004	-2.479593	0.000000
H	2.452720	2.479906	0.000000
H	2.452718	-2.479909	0.000000
H	4.908129	2.483790	0.000000
H	4.908130	-2.483790	0.000000
H	7.014138	1.242866	0.000000
H	7.014137	-1.242864	0.000000

Rings 33, 34, 35, 36, 37

C	-4.356439	-1.189318	0.000000
C	-3.031656	-1.516164	0.000000
C	-2.026817	-0.522105	0.000000
C	-2.437716	0.834164	0.000000
C	-3.818324	1.142565	0.000000
C	-4.758769	0.158247	0.000000
C	-0.625743	-0.824758	0.000000
C	0.308111	0.221286	0.000000
C	-0.131149	1.583962	0.000000
C	-1.471333	1.858514	0.000000
C	0.857446	2.631584	0.000000
C	2.169548	2.357090	0.000000
C	2.649446	0.999344	0.000000
C	1.705247	-0.057937	0.000000
C	2.160095	-1.393776	0.000000
C	4.001971	0.701194	0.000000
C	4.442082	-0.617530	0.000000
C	3.535784	-1.652056	0.000000
C	-0.132850	-2.164111	0.000000
C	1.190425	-2.436050	0.000000
H	-5.102466	-1.972001	0.000000
H	-2.756452	-2.559482	0.000000
H	-4.113679	2.183710	0.000000
H	-5.810923	0.407191	0.000000
H	-1.805160	2.888725	0.000000
H	0.509593	3.656344	0.000000
H	2.898847	3.156609	0.000000
H	4.720109	1.510724	0.000000
H	5.502621	-0.828574	0.000000
H	3.877819	-2.678626	0.000000
H	1.533820	-3.462321	0.000000
H	-0.830280	-2.987171	0.000000

Ring 38

C	0.423228	-1.540561	0.000000
C	1.468853	-0.630011	0.000000
C	1.408334	0.755367	0.000000
C	0.287493	1.571552	0.000000
C	-1.050000	1.204358	0.000000
C	-1.597006	-0.069635	0.000000
C	-0.941107	-1.291111	0.000000
H	-2.678694	-0.116849	0.000000
H	-1.578180	-2.166913	0.000000
H	0.710321	-2.584805	0.000000
H	2.464173	-1.056649	0.000000
H	2.362343	1.267636	0.000000
H	0.482685	2.636809	0.000000
H	-1.761420	2.021013	0.000000

Ring 39

C	1.561391	0.816760	0.000000
C	0.701021	1.880685	0.000000
C	-0.702808	1.880302	0.000000
C	-1.562140	0.815642	0.000000
C	-1.229249	-0.541581	0.000000
C	0.000516	-1.164282	0.000000
C	1.229915	-0.541055	0.000000
F	2.260783	-1.354014	0.000000
F	-2.259523	-1.355488	0.000000
H	0.000480	-2.247534	0.000000
H	2.625239	1.020255	0.000000
H	1.165006	2.858709	0.000000
H	-1.167592	2.857961	0.000000
H	-2.626348	1.017305	0.000000

Ring 40

C	1.562069	-0.860980	0.000000
C	0.712786	-1.903574	0.000000
C	-0.712955	-1.903500	0.000000
C	-1.562012	-0.860752	0.000000
C	-1.262244	0.544332	0.000000
C	0.000067	1.128391	0.000000
C	1.262343	0.544082	0.000000
N	2.329028	1.353610	0.000000
N	-2.329154	1.353597	0.000000
H	0.001144	2.212304	0.000000
H	2.618407	-1.099788	0.000000
H	1.169188	-2.884900	0.000000
H	-1.169665	-2.884736	0.000000
H	-2.618513	-1.098392	0.000000
H	-2.232512	2.353620	0.000000
H	-3.263332	0.984443	0.000000
H	2.232321	2.353678	0.000000
H	3.263520	0.985319	0.000000

Ring 41

C	-0.709498	1.555174	0.000000
C	-1.835835	0.672945	0.000000
C	-1.835746	-0.673562	0.000000
C	-0.709174	-1.555265	0.000000
C	0.607005	-1.280566	0.000000
C	1.316301	0.000543	0.000000
C	0.606957	1.281434	0.000000
O	2.538027	-0.000555	0.000000
H	1.295669	2.117136	0.000000
H	1.295689	-2.116282	0.000000
H	-0.965683	2.608066	0.000000
H	-2.802550	1.160051	0.000000
H	-2.802515	-1.160504	0.000000
H	-0.964887	-2.608248	0.000000

Ring 42

C	1.103153	-1.578140	0.000000
C	2.243303	-0.666792	0.000000
C	2.243216	0.666838	0.000000
C	1.103028	1.578067	0.000000
C	-0.201864	1.307208	0.000000
C	-0.868215	0.000009	0.000000
C	-0.201647	-1.307089	0.000000
C	-2.190844	0.000023	0.000000
O	-3.347110	-0.000102	0.000000
H	-0.874374	-2.156120	0.000000
H	-0.873926	2.156714	0.000000
H	1.362038	-2.629176	0.000000
H	3.209835	-1.154734	0.000000
H	3.209886	1.154441	0.000000
H	1.362644	2.628951	0.000000

Ring 43

C	1.071301	-1.581783	0.000000
C	2.209493	-0.667291	0.000000
C	2.209278	0.667349	0.000000
C	1.071144	1.581849	0.000000
C	-0.234037	1.304451	0.000000
C	-0.879549	0.000072	0.000000
C	-0.233881	-1.304300	0.000000
N	-2.181738	-0.000356	0.000000
N	-3.312292	0.000079	0.000000
H	-0.919497	-2.142823	0.000000
H	-0.919519	2.143107	0.000000
H	1.330206	-2.632355	0.000000
H	3.177007	-1.153334	0.000000
H	3.176960	1.153001	0.000000
H	1.330560	2.632260	0.000000

Ring 44

C	0.738504	1.558081	0.000000
C	1.878763	0.669349	0.000000
C	1.878693	-0.669455	0.000000
C	0.738369	-1.558024	0.000000
C	-0.571293	-1.279634	0.000000
C	-1.278385	0.000043	0.000000
C	-0.571182	1.279656	0.000000
C	-2.619736	0.000116	0.000000
H	-1.235418	2.136271	0.000000
H	0.993593	2.611053	0.000000
H	2.843858	1.160604	0.000000
H	2.843277	-1.161512	0.000000
H	0.992948	-2.611101	0.000000
H	-1.236118	-2.135868	0.000000
H	-3.181890	-0.922240	0.000000
H	-3.182644	0.922011	0.000000

Ring 45

C	0.377842	1.570296	-0.007046
C	1.519921	0.666172	0.004130
C	1.520538	-0.667869	0.005954
C	0.376305	-1.569425	-0.007558
C	-0.926235	-1.300559	-0.005440
C	-1.672787	0.000569	0.011528
C	-0.924661	1.300854	-0.004627
H	-2.334259	-0.002262	0.886695
H	-1.586232	2.160690	-0.014409
H	0.642203	2.621698	-0.015645
H	2.485736	1.156250	0.009862
H	2.486087	-1.158494	0.017598
H	0.641074	-2.621116	-0.017261
H	-1.587437	-2.160532	-0.015382
H	-2.372711	0.003545	-0.833105