The Description of Aromaticity in Porphyrinoids

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Supporting Information

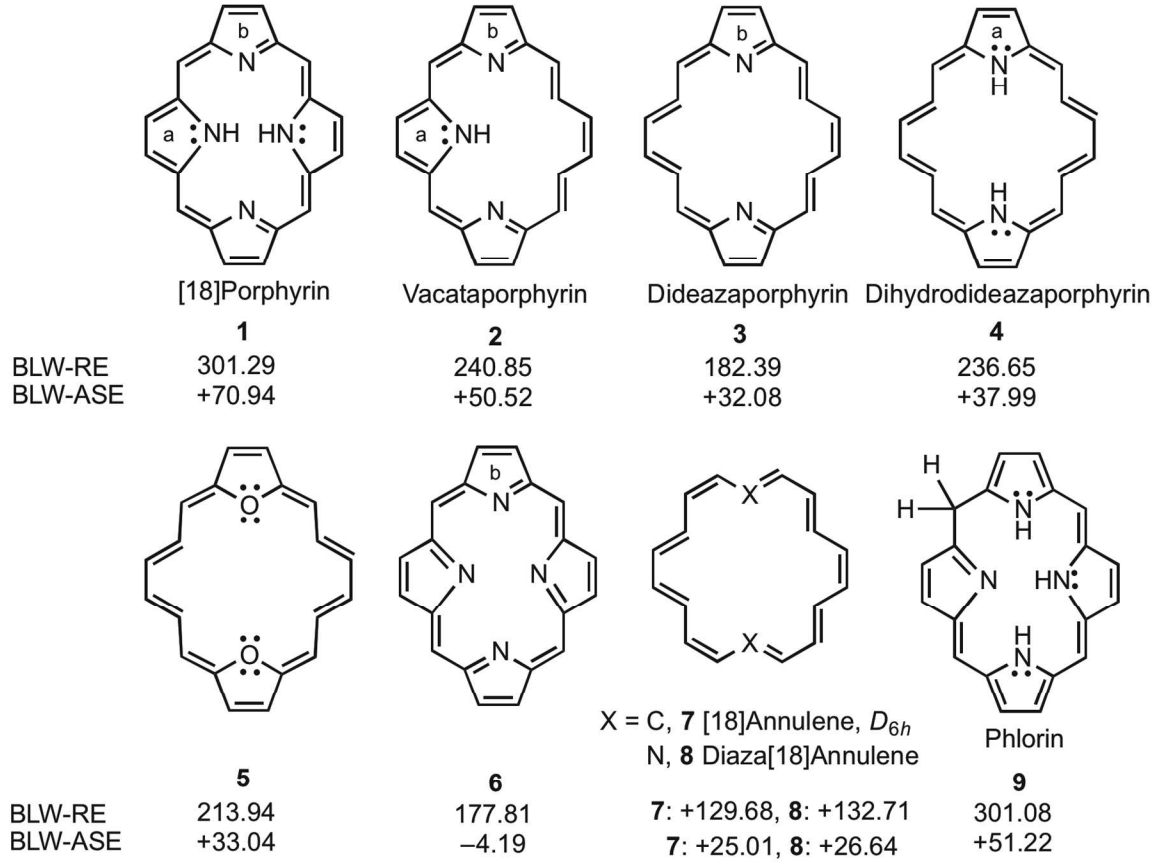

Figure S1. Block-localized wavefunction computed RE's (resonance energies) and ASE's (aromatic stabilization energies, see Computational Methods section) for **1**-**9** (in kcal/mol, at the B3LYP/6-31G* level).

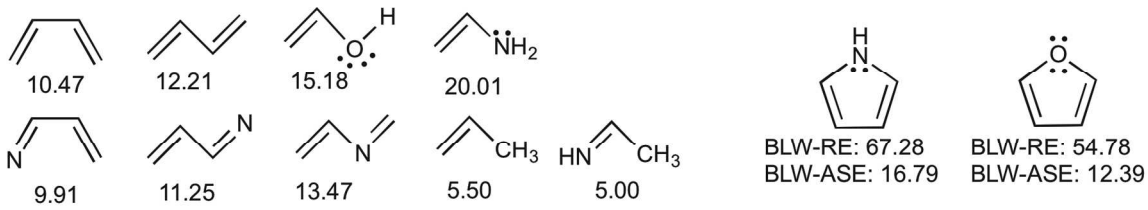

Figure S2. Computed BLW-RE's (in kcal/mol) for all reference compounds used to evaluate the BLW-ASE's of **1**-**9**. The BLW-RE's and BLW-ASE's of pyrrole and furan also are listed. All BLW computations were performed at the B3LYP/6-31G* level.

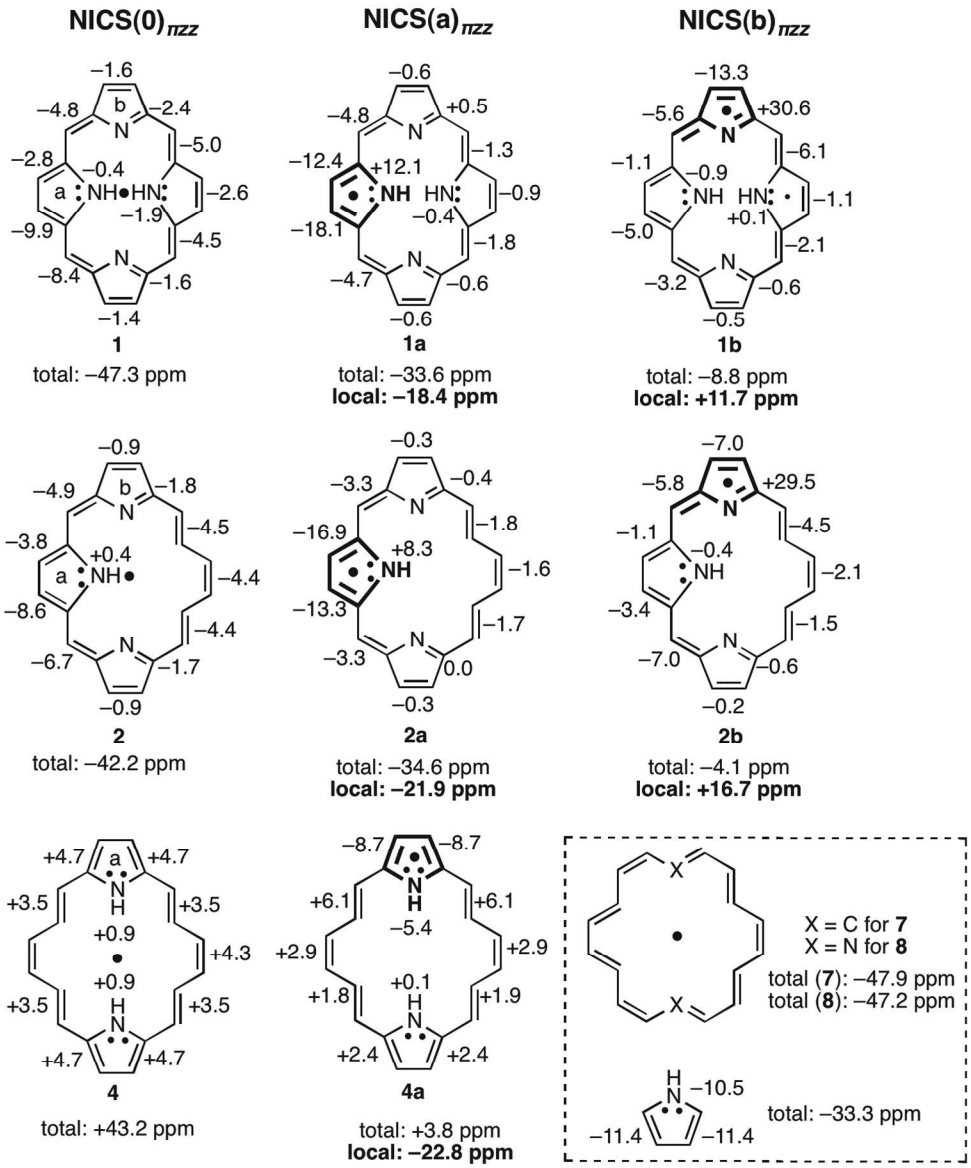

Figure S3. Dissected $NICS_{\pi zz}$ computed at the heavy atom centers "0", as well as at the "**a**" and "**b**" ring centers (position of NICS points are indicated by the black "dots") for **1**, **2**, **4**, **7**, and **8**. The *total* $NICS_{\pi zz}$ include the *zz* tensor components of all π (and lone pair) MO contributions; *local* $NICS_{\pi zz}$ consider only contributions from the highlighted π and lone pairs MO's (in bold). Computations were performed at the PW91/IGLOIII//B3LYP/6-31G* level.

Optimized coordinates and total electronic energies for compounds **1**-**9** at B3LYP/6-31G*

1 (Total electronic energy: -989.5512503 a.u.)

N	0.00000	2.12367	0.00000
C	1.12893	2.90112	0.00000
C	0.68754	4.26939	0.00000
C	-0.68754	4.26939	0.00000
C	-1.12893	2.90112	0.00000
C	2.44248	2.42583	0.00000
C	2.85697	1.08503	0.00000
N	2.03694	0.00000	0.00000
C	2.85697	-1.08503	0.00000
C	4.26263	-0.67965	0.00000
C	4.26263	0.67965	0.00000
N	-2.03694	0.00000	0.00000
C	-2.85697	-1.08503	0.00000
C	-4.26263	-0.67965	0.00000
C	-4.26263	0.67965	0.00000
C	-2.85697	1.08503	0.00000
C	2.44248	-2.42583	0.00000
C	1.12893	-2.90112	0.00000
C	0.68754	-4.26939	0.00000
C	-0.68754	-4.26939	0.00000
C	-1.12893	-2.90112	0.00000
N	0.00000	-2.12367	0.00000
C	-2.44248	-2.42583	0.00000
C	-2.44248	2.42583	0.00000
H	-1.35350	-5.13056	0.00000
H	1.35350	-5.13056	0.00000
H	5.11609	-1.35724	0.00000
H	5.11609	1.35724	0.00000
H	1.35350	5.13056	0.00000
H	-1.35350	5.13056	0.00000
H	-5.11609	1.35724	0.00000
H	-5.11609	-1.35724	0.00000
H	3.22586	-3.18690	0.00000
H	3.22586	3.18690	0.00000
H	-3.22586	3.18690	0.00000
H	-3.22586	-3.18690	0.00000
H	0.00000	-1.10467	0.00000
H	0.00000	1.10467	0.00000

2 (-935.3460441 a.u.)

C	-3.18147	1.17909	0.00000
C	-4.55253	0.67324	0.00000
C	-4.45472	-0.68215	0.00000
C	-2.47937	-2.26377	0.00000
C	-1.13192	-2.66478	0.00000
C	-0.68703	-4.02186	0.00000
C	0.68703	-4.02186	0.00000
C	1.13192	-2.66478	0.00000
C	-2.77910	2.54784	0.00000
C	-3.02136	-0.98220	0.00000
C	3.02136	-0.98220	0.00000
C	4.45472	-0.68215	0.00000
C	4.55253	0.67324	0.00000
C	2.77910	2.54784	0.00000
C	1.43147	2.81776	0.00000
C	0.69900	4.01989	0.00000
C	-0.69900	4.01989	0.00000
C	-1.43147	2.81776	0.00000
C	2.47937	-2.26377	0.00000
C	3.18147	1.17909	0.00000
N	-2.28817	0.16545	0.00000
N	0.00000	-1.87662	0.00000
N	2.28817	0.16545	0.00000
H	-5.44980	1.28021	0.00000
H	-5.25433	-1.41320	0.00000
H	-3.18719	-3.08871	0.00000
H	-1.34915	-4.87751	0.00000
H	1.34915	-4.87751	0.00000
H	-3.54057	3.32486	0.00000
H	5.25433	-1.41320	0.00000
H	5.44980	1.28021	0.00000
H	3.54057	3.32486	0.00000
H	1.22470	4.97328	0.00000
H	-1.22470	4.97328	0.00000
H	3.18719	-3.08871	0.00000
H	0.85629	1.90294	0.00000
H	-0.85629	1.90294	0.00000
H	0.00000	-0.86033	0.00000

3 (-881.1558256 a.u.)

C	1.08573	3.39889	0.00000
C	0.68224	4.81135	0.00000
C	-0.68224	4.81135	0.00000
C	-2.39605	2.85361	0.00000
C	-2.55308	1.47188	0.00014
C	-3.72517	0.70459	0.00025
C	-3.72517	-0.70459	0.00025
C	-2.55308	-1.47188	0.00014
C	2.39605	2.85361	0.00000
C	-1.08573	3.39889	-0.00000
C	-1.08573	-3.39889	-0.00000
C	-0.68224	-4.81135	0.00000
C	0.68224	-4.81135	0.00000
C	2.39605	-2.85361	0.00000
C	2.55308	-1.47188	-0.00014
C	3.72517	-0.70459	-0.00025
C	3.72517	0.70459	-0.00025
C	2.55308	1.47188	-0.00014
C	-2.39605	-2.85361	0.00000
C	1.08573	-3.39889	0.00000
N	0.00000	2.60141	0.00000
N	0.00000	-2.60141	0.00000
H	1.35223	5.67119	0.00016
H	-1.35223	5.67119	-0.00016
H	-3.25701	3.52944	-0.00012
H	-4.69363	1.21670	0.00037
H	-4.69363	-1.21670	0.00037
H	3.25701	3.52944	0.00012
H	-1.59951	0.94091	0.00018
H	-1.59951	-0.94091	0.00018
H	-1.35223	-5.67119	-0.00016
H	1.35223	-5.67119	0.00016
H	3.25701	-3.52944	0.00012
H	4.69363	-1.21670	-0.00037
H	4.69363	1.21670	-0.00037
H	-3.25701	-3.52944	-0.00012
H	1.59951	-0.94091	-0.00018
H	1.59951	0.94091	-0.00018

4 (-882.380304 a.u., Nlm=4)

C	1.14238	3.45157	0.00000
C	-1.14238	3.45157	0.00000
C	1.14238	-3.45157	0.00000
C	-1.14238	-3.45157	0.00000
C	0.70752	4.78076	0.00000
C	-0.70752	4.78076	0.00000
C	0.70752	-4.78076	0.00000
C	-0.70752	-4.78076	0.00000
C	-2.45554	2.83845	0.00000
C	2.45554	2.83845	0.00000
C	-2.45554	-2.83845	0.00000
C	2.45554	-2.83845	0.00000
C	-2.62240	1.48897	0.00000
C	2.62240	1.48897	0.00000
C	-2.62240	-1.48897	0.00000
C	2.62240	-1.48897	0.00000
C	-3.81972	0.68601	0.00000
C	3.81972	0.68601	0.00000
C	-3.81972	-0.68601	0.00000
C	3.81972	-0.68601	0.00000
N	0.00000	2.68380	0.00000
N	0.00000	-2.68380	0.00000
H	1.35412	5.64818	0.00000
H	-1.35412	5.64818	0.00000
H	1.35412	-5.64818	0.00000
H	-1.35412	-5.64818	0.00000
H	-3.31092	3.51058	0.00000
H	3.31092	3.51058	0.00000
H	-3.31092	-3.51058	0.00000
H	3.31092	-3.51058	0.00000
H	-4.77704	1.20410	0.00000
H	4.77704	1.20410	0.00000
H	-4.77704	-1.20410	0.00000
H	4.77704	-1.20410	0.00000
H	-1.70820	0.90553	0.00000
H	1.70820	0.90553	0.00000
H	-1.70820	-0.90553	0.00000
H	1.70820	-0.90553	0.00000
H	0.00000	1.67975	0.00000
H	0.00000	-1.67975	0.00000

5 (-922.1134742 a.u.)

C	1.11421	3.52689	0.00000
C	-1.11421	3.52689	0.00000
C	1.11421	-3.52689	0.00000
C	-1.11421	-3.52689	0.00000
C	0.71249	4.84574	0.00000
C	-0.71249	4.84574	0.00000
C	0.71249	-4.84574	0.00000
C	-0.71249	-4.84574	0.00000
C	-2.38631	2.84951	0.00000
C	2.38631	2.84951	0.00000
C	-2.38631	-2.84951	0.00000
C	2.38631	-2.84951	0.00000
C	-2.47077	1.49350	0.00000
C	2.47077	1.49350	0.00000
C	-2.47077	-1.49350	0.00000
C	2.47077	-1.49350	0.00000
C	-3.66179	0.68430	0.00000
C	3.66179	0.68430	0.00000
C	-3.66179	-0.68430	0.00000
C	3.66179	-0.68430	0.00000
O	0.00000	2.72924	0.00000
O	0.00000	-2.72924	0.00000
H	1.36546	5.70777	0.00000
H	-1.36546	5.70777	0.00000
H	1.36546	-5.70777	0.00000
H	-1.36546	-5.70777	0.00000
H	-3.27455	3.47750	0.00000
H	3.27455	3.47750	0.00000
H	-3.27455	-3.47750	0.00000
H	3.27455	-3.47750	0.00000
H	-4.62007	1.20169	0.00000
H	4.62007	1.20169	0.00000
H	-4.62007	-1.20169	0.00000
H	4.62007	-1.20169	0.00000
H	-1.52375	0.96602	0.00000
H	1.52375	0.96602	0.00000
H	-1.52375	-0.96602	0.00000
H	1.52375	-0.96602	0.00000

6 (-988.1826734 a.u.)

N	0.00000	-2.06530	0.00000
N	0.00000	2.06530	0.00000
N	2.06653	0.00000	0.00000
N	-2.06653	0.00000	0.00000
C	-2.88467	1.08060	0.00000
C	2.88467	-1.08060	0.00000
C	2.88467	1.08060	0.00000
C	-2.88467	-1.08060	0.00000
C	-1.08064	-2.88345	0.00000
C	1.08064	2.88345	0.00000
C	1.08064	-2.88345	0.00000
C	-1.08064	2.88345	0.00000
C	-0.68108	4.28854	0.00000
C	0.68108	-4.28854	0.00000
C	0.68108	4.28854	0.00000
C	-0.68108	-4.28854	0.00000
C	-4.28980	-0.68105	0.00000
C	4.28980	0.68105	0.00000
C	4.28980	-0.68105	0.00000
C	-4.28980	0.68105	0.00000
C	-2.40670	2.40629	0.00000
C	2.40670	-2.40629	0.00000
C	2.40670	2.40629	0.00000
C	-2.40670	-2.40629	0.00000
H	-3.17714	3.17761	0.00000
H	3.17714	-3.17761	0.00000
H	3.17714	3.17761	0.00000
H	-3.17714	-3.17761	0.00000
H	1.34831	5.14232	0.00000
H	-1.34831	-5.14232	0.00000
H	-1.34831	5.14232	0.00000
H	1.34831	-5.14232	0.00000
H	-5.14370	1.34812	0.00000
H	5.14370	-1.34812	0.00000
H	5.14370	1.34812	0.00000
H	-5.14370	-1.34812	0.00000

7 (-696.6407759 a.u.)

H	0.35268	-1.86848	0.00000
H	-0.35268	1.86848	0.00000
H	-1.44181	-1.23967	0.00000
H	1.79449	-0.62881	0.00000
H	-1.79449	0.62881	0.00000
H	1.44181	1.23967	0.00000
C	0.55381	-2.93404	0.00000
C	-2.26405	-1.94663	0.00000
C	2.81786	-0.98741	0.00000
C	-2.81786	0.98741	0.00000
C	2.26405	1.94663	0.00000
C	-0.55381	2.93404	0.00000
C	-0.57020	-3.76047	0.00000
C	1.90173	-3.29389	0.00000
C	-1.90173	-3.29389	0.00000
C	-3.54176	-1.38642	0.00000
C	-3.80345	-0.00000	0.00000
C	-2.97156	2.37405	0.00000
C	-1.90173	3.29389	0.00000
C	0.57020	3.76047	0.00000
C	1.90173	3.29389	0.00000
C	3.54176	1.38642	0.00000
C	3.80345	0.00000	0.00000
C	2.97156	-2.37405	0.00000
H	-0.41649	-4.83890	0.00000
H	2.15170	-4.35415	0.00000
H	-2.69495	-4.04050	0.00000
H	-4.39886	-2.05876	0.00000
H	-4.84665	0.31365	0.00000
H	-3.98236	2.78014	0.00000
H	-2.15170	4.35415	0.00000
H	0.41649	4.83890	0.00000
H	2.69495	4.04050	0.00000
H	4.39886	2.05876	0.00000
H	4.84665	-0.31365	0.00000
H	3.98236	-2.78014	0.00000

8 (-728.73568 a.u.)

N	-2.95523	0.00000	0.00000
N	2.95523	0.00000	0.00000
C	-1.49910	-2.43123	-0.00000
C	1.49910	-2.43123	-0.00000
C	-1.49910	2.43123	0.00000
C	1.49910	2.43123	0.00000
C	-2.89186	-2.38008	-0.00000
C	2.89186	-2.38008	-0.00000
C	-2.89186	2.38008	0.00000
C	2.89186	2.38008	0.00000
C	-3.59754	-1.16312	-0.00000
C	3.59754	-1.16312	-0.00000
C	-3.59754	1.16312	0.00000
C	3.59754	1.16312	0.00000
C	0.70385	-3.57678	-0.00000
C	-0.70385	-3.57678	-0.00000
C	0.70385	3.57678	0.00000
C	-0.70385	3.57678	0.00000
H	-1.01060	-1.46202	-0.00000
H	1.01060	-1.46202	-0.00000
H	-1.01060	1.46202	0.00000
H	1.01060	1.46202	0.00000
H	-3.46826	-3.30349	-0.00000
H	3.46826	-3.30349	-0.00000
H	-3.46826	3.30349	0.00000
H	3.46826	3.30349	0.00000
H	-4.69596	-1.19095	-0.00000
H	4.69596	-1.19095	-0.00000
H	-4.69596	1.19095	0.00000
H	4.69596	1.19095	0.00000
H	1.20312	-4.54536	-0.00000
H	-1.20312	-4.54536	-0.00000
H	1.20312	4.54536	0.00000
H	-1.20312	4.54536	0.00000

9 (-990.7228707 a.u., NIm=3)

N	-0.06743	2.18286	0.00000
C	1.11958	2.91161	0.00000
C	0.73748	4.26029	0.00000
C	-0.66736	4.32668	0.00000
C	-1.14389	3.01923	0.00000
C	2.45782	2.41304	0.00000
C	2.92840	1.12708	0.00000
N	2.15587	-0.03493	0.00000
C	2.93053	-1.17793	0.00000
C	4.29900	-0.70266	0.00000
C	4.29418	0.66133	0.00000
N	-2.03026	0.01943	0.00000
C	-2.84575	-1.13274	0.00000
C	-4.23054	-0.74983	0.00000
C	-4.25728	0.61760	0.00000
C	-2.88276	1.04716	0.00000
C	2.47986	-2.48272	0.00000
C	1.13843	-2.95087	0.00000
C	0.70532	-4.30719	0.00000
C	-0.68196	-4.32909	0.00000
C	-1.13797	-2.99124	0.00000
N	-0.00592	-2.19366	0.00000
C	-2.43308	-2.45965	0.00000
C	-2.56608	2.53148	0.00000
H	-1.32260	-5.20125	0.00000
H	1.37481	-5.15684	0.00000
H	1.43017	5.09186	0.00000
H	-1.27871	5.21931	0.00000
H	-5.12139	1.27103	0.00000
H	-5.06805	-1.43705	0.00000
H	-0.13882	-1.19305	0.00000
H	-0.24173	1.18419	0.00000
H	5.15379	1.31914	0.00000
H	5.16060	-1.35716	0.00000
H	-3.08065	2.97179	0.86787
H	-3.08065	2.97179	-0.86787
H	1.15688	-0.02705	0.00000
H	3.21800	3.18875	0.00000
H	-3.23310	-3.19633	0.00000
H	3.24190	-3.25441	0.00000

9 (-990.7351226 a.u., minimum)

N	-2.12629	-0.47031	-0.24546
C	-2.53000	-1.22976	-1.33577
C	-3.52095	-2.09621	-0.85833
C	-3.69592	-1.84197	0.51807
C	-2.83225	-0.80942	0.87208
C	-2.01327	-1.04291	-2.65224
C	-0.86931	-0.36839	-2.99302
N	0.09546	0.11078	-2.07389
C	1.14705	0.72081	-2.77169
C	0.76280	0.71818	-4.16134
C	-0.42073	0.05031	-4.29304
N	-0.17521	0.24272	2.03017
C	0.89105	0.14935	2.93432
C	0.41106	-0.28030	4.22366
C	-0.94024	-0.46002	4.08664
C	-1.25413	-0.10605	2.72438
C	2.32561	1.18305	-2.23009
C	2.74526	1.13694	-0.87405
C	4.06131	1.34278	-0.38008
C	4.05330	1.11428	0.98869
C	2.73287	0.78194	1.36755
N	1.97022	0.80256	0.20983
C	2.20955	0.44473	2.62591
C	-2.65452	-0.05387	2.15559
H	4.89640	1.16284	1.66553
H	4.91243	1.59414	-0.99880
H	-4.04024	-2.83360	-1.45624
H	-4.38298	-2.33965	1.18940
H	-1.65194	-0.78235	4.83708
H	1.02229	-0.43445	5.10483
H	0.95770	0.74390	0.28923
H	-1.47783	0.30285	-0.28121
H	-0.98011	-0.11323	-5.20558
H	1.34503	1.18109	-4.94764
H	-2.94043	0.99969	2.00257
H	-3.35581	-0.45554	2.89335
H	0.30906	-0.45870	-1.26175
H	-2.60117	-1.45598	-3.46651
H	2.92866	0.40154	3.44040
H	3.05846	1.56642	-2.93264

Full citation for reference 43:

Gaussian 03, Revision C.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
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