

Supporting Information For “A Hückel Theory Perspective on Möbius Aromaticity”

William C. McKee,* Judy, I. Wu, Henry S. Rzepa, Paul von Ragué Schleyer*

*Center for Computational Chemistry, Department of Chemistry, University of Georgia,
Athens, Georgia 30602-2525, United States, and Department of Chemistry, Imperial College London,
South Kensington Campus, Exhibition Road, London, SW7 2AY, U. K.
schleyer@chem.uga.edu, chadm@uga.edu*

Contents

March 21, 1998 letter from E. Heilbronner to P. v. R. Schleyer (S2-S3)

B3LYP/6-311+G** geometries, HF/6-31G**/B3LYP/6-311+G** p-NHOs twist angles (degrees), and p-NHO basis depictions for Möbius and Hückel conformations of [8], [12], [16], [20]annulene. (S4-S15)

N. v. E. Heilbronner
Grutstrasse 10
CH-8704 HERALIBERG
Switzerland

21. March 1998

Dear Paul :

Reading the title of your preprint reminded me of a story told about Adele Sandrock, a german actress who, nearing 70 after a rather chequered career, became famous for her portrayal of crusty old dowagers. When a young actress asked her to become her child's godmother, she agreed and asked to see the child which was just being bathed. Sandrock lifted the baby out of the tub, looked closely at it and said : "Aha ! Ein Knabe wenn ich mich recht erinnere."

Although this story neatly describes my first reaction, my second reaction was one of considerable surprise. I am of course extremely grateful to you for dedicating such a nice paper to me and for letting me have a preprint. However pleasant it is to have one's prediction verified and to see one's name quoted, I feel that including my name in the title and in the summary is overdoing it. "Möbius" by itself is quite enough and in fact the nomenclature generally used. Apart from this the manuscript seems to be in good shape and can be read, even by rather old chemists, without too much trouble.

If you are interested, I can tell you how reference [1] of your paper came about. After a few glasses of Remy Martin in our home in Rüschlikon, F. Feichtmayr, on leave from the BASF, H. Preuss

"Aha! A boy...if I remember correctly."

who had given a talk at the ETH, and myself tried to think up crazy titles for a theoretical paper. My suggestion was "Electron in a Möbius Band" as an extension of "Electron in a Box". The next morning, remembering my proposal, I solved the problem for fun, using first the free electron approximation and then the HMO formalism. I showed the result to Feichtmayr who remarked: "Sehr lustig, aber Sie würden sich natürlich nie trauen so etwas Unsinniges zu veröffentlichen !". All I said was "Wollen wir wetten ?", which we did. In the afternoon I wrote the note and sent it off to Tetrahedron Letters, where it was accepted and published, much to my surprise.

I include the reprint of a paper just published. It also deals with "aromaticity", albeit with a prediction published almost exactly 100 years before mine.

Once again many thanks for your kindness and congratulations for having solved a problem which I would not have thought to be soluble in this manner.

With kindest regards,

Cordially yours,

Edgar

"Very amusing, but you naturally never would presume to publish such nonsense."

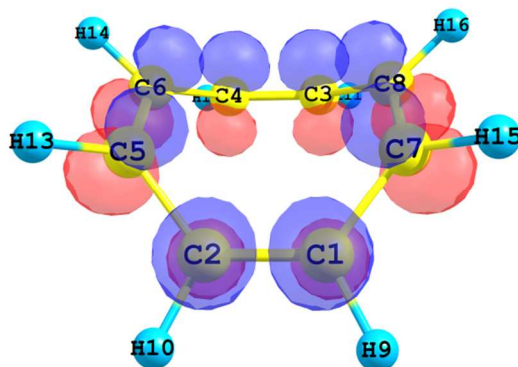
"Shall we bet?"

Hückel [8]annulene, D_{2d}

C	1.580383811	0.633192359	0.375189772
C	0.633192359	1.580383811	0.375189772
C	-0.633192359	-1.580383811	0.375189772
C	-1.580383811	-0.633192359	0.375189772
C	-0.633192359	1.580383811	-0.375189772
C	-1.580383811	0.633192359	-0.375189772
C	1.580383811	-0.633192359	-0.375189772
C	0.633192359	-1.580383811	-0.375189772
H	2.495236011	0.838930250	0.928830746
H	0.838930250	2.495236011	0.928830746
H	-0.838930250	-2.495236011	0.928830746
H	-2.495236011	-0.838930250	0.928830746
H	-0.838930250	2.495236011	-0.928830746
H	-2.495236011	0.838930250	-0.928830746
H	2.495236011	-0.838930250	-0.928830746
H	0.838930250	-2.495236011	-0.928830746

p NHO twist angles:

C1- C2	0
C2- C5	36.819
C5- C6	0
C6- C4	-36.819
C4- C3	0
C3- C8	36.819
C8- C7	0
C7- C1	-36.819

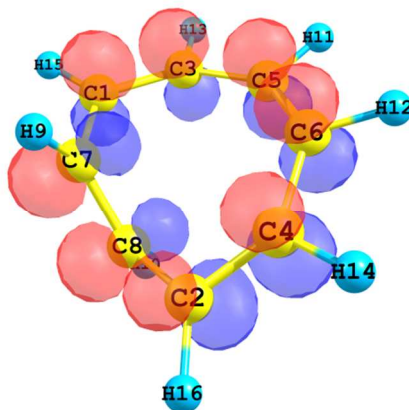


Möbius [8]annulene, C₂

C	-0.370739412	1.761587527	-0.788207586
C	0.370739412	-1.761587527	-0.788207586
C	0.000000000	1.792582158	0.518887098
C	0.000000000	-1.792582158	0.518887098
C	0.058785589	0.685168134	1.473218179
C	-0.058785589	-0.685168134	1.473218179
C	-0.525911256	0.426695893	-1.327885283
C	0.525911256	-0.426695893	-1.327885283
H	-1.533587932	0.027427558	-1.426563156
H	1.533587932	-0.027427558	-1.426563156
H	0.128455798	1.074074079	2.487528270
H	-0.128455798	-1.074074079	2.487528270
H	0.105436134	2.768961829	0.987879259
H	-0.105436134	-2.768961829	0.987879259
H	-0.645771433	2.676763695	-1.304918800
H	0.645771433	-2.676763695	-1.304918800

p NHO twist angles:

C1-C3	-4.235
C3-C5	0.25
C5-C6	3.763
C6-C4	0.25
C4-C2	-4.235
C2-C8	-54.669
C8-C7	-16.566
C7-C1	-54.669 (phase shift)

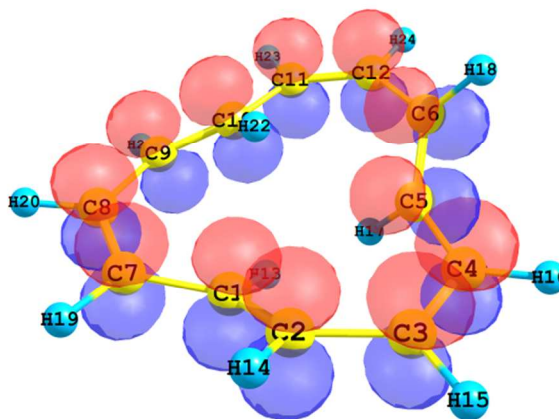


Hückel [12]annulene, C_1

C	0.607814110	-1.590779461	0.251148081
C	-0.390603941	-2.358507142	-0.231649537
C	-1.824153931	-2.107168348	-0.035063756
C	-2.443184757	-0.931663596	0.216033800
C	-1.763311168	0.364463300	0.433331006
C	-1.852585566	1.478153879	-0.313082365
C	2.024379668	-1.618843202	-0.072640311
C	2.800945429	-0.504289357	-0.038096806
C	2.311658164	0.858255387	0.189939627
C	1.094028210	1.263212701	-0.233996613
C	0.395079767	2.518708505	-0.011694300
C	-0.951945521	2.627977622	-0.111250814
H	0.341304687	-0.787702344	0.920798539
H	-0.149021869	-3.194807409	-0.885853653
H	-2.470809312	-2.964777573	-0.206205738
H	-3.530583064	-0.935007716	0.248631799
H	-1.082512678	0.414704253	1.278257247
H	-2.574476225	1.536369589	-1.126791214
H	2.476730721	-2.563545164	-0.363766753
H	3.869444509	-0.619912340	-0.202881280
H	2.966755627	1.545606230	0.722774063
H	0.527860730	0.550179675	-0.818798307
H	0.978942424	3.406256790	0.220176568
H	-1.402358313	3.615514303	-0.044209340

p NHO twist angles:

C1- C2	3.578
C2- C3	20.361
C3- C4	-0.149
C4- C5	-56.057
C5- C6	4.36
C6- C12	49.477
C12-C11	3.667
C11-C10	24.287
C10-C9	-3.415
C9- C8	-34.047
C8- C7	-4.005
C7- C1	-26.73

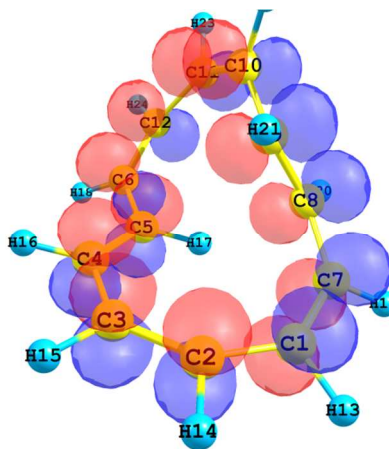


Möbius [12]annulene, C₁

C	-2.595081445	-0.815568489	-0.341594041
C	-2.709119460	0.433614816	0.356548866
C	-1.933350714	1.552641985	0.597198306
C	-0.600768380	1.936648208	0.265320845
C	0.285182251	1.226586253	-0.490551918
C	1.678876530	1.512124756	-0.702650277
C	-1.579711222	-1.635496764	-0.778567824
C	-0.189153079	-1.661634983	-0.461694352
C	0.389243917	-1.329515298	0.732907590
C	1.809604409	-1.286717331	0.958461375
C	2.766736237	-0.578525149	0.286579984
C	2.706830716	0.633537390	-0.503855250
H	-3.580315602	-1.185139546	-0.624672533
H	-3.729411191	0.575605451	0.708739282
H	-2.460614607	2.309590764	1.173339380
H	-0.251570638	2.851506384	0.740521694
H	-0.077841832	0.336954571	-0.971425752
H	1.954818726	2.522789398	-0.999244198
H	-1.890679412	-2.391196622	-1.498012128
H	0.472167315	-2.036254004	-1.241347790
H	-0.260570153	-1.223528900	1.600645632
H	2.167714835	-1.863489988	1.811616933
H	3.788820233	-0.831173419	0.562084052
H	3.691743762	1.008163592	-0.770864458

p NHO twist angles:

C1-C2	20.81 (phase shift)
C2-C3	2.921
C3-C4	10.767
C4-C5	3.313
C5-C6	-44.057
C6-C12	-5.526
C12-C11	6.163
C11-C10	8.553
C10-C9	44.723
C9-C8	7.585
C8-C7	28.251
C7-C1	7.852

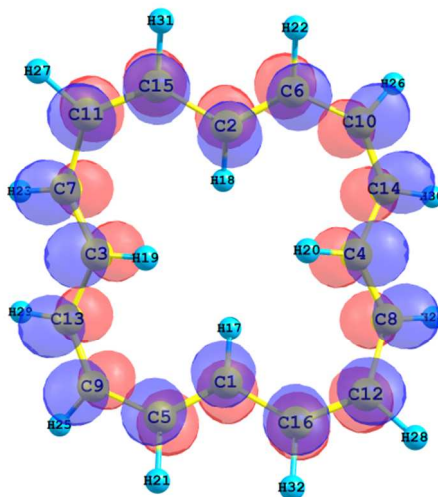


Hückel [16]annulene, S_4

C	0.000000000	2.366656815	0.030736614
C	0.000000000	-2.366656815	0.030736614
C	-2.366656815	0.000000000	-0.030736614
C	2.366656815	0.000000000	-0.030736614
C	-1.204200479	2.968092911	-0.118041030
C	1.204200479	-2.968092911	-0.118041030
C	-2.968092911	-1.204200479	0.118041030
C	2.968092911	1.204200479	0.118041030
C	-2.510138157	2.494772151	0.311385454
C	2.510138157	-2.494772151	0.311385454
C	-2.494772151	-2.510138157	-0.311385454
C	2.494772151	2.510138157	-0.311385454
C	-2.996246151	1.231137447	0.388963457
C	2.996246151	-1.231137447	0.388963457
C	-1.231137447	-2.996246151	-0.388963457
C	1.231137447	2.996246151	-0.388963457
H	0.064124005	1.413332269	0.542491576
H	-0.064124005	-1.413332269	0.542491576
H	-1.413332269	0.064124005	-0.542491576
H	1.413332269	-0.064124005	-0.542491576
H	-1.206396765	3.962575297	-0.563780980
H	1.206396765	-3.962575297	-0.563780980
H	-3.962575297	-1.206396765	0.563780980
H	3.962575297	1.206396765	0.563780980
H	-3.203866474	3.288776202	0.578692687
H	3.203866474	-3.288776202	0.578692687
H	-3.288776202	-3.203866474	-0.578692687
H	3.288776202	3.203866474	-0.578692687
H	-4.009241253	1.123475013	0.770939474
H	4.009241253	-1.123475013	0.770939474
H	-1.123475013	-4.009241253	-0.770939474
H	1.123475013	4.009241253	-0.770939474

p NHO twist angles:

C1-C5	-1.337
C5-C9	-27.551
C9-C13	-2.34
C13-C3	-8.661
C3-C7	1.337
C7-C11	27.551
C11-C15	2.34
C15-C2	8.661
C2-C6	-1.337
C6-C10	-27.551
C10-C14	-2.34
C14-C4	-8.661
C4-C8	1.337



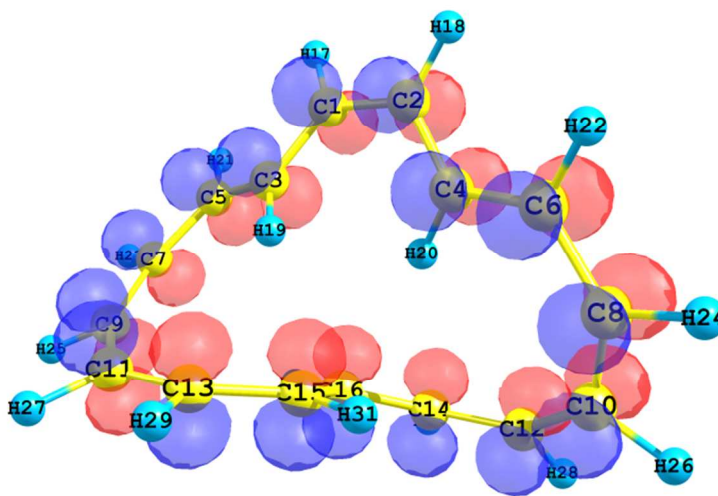
C8-C12	27.551
C12-C16	2.34
C16-C1	8.661

Möbius [16]annulene, C₂

C	0.081702765	0.694551564	2.653866275
C	-0.081702765	-0.694551564	2.653866275
C	-0.061268160	1.432432044	1.472443728
C	0.061268160	-1.432432044	1.472443728
C	0.303673565	2.753753561	1.244856743
C	-0.303673565	-2.753753561	1.244856743
C	0.000000000	3.515776806	0.112126408
C	0.000000000	-3.515776806	0.112126408
C	-0.851120273	3.313027295	-0.992433713
C	0.851120273	-3.313027295	-0.992433713
C	-1.655191435	2.285167578	-1.507609435
C	1.655191435	-2.285167578	-1.507609435
C	-1.683125432	0.878727853	-1.512807289
C	1.683125432	-0.878727853	-1.512807289
C	-0.691418437	-0.101840681	-1.400602239
C	0.691418437	0.101840681	-1.400602239
H	0.272947341	1.211187232	3.591379058
H	-0.272947341	-1.211187232	3.591379058
H	-0.545628338	0.915861755	0.661051421
H	0.545628338	-0.915861755	0.661051421
H	0.873106773	3.264596919	2.018564513
H	-0.873106773	-3.264596919	2.018564513
H	0.399111891	4.526510432	0.145853607
H	-0.399111891	-4.526510432	0.145853607
H	-1.047340462	4.254216129	-1.504244572
H	1.047340462	-4.254216129	-1.504244572
H	-2.487535473	2.693881960	-2.081278854
H	2.487535473	-2.693881960	-2.081278854
H	-2.655677834	0.478073793	-1.792123996
H	2.655677834	-0.478073793	-1.792123996
H	-1.039438147	-1.129080323	-1.458244077
H	1.039438147	1.129080323	-1.458244077

p NHO twist angles:

C1-C2	17.529
C2-C4	8.712
C4-C6	7.446
C6-C8	0.725
C8-C10	-10.222
C10-C12	-11.15
C12-C14	-23.277
C14-C16	-4.82
C16-C15	-5.474
C15-C13	-4.82
C13-C11	-23.277 (phase shift)
C11-C9	-11.15
C9-C7	-10.222



C7-C5	0.725
C5-C3	7.446
C3-C1	8.72

Hückel [20]annulene, C₁

C	3.548449400	-0.017776627	0.067505279
C	4.178538776	-1.309137274	0.019445902
C	3.508955415	-2.499873939	-0.000098987
C	2.077687751	-2.635538025	-0.040515777
C	1.366231319	-3.790960601	-0.069155585
C	-0.085267318	-3.840699156	-0.135437210
C	-0.901516072	-2.827115440	0.248051948
C	-2.316647983	-2.708682349	0.018263328
C	-2.971712848	-1.549907049	0.289290124
C	-4.351262172	-1.246048609	0.002959369
C	4.159575503	1.193316641	0.023046997
C	3.457846359	2.465621454	0.073202064
C	2.123817614	2.620737927	-0.123058994
C	1.369139275	3.831159636	0.060185489
C	0.007503746	3.915277016	0.018499413
C	-0.877473655	2.816120026	-0.270960637
C	-2.213317727	2.758679587	-0.035069303
C	-2.952416918	1.542556877	-0.262604400
C	-4.225303953	1.278036194	0.122965590
C	-4.903261698	-0.001407897	-0.017481899
H	2.469613419	-0.017770086	0.171873660
H	5.265101697	-1.330643794	0.004140391
H	4.093403799	-3.416308120	-0.008184292
H	1.508287004	-1.714761611	-0.094819470
H	1.898070361	-4.739577772	-0.096652817
H	-0.527109207	-4.742973883	-0.552859809
H	-0.447657712	-1.967308463	0.736662679
H	-2.838091206	-3.534898197	-0.461057633
H	-2.391929506	-0.754397388	0.748212534
H	-5.008960208	-2.089043006	-0.196052126
H	5.245389681	1.233538372	-0.023834367
H	4.057075262	3.343363153	0.305440433
H	1.558048187	1.738798731	-0.401761730
H	1.929098209	4.728444337	0.310998573
H	-0.453383197	4.868779011	0.262656665
H	-0.426385640	1.916828525	-0.680638208
H	-2.731416195	3.611180092	0.399799185
H	-2.401711368	0.760847212	-0.777690194
H	-4.812391164	2.085456349	0.558215618
H	-5.982441088	0.054296191	-0.138645365

p NHO twist angles:

C1-C2	4.993
C2-C3	1.106
C3-C4	3.589
C4-C5	-1.602
C5-C6	-20.214
C6-C7	-3.779

Möbius [20]annulene, C₂

C	0.130296202	0.677061038	3.420499876
C	-0.130296202	-0.677061038	3.420499876
C	0.206708216	1.560641695	2.312704761
C	-0.206708216	-1.560641695	2.312704761
C	0.493394358	2.897112885	2.469533408
C	-0.493394358	-2.897112885	2.469533408
C	0.469589638	3.990850624	1.551678962
C	-0.469589638	-3.990850624	1.551678962
C	0.001390789	4.122570355	0.261319065
C	-0.001390789	-4.122570355	0.261319065
C	-0.549136423	3.131873015	-0.591060311
C	0.549136423	-3.131873015	-0.591060311
C	-1.311217983	3.403955509	-1.700449896
C	1.311217983	-3.403955509	-1.700449896
C	-1.959388717	2.408719903	-2.494823349
C	1.959388717	-2.408719903	-2.494823349
C	-1.525146279	1.124346018	-2.714714377
C	1.525146279	-1.124346018	-2.714714377
C	-0.186838126	0.659339977	-2.564228078
C	0.186838126	-0.659339977	-2.564228078
H	0.254412106	1.140230760	4.397001756
H	-0.254412106	-1.140230760	4.397001756
H	-0.006863832	1.158000003	1.330362304
H	0.006863832	-1.158000003	1.330362304
H	0.750782335	3.193778916	3.485179820
H	-0.750782335	-3.193778916	3.485179820
H	0.807891805	4.923216295	1.996426764
H	-0.807891805	-4.923216295	1.996426764
H	0.000000000	5.136406843	-0.133731861
H	0.000000000	-5.136406843	-0.133731861
H	-0.445587083	2.091237795	-0.313312800
H	0.445587083	-2.091237795	-0.313312800
H	-1.555657417	4.444478036	-1.907323856
H	1.555657417	-4.444478036	-1.907323856
H	-2.914065205	2.693510658	-2.931311525
H	2.914065205	-2.693510658	-2.931311525
H	-2.241321798	0.417606905	-3.128522905
H	2.241321798	-0.417606905	-3.128522905
H	0.591740732	1.416484425	-2.497528017
H	-0.591740732	-1.416484425	-2.497528017

p NHO twist angles:

C1-C2	3.121
C2-C4	4.55
C4-C6	2.726
C6-C8	5.766
C8-C10	-1.433
C10-C12	-8.287

C12-C14	-2.463
C14-C16	-25.469
C16-C18	-8.62
C18-C20	-19.659
C20-C19	-4.779
C19-C17	-19.659
C17-C15	-8.62
C15-C13	-25.469
C13-C11	-2.463
C11-C9	-8.287 (phase shift)
C9-C7	-1.433
C7-C5	5.766
C5-C3	2.726
C3-C1	4.55

