Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:
Switching between Hückel Aromaticity and Möbius Aromaticity: A Density Functional Theory and Information-Theoretic Approach Study

Donghai Yu,[1,2] Chunying Rong,[1*] Tian Lu,[3] Paul Geerlings,[2] Frank De Proft,[2*] Mercedes Alonso,[2* 2] and Shubin Liu[4*]

[1] Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research (Ministry of Education of China), College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha, 410081, China

[2] Research Group of General Chemistry (ALGC), Vrije Universiteit Brussel (VUB), Pleinlaan 2, 1050 Brussels, Belgium

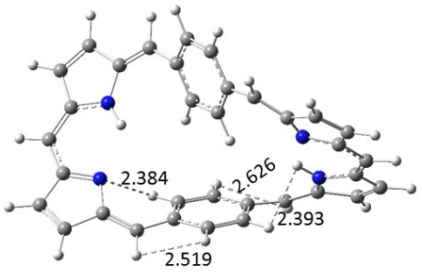
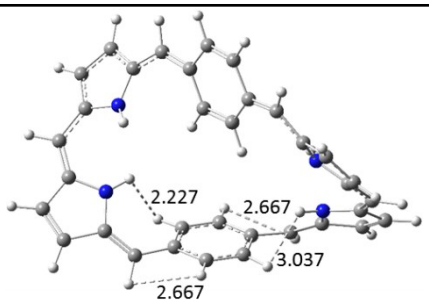
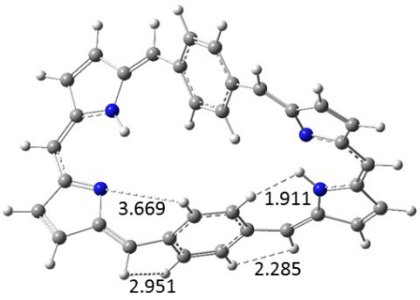
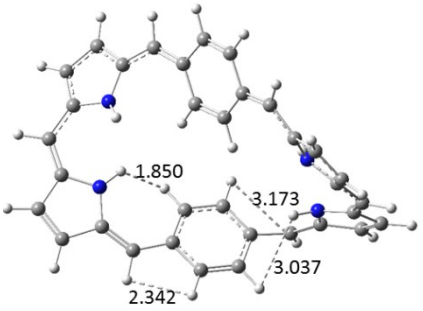
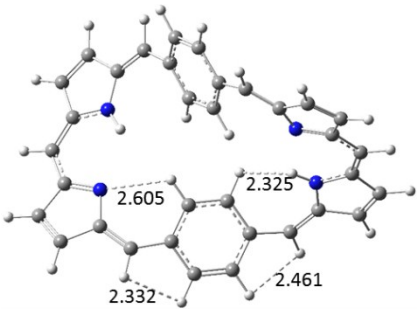
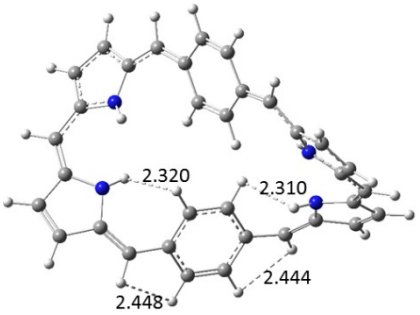
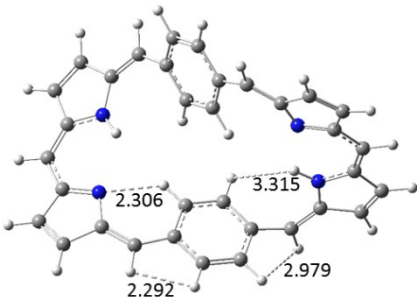
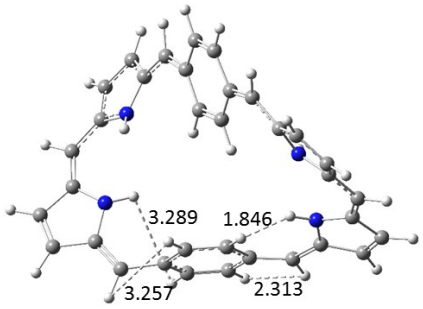
[3] Beijing Kein Research Center for Natural Sciences, Beijing 100022, China

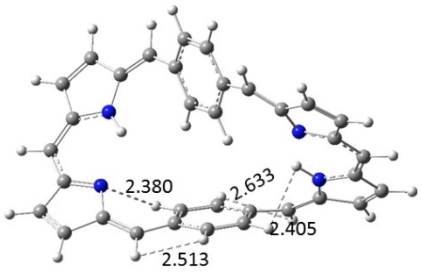
[4] Research Computing Center, University of North Carolina, Chapel Hill, North Carolina 27599-3420, USA

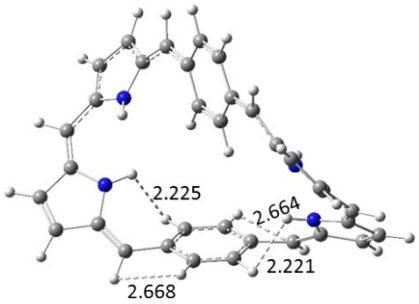
Content

1. The representative molecular structures

Table S1. 3D structures of intermediates and transition state along the conformational interconversion of [28] and [30]benzihexaphyrins, together with selected structural parameters and relative energy (Δ*E* with kJ/mol).

	Natural state	Δ*E*	Reduced state	Δ*E*
Möbius start		0.00		0.00
TS1		28.03		9.47
Hückel		11.65		-17.41
TS2		16.90		9.82

Möbius end 

0.01 

0.01

2. The Cartesian coordinates of Möbius and Hückel conformation

Table S2. The Cartesian coordinates of Möbius and Hückel conformation of natural and reduced states

	Natural state					
	Möbius			Hückel		
C	0.423577	3.894344	0.460349	0.371916	4.132114	-0.826814
C	-0.678744	3.899541	-0.365850	-0.749150	4.210820	-0.026152
C	-1.240989	2.699688	-0.835525	-1.246966	3.075187	0.629360
C	-0.612261	1.495644	-0.471675	-0.561740	1.861813	0.463418
C	0.541825	1.495080	0.305946	0.594414	1.792721	-0.304119
C	1.079636	2.696515	0.794953	1.085608	2.930584	-0.959305
C	2.289385	2.829728	1.594955	2.331523	2.986034	-1.710630
C	-2.450185	2.819012	-1.642123	-2.450779	3.234298	1.440550
C	3.448071	2.123181	1.553946	3.468851	2.268932	-1.543595
C	-3.566067	2.051737	-1.623901	-3.520443	2.413335	1.510868
N	3.737026	1.044750	0.730529	3.689439	1.238062	-0.630328
C	5.053092	0.892937	0.772447	4.999382	1.078544	-0.586655
C	5.680102	1.842743	1.701894	5.700280	1.968671	-1.524319
C	4.679054	2.586905	2.206033	4.743586	2.680012	-2.144495
C	-4.837158	2.400186	-2.254387	-4.781994	2.743906	2.171927
C	-5.787562	1.559604	-1.802797	-5.701508	1.825035	1.832256
C	-5.163316	0.614684	-0.884355	-5.067670	0.843561	0.957754
N	-3.822778	0.911544	-0.883118	-3.744237	1.201574	0.868834
C	5.779275	-0.027856	-0.045140	5.679531	0.169819	0.284061
C	-5.773959	-0.317418	-0.088548	-5.679531	-0.169819	0.284061
N	-3.718474	-1.259491	0.739533	-3.689439	-1.238062	-0.630329
C	-5.029516	-1.133668	0.817371	-4.999382	-1.078544	-0.586655
C	-5.570923	-1.876686	1.966921	-5.700280	-1.968671	-1.524319
C	-4.508891	-2.412850	2.601542	-4.743586	-2.680012	-2.144495
C	4.693125	-2.556688	-2.384768	4.781994	-2.743906	2.171927
C	5.707893	-1.865032	-1.825833	5.701508	-1.825035	1.832256
C	5.151470	-0.960703	-0.824330	5.067670	-0.843561	0.957754
N	3.807547	-1.204775	-0.798818	3.744237	-1.201574	0.868834
C	-3.332487	-2.068328	1.797517	-3.468851	-2.268932	-1.543595
C	3.453848	-2.185612	-1.709070	3.520443	-2.413335	1.510868
C	-2.067816	-2.527645	1.968846	-2.331523	-2.986034	-1.710630
C	2.218984	-2.723573	-1.839395	2.450779	-3.234298	1.440550

H	0.817581	4.834775	0.832700	0.732014	5.021285	-1.334718
H	-1.146618	4.841701	-0.632614	-1.268826	5.156821	0.085582
H	-0.993977	0.547145	-0.838247	-0.905883	0.979700	0.996617
H	1.020779	0.553948	0.552453	1.135103	0.859836	-0.401536
H	6.739666	1.911467	1.905815	6.771932	2.015345	-1.659510
H	4.737579	3.406469	2.909048	4.854681	3.450540	-2.894962
H	-4.958180	3.237451	-2.926816	-4.914508	3.621145	2.788853
H	-6.842929	1.564919	-2.033458	-6.743689	1.788838	2.114305
H	-3.186935	0.404638	-0.275512	-3.110752	0.700828	0.257469
H	-6.615095	-1.938068	2.240984	-6.771932	-2.015345	-1.659510
H	-4.500445	-3.025595	3.492394	-4.854681	-3.450540	-2.894962
H	4.754421	-3.312631	-3.154443	4.914508	-3.621145	2.788853
H	6.760122	-1.929175	-2.062210	6.743689	-1.788838	2.114305
H	3.182185	-0.574836	-0.302809	3.110752	-0.700828	0.257469
C	1.130394	-2.524738	-0.884580	1.246966	-3.075187	0.629360
C	-0.207805	-2.509642	-1.304678	0.561740	-1.861813	0.463418
C	-1.246875	-2.441572	-0.393424	-0.594414	-1.792721	-0.304119
C	-0.992160	-2.428940	0.990663	-1.085608	-2.930584	-0.959305
C	0.345999	-2.452137	1.411453	-0.371916	-4.132114	-0.826814
C	1.384821	-2.473589	0.498319	0.749150	-4.210820	-0.026152
H	2.406813	-2.519901	0.856415	1.268826	-5.156821	0.085582
H	0.569234	-2.466284	2.473826	-0.732014	-5.021285	-1.334718
H	-0.429911	-2.565857	-2.365751	0.905883	-0.979700	0.996617
H	-2.271407	-2.442277	-0.740192	-1.135103	-0.859836	-0.401536
H	6.858680	0.044494	-0.082453	6.752984	0.268300	0.388471
H	2.043310	-3.390506	-2.677166	2.559432	-4.184376	1.954624
H	-6.854191	-0.385487	-0.107464	-6.752984	-0.268300	0.388471
H	-2.533136	3.729810	-2.227772	-2.559432	4.184376	1.954624
H	-1.842903	-3.059947	2.889715	-2.404652	-3.814086	-2.411902
H	2.317161	3.717894	2.222458	2.404652	3.814086	-2.411902

Reduced state

		Möbius			Hückel	
C	2.504733	1.274025	-3.337040	2.432211	1.151811	-3.478525
C	-2.504606	-1.273643	-3.337098	-2.543509	-1.459533	-3.273426
C	3.570805	1.436535	-2.388006	3.514628	1.317864	-2.560667
C	-3.570571	-1.436512	-2.388000	-3.593350	-1.541097	-2.307645
N	3.810240	0.608831	-1.306735	3.734064	0.553288	-1.429900
C	5.069179	0.856702	-0.793007	5.017407	0.760761	-0.964955
C	5.596953	1.925557	-1.502851	5.586860	1.751765	-1.758476
C	4.668743	2.281695	-2.497076	4.657331	2.093988	-2.748775
C	-4.668353	-2.281869	-2.497117	-4.739250	-2.331299	-2.385177
C	-5.596556	-1.926065	-1.502769	-5.635895	-1.900231	-1.399334
C	-5.068942	-0.857206	-0.792809	-5.043193	-0.840629	-0.719503
N	-3.810089	-0.609017	-1.306589	-3.776961	-0.676402	-1.244717
C	5.704927	0.003197	0.180584	5.641671	-0.053847	0.036770
C	-5.704845	-0.003889	0.180849	-5.636115	0.062477	0.223621
N	-3.709230	0.760874	1.386023	-3.605757	0.920817	1.324701

C	-5.070561	0.775500	1.086471	-4.985425	0.903365	1.062856
C	-5.640313	1.832740	1.910221	-5.564939	1.961188	1.867953
C	-4.661288	2.387930	2.648411	-4.594155	2.519788	2.616590
C	4.660932	-2.388102	2.648465	4.679039	-2.278029	2.678211
C	5.640046	-1.833254	1.910135	5.624701	-1.793618	1.849973
C	5.070493	-0.776006	1.086262	5.019270	-0.811688	0.971207
N	3.709176	-0.761052	1.385860	3.649124	-0.799796	1.279452
C	-3.416006	1.665328	2.406665	-3.347608	1.807570	2.379300
C	3.415793	-1.665280	2.406645	3.425716	-1.585921	2.418356
C	-2.245768	1.805759	3.064058	-2.233079	1.888219	3.140614
C	2.245562	-1.805429	3.064125	2.336972	-1.593898	3.220187
H	6.559459	2.376532	-1.313364	6.578805	2.155522	-1.621428
H	4.769549	3.064251	-3.234484	4.781250	2.818213	-3.540287
H	-4.769061	-3.064331	-3.234638	-4.887490	-3.124797	-3.102636
H	-6.558967	-2.377245	-1.313290	-6.621385	-2.289923	-1.192690
H	-3.327977	0.268863	-1.170958	-3.246401	0.175941	-1.126891
H	-6.682249	2.117349	1.874239	-6.609814	2.234667	1.829699
H	-4.746788	3.203229	3.352386	-4.689080	3.332683	3.322215
H	4.746284	-3.203298	3.352577	4.796787	-3.023780	3.451316
H	6.681920	-2.118090	1.874161	6.667510	-2.073388	1.802116
H	3.114244	0.020330	1.158318	3.125128	0.059654	1.164380
C	1.104969	-0.890315	2.956514	1.166465	-0.734732	3.117093
C	-1.105136	0.890657	2.956489	-1.064516	1.022387	3.076072
C	0.209917	1.371156	2.957415	-0.464536	0.630535	4.285702
C	1.289427	0.501197	2.956268	0.602455	-0.241028	4.306629
C	-1.289598	-0.500852	2.957240	-0.515448	0.520712	1.885832
C	-0.210093	-1.370808	2.958432	0.582368	-0.333441	1.905576
H	-0.382214	-2.442030	2.987472	0.964277	-0.733404	0.970253
H	-2.294891	-0.904645	3.031318	-0.925841	0.840860	0.931986
H	2.294737	0.905071	3.029653	1.036726	-0.537471	5.256191
H	0.382051	2.442397	2.985664	-0.870663	1.006555	5.219415
H	6.785792	-0.058593	0.138204	6.724171	-0.097528	0.008368
H	2.163829	-2.636262	3.757039	2.416790	-2.200985	4.116332
H	-6.785725	0.057662	0.138495	-6.719109	0.102958	0.227833
H	-2.770608	-1.641973	-4.325026	-2.822607	-1.892319	-4.230900
H	-2.164079	2.636690	3.756859	-2.284785	2.573721	3.980505
H	2.770685	1.642551	-4.324908	2.677984	1.494739	-4.480496
H	-3.114173	-0.020480	1.158694	-3.082293	0.055037	1.270811
H	3.327993	-0.268995	-1.171238	3.208016	-0.283365	-1.217361
C	-1.288512	-0.658100	-3.238032	-1.327176	-0.829672	-3.229606
C	1.288587	0.658580	-3.238000	1.218366	0.531902	-3.335687
C	0.582564	0.335178	-4.466374	0.500021	0.143083	-4.533129
C	-0.582626	-0.334363	-4.466398	-0.651579	-0.551529	-4.481596
C	-0.613914	-0.285072	-2.004254	-0.641143	-0.392058	-2.028157
C	0.614078	0.285309	-2.004245	0.574742	0.206488	-2.076472
H	1.056109	0.601936	-5.406091	0.951354	0.376204	-5.492474
H	-1.056266	-0.600887	-5.406134	-1.135796	-0.869487	-5.399656
H	-1.082872	-0.531690	-1.056084	-1.086335	-0.616885	-1.062640

H	1.083102	0.531741	-1.056059	1.053024	0.517017	-1.151370

3. The global and local aromaticity indexes of porphyrinoids

Table S3. The global and local aromaticity indexes of porphyrinoids at different rotation angles (RD).

Macrocycle										
	Natural state					Reduced state				
RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-3.083	-3.671	-10.659	0.4300	0.02700	1.528	1.476	12.413	0.4505	0.08403
5	-3.042	-3.674	-10.668	0.4297	0.02699	1.493	1.445	12.342	0.4500	0.08404
10	-3.028	-3.666	-10.743	0.4300	0.02699	1.413	1.374	12.146	0.4492	0.08405
15	-3.006	-3.617	-10.749	0.4274	0.02704	1.308	1.267	11.815	0.4480	0.08407
20	-2.944	-3.530	-10.664	0.4253	0.02710	1.152	1.111	11.292	0.4467	0.08410
25	-2.823	-3.369	-10.455	0.4212	0.02719	0.960	0.923	10.566	0.4454	0.08413
30	-2.631	-3.112	-10.233	0.4154	0.02734	0.673	0.670	9.477	0.4446	0.08419
35	-2.336	-2.792	-9.948	0.4076	0.02753	0.304	0.307	7.816	0.4464	0.08432
40	-1.821	-2.295	-9.472	0.3962	0.02781	-2.576	-2.553	-4.814	0.5225	0.08375
45	-0.845	-1.297	-8.604	0.3795	0.02821	-2.796	-2.800	-4.623	0.5355	0.08342
50	1.421	0.948	8.824	0.3683	0.02847	-2.652	-2.714	-4.515	0.5393	0.08323
55	3.697	2.920	13.773	0.3928	0.02796	-2.510	-2.614	-4.436	0.5417	0.08307
60	4.352	3.423	15.060	0.4014	0.02775	-2.403	-2.547	-4.355	0.5446	0.08289
65	4.626	3.591	15.443	0.4042	0.02769	-2.266	-2.464	-4.225	0.5473	0.08271
70	4.727	3.639	15.473	0.4056	0.02770	-2.093	-2.346	-4.218	0.5475	0.08253
75	4.790	3.669	15.469	0.4066	0.02775	-1.986	-2.289	-4.245	0.5477	0.08238
80	4.828	3.682	15.408	0.4071	0.02780	-1.887	-2.255	-4.278	0.5478	0.08226
85	4.847	3.699	15.332	0.4074	0.02783	-1.813	-2.222	-4.347	0.5476	0.08215
90	4.813	3.680	15.186	0.4075	0.02783	-1.717	-2.164	-4.414	0.5466	0.08206
95	4.736	3.613	14.968	0.4071	0.02781	-1.668	-2.141	-4.486	0.5449	0.08200
100	4.624	3.525	14.728	0.4067	0.02778	-1.672	-2.132	-4.604	0.5423	0.08193
105	4.443	3.408	14.447	0.4060	0.02775	-1.672	-2.076	-4.719	0.5384	0.08189
110	4.198	3.248	14.087	0.4046	0.02774	-1.680	-1.989	-4.805	0.5332	0.08189
115	3.828	2.980	13.532	0.4018	0.02778	-1.728	-1.903	-4.917	0.5259	0.08198
120	3.394	2.675	12.886	0.3991	0.02782	-1.727	-1.790	-5.083	0.5165	0.08216
125	2.875	2.281	12.071	0.3938	0.02791	-1.584	-1.565	-5.349	0.5036	0.08245
130	2.134	1.678	10.769	0.3863	0.02803	-1.246	-1.170	-5.710	0.4855	0.08289
135	0.935	0.603	8.345	0.3768	0.02820	-0.728	-0.646	-6.062	0.4670	0.08347
140	-0.599	-0.837	-8.473	0.3856	0.02800	-0.029	-0.029	-6.187	0.4521	0.08415
145	-1.589	-1.758	-9.032	0.3990	0.02774	0.481	0.450	7.991	0.4452	0.08437
150	-2.200	-2.360	-9.457	0.4096	0.02750	0.781	0.749	9.290	0.4438	0.08440
155	-2.596	-2.778	-9.815	0.4168	0.02734	1.027	0.989	10.287	0.4446	0.08436
160	-2.850	-3.079	-10.092	0.4224	0.02722	1.249	1.196	11.084	0.4460	0.08430
165	-3.022	-3.312	-10.396	0.4258	0.02713	1.380	1.331	11.674	0.4477	0.08422
170	-3.105	-3.484	-10.594	0.4276	0.02706	1.463	1.416	12.057	0.4492	0.08414
175	-3.104	-3.593	-10.652	0.4291	0.02702	1.499	1.454	12.271	0.4504	0.08406
180	-3.071	-3.662	-10.664	0.4297	0.02700	1.513	1.456	12.372	0.4511	0.08399
Cycle A										
	Natural state					Reduced state				
RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-7.789	-10.257	-18.544	0.9415	0.00424	-5.631	-7.995	-25.417	0.9661	0.00429
5	-7.786	-10.258	-18.516	0.9418	0.00422	-5.651	-8.005	-25.300	0.9662	0.00422
10	-7.785	-10.260	-18.492	0.9419	0.00420	-5.686	-8.034	-24.921	0.9660	0.00415

15	-7.756	-10.237	-18.446	0.9426	0.00419	-5.766	-8.137	-24.287	0.9657	0.00422
20	-7.691	-10.193	-18.405	0.9431	0.00419	-5.876	-8.272	-23.390	0.9651	0.00428
25	-7.573	-10.113	-18.330	0.9437	0.00418	-6.001	-8.332	-22.182	0.9645	0.00422
30	-7.439	-10.017	-18.254	0.9445	0.00419	-6.191	-8.441	-20.686	0.9642	0.00411
35	-7.280	-9.893	-18.115	0.9456	0.00421	-6.552	-8.816	-18.797	0.9637	0.00406
40	-7.065	-9.715	-17.813	0.9469	0.00423	-7.372	-9.616	-13.362	0.9492	0.00483
45	-6.681	-9.388	-17.192	0.9488	0.00424	-7.478	-9.696	-12.944	0.9450	0.00514
50	-5.779	-8.627	-15.788	0.9521	0.00416	-7.507	-9.697	-14.045	0.9441	0.00523
55	-5.044	-7.980	-14.551	0.9532	0.00412	-7.556	-9.714	-14.984	0.9436	0.00524
60	-4.887	-7.837	-13.798	0.9543	0.00419	-7.590	-9.740	-15.813	0.9434	0.00529
65	-4.817	-7.782	-13.307	0.9555	0.00418	-7.602	-9.760	-16.530	0.9434	0.00528
70	-4.778	-7.764	-13.021	0.9566	0.00411	-7.597	-9.757	-16.891	0.9440	0.00519
75	-4.708	-7.744	-12.792	0.9576	0.00403	-7.577	-9.741	-17.230	0.9447	0.00529
80	-4.638	-7.697	-12.523	0.9584	0.00404	-7.576	-9.732	-17.438	0.9455	0.00538
85	-4.605	-7.674	-12.302	0.9589	0.00411	-7.631	-9.757	-17.549	0.9460	0.00533
90	-4.624	-7.690	-12.125	0.9590	0.00416	-7.677	-9.811	-17.544	0.9467	0.00521
95	-4.669	-7.731	-11.962	0.9590	0.00418	-7.647	-9.785	-17.344	0.9472	0.00519
100	-4.710	-7.771	-11.789	0.9590	0.00416	-7.583	-9.713	-16.914	0.9478	0.00523
105	-4.759	-7.816	-11.666	0.9588	0.00411	-7.508	-9.668	-16.251	0.9486	0.00522
110	-4.828	-7.879	-11.638	0.9583	0.00406	-7.453	-9.664	-15.426	0.9493	0.00511
115	-4.918	-7.949	-11.691	0.9577	0.00402	-7.422	-9.704	-14.403	0.9504	0.00496
120	-5.053	-8.065	-11.980	0.9568	0.00401	-7.352	-9.633	-13.235	0.9516	0.00486
125	-5.211	-8.200	-12.461	0.9561	0.00402	-7.294	-9.534	-11.877	0.9536	0.00467
130	-5.461	-8.406	-13.207	0.9552	0.00406	-7.237	-9.447	-10.138	0.9562	0.00441
135	-5.953	-8.780	-14.753	0.9532	0.00418	-7.085	-9.310	-12.383	0.9597	0.00420
140	-6.632	-9.308	-16.931	0.9485	0.00430	-6.832	-9.119	-15.016	0.9635	0.00405
145	-6.995	-9.617	-17.877	0.9456	0.00433	-6.544	-8.870	-17.034	0.9650	0.00402
150	-7.237	-9.817	-18.311	0.9438	0.00434	-6.242	-8.581	-18.820	0.9656	0.00403
155	-7.420	-9.963	-18.479	0.9428	0.00434	-6.025	-8.361	-20.402	0.9659	0.00407
160	-7.559	-10.070	-18.556	0.9421	0.00433	-5.870	-8.246	-21.766	0.9661	0.00417
165	-7.684	-10.162	-18.616	0.9417	0.00431	-5.723	-8.142	-22.908	0.9662	0.00423
170	-7.761	-10.222	-18.594	0.9415	0.00428	-5.631	-8.064	-23.862	0.9663	0.00421
175	-7.793	-10.252	-18.571	0.9414	0.00426	-5.591	-7.990	-24.587	0.9662	0.00416
180	-7.795	-10.262	-18.552	0.9414	0.00423	-5.594	-7.964	-25.077	0.9660	0.00423

Cycle B

	Natural state					Reduced state				
RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-3.465	-4.785	-7.296	0.3094	0.04383	-1.548	-2.615	-3.907	0.2651	0.04351
5	-3.489	-4.832	-7.416	0.3067	0.04390	-1.611	-2.653	-3.876	0.2692	0.04328
10	-3.521	-4.858	-7.434	0.3042	0.04397	-1.688	-2.703	-3.828	0.2729	0.04306
15	-3.537	-4.870	-7.432	0.3005	0.04408	-1.790	-2.756	-3.752	0.2765	0.04285
20	-3.551	-4.872	-7.424	0.2975	0.04418	-1.932	-2.841	-3.711	0.2802	0.04265
25	-3.549	-4.857	-7.386	0.2939	0.04429	-2.104	-2.963	-3.707	0.2836	0.04249
30	-3.519	-4.824	-7.345	0.2897	0.04444	-2.325	-3.153	-3.761	0.2867	0.04239
35	-3.464	-4.777	-7.278	0.2855	0.04460	-2.607	-3.438	-4.375	0.2903	0.04238
40	-3.375	-4.695	-7.148	0.2812	0.04477	-4.765	-5.348	-9.584	0.3210	0.04157
45	-3.162	-4.498	-6.625	0.2770	0.04493	-4.956	-5.613	-10.100	0.3237	0.04181
50	-2.494	-3.917	-5.035	0.2725	0.04504	-4.902	-5.626	-9.873	0.3227	0.04214
55	-1.776	-3.243	-3.819	0.2760	0.04496	-4.863	-5.607	-9.591	0.3219	0.04233
60	-1.614	-3.037	-4.061	0.2797	0.04483	-4.857	-5.609	-9.406	0.3214	0.04244
65	-1.566	-3.092	-3.907	0.2803	0.04483	-4.856	-5.616	-9.280	0.3202	0.04251
70	-1.524	-3.003	-3.932	0.2787	0.04493	-4.769	-5.552	-8.959	0.3183	0.04263

75	-1.485	-3.069	-3.639	0.2763	0.04507	-4.694	-5.505	-8.722	0.3156	0.04276
80	-1.456	-2.970	-3.633	0.2734	0.04523	-4.612	-5.453	-8.497	0.3125	0.04292
85	-1.455	-2.967	-3.448	0.2709	0.04537	-4.526	-5.411	-8.340	0.3085	0.04309
90	-1.492	-3.068	-3.380	0.2685	0.04550	-4.438	-5.373	-8.221	0.3038	0.04328
95	-1.540	-3.102	-3.452	0.2668	0.04558	-4.346	-5.339	-8.172	0.2979	0.04350
100	-1.575	-3.062	-3.277	0.2661	0.04564	-4.265	-5.302	-8.182	0.2913	0.04372
105	-1.603	-3.153	-3.566	0.2662	0.04567	-4.205	-5.262	-8.202	0.2836	0.04395
110	-1.636	-3.182	-3.721	0.2671	0.04568	-4.146	-5.209	-8.146	0.2751	0.04420
115	-1.695	-3.228	-3.941	0.2687	0.04565	-4.032	-5.104	-7.909	0.2650	0.04450
120	-1.772	-3.283	-4.171	0.2709	0.04559	-3.859	-4.951	-7.529	0.2537	0.04482
125	-1.874	-3.379	-4.498	0.2740	0.04548	-3.583	-4.713	-6.872	0.2404	0.04521
130	-2.056	-3.477	-4.696	0.2783	0.04531	-3.131	-4.307	-5.618	0.2256	0.04563
135	-2.335	-3.777	-5.352	0.2858	0.04502	-2.644	-3.847	-4.295	0.2139	0.04582
140	-2.775	-4.171	-6.190	0.3005	0.04451	-2.228	-3.418	-4.267	0.2085	0.04579
145	-3.043	-4.397	-6.729	0.3085	0.04421	-1.911	-3.094	-4.335	0.2137	0.04559
150	-3.201	-4.533	-7.042	0.3128	0.04402	-1.721	-2.896	-4.380	0.2221	0.04533
155	-3.296	-4.616	-7.209	0.3147	0.04391	-1.597	-2.760	-4.395	0.2309	0.04502
160	-3.359	-4.673	-7.310	0.3154	0.04383	-1.529	-2.675	-4.418	0.2393	0.04470
165	-3.402	-4.719	-7.369	0.3151	0.04378	-1.522	-2.640	-4.422	0.2471	0.04437
170	-3.423	-4.753	-7.386	0.3141	0.04376	-1.549	-2.631	-4.359	0.2536	0.04407
175	-3.440	-4.779	-7.389	0.3126	0.04377	-1.581	-2.622	-4.294	0.2598	0.04376
180	-3.461	-4.804	-7.390	0.3105	0.04380	-1.620	-2.622	-4.211	0.2653	0.04348

Cycle C

	Natural state					Reduced state				
RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-1.036	-5.284	-7.577	0.1868	0.03692	-8.284	-7.257	-9.751	0.8956	0.01417
5	-1.075	-5.297	-7.798	0.1823	0.03728	-8.271	-7.244	-10.126	0.8944	0.01427
10	-1.080	-5.313	-8.020	0.1782	0.03765	-8.270	-7.234	-10.470	0.8932	0.01439
15	-1.073	-5.324	-8.213	0.1694	0.03811	-8.280	-7.230	-10.747	0.8920	0.01453
20	-1.046	-5.329	-8.385	0.1613	0.03852	-8.325	-7.247	-10.965	0.8910	0.01467
25	-1.015	-5.313	-8.463	0.1501	0.03897	-8.418	-7.301	-11.102	0.8903	0.01480
30	-0.983	-5.282	-8.477	0.1360	0.03948	-8.599	-7.428	-11.056	0.8902	0.01489
35	-0.879	-5.245	-8.449	0.1191	0.04007	-8.968	-7.702	-10.599	0.8916	0.01488
40	-0.739	-5.112	-8.155	0.0974	0.04080	-11.335	-9.394	-17.832	0.8980	0.01461
45	-0.563	-4.942	-7.419	0.0664	0.04172	-11.545	-9.576	-18.448	0.9004	0.01453
50	-0.335	-4.761	-5.948	0.0383	0.04208	-11.529	-9.582	-18.177	0.9021	0.01446
55	-0.382	-4.910	-7.307	0.0648	0.04111	-11.505	-9.579	-17.761	0.9030	0.01445
60	-0.517	-4.966	-7.376	0.0818	0.04054	-11.505	-9.587	-17.339	0.9034	0.01447
65	-0.490	-4.953	-7.171	0.0914	0.04022	-11.527	-9.607	-16.924	0.9036	0.01450
70	-0.413	-4.934	-6.911	0.0988	0.03996	-11.517	-9.601	-16.253	0.9038	0.01453
75	-0.335	-4.927	-6.683	0.1066	0.03970	-11.545	-9.625	-15.694	0.9040	0.01456
80	-0.287	-4.917	-6.443	0.1135	0.03946	-11.569	-9.644	-15.147	0.9043	0.01458
85	-0.311	-4.903	-6.225	0.1207	0.03918	-11.576	-9.650	-14.619	0.9045	0.01460
90	-0.357	-4.885	-6.061	0.1286	0.03885	-11.556	-9.637	-14.095	0.9046	0.01462
95	-0.368	-4.845	-6.108	0.1363	0.03852	-11.540	-9.629	-13.641	0.9047	0.01465
100	-0.358	-4.718	-6.230	0.1440	0.03818	-11.515	-9.607	-13.196	0.9046	0.01468
105	-0.343	-4.725	-6.206	0.1511	0.03787	-11.474	-9.569	-12.775	0.9045	0.01469
110	-0.319	-4.659	-6.203	0.1579	0.03759	-11.422	-9.529	-12.400	0.9043	0.01467
115	-0.284	-4.609	-6.196	0.1635	0.03735	-11.342	-9.476	-12.564	0.9040	0.01462
120	-0.282	-4.575	-6.172	0.1682	0.03715	-11.234	-9.403	-12.627	0.9039	0.01453
125	-0.273	-4.567	-6.146	0.1712	0.03701	-11.050	-9.282	-12.463	0.9039	0.01440
130	-0.283	-4.572	-6.083	0.1720	0.03692	-10.740	-9.075	-11.875	0.9040	0.01420

135	-0.366	-4.618	-6.016	0.1712	0.03689	-10.354	-8.786	-10.814	0.9038	0.01399
140	-0.559	-4.734	-6.374	0.1773	0.03673	-9.923	-8.452	-9.627	0.9033	0.01384
145	-0.676	-4.818	-6.587	0.1848	0.03652	-9.488	-8.130	-9.026	0.9026	0.01378
150	-0.776	-4.880	-6.693	0.1901	0.03637	-9.163	-7.887	-8.859	0.9017	0.01377
155	-0.869	-4.955	-6.758	0.1936	0.03628	-8.878	-7.675	-8.927	0.9009	0.01380
160	-0.931	-5.048	-6.788	0.1952	0.03625	-8.694	-7.538	-9.142	0.8998	0.01386
165	-0.953	-5.135	-6.970	0.1955	0.03628	-8.547	-7.424	-9.466	0.8988	0.01393
170	-0.964	-5.199	-7.182	0.1940	0.03639	-8.403	-7.316	-9.837	0.8979	0.01401
175	-0.997	-5.246	-7.358	0.1911	0.03659	-8.309	-7.239	-10.257	0.8968	0.01411
180	-1.023	-5.277	-7.536	0.1871	0.03688	-8.238	-7.175	-10.690	0.8958	0.01421

Cycle D

	Natural state					Reduced state				
RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-5.445	-8.587	-24.697	0.9477	0.00484	3.530	-0.899	-3.553	0.1175	0.03306
5	-5.465	-8.621	-24.540	0.9476	0.00478	3.522	-0.910	-3.547	0.1180	0.03304
10	-5.554	-8.740	-24.143	0.9473	0.00472	3.520	-0.928	-3.529	0.1186	0.03300
15	-5.651	-8.849	-23.546	0.9482	0.00474	3.498	-0.961	-3.504	0.1192	0.03297
20	-5.750	-8.901	-22.747	0.9490	0.00473	3.466	-1.010	-3.471	0.1199	0.03293
25	-5.792	-8.918	-21.715	0.9506	0.00461	3.399	-1.082	-3.433	0.1219	0.03287
30	-5.813	-8.945	-20.359	0.9527	0.00451	3.282	-1.193	-3.384	0.1261	0.03276
35	-5.906	-9.041	-18.748	0.9556	0.00437	3.044	-1.385	-3.318	0.1346	0.03253
40	-6.042	-9.116	-16.916	0.9593	0.00416	1.189	-2.863	-4.033	0.1931	0.03103
45	-6.065	-9.035	-14.530	0.9644	0.00384	1.029	-2.999	-4.480	0.1996	0.03086
50	-5.711	-8.584	-10.854	0.9676	0.00350	1.069	-2.969	-4.473	0.2025	0.03083
55	-5.174	-8.038	-10.204	0.9620	0.00380	1.112	-2.924	-4.432	0.2047	0.03083
60	-5.025	-7.834	-10.888	0.9606	0.00389	1.126	-2.891	-4.414	0.2070	0.03080
65	-4.901	-7.772	-11.438	0.9601	0.00391	1.108	-2.878	-4.440	0.2095	0.03076
70	-4.831	-7.765	-11.874	0.9601	0.00400	1.107	-2.837	-4.392	0.2098	0.03073
75	-4.787	-7.766	-12.190	0.9600	0.00408	1.084	-2.816	-4.383	0.2109	0.03068
80	-4.748	-7.755	-12.403	0.9599	0.00406	1.088	-2.784	-4.359	0.2116	0.03059
85	-4.712	-7.735	-12.511	0.9596	0.00397	1.115	-2.742	-4.318	0.2125	0.03050
90	-4.696	-7.729	-12.474	0.9594	0.00402	1.160	-2.696	-4.252	0.2126	0.03043
95	-4.704	-7.744	-12.222	0.9591	0.00415	1.216	-2.662	-4.168	0.2120	0.03043
100	-4.719	-7.775	-11.859	0.9590	0.00417	1.283	-2.627	-4.032	0.2112	0.03047
105	-4.723	-7.806	-11.360	0.9588	0.00405	1.348	-2.591	-3.875	0.2098	0.03053
110	-4.757	-7.839	-10.703	0.9589	0.00399	1.424	-2.552	-3.707	0.2078	0.03059
115	-4.798	-7.873	-9.829	0.9592	0.00403	1.532	-2.503	-3.523	0.2047	0.03067
120	-4.860	-7.986	-8.858	0.9601	0.00400	1.634	-2.452	-3.289	0.1997	0.03078
125	-4.949	-8.109	-9.960	0.9615	0.00389	1.796	-2.347	-2.979	0.1915	0.03097
130	-5.122	-8.294	-12.172	0.9636	0.00377	2.021	-2.167	-3.087	0.1779	0.03125
135	-5.480	-8.688	-14.733	0.9666	0.00362	2.314	-1.914	-3.195	0.1605	0.03170
140	-5.772	-9.003	-17.233	0.9649	0.00379	2.651	-1.629	-3.301	0.1455	0.03225
145	-5.715	-8.935	-18.945	0.9607	0.00403	2.956	-1.376	-3.371	0.1344	0.03260
150	-5.655	-8.836	-20.365	0.9569	0.00414	3.153	-1.223	-3.452	0.1276	0.03280
155	-5.633	-8.833	-21.605	0.9539	0.00434	3.282	-1.111	-3.499	0.1233	0.03291
160	-5.646	-8.878	-22.699	0.9515	0.00456	3.375	-1.026	-3.519	0.1206	0.03298
165	-5.626	-8.820	-23.576	0.9498	0.00462	3.448	-0.964	-3.531	0.1189	0.03301
170	-5.571	-8.714	-24.205	0.9486	0.00460	3.517	-0.920	-3.522	0.1183	0.03300
175	-5.502	-8.641	-24.588	0.9479	0.00472	3.577	-0.889	-3.495	0.1176	0.03300
180	-5.442	-8.581	-24.706	0.9476	0.00483	3.630	-0.870	-3.460	0.1171	0.03300

Cycle E

	Natural state					Reduced state				

RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-3.293	-4.723	-7.516	0.3289	0.04381	-8.284	-7.257	-9.755	0.8956	0.01417
5	-3.299	-4.719	-7.648	0.3323	0.04366	-8.327	-7.290	-9.458	0.8968	0.01408
10	-3.314	-4.707	-7.744	0.3350	0.04353	-8.403	-7.349	-9.186	0.8980	0.01401
15	-3.330	-4.684	-7.822	0.3361	0.04344	-8.548	-7.445	-8.917	0.8991	0.01394
20	-3.339	-4.663	-7.889	0.3369	0.04338	-8.692	-7.555	-8.720	0.9003	0.01388
25	-3.314	-4.619	-7.885	0.3368	0.04334	-8.889	-7.697	-8.504	0.9014	0.01383
30	-3.263	-4.549	-7.819	0.3357	0.04333	-9.148	-7.886	-8.652	0.9024	0.01380
35	-3.207	-4.472	-7.708	0.3337	0.04333	-9.514	-8.153	-9.770	0.9031	0.01381
40	-3.123	-4.372	-7.480	0.3302	0.04336	-11.848	-9.957	-19.331	0.9008	0.01455
45	-2.930	-4.185	-6.914	0.3247	0.04343	-12.077	-10.157	-19.955	0.9008	0.01463
50	-2.382	-3.615	-5.057	0.3147	0.04365	-12.045	-10.129	-19.512	0.9011	0.01466
55	-1.847	-3.134	-3.390	0.3088	0.04388	-12.010	-10.095	-19.035	0.9015	0.01469
60	-1.691	-3.038	-3.567	0.3054	0.04392	-11.997	-10.074	-18.661	0.9018	0.01472
65	-1.632	-3.025	-3.631	0.3018	0.04404	-11.984	-10.051	-18.368	0.9022	0.01473
70	-1.594	-3.026	-3.604	0.2976	0.04423	-11.909	-9.979	-17.793	0.9030	0.01472
75	-1.564	-3.029	-3.529	0.2928	0.04445	-11.836	-9.906	-17.303	0.9035	0.01470
80	-1.551	-3.041	-3.411	0.2880	0.04469	-11.746	-9.821	-16.826	0.9039	0.01469
85	-1.549	-3.059	-3.260	0.2833	0.04492	-11.627	-9.709	-16.420	0.9042	0.01468
90	-1.550	-3.077	-3.311	0.2782	0.04516	-11.495	-9.585	-16.062	0.9045	0.01468
95	-1.559	-3.102	-3.405	0.2727	0.04538	-11.378	-9.475	-15.854	0.9046	0.01467
100	-1.576	-3.129	-3.506	0.2675	0.04560	-11.263	-9.371	-15.715	0.9048	0.01464
105	-1.604	-3.097	-3.359	0.2620	0.04581	-11.135	-9.260	-15.622	0.9049	0.01460
110	-1.628	-3.134	-3.453	0.2562	0.04602	-11.001	-9.148	-15.587	0.9049	0.01456
115	-1.642	-3.136	-3.602	0.2498	0.04623	-10.855	-9.036	-15.551	0.9050	0.01451
120	-1.646	-3.200	-4.041	0.2424	0.04643	-10.686	-8.903	-15.434	0.9051	0.01446
125	-1.728	-3.207	-4.085	0.2339	0.04662	-10.445	-8.723	-15.109	0.9052	0.01440
130	-1.860	-3.309	-4.315	0.2249	0.04677	-10.102	-8.490	-14.463	0.9048	0.01436
135	-2.077	-3.484	-4.529	0.2208	0.04675	-9.759	-8.268	-13.630	0.9013	0.01449
140	-2.467	-3.895	-4.964	0.2417	0.04626	-9.287	-7.935	-12.249	0.8936	0.01481
145	-2.796	-4.218	-5.431	0.2647	0.04572	-8.865	-7.638	-10.932	0.8910	0.01486
150	-3.006	-4.438	-5.859	0.2830	0.04529	-8.571	-7.431	-10.003	0.8903	0.01481
155	-3.128	-4.569	-6.231	0.2962	0.04495	-8.382	-7.294	-9.332	0.8904	0.01473
160	-3.238	-4.627	-6.587	0.3065	0.04466	-8.267	-7.214	-9.170	0.8909	0.01464
165	-3.283	-4.672	-6.873	0.3141	0.04442	-8.195	-7.167	-9.127	0.8918	0.01454
170	-3.284	-4.710	-7.090	0.3199	0.04420	-8.170	-7.151	-9.011	0.8930	0.01445
175	-3.290	-4.715	-7.278	0.3247	0.04401	-8.167	-7.146	-8.840	0.8944	0.01435
180	-3.293	-4.709	-7.441	0.3283	0.04384	-8.191	-7.157	-8.663	0.8957	0.01427

Cycle F

	Natural state					Reduced state				
RD(°)	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU	NICS(0)	NICS(1)	$NICS(1)_{zz}$	HOMA	FLU
0	-1.050	-5.086	-6.913	0.1790	0.03648	-1.549	-2.726	-3.741	0.2652	0.04350
5	-1.017	-5.053	-6.879	0.1810	0.03645	-1.500	-2.726	-3.772	0.2603	0.04375
10	-0.998	-5.019	-6.851	0.1829	0.03644	-1.465	-2.738	-3.805	0.2550	0.04401
15	-0.982	-4.984	-6.811	0.1834	0.03648	-1.464	-2.762	-3.854	0.2489	0.04427
20	-0.974	-4.955	-6.775	0.1841	0.03652	-1.483	-2.811	-3.870	0.2427	0.04455
25	-0.965	-4.928	-6.734	0.1837	0.03659	-1.531	-2.892	-3.860	0.2353	0.04485
30	-0.952	-4.902	-6.676	0.1828	0.03667	-1.630	-3.013	-3.802	0.2265	0.04517
35	-0.928	-4.878	-6.620	0.1814	0.03675	-1.870	-3.279	-3.616	0.2159	0.04554
40	-0.863	-4.833	-6.517	0.1783	0.03687	-4.290	-5.347	-10.578	0.2473	0.04450
45	-0.703	-4.735	-6.366	0.1730	0.03705	-4.711	-5.631	-11.392	0.2610	0.04412
50	-0.422	-4.615	-6.525	0.1606	0.03741	-4.715	-5.620	-11.314	0.2655	0.04398

55	-0.434	-4.638	-6.966	0.1496	0.03783	-4.687	-5.600	-11.158	0.2693	0.04389
60	-0.442	-4.658	-7.008	0.1412	0.03816	-4.682	-5.604	-11.045	0.2742	0.04378
65	-0.417	-4.682	-6.940	0.1364	0.03835	-4.690	-5.621	-10.935	0.2796	0.04367
70	-0.375	-4.705	-6.786	0.1344	0.03846	-4.619	-5.582	-10.576	0.2836	0.04366
75	-0.333	-4.722	-6.585	0.1346	0.03851	-4.564	-5.556	-10.242	0.2879	0.04363
80	-0.296	-4.725	-6.360	0.1362	0.03850	-4.512	-5.534	-9.936	0.2933	0.04356
85	-0.278	-4.721	-6.141	0.1383	0.03845	-4.449	-5.504	-9.619	0.2990	0.04346
90	-0.286	-4.719	-5.939	0.1408	0.03835	-4.399	-5.464	-9.309	0.3041	0.04335
95	-0.316	-4.718	-6.022	0.1429	0.03825	-4.386	-5.429	-9.084	0.3090	0.04322
100	-0.350	-4.708	-6.208	0.1450	0.03814	-4.355	-5.373	-8.872	0.3132	0.04308
105	-0.380	-4.696	-6.389	0.1468	0.03804	-4.295	-5.296	-8.639	0.3166	0.04296
110	-0.405	-4.691	-6.553	0.1486	0.03797	-4.210	-5.211	-8.426	0.3187	0.04291
115	-0.392	-4.694	-6.696	0.1496	0.03793	-4.093	-5.108	-8.180	0.3191	0.04293
120	-0.410	-4.702	-6.775	0.1506	0.03790	-3.918	-4.973	-7.905	0.3181	0.04300
125	-0.463	-4.734	-6.829	0.1497	0.03790	-3.648	-4.761	-7.450	0.3147	0.04312
130	-0.540	-4.803	-6.826	0.1477	0.03787	-3.249	-4.432	-6.709	0.3082	0.04325
135	-0.620	-4.913	-6.633	0.1460	0.03778	-2.934	-4.107	-6.037	0.3007	0.04300
140	-0.846	-5.041	-6.679	0.1491	0.03761	-2.845	-3.806	-5.610	0.2926	0.04245
145	-0.984	-5.087	-6.906	0.1536	0.03738	-2.533	-3.466	-4.766	0.2870	0.04240
150	-1.053	-5.110	-6.980	0.1585	0.03716	-2.298	-3.242	-4.130	0.2834	0.04246
155	-1.090	-5.126	-6.974	0.1628	0.03699	-2.104	-3.084	-3.639	0.2807	0.04256
160	-1.107	-5.132	-6.951	0.1668	0.03685	-1.920	-2.955	-3.226	0.2778	0.04270
165	-1.111	-5.132	-6.955	0.1701	0.03675	-1.779	-2.866	-3.117	0.2751	0.04287
170	-1.109	-5.133	-6.947	0.1733	0.03665	-1.672	-2.813	-3.200	0.2721	0.04307
175	-1.085	-5.118	-6.927	0.1761	0.03657	-1.564	-2.776	-3.278	0.2687	0.04329
180	-1.053	-5.093	-6.902	0.1785	0.03651	-1.481	-2.746	-3.347	0.2652	0.04352

4. The ITA quantities of two porphyrinoids

Table S4. The ITA quantities of two porphyrinoids, both global and local descriptors are given. For the small rings. For the global quantities, the average values of four own the best correlation with conventional aromaticity indexes, for the local, the averaged values of carbons carried hydrogen own the best correlation with conventional aromaticity indexes, and collected here.

Natural state								
Averaged values of four nitrogens of natural state								
RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	3.59159	337.63706	46.04461	0.20962	52.25387	2993.21587	7.41909	7.77912
5	3.59098	337.63747	46.04377	0.20947	52.25423	2993.26501	7.41878	7.77863
10	3.59084	337.63906	46.04330	0.20938	52.25428	2993.26962	7.41859	7.77836
15	3.59329	337.64628	46.04468	0.20950	52.25404	2993.27729	7.41886	7.77895
20	3.59693	337.65597	46.04702	0.20975	52.25377	2993.30121	7.41938	7.78003
25	3.60182	337.66814	46.05046	0.21014	52.25328	2993.30432	7.42017	7.78162
30	3.60917	337.68565	46.05572	0.21075	52.25247	2993.30319	7.42144	7.78412
35	3.61834	337.70599	46.06252	0.21154	52.25137	2993.28575	7.42308	7.78731
40	3.62931	337.72921	46.07084	0.21252	52.25001	2993.25434	7.42510	7.79121
45	3.64593	337.76196	46.08367	0.21406	52.24747	2993.13172	7.42826	7.79722
50	3.67946	337.82453	46.10830	0.21712	52.24152	2992.82515	7.43454	7.80910
55	3.70177	337.86695	46.12315	0.21912	52.23718	2992.62578	7.43864	7.81720
60	3.70113	337.86379	46.12228	0.21901	52.23692	2992.58536	7.43842	7.81682

Comment [MAG]: Clarify, this is not understandable !!

the average values of four own the best correlation with conventional aromaticity indexes,

you mean the average values of the four nitrogen atoms in the macrocycle

for the local, I don´t know what you mean

Comment [□]: The local ITA quantities refer to the averaged values of carbons carried hydrogen. This is also the mathematical reasons, this average values could obtain the best correlation.

65	3.69878	337.85997	46.12046	0.21874	52.23741	2992.61376	7.43789	7.81589
70	3.69708	337.85937	46.11912	0.21854	52.23774	2992.63349	7.43751	7.81527
75	3.69616	337.86127	46.11818	0.21841	52.23791	2992.65336	7.43726	7.81492
80	3.69527	337.86376	46.11723	0.21830	52.23815	2992.68916	7.43702	7.81457
85	3.69394	337.86499	46.11599	0.21815	52.23839	2992.71514	7.43672	7.81406
90	3.69224	337.86494	46.11452	0.21799	52.23883	2992.77190	7.43638	7.81344
95	3.69014	337.86388	46.11279	0.21780	52.23900	2992.76728	7.43598	7.81267
100	3.68769	337.86143	46.11088	0.21759	52.23940	2992.79581	7.43554	7.81177
105	3.68500	337.85816	46.10873	0.21735	52.23995	2992.85354	7.43502	7.81069
110	3.68212	337.85465	46.10636	0.21707	52.23999	2992.82033	7.43443	7.80945
115	3.67843	337.84872	46.10342	0.21670	52.24041	2992.83552	7.43365	7.80783
120	3.67495	337.84253	46.10047	0.21632	52.24077	2992.84968	7.43284	7.80611
125	3.67102	337.83381	46.09739	0.21588	52.24110	2992.83977	7.43193	7.80422
130	3.66508	337.81790	46.09312	0.21526	52.24161	2992.80495	7.43063	7.80154
135	3.65538	337.78826	46.08670	0.21435	52.24279	2992.79874	7.42876	7.79771
140	3.64522	337.75889	46.08141	0.21391	52.24476	2992.86682	7.42785	7.79574
145	3.63605	337.73706	46.07612	0.21346	52.24663	2992.95685	7.42693	7.79388
150	3.62688	337.71567	46.07026	0.21286	52.24836	2993.04530	7.42569	7.79147
155	3.61811	337.69508	46.06432	0.21218	52.24978	2993.08980	7.42429	7.78879
160	3.61042	337.67736	46.05891	0.21152	52.25102	2993.13533	7.42295	7.78623
165	3.60409	337.66295	46.05427	0.21093	52.25211	2993.19037	7.42175	7.78400
170	3.59800	337.64956	46.04988	0.21036	52.25293	2993.18989	7.42058	7.78181
175	3.59399	337.64125	46.04681	0.20994	52.25349	2993.20092	7.41973	7.78026
180	3.59149	337.63678	46.04466	0.20963	52.25393	2993.21898	7.41911	7.77915

Cycle A of natural state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.80541	245.55224	39.14056	0.09186	31.52509	1121.00207	6.18522	6.47929
5	4.80571	245.55172	39.14131	0.09198	31.52513	1121.00765	6.18546	6.47965
10	4.80597	245.55054	39.14221	0.09212	31.52520	1121.01733	6.18576	6.48008
15	4.80590	245.54895	39.14294	0.09226	31.52532	1121.02505	6.18605	6.48048
20	4.80575	245.54707	39.14362	0.09240	31.52546	1121.03512	6.18633	6.48090
25	4.80536	245.54481	39.14421	0.09255	31.52559	1121.03975	6.18663	6.48134
30	4.80451	245.54227	39.14436	0.09265	31.52576	1121.03926	6.18685	6.48171
35	4.80331	245.54014	39.14406	0.09272	31.52592	1121.02983	6.18697	6.48198
40	4.80170	245.53816	39.14313	0.09271	31.52595	1120.99731	6.18693	6.48205
45	4.79951	245.53749	39.14084	0.09251	31.52599	1120.96602	6.18649	6.48155
50	4.79701	245.54106	39.13636	0.09192	31.52654	1121.01382	6.18521	6.47977
55	4.79586	245.54143	39.13445	0.09169	31.52630	1120.96738	6.18465	6.47887
60	4.79351	245.53386	39.13323	0.09176	31.52658	1121.02063	6.18475	6.47904
65	4.79073	245.52658	39.13175	0.09184	31.52649	1120.99507	6.18490	6.47939
70	4.78855	245.52113	39.13069	0.09194	31.52631	1120.95428	6.18507	6.47979
75	4.78711	245.51773	39.13004	0.09201	31.52650	1120.97161	6.18521	6.48012
80	4.78606	245.51605	39.12954	0.09205	31.52670	1120.99463	6.18529	6.48035
85	4.78548	245.51544	39.12923	0.09206	31.52661	1120.97644	6.18531	6.48049
90	4.78535	245.51605	39.12905	0.09204	31.52678	1120.99519	6.18528	6.48051
95	4.78555	245.51772	39.12901	0.09200	31.52662	1120.97455	6.18520	6.48044

100	4.78607	245.52002	39.12912	0.09194	31.52662	1120.97844	6.18510	6.48029
105	4.78701	245.52313	39.12946	0.09187	31.52668	1120.98885	6.18497	6.48008
110	4.78842	245.52727	39.13006	0.09179	31.52668	1120.99795	6.18484	6.47984
115	4.79000	245.53120	39.13084	0.09172	31.52658	1120.99192	6.18472	6.47959
120	4.79198	245.53575	39.13187	0.09165	31.52665	1121.01809	6.18461	6.47932
125	4.79393	245.53952	39.13292	0.09159	31.52658	1121.02367	6.18451	6.47906
130	4.79568	245.54224	39.13389	0.09154	31.52652	1121.02994	6.18444	6.47880
135	4.79752	245.54448	39.13498	0.09154	31.52608	1120.98014	6.18449	6.47865
140	4.79906	245.54592	39.13587	0.09155	31.52619	1121.01372	6.18455	6.47862
145	4.80007	245.54699	39.13648	0.09156	31.52589	1120.98833	6.18458	6.47861
150	4.80103	245.54797	39.13702	0.09156	31.52572	1120.98524	6.18461	6.47858
155	4.80192	245.54885	39.13753	0.09157	31.52559	1120.99001	6.18464	6.47856
160	4.80278	245.54978	39.13801	0.09158	31.52551	1121.00491	6.18466	6.47853
165	4.80358	245.55085	39.13854	0.09161	31.52545	1121.02255	6.18472	6.47859
170	4.80430	245.55090	39.13918	0.09168	31.52533	1121.02915	6.18486	6.47876
175	4.80490	245.55176	39.13984	0.09176	31.52515	1121.00883	6.18502	6.47899
180	4.80544	245.55191	39.14061	0.09187	31.52507	1121.00310	6.18524	6.47931

Cycle B of natural state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.81972	245.72343	39.14924	0.09390	31.53336	1121.26799	6.18894	6.50258
5	4.81969	245.72247	39.14977	0.09399	31.53375	1121.31466	6.18912	6.50282
10	4.81956	245.72168	39.15025	0.09407	31.53376	1121.29893	6.18928	6.50303
15	4.81907	245.72048	39.15057	0.09415	31.53389	1121.29149	6.18944	6.50324
20	4.81845	245.71917	39.15079	0.09421	31.53444	1121.35341	6.18956	6.50342
25	4.81778	245.71828	39.15088	0.09426	31.53459	1121.34459	6.18966	6.50357
30	4.81681	245.71722	39.15072	0.09428	31.53475	1121.33311	6.18970	6.50364
35	4.81563	245.71608	39.15029	0.09427	31.53528	1121.37531	6.18968	6.50363
40	4.81421	245.71529	39.14944	0.09421	31.53555	1121.37921	6.18954	6.50345
45	4.81200	245.71447	39.14757	0.09402	31.53569	1121.34484	6.18914	6.50290
50	4.80722	245.71168	39.14350	0.09362	31.53640	1121.36245	6.18825	6.50147
55	4.80451	245.70806	39.14231	0.09353	31.53688	1121.36827	6.18805	6.50089
60	4.80522	245.70913	39.14211	0.09346	31.53704	1121.43257	6.18790	6.50062
65	4.80604	245.71112	39.14154	0.09333	31.53686	1121.44821	6.18764	6.50027
70	4.80656	245.71297	39.14093	0.09321	31.53615	1121.36605	6.18740	6.49999
75	4.80675	245.71412	39.14044	0.09312	31.53611	1121.37329	6.18723	6.49982
80	4.80680	245.71494	39.14001	0.09306	31.53615	1121.39165	6.18709	6.49969
85	4.80684	245.71565	39.13969	0.09301	31.53577	1121.33460	6.18699	6.49960
90	4.80682	245.71618	39.13939	0.09296	31.53582	1121.34504	6.18690	6.49949
95	4.80685	245.71633	39.13914	0.09292	31.53631	1121.43240	6.18682	6.49940
100	4.80698	245.71724	39.13892	0.09288	31.53607	1121.40074	6.18673	6.49928
105	4.80719	245.71809	39.13876	0.09284	31.53594	1121.38878	6.18666	6.49917
110	4.80740	245.71877	39.13874	0.09283	31.53582	1121.37268	6.18664	6.49911
115	4.80772	245.71909	39.13888	0.09283	31.53570	1121.36401	6.18664	6.49917
120	4.80799	245.71900	39.13923	0.09287	31.53607	1121.43039	6.18673	6.49928
125	4.80843	245.71840	39.13973	0.09292	31.53599	1121.43678	6.18683	6.49940
130	4.80920	245.71919	39.14035	0.09298	31.53539	1121.34869	6.18696	6.49961

135	4.81037	245.71989	39.14124	0.09306	31.53520	1121.34682	6.18714	6.49989
140	4.81225	245.72006	39.14276	0.09320	31.53474	1121.32563	6.18742	6.50015
145	4.81403	245.72091	39.14396	0.09330	31.53453	1121.34668	6.18764	6.50044
150	4.81549	245.72189	39.14492	0.09338	31.53421	1121.33358	6.18783	6.50075
155	4.81675	245.72290	39.14574	0.09346	31.53394	1121.32141	6.18799	6.50104
160	4.81777	245.72358	39.14654	0.09354	31.53379	1121.31953	6.18817	6.50136
165	4.81859	245.72394	39.14730	0.09363	31.53363	1121.30713	6.18836	6.50168
170	4.81933	245.72435	39.14795	0.09371	31.53341	1121.28560	6.18852	6.50196
175	4.81970	245.72436	39.14856	0.09379	31.53319	1121.25507	6.18870	6.50224
180	4.81984	245.72378	39.14917	0.09389	31.53324	1121.25597	6.18890	6.50251

Cycle C of natural state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.89449	245.75056	39.24215	0.10493	31.53180	1121.43709	6.21184	6.53150
5	4.89477	245.75199	39.24160	0.10482	31.53191	1121.47854	6.21162	6.53129
10	4.89499	245.75455	39.24093	0.10469	31.53141	1121.40424	6.21136	6.53104
15	4.89482	245.75614	39.24016	0.10458	31.53161	1121.43947	6.21112	6.53084
20	4.89439	245.75795	39.23923	0.10444	31.53177	1121.44647	6.21085	6.53058
25	4.89370	245.75991	39.23794	0.10427	31.53147	1121.38987	6.21050	6.53019
30	4.89257	245.76125	39.23651	0.10411	31.53203	1121.44665	6.21015	6.52977
35	4.89083	245.76285	39.23462	0.10391	31.53241	1121.45661	6.20974	6.52923
40	4.88832	245.76351	39.23223	0.10368	31.53317	1121.50864	6.20924	6.52861
45	4.88399	245.76220	39.22912	0.10345	31.53413	1121.52662	6.20878	6.52869
50	4.87492	245.74636	39.22789	0.10381	31.53720	1121.67669	6.20952	6.53119
55	4.87077	245.72725	39.23348	0.10488	31.53843	1121.61503	6.21172	6.53431
60	4.87112	245.72385	39.23521	0.10511	31.53825	1121.58178	6.21219	6.53458
65	4.87208	245.72270	39.23658	0.10527	31.53832	1121.61726	6.21252	6.53490
70	4.87320	245.72166	39.23818	0.10547	31.53803	1121.59673	6.21292	6.53533
75	4.87434	245.72031	39.24009	0.10571	31.53770	1121.55685	6.21342	6.53588
80	4.87539	245.71880	39.24207	0.10597	31.53746	1121.53035	6.21395	6.53648
85	4.87646	245.71674	39.24396	0.10622	31.53804	1121.64069	6.21444	6.53701
90	4.87763	245.71587	39.24592	0.10647	31.53762	1121.58018	6.21495	6.53753
95	4.87876	245.71492	39.24773	0.10670	31.53724	1121.53584	6.21541	6.53798
100	4.87985	245.71394	39.24938	0.10690	31.53705	1121.52162	6.21583	6.53837
105	4.88087	245.71332	39.25079	0.10707	31.53689	1121.51688	6.21618	6.53866
110	4.88182	245.71277	39.25187	0.10720	31.53723	1121.59190	6.21642	6.53881
115	4.88273	245.71264	39.25248	0.10724	31.53739	1121.65585	6.21652	6.53877
120	4.88341	245.71383	39.25250	0.10721	31.53695	1121.60683	6.21644	6.53848
125	4.88401	245.71579	39.25192	0.10708	31.53625	1121.53293	6.21617	6.53791
130	4.88466	245.71930	39.25043	0.10681	31.53560	1121.48720	6.21562	6.53699
135	4.88562	245.72506	39.24779	0.10636	31.53521	1121.51817	6.21468	6.53561
140	4.88676	245.72986	39.24565	0.10595	31.53434	1121.47504	6.21386	6.53435
145	4.88804	245.73274	39.24505	0.10578	31.53371	1121.44106	6.21352	6.53375
150	4.88931	245.73526	39.24475	0.10566	31.53316	1121.41547	6.21327	6.53334
155	4.89055	245.73797	39.24450	0.10555	31.53273	1121.40284	6.21305	6.53300
160	4.89161	245.74033	39.24419	0.10544	31.53263	1121.43523	6.21284	6.53269
165	4.89258	245.74294	39.24384	0.10532	31.53235	1121.42966	6.21261	6.53240

170	4.89343	245.74565	39.24336	0.10520	31.53180	1121.38695	6.21236	6.53209
175	4.89403	245.74803	39.24284	0.10508	31.53149	1121.36487	6.21212	6.53182
180	4.89443	245.75041	39.24216	0.10494	31.53172	1121.42119	6.21185	6.53151

Cycle D of natural state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.75203	245.48779	39.10240	0.09041	31.52840	1121.03936	6.18196	6.47725
5	4.75182	245.48595	39.10222	0.09038	31.52822	1121.03088	6.18189	6.47708
10	4.75158	245.48320	39.10230	0.09039	31.52812	1121.03742	6.18189	6.47707
15	4.75226	245.48122	39.10337	0.09047	31.52781	1120.99751	6.18203	6.47726
20	4.75331	245.47940	39.10482	0.09057	31.52755	1120.97548	6.18223	6.47751
25	4.75443	245.47738	39.10647	0.09069	31.52739	1120.96455	6.18246	6.47778
30	4.75659	245.47690	39.10889	0.09084	31.52753	1121.00352	6.18276	6.47804
35	4.75945	245.47802	39.11170	0.09100	31.52748	1121.00219	6.18310	6.47824
40	4.76317	245.48128	39.11509	0.09120	31.52703	1120.94853	6.18352	6.47850
45	4.76973	245.48914	39.12023	0.09150	31.52696	1120.97724	6.18416	6.47905
50	4.78236	245.51019	39.12829	0.09185	31.52582	1120.89075	6.18491	6.47960
55	4.78801	245.52318	39.13012	0.09163	31.52565	1120.91443	6.18444	6.47861
60	4.78819	245.52001	39.13077	0.09173	31.52601	1120.97155	6.18464	6.47888
	4.78807	245.51573	39.13149	0.09196	31.52551	1120.88950	6.18509	6.47953
70	4.78762	245.51240	39.13161	0.09211	31.52589	1120.94642	6.18541	6.48003
75	4.78738	245.51097	39.13150	0.09219	31.52635	1121.01947	6.18557	6.48034
80	4.78722	245.51199	39.13127	0.09222	31.52598	1120.93876	6.18563	6.48053
85	4.78702	245.51324	39.13088	0.09220	31.52601	1120.92636	6.18559	6.48058
90	4.78682	245.51515	39.13044	0.09214	31.52630	1120.95847	6.18547	6.48054
95	4.78661	245.51735	39.12991	0.09205	31.52661	1120.99510	6.18531	6.48042
100	4.78620	245.51992	39.12929	0.09195	31.52667	1120.98716	6.18512	6.48030
105	4.78587	245.52281	39.12869	0.09185	31.52664	1120.96282	6.18492	6.48016
110	4.78552	245.52594	39.12815	0.09176	31.52704	1121.00340	6.18475	6.48006
115	4.78499	245.52852	39.12757	0.09168	31.52738	1121.04106	6.18461	6.48003
120	4.78476	245.53198	39.12724	0.09164	31.52771	1121.07259	6.18455	6.48010
125	4.78431	245.53470	39.12694	0.09164	31.52812	1121.10684	6.18456	6.48029
130	4.78360	245.53640	39.12684	0.09171	31.52849	1121.13179	6.18473	6.48074
135	4.78144	245.53539	39.12647	0.09184	31.52901	1121.14210	6.18504	6.48139
140	4.77592	245.52827	39.12313	0.09167	31.52949	1121.16472	6.18470	6.48086
145	4.77081	245.52010	39.11930	0.09143	31.52941	1121.14394	6.18418	6.48018
150	4.76656	245.51284	39.11591	0.09124	31.52924	1121.12047	6.18375	6.47968
155	4.76292	245.50699	39.11284	0.09107	31.52896	1121.07614	6.18339	6.47926
160	4.76007	245.50250	39.11019	0.09093	31.52875	1121.05204	6.18307	6.47887
165	4.75770	245.49869	39.10788	0.09079	31.52874	1121.05861	6.18277	6.47848
170	4.75505	245.49433	39.10534	0.09063	31.52871	1121.06156	6.18243	6.47801
175	4.75321	245.49090	39.10352	0.09050	31.52861	1121.05589	6.18215	6.47758
180	4.75193	245.48783	39.10229	0.09041	31.52836	1121.03241	6.18195	6.47725

Cycle E of natural state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.82269	245.75025	39.13551	0.09142	31.53094	1121.28245	6.18379	6.49343
5	4.82281	245.74877	39.13661	0.09158	31.53071	1121.23504	6.18411	6.49373

10	4.82286	245.74672	39.13766	0.09174	31.53078	1121.23338	6.18442	6.49402
15	4.82271	245.74437	39.13877	0.09191	31.53124	1121.28588	6.18478	6.49441
20	4.82247	245.74214	39.13982	0.09209	31.53154	1121.31821	6.18514	6.49480
25	4.82215	245.74015	39.14079	0.09226	31.53131	1121.24646	6.18548	6.49520
30	4.82172	245.73778	39.14176	0.09245	31.53160	1121.25927	6.18585	6.49566
35	4.82121	245.73563	39.14270	0.09264	31.53232	1121.34301	6.18622	6.49616
40	4.82059	245.73313	39.14361	0.09283	31.53223	1121.28353	6.18661	6.49671
45	4.81937	245.72942	39.14455	0.09306	31.53256	1121.26501	6.18708	6.49748
50	4.81496	245.72052	39.14533	0.09342	31.53396	1121.29218	6.18780	6.49867
55	4.80983	245.71131	39.14513	0.09364	31.53610	1121.44266	6.18823	6.49947
60	4.80921	245.71116	39.14465	0.09361	31.53545	1121.31790	6.18818	6.49962
65	4.80898	245.71200	39.14373	0.09349	31.53528	1121.30221	6.18793	6.49950
70	4.80867	245.71310	39.14286	0.09338	31.53527	1121.30013	6.18771	6.49942
75	4.80812	245.71309	39.14214	0.09330	31.53555	1121.33015	6.18756	6.49944
80	4.80770	245.71372	39.14146	0.09322	31.53561	1121.33266	6.18740	6.49944
85	4.80740	245.71424	39.14082	0.09314	31.53611	1121.40721	6.18724	6.49943
90	4.80716	245.71507	39.14023	0.09306	31.53589	1121.36976	6.18709	6.49941
95	4.80700	245.71560	39.13963	0.09298	31.53632	1121.43982	6.18693	6.49937
100	4.80695	245.71701	39.13901	0.09289	31.53606	1121.39719	6.18676	6.49928
105	4.80703	245.71850	39.13839	0.09280	31.53595	1121.38584	6.18657	6.49918
110	4.80718	245.72007	39.13781	0.09271	31.53579	1121.36876	6.18640	6.49908
115	4.80754	245.72173	39.13729	0.09263	31.53556	1121.35371	6.18624	6.49910
120	4.80780	245.72369	39.13675	0.09255	31.53565	1121.37785	6.18609	6.49904
125	4.80818	245.72602	39.13606	0.09245	31.53545	1121.36487	6.18589	6.49899
130	4.80891	245.72967	39.13506	0.09229	31.53516	1121.35208	6.18557	6.49879
135	4.81068	245.73739	39.13303	0.09191	31.53462	1121.36480	6.18477	6.49739
140	4.81334	245.74666	39.13052	0.09130	31.53328	1121.30950	6.18351	6.49470
145	4.81550	245.75049	39.12991	0.09104	31.53269	1121.32011	6.18298	6.49351
150	4.81726	245.75229	39.13004	0.09093	31.53221	1121.32293	6.18277	6.49289
155	4.81870	245.75327	39.13058	0.09091	31.53161	1121.28181	6.18274	6.49262
160	4.81990	245.75347	39.13137	0.09096	31.53143	1121.29679	6.18283	6.49260
165	4.82080	245.75304	39.13231	0.09104	31.53128	1121.30376	6.18302	6.49273
170	4.82171	245.75275	39.13326	0.09114	31.53090	1121.26238	6.18321	6.49289
175	4.82231	245.75181	39.13427	0.09125	31.53115	1121.32008	6.18345	6.49310
180	4.82266	245.75039	39.13536	0.09140	31.53103	1121.29642	6.18374	6.49339

Cycle F of natural state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	$R_2{}^r$	$R_3{}^r$
0	4.88591	245.71943	39.25149	0.10701	31.53562	1121.49300	6.21612	6.53949
5	4.88621	245.72076	39.25085	0.10689	31.53530	1121.46997	6.21588	6.53914
10	4.88642	245.72166	39.25013	0.10676	31.53560	1121.55434	6.21562	6.53878
15	4.88634	245.72252	39.24941	0.10664	31.53557	1121.56105	6.21537	6.53843
20	4.88612	245.72340	39.24875	0.10654	31.53498	1121.46517	6.21516	6.53812
25	4.88568	245.72367	39.24808	0.10644	31.53497	1121.46318	6.21496	6.53782
30	4.88502	245.72307	39.24757	0.10638	31.53541	1121.52529	6.21483	6.53761
35	4.88411	245.72222	39.24712	0.10634	31.53571	1121.54804	6.21474	6.53743
40	4.88294	245.72117	39.24672	0.10632	31.53588	1121.53291	6.21470	6.53734

45	4.88094	245.71817	39.24639	0.10635	31.53657	1121.57300	6.21474	6.53734
50	4.87649	245.71119	39.24620	0.10652	31.53829	1121.65985	6.21508	6.53766
55	4.87313	245.70771	39.24549	0.10658	31.53857	1121.56155	6.21518	6.53784
60	4.87263	245.70926	39.24439	0.10645	31.53869	1121.57263	6.21490	6.53746
65	4.87320	245.71046	39.24447	0.10644	31.53836	1121.54476	6.21489	6.53750
70	4.87413	245.71071	39.24502	0.10649	31.53873	1121.63538	6.21499	6.53767
75	4.87513	245.71169	39.24572	0.10655	31.53824	1121.58797	6.21512	6.53781
80	4.87625	245.71221	39.24655	0.10663	31.53786	1121.54823	6.21528	6.53795
85	4.87731	245.71279	39.24732	0.10670	31.53773	1121.56171	6.21543	6.53805
90	4.87828	245.71257	39.24806	0.10677	31.53814	1121.66591	6.21557	6.53814
95	4.87912	245.71365	39.24876	0.10684	31.53724	1121.53448	6.21571	6.53824
100	4.87987	245.71375	39.24948	0.10692	31.53706	1121.52335	6.21586	6.53838
105	4.88057	245.71378	39.25026	0.10700	31.53689	1121.51176	6.21604	6.53856
110	4.88120	245.71317	39.25108	0.10710	31.53741	1121.61464	6.21624	6.53879
115	4.88185	245.71334	39.25185	0.10719	31.53697	1121.54761	6.21642	6.53904
120	4.88223	245.71299	39.25259	0.10729	31.53679	1121.51587	6.21663	6.53932
125	4.88248	245.71262	39.25317	0.10737	31.53680	1121.51444	6.21680	6.53960
130	4.88248	245.71244	39.25331	0.10741	31.53713	1121.55770	6.21688	6.53982
135	4.88203	245.71202	39.25313	0.10743	31.53748	1121.59461	6.21694	6.54019
140	4.88118	245.71024	39.25358	0.10756	31.53747	1121.53289	6.21723	6.54101
145	4.88149	245.71002	39.25384	0.10759	31.53781	1121.59281	6.21730	6.54125
150	4.88210	245.71065	39.25383	0.10756	31.53766	1121.59681	6.21725	6.54122
155	4.88283	245.71168	39.25363	0.10749	31.53747	1121.60593	6.21711	6.54105
160	4.88358	245.71351	39.25330	0.10740	31.53691	1121.55208	6.21694	6.54080
165	4.88423	245.71509	39.25292	0.10731	31.53639	1121.50749	6.21676	6.54051
170	4.88496	245.71678	39.25241	0.10720	31.53617	1121.51804	6.21652	6.54014
175	4.88551	245.71812	39.25190	0.10709	31.53617	1121.55779	6.21630	6.53978
180	4.88587	245.71964	39.25132	0.10698	31.53572	1121.50858	6.21608	6.53943

Reduced state

Averaged values of four nitrogens of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	3.27229	336.47605	45.46810	0.11972	52.33765	3000.51581	7.23523	7.47224
5	3.27209	336.47596	45.46811	0.11973	52.33790	3000.54882	7.23527	7.47232
10	3.27199	336.47700	45.46824	0.11978	52.33821	3000.58590	7.23536	7.47251
15	3.27223	336.47972	45.46854	0.11983	52.33842	3000.61312	7.23549	7.47275
20	3.27266	336.48365	45.46908	0.11992	52.33880	3000.66255	7.23567	7.47313
25	3.27441	336.49215	45.47044	0.12009	52.33923	3000.75030	7.23604	7.47382
30	3.27829	336.50791	45.47319	0.12042	52.33925	3000.81531	7.23670	7.47505
35	3.28657	336.53796	45.47896	0.12110	52.33889	3000.90449	7.23808	7.47758
40	3.32444	336.65806	45.50040	0.12327	52.33282	3000.82624	7.24229	7.48522
45	3.32542	336.66881	45.50077	0.12354	52.33370	3000.98856	7.24285	7.48643
50	3.32447	336.67194	45.50019	0.12368	52.33496	3001.16363	7.24318	7.48719
55	3.32221	336.66909	45.49846	0.12363	52.33574	3001.24003	7.24311	7.48719
60	3.31974	336.66409	45.49645	0.12350	52.33645	3001.30489	7.24288	7.48688
65	3.31779	336.65948	45.49477	0.12337	52.33686	3001.33514	7.24263	7.48653
70	3.31450	336.65119	45.49261	0.12323	52.33770	3001.39601	7.24237	7.48615

75	3.31158	336.64321	45.49066	0.12308	52.33856	3001.46900	7.24209	7.48572
80	3.30838	336.63454	45.48863	0.12291	52.33916	3001.49170	7.24179	7.48525
85	3.30569	336.62708	45.48699	0.12278	52.33973	3001.51836	7.24153	7.48484
90	3.30325	336.62051	45.48563	0.12267	52.34035	3001.56074	7.24133	7.48453
95	3.30150	336.61612	45.48474	0.12261	52.34076	3001.58253	7.24121	7.48433
100	3.30002	336.61292	45.48411	0.12257	52.34107	3001.59072	7.24114	7.48423
105	3.29893	336.61067	45.48385	0.12257	52.34156	3001.63378	7.24115	7.48424
110	3.29857	336.61036	45.48422	0.12262	52.34191	3001.66541	7.24125	7.48440
115	3.29866	336.61101	45.48507	0.12271	52.34198	3001.65925	7.24142	7.48466
120	3.29910	336.61201	45.48635	0.12283	52.34199	3001.64571	7.24165	7.48499
125	3.29932	336.61152	45.48765	0.12292	52.34187	3001.59592	7.24184	7.48523
130	3.29845	336.60589	45.48826	0.12291	52.34201	3001.57144	7.24180	7.48503
135	3.29885	336.59589	45.48891	0.12270	52.34044	3001.32377	7.24135	7.48392
140	3.29720	336.57257	45.48603	0.12189	52.33773	3000.93280	7.23965	7.48040
145	3.29115	336.54721	45.48116	0.12120	52.33743	3000.80371	7.23824	7.47770
150	3.28623	336.52789	45.47744	0.12073	52.33725	3000.70045	7.23729	7.47591
155	3.28232	336.51277	45.47463	0.12040	52.33724	3000.63754	7.23662	7.47468
160	3.27938	336.50110	45.47257	0.12017	52.33715	3000.57634	7.23614	7.47381
165	3.27692	336.49173	45.47096	0.12000	52.33734	3000.56341	7.23581	7.47321
170	3.27524	336.48555	45.46990	0.11989	52.33751	3000.56297	7.23559	7.47283
175	3.27371	336.48060	45.46900	0.11981	52.33749	3000.52374	7.23542	7.47256
180	3.27221	336.47620	45.46812	0.11974	52.33790	3000.55558	7.23527	7.47232

Cycle A of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.78093	245.04099	39.20719	0.10440	31.58911	1124.61941	6.20749	6.49347
5	4.78066	245.04043	39.20702	0.10440	31.58911	1124.61490	6.20748	6.49346
10	4.78060	245.04032	39.20676	0.10436	31.58908	1124.61365	6.20741	6.49335
15	4.78089	245.04121	39.20663	0.10430	31.58903	1124.60920	6.20731	6.49317
20	4.78146	245.04275	39.20648	0.10420	31.58878	1124.57513	6.20714	6.49286
25	4.78260	245.04598	39.20668	0.10408	31.58867	1124.56223	6.20693	6.49245
30	4.78464	245.05114	39.20756	0.10395	31.58868	1124.56929	6.20671	6.49197
35	4.78852	245.06013	39.20998	0.10385	31.58902	1124.64163	6.20656	6.49153
40	4.80113	245.07690	39.22255	0.10430	31.58777	1124.50805	6.20754	6.49218
45	4.80042	245.07312	39.22196	0.10427	31.58780	1124.53078	6.20748	6.49207
50	4.79960	245.06926	39.22144	0.10432	31.58776	1124.53309	6.20760	6.49225
55	4.79889	245.06480	39.22104	0.10443	31.58751	1124.50554	6.20782	6.49255
60	4.79805	245.05944	39.22055	0.10452	31.58765	1124.54042	6.20802	6.49281
65	4.79727	245.05492	39.22007	0.10460	31.58719	1124.46831	6.20819	6.49301
70	4.79602	245.04912	39.21895	0.10462	31.58802	1124.61647	6.20824	6.49303
75	4.79465	245.04394	39.21770	0.10461	31.58729	1124.48948	6.20824	6.49297
80	4.79321	245.03840	39.21623	0.10455	31.58739	1124.50898	6.20815	6.49276
85	4.79194	245.03407	39.21492	0.10450	31.58729	1124.49772	6.20805	6.49257
90	4.79071	245.03009	39.21374	0.10444	31.58724	1124.49114	6.20794	6.49238
95	4.78975	245.02816	39.21296	0.10440	31.58741	1124.50711	6.20786	6.49229
100	4.78896	245.02746	39.21247	0.10437	31.58729	1124.47249	6.20780	6.49226
105	4.78851	245.02811	39.21231	0.10434	31.58746	1124.48795	6.20774	6.49226

110	4.78863	245.03076	39.21255	0.10432	31.58783	1124.54311	6.20768	6.49229
115	4.78893	245.03494	39.21285	0.10427	31.58779	1124.52225	6.20757	6.49225
120	4.78977	245.04162	39.21318	0.10419	31.58783	1124.51598	6.20739	6.49209
125	4.79045	245.04867	39.21318	0.10406	31.58801	1124.52631	6.20711	6.49182
130	4.79080	245.05596	39.21257	0.10388	31.58824	1124.53975	6.20673	6.49139
135	4.79154	245.06446	39.21226	0.10368	31.58873	1124.59941	6.20629	6.49086
140	4.79278	245.06914	39.21359	0.10391	31.58879	1124.59721	6.20672	6.49155
145	4.79081	245.06509	39.21242	0.10406	31.58857	1124.55373	6.20697	6.49209
150	4.78855	245.05912	39.21115	0.10417	31.58892	1124.60465	6.20716	6.49251
155	4.78641	245.05364	39.21001	0.10425	31.58918	1124.64232	6.20729	6.49284
160	4.78468	245.04955	39.20918	0.10432	31.58889	1124.58428	6.20739	6.49311
165	4.78320	245.04613	39.20844	0.10437	31.58849	1124.51926	6.20746	6.49329
170	4.78204	245.04353	39.20790	0.10440	31.58837	1124.49830	6.20749	6.49341
175	4.78120	245.04169	39.20742	0.10440	31.58832	1124.48866	6.20750	6.49346
180	4.78065	245.04053	39.20702	0.10440	31.58831	1124.48561	6.20748	6.49346

Cycle B of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.82907	245.24429	39.25329	0.10719	31.59493	1124.82859	6.21276	6.50790
5	4.82847	245.24302	39.25308	0.10718	31.59488	1124.81753	6.21274	6.50786
10	4.82794	245.24178	39.25288	0.10717	31.59452	1124.75092	6.21272	6.50781
15	4.82751	245.24067	39.25279	0.10717	31.59493	1124.80932	6.21272	6.50781
20	4.82720	245.23985	39.25276	0.10718	31.59468	1124.76425	6.21274	6.50780
25	4.82685	245.23863	39.25280	0.10720	31.59464	1124.75225	6.21278	6.50782
30	4.82630	245.23666	39.25310	0.10728	31.59495	1124.78701	6.21292	6.50799
35	4.82539	245.23332	39.25395	0.10744	31.59539	1124.81112	6.21325	6.50844
40	4.82206	245.20758	39.26661	0.10948	31.59800	1124.85746	6.21744	6.51397
45	4.82231	245.20816	39.26690	0.10950	31.59816	1124.86925	6.21748	6.51391
50	4.82290	245.21057	39.26614	0.10935	31.59811	1124.90258	6.21717	6.51340
55	4.82355	245.21344	39.26544	0.10921	31.59757	1124.83907	6.21688	6.51294
60	4.82398	245.21459	39.26488	0.10910	31.59766	1124.87538	6.21665	6.51260
65	4.82411	245.21554	39.26428	0.10900	31.59757	1124.87184	6.21644	6.51235
70	4.82448	245.21779	39.26318	0.10881	31.59713	1124.83687	6.21606	6.51185
75	4.82459	245.21950	39.26208	0.10864	31.59694	1124.82928	6.21571	6.51142
80	4.82464	245.22124	39.26094	0.10846	31.59682	1124.83320	6.21534	6.51099
85	4.82456	245.22294	39.25970	0.10827	31.59666	1124.82156	6.21496	6.51055
90	4.82445	245.22448	39.25848	0.10809	31.59691	1124.87307	6.21460	6.51014
95	4.82422	245.22593	39.25726	0.10792	31.59713	1124.91491	6.21424	6.50976
100	4.82396	245.22825	39.25599	0.10774	31.59650	1124.80698	6.21388	6.50937
105	4.82375	245.22998	39.25473	0.10756	31.59659	1124.82256	6.21352	6.50900
110	4.82361	245.23217	39.25364	0.10741	31.59666	1124.83518	6.21322	6.50871
115	4.82356	245.23423	39.25269	0.10729	31.59685	1124.86927	6.21296	6.50849
120	4.82362	245.23648	39.25184	0.10717	31.59693	1124.89055	6.21274	6.50833
125	4.82394	245.23961	39.25108	0.10707	31.59690	1124.88743	6.21253	6.50820
130	4.82496	245.24345	39.25073	0.10700	31.59648	1124.84711	6.21238	6.50810
135	4.82606	245.24573	39.25130	0.10706	31.59645	1124.86062	6.21251	6.50833
140	4.82684	245.24663	39.25247	0.10722	31.59642	1124.85909	6.21285	6.50880

145	4.82857	245.24873	39.25328	0.10728	31.59583	1124.83710	6.21296	6.50877
150	4.82969	245.24930	39.25366	0.10728	31.59592	1124.90603	6.21297	6.50862
155	4.83024	245.24914	39.25379	0.10727	31.59572	1124.91553	6.21293	6.50844
160	4.83040	245.24892	39.25388	0.10726	31.59512	1124.83596	6.21292	6.50832
165	4.83033	245.24806	39.25384	0.10724	31.59487	1124.81010	6.21289	6.50819
170	4.83001	245.24698	39.25373	0.10723	31.59467	1124.78135	6.21285	6.50809
175	4.82963	245.24579	39.25355	0.10721	31.59452	1124.76562	6.21281	6.50798
180	4.82920	245.24474	39.25332	0.10718	31.59443	1124.75217	6.21276	6.50788

Cycle C of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.92863	245.02883	39.47474	0.13832	31.58191	1123.64952	6.27585	6.58562
5	4.92838	245.03006	39.47377	0.13817	31.58162	1123.61615	6.27553	6.58518
10	4.92789	245.03123	39.47246	0.13797	31.58173	1123.63846	6.27512	6.58460
15	4.92720	245.03237	39.47090	0.13773	31.58194	1123.67184	6.27465	6.58394
20	4.92654	245.03325	39.46927	0.13749	31.58263	1123.79604	6.27415	6.58323
25	4.92563	245.03460	39.46740	0.13721	31.58220	1123.72250	6.27358	6.58245
30	4.92445	245.03554	39.46536	0.13692	31.58192	1123.66909	6.27299	6.58164
35	4.92280	245.03560	39.46324	0.13663	31.58247	1123.73288	6.27241	6.58086
40	4.91214	245.02961	39.45442	0.13557	31.58500	1123.83022	6.27028	6.57830
45	4.91176	245.03056	39.45324	0.13540	31.58498	1123.82861	6.26993	6.57780
50	4.91223	245.03137	39.45306	0.13535	31.58479	1123.81703	6.26984	6.57766
55	4.91271	245.03283	39.45283	0.13530	31.58422	1123.75062	6.26973	6.57747
60	4.91304	245.03386	39.45246	0.13523	31.58438	1123.80286	6.26958	6.57723
65	4.91321	245.03462	39.45208	0.13516	31.58422	1123.78743	6.26944	6.57702
70	4.91379	245.03544	39.45208	0.13514	31.58432	1123.82924	6.26939	6.57692
75	4.91414	245.03628	39.45195	0.13510	31.58385	1123.76853	6.26931	6.57678
80	4.91459	245.03711	39.45184	0.13507	31.58353	1123.74266	6.26923	6.57663
85	4.91485	245.03773	39.45165	0.13502	31.58349	1123.74746	6.26914	6.57647
90	4.91500	245.03761	39.45153	0.13499	31.58408	1123.86755	6.26908	6.57635
95	4.91493	245.03759	39.45147	0.13498	31.58321	1123.71823	6.26905	6.57630
100	4.91481	245.03687	39.45150	0.13499	31.58325	1123.72158	6.26907	6.57631
105	4.91470	245.03608	39.45180	0.13504	31.58321	1123.71152	6.26918	6.57646
110	4.91460	245.03468	39.45241	0.13514	31.58367	1123.76982	6.26939	6.57678
115	4.91464	245.03280	39.45347	0.13531	31.58375	1123.77285	6.26974	6.57729
120	4.91478	245.03104	39.45492	0.13555	31.58372	1123.74857	6.27023	6.57800
125	4.91538	245.02913	39.45711	0.13590	31.58348	1123.69893	6.27094	6.57902
130	4.91701	245.02701	39.46054	0.13642	31.58414	1123.79701	6.27199	6.58050
135	4.91873	245.02478	39.46451	0.13702	31.58372	1123.72528	6.27322	6.58225
140	4.92056	245.02268	39.46828	0.13759	31.58370	1123.73264	6.27437	6.58386
145	4.92332	245.02305	39.47161	0.13803	31.58303	1123.66893	6.27528	6.58504
150	4.92513	245.02350	39.47359	0.13829	31.58283	1123.67513	6.27579	6.58570
155	4.92634	245.02395	39.47471	0.13843	31.58246	1123.64912	6.27607	6.58605
160	4.92728	245.02475	39.47543	0.13850	31.58214	1123.62287	6.27623	6.58623
165	4.92797	245.02579	39.47572	0.13852	31.58224	1123.65868	6.27626	6.58625
170	4.92836	245.02659	39.47563	0.13849	31.58229	1123.68803	6.27619	6.58613
175	4.92861	245.02758	39.47528	0.13842	31.58223	1123.69010	6.27604	6.58590

180	4.92865	245.02889	39.47463	0.13830	31.58203	1123.67690	6.27581	6.58556

Cycle D of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.82605	245.12829	39.23124	0.10599	31.58572	1124.54342	6.21113	6.50178
5	4.82609	245.12819	39.23122	0.10598	31.58574	1124.54996	6.21112	6.50173
10	4.82619	245.12796	39.23120	0.10596	31.58571	1124.55058	6.21109	6.50165
15	4.82633	245.12784	39.23126	0.10595	31.58570	1124.54502	6.21108	6.50158
20	4.82644	245.12726	39.23128	0.10593	31.58569	1124.54484	6.21106	6.50148
25	4.82650	245.12634	39.23126	0.10590	31.58582	1124.56258	6.21101	6.50133
30	4.82647	245.12520	39.23130	0.10588	31.58588	1124.57057	6.21099	6.50121
35	4.82636	245.12406	39.23159	0.10590	31.58599	1124.58054	6.21104	6.50122
40	4.82597	245.12218	39.23514	0.10625	31.58650	1124.57545	6.21165	6.50191
45	4.82534	245.12090	39.23457	0.10620	31.58658	1124.58392	6.21155	6.50173
50	4.82457	245.11862	39.23384	0.10618	31.58661	1124.59671	6.21151	6.50166
55	4.82380	245.11575	39.23320	0.10619	31.58654	1124.58597	6.21153	6.50166
60	4.82306	245.11259	39.23264	0.10622	31.58638	1124.56598	6.21160	6.50171
65	4.82235	245.10931	39.23217	0.10628	31.58638	1124.57403	6.21170	6.50183
70	4.82159	245.10545	39.23132	0.10629	31.58655	1124.61142	6.21174	6.50182
75	4.82083	245.10198	39.23049	0.10631	31.58617	1124.56297	6.21178	6.50182
80	4.82004	245.09803	39.22960	0.10632	31.58623	1124.58703	6.21181	6.50179
85	4.81932	245.09430	39.22879	0.10632	31.58615	1124.59129	6.21182	6.50174
90	4.81873	245.09162	39.22809	0.10630	31.58616	1124.60422	6.21180	6.50166
95	4.81846	245.09059	39.22769	0.10628	31.58587	1124.56055	6.21177	6.50158
100	4.81845	245.09066	39.22747	0.10624	31.58573	1124.54158	6.21168	6.50144
105	4.81876	245.09196	39.22749	0.10618	31.58576	1124.55009	6.21157	6.50126
110	4.81956	245.09477	39.22793	0.10612	31.58575	1124.55288	6.21146	6.50111
115	4.82060	245.09841	39.22854	0.10606	31.58573	1124.55468	6.21135	6.50095
120	4.82192	245.10305	39.22935	0.10601	31.58582	1124.57301	6.21125	6.50085
125	4.82326	245.10827	39.23002	0.10594	31.58589	1124.58643	6.21113	6.50074
130	4.82456	245.11403	39.23038	0.10584	31.58578	1124.57146	6.21096	6.50059
135	4.82584	245.12023	39.23126	0.10585	31.58569	1124.54963	6.21096	6.50082
140	4.82628	245.12372	39.23223	0.10598	31.58657	1124.66863	6.21118	6.50143
145	4.82613	245.12529	39.23194	0.10596	31.58647	1124.63533	6.21112	6.50150
150	4.82600	245.12639	39.23170	0.10595	31.58650	1124.63127	6.21109	6.50155
155	4.82597	245.12726	39.23155	0.10595	31.58652	1124.63291	6.21107	6.50159
160	4.82595	245.12792	39.23145	0.10595	31.58649	1124.63246	6.21108	6.50165
165	4.82596	245.12837	39.23137	0.10597	31.58624	1124.59694	6.21109	6.50171
170	4.82590	245.12827	39.23128	0.10598	31.58587	1124.55031	6.21111	6.50174
175	4.82597	245.12840	39.23126	0.10599	31.58591	1124.56661	6.21112	6.50177
180	4.82608	245.12839	39.23124	0.10599	31.58585	1124.56494	6.21113	6.50177

Cycle E of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.92863	245.02884	39.47473	0.13832	31.58190	1123.64851	6.27585	6.58562
5	4.92887	245.02798	39.47539	0.13842	31.58219	1123.69331	6.27606	6.58591
10	4.92911	245.02756	39.47588	0.13850	31.58176	1123.63309	6.27621	6.58612
15	4.92913	245.02742	39.47604	0.13853	31.58194	1123.65354	6.27627	6.58620

20	4.92886	245.02681	39.47581	0.13850	31.58235	1123.71795	6.27622	6.58614
25	4.92819	245.02655	39.47520	0.13843	31.58225	1123.68207	6.27607	6.58596
30	4.92686	245.02591	39.47397	0.13828	31.58243	1123.68647	6.27577	6.58558
35	4.92412	245.02467	39.47143	0.13797	31.58292	1123.68533	6.27514	6.58480
40	4.90279	245.01749	39.44940	0.13511	31.58669	1123.84557	6.26936	6.57736
45	4.90225	245.01910	39.44778	0.13486	31.58671	1123.85351	6.26885	6.57664
50	4.90358	245.02151	39.44805	0.13485	31.58621	1123.82237	6.26884	6.57656
55	4.90498	245.02339	39.44834	0.13485	31.58593	1123.82750	6.26883	6.57648
60	4.90616	245.02549	39.44842	0.13482	31.58561	1123.81667	6.26876	6.57632
65	4.90721	245.02757	39.44847	0.13479	31.58505	1123.76851	6.26869	6.57617
70	4.90902	245.02996	39.44909	0.13482	31.58453	1123.74761	6.26875	6.57616
75	4.91070	245.03222	39.44971	0.13486	31.58432	1123.76216	6.26882	6.57619
80	4.91230	245.03453	39.45026	0.13489	31.58405	1123.77206	6.26888	6.57618
85	4.91371	245.03617	39.45085	0.13493	31.58387	1123.79025	6.26895	6.57622
90	4.91507	245.03777	39.45152	0.13499	31.58385	1123.82100	6.26907	6.57633
95	4.91622	245.03902	39.45225	0.13506	31.58323	1123.75366	6.26922	6.57650
100	4.91739	245.04021	39.45317	0.13517	31.58271	1123.70072	6.26944	6.57677
105	4.91855	245.04077	39.45420	0.13529	31.58312	1123.79561	6.26969	6.57709
110	4.91954	245.04144	39.45519	0.13542	31.58288	1123.76873	6.26995	6.57742
115	4.92047	245.04138	39.45627	0.13556	31.58283	1123.77736	6.27024	6.57780
120	4.92133	245.04128	39.45746	0.13572	31.58280	1123.78485	6.27056	6.57823
125	4.92228	245.04077	39.45894	0.13593	31.58255	1123.75140	6.27099	6.57880
130	4.92334	245.03986	39.46083	0.13620	31.58220	1123.71901	6.27155	6.57956
135	4.92325	245.03737	39.46222	0.13645	31.58209	1123.67311	6.27204	6.58028
140	4.92098	245.03402	39.46194	0.13649	31.58280	1123.72264	6.27212	6.58054
145	4.92136	245.03273	39.46327	0.13669	31.58325	1123.79824	6.27254	6.58114
150	4.92240	245.03212	39.46508	0.13695	31.58308	1123.78297	6.27306	6.58186
155	4.92365	245.03160	39.46704	0.13723	31.58270	1123.72806	6.27363	6.58262
160	4.92476	245.03083	39.46886	0.13749	31.58228	1123.66681	6.27416	6.58334
165	4.92586	245.03041	39.47054	0.13773	31.58200	1123.63898	6.27464	6.58400
170	4.92689	245.02966	39.47211	0.13795	31.58203	1123.65178	6.27509	6.58460
175	4.92773	245.02942	39.47343	0.13814	31.58224	1123.69880	6.27547	6.58511
180	4.92857	245.02904	39.47460	0.13830	31.58200	1123.66792	6.27581	6.58556

Cycle F of reduced state

RD(°)	S_S	I_F	S_{GBP}	I_G	E_2	E_3	R_2^r	R_3^r
0	4.82907	245.24428	39.25329	0.10719	31.59493	1124.82933	6.21276	6.50790
5	4.82977	245.24637	39.25327	0.10716	31.59457	1124.78480	6.21271	6.50783
10	4.83042	245.24827	39.25321	0.10712	31.59445	1124.77975	6.21264	6.50776
15	4.83097	245.25017	39.25318	0.10711	31.59438	1124.77409	6.21260	6.50774
20	4.83141	245.25185	39.25305	0.10708	31.59438	1124.77588	6.21255	6.50770
25	4.83152	245.25262	39.25301	0.10708	31.59489	1124.85129	6.21254	6.50777
30	4.83112	245.25221	39.25293	0.10709	31.59570	1124.95799	6.21258	6.50793
35	4.82956	245.25114	39.25273	0.10714	31.59545	1124.82510	6.21268	6.50829
40	4.81737	245.22300	39.25445	0.10790	31.59934	1124.95557	6.21424	6.51090
45	4.81747	245.22111	39.25536	0.10802	31.59924	1124.93618	6.21447	6.51105
50	4.81796	245.22120	39.25553	0.10801	31.59901	1124.91546	6.21445	6.51095

55	4.81847	245.22134	39.25567	0.10800	31.59869	1124.89818	6.21443	6.51083
60	4.81895	245.22118	39.25591	0.10800	31.59851	1124.89410	6.21443	6.51073
65	4.81944	245.22071	39.25634	0.10803	31.59876	1124.96411	6.21450	6.51071
70	4.82026	245.22157	39.25646	0.10801	31.59785	1124.85361	6.21443	6.51050
75	4.82106	245.22170	39.25683	0.10801	31.59777	1124.87227	6.21445	6.51040
80	4.82213	245.22277	39.25723	0.10802	31.59749	1124.87240	6.21445	6.51026
85	4.82329	245.22358	39.25787	0.10806	31.59708	1124.84666	6.21453	6.51020
90	4.82440	245.22443	39.25851	0.10810	31.59672	1124.83771	6.21461	6.51015
95	4.82549	245.22524	39.25928	0.10816	31.59623	1124.79677	6.21474	6.51017
100	4.82664	245.22581	39.26005	0.10823	31.59651	1124.88786	6.21486	6.51017
105	4.82771	245.22735	39.26071	0.10828	31.59576	1124.79487	6.21496	6.51016
110	4.82850	245.22879	39.26109	0.10830	31.59554	1124.78696	6.21501	6.51011
115	4.82901	245.22982	39.26103	0.10827	31.59548	1124.80468	6.21494	6.50993
120	4.82915	245.23156	39.26056	0.10820	31.59540	1124.80172	6.21479	6.50970
125	4.82887	245.23339	39.25948	0.10805	31.59562	1124.84005	6.21449	6.50934
130	4.82804	245.23556	39.25748	0.10780	31.59546	1124.82045	6.21397	6.50877
135	4.82597	245.23369	39.25567	0.10764	31.59605	1124.88686	6.21366	6.50866
140	4.82419	245.22919	39.25537	0.10771	31.59573	1124.78359	6.21380	6.50921
145	4.82440	245.23081	39.25456	0.10759	31.59545	1124.76308	6.21356	6.50897
150	4.82490	245.23269	39.25406	0.10750	31.59530	1124.76409	6.21337	6.50875
155	4.82551	245.23468	39.25373	0.10742	31.59553	1124.82345	6.21322	6.50855
160	4.82613	245.23658	39.25352	0.10736	31.59549	1124.83785	6.21310	6.50840
165	4.82682	245.23899	39.25338	0.10730	31.59491	1124.76509	6.21299	6.50824
170	4.82749	245.24032	39.25330	0.10726	31.59495	1124.79434	6.21290	6.50811
175	4.82822	245.24225	39.25327	0.10722	31.59465	1124.76478	6.21283	6.50800
180	4.82903	245.24435	39.25326	0.10718	31.59458	1124.77095	6.21275	6.50789