SUPPORTING INFORMATION/1

Dibenzo[*a,o*]phenanthro[3,4-*s*]pycene, a Configurationally Stable Double Helicene: Synthesis, and Determination of its Conformation by NMR and GIAO Calculations

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Table. Shielding constants (σ) for H1-H24; *relative chemical shift increments* ($\Delta\delta_{\text{H}}$) for H1-H16 calculated for **5-PP** and **5-PM**, and experimentally observed $\Delta\delta_{\text{H}}$ values.

H	5-PP		5-PM		exp. $\Delta\delta_{\text{H}}$
	calcd. σ	calcd. $\Delta\delta_{\text{H}}$	calcd. σ	calcd. $\Delta\delta_{\text{H}}$	
H1	26.05	-0.66	24.97	1.04	1.03
H2	26.24	-0.19	25.92	0.27	0.29
H3	25.75	-0.08	25.58	0.14	0.15
H4	25.41	-0.08	25.28	0.12	0.12
H5	25.21	-0.05	25.16	0.10	0.10
H6	25.02	-0.01	24.95	0.20	0.21
H7	24.61	0.49	24.42	0.54	0.52
H8	23.93	0.40	23.87	0.28	0.30
H9	23.98	0.35	23.94	0.21	0.24
H10	24.64	0.46	24.61	0.35	0.42
H11	24.80	0.21	24.80	0.35	0.39
H12	24.74	0.42	24.79	0.47	0.56
H13	24.74	0.59	24.68	0.72	0.77
H14	25.16	0.51	25.01	0.71	0.75
H15	25.57	0.48	25.12	1.07	1.16
H16	24.73	0.66	23.61	2.40	2.30
H17	24.33		24.15		
H18	25.10		24.96		
H19	25.01		25.15		
H20	25.16		25.26		
H21	25.33		25.40		
H22	25.67		25.72		
H23	26.05		26.19		
H24	25.39		26.01		

Chart. Calculated and experimental *relative chemical shift increment* (Δd_H , as defined in the main text of the manuscript) for hydrogens H1-H16.

Calculated absolute electronic energies (hartree/particle) and relative electronic energies (kcal/mol) for the conformations PM, PP and the transition state.

	PM	PP	PP-PM	TS	TS-PP
AM1	0.340091	0.345033	3.10	0.381023	22.58
RHF/6-31G(d)	-1604.509039	-1604.501106	4.98	-	-
B3LYP/6-31G(d)	-1614.991176	-1614.983778	4.64	-	-

Calculated zero-point energies (unscaled), thermal corrections to energy (including ZPE), Enthalpies and free Energies at AM1 level (Temperature 298.15 k).

		ZPE	Thermal Ener.	Enthalpies	Free Energies
Absolutes (Hartrees)	PM	0.543551	0.570912	0.911947	0.826694
	PP	0.543609	0.570907	0.916885	0.831972
	TS	0.543068	0.569655	0.951622	0.868511
Relatives (Kcal/mol)	PP-PM	0.036	-0.003	3.10	3.31
	TS-PP	-0.34	-0.79	21.80	22.93

5-PP, B3LYP/6-31G(d) geometry:

C	3.766048	3.214773	0.157713
C	2.447470	3.319204	-0.186100
C	1.604574	2.169987	-0.207151
C	2.156913	0.904890	0.106121
C	3.603004	0.764415	0.124380
C	4.380290	1.942179	0.294880
C	4.336617	-0.474395	-0.124305
C	5.737003	-0.530039	0.168163
C	6.423638	0.654190	0.581861
C	5.781657	1.854046	0.572306
C	3.769378	-1.601420	-0.774996
C	4.501684	-2.747995	-1.013650
C	5.850068	-2.832981	-0.613931
C	6.455175	-1.732237	-0.045582
C	0.172229	2.318810	-0.407106
C	-0.712733	1.256634	-0.091749
C	-0.143954	-0.074592	0.085456
C	1.234355	-0.178112	0.417803
C	-0.894927	-1.315986	-0.027241
C	-0.452109	-2.430687	0.730109
C	0.796984	-2.360367	1.409601
C	1.646285	-1.316115	1.179602
C	-0.363029	3.521625	-0.955987
C	-1.709286	3.675061	-1.133793
C	-2.619079	2.739578	-0.570897
C	-2.119478	1.583515	0.084399
C	-2.022812	-1.513733	-0.925266
C	-2.798071	-2.711965	-0.819130
C	-2.410093	-3.729450	0.106645
C	-1.251502	-3.613175	0.812872
C	-4.028151	2.980346	-0.642509
C	-4.913270	2.164493	-0.007609
C	-4.442847	1.130440	0.861135
C	-3.039843	0.867879	0.958545
C	-5.350412	0.429201	1.691687
C	-4.901592	-0.451448	2.652894
C	-3.515662	-0.632237	2.828896
C	-2.612868	0.011273	2.004803
C	-2.335388	-0.630564	-1.990342
C	-3.401397	-0.864163	-2.836537
C	-4.214830	-2.002295	-2.667312
C	-3.903876	-2.913708	-1.681008
H	4.375915	4.106381	0.279553
H	2.020155	4.303014	-0.337430
H	7.482813	0.589474	0.818355
H	6.321211	2.775023	0.779382
H	2.743870	-1.554865	-1.118158
H	4.033278	-3.584808	-1.524548
H	6.416083	-3.744184	-0.787056
H	7.510941	-1.756321	0.214402
H	1.096740	-3.184139	2.052265
H	2.636101	-1.319071	1.617803
H	0.309231	4.290318	-1.318244
H	-2.103459	4.550724	-1.643317
H	-3.023315	-4.623735	0.186544

H	-0.909901	-4.419978	1.456924
H	-4.373466	3.833655	-1.221304
H	-5.984145	2.336189	-0.084013
H	-6.413792	0.627328	1.578518
H	-5.607208	-0.973556	3.293439
H	-3.149393	-1.273432	3.625963
H	-1.554096	-0.118145	2.187198
H	-1.709196	0.234949	-2.163258
H	-3.604953	-0.168029	-3.645682
H	-5.059944	-2.173820	-3.328472
H	-4.490442	-3.822223	-1.564897

5-PM, B3LYP/6-31G(d) geometry:

C	3.796048	2.828414	-1.299308
C	2.456273	3.055045	-1.125049
C	1.602245	2.018666	-0.663808
C	2.140759	0.727296	-0.439903
C	3.572469	0.593059	-0.298826
C	4.389745	1.620781	-0.848835
C	4.242769	-0.471787	0.440171
C	5.663175	-0.608124	0.340997
C	6.417847	0.348776	-0.408890
C	5.808672	1.447453	-0.931742
C	3.571274	-1.316183	1.361697
C	4.241005	-2.295817	2.068865
C	5.626520	-2.482863	1.894399
C	6.321478	-1.641917	1.050602
C	0.204636	2.253003	-0.322467
C	-0.630963	1.155036	-0.001020
C	-0.200203	-0.142656	-0.531591
C	1.198636	-0.387127	-0.570648
C	-1.108890	-1.136389	-1.061422
C	-0.620909	-2.461692	-1.225422
C	0.774258	-2.706776	-1.153743
C	1.656800	-1.686832	-0.930074
C	-0.308048	3.571825	-0.189466
C	-1.570845	3.783574	0.295581
C	-2.336712	2.712229	0.824181
C	-1.825628	1.384843	0.775703
C	-2.476050	-0.875102	-1.507849
C	-3.351528	-1.979923	-1.755246
C	-2.848235	-3.317678	-1.688386
C	-1.519622	-3.540894	-1.503011
C	-3.615756	2.978030	1.409711
C	-4.345220	1.985266	1.985339
C	-3.800261	0.669138	2.119338
C	-2.518819	0.366507	1.559593
C	-4.494938	-0.312721	2.865628
C	-3.933493	-1.546761	3.118269
C	-2.635927	-1.821176	2.646904
C	-1.950157	-0.888678	1.891708
C	-2.964755	0.415623	-1.831237
C	-4.264243	0.616659	-2.257618
C	-5.151295	-0.468166	-2.388705

C	-4.689176	-1.746303	-2.155154
H	4.434216	3.598247	-1.725616
H	2.040200	4.019638	-1.393343
H	7.494020	0.217164	-0.489627
H	6.390622	2.221853	-1.425578
H	2.510156	-1.178544	1.529012
H	3.694341	-2.917430	2.772825
H	6.146303	-3.263282	2.443390
H	7.399020	-1.739820	0.940491
H	1.138704	-3.710071	-1.360779
H	2.718635	-1.871523	-1.018069
H	0.305519	4.423022	-0.461273
H	-1.975577	4.791089	0.351713
H	-3.533534	-4.142619	-1.867308
H	-1.111351	-4.547570	-1.550688
H	-3.993606	3.997034	1.374824
H	-5.326408	2.188166	2.407515
H	-5.476671	-0.062368	3.261115
H	-4.473730	-2.288925	3.699735
H	-2.161942	-2.769776	2.884107
H	-0.944441	-1.119481	1.568387
H	-2.299523	1.266361	-1.777691
H	-4.595875	1.621862	-2.503152
H	-6.177155	-0.302618	-2.706494
H	-5.339554	-2.604346	-2.309079

5-TS, AM1 geometry:

C	-3.862700	-3.042526	-1.424072
C	-3.862700	-1.677155	-1.424072
C	-2.627808	-0.973618	-1.424072
C	-1.444626	-1.635986	-1.832138
C	-1.431747	-3.078979	-1.824265
C	-2.625214	-3.734863	-1.431839
C	-0.279449	-3.957703	-1.976547
C	-0.228378	-5.154556	-1.208221
C	-1.434174	-5.693161	-0.652679
C	-2.611267	-5.061188	-0.885345
C	0.774002	-3.784027	-2.899887
C	1.931046	-4.539413	-2.840652
C	2.062927	-5.563644	-1.889084
C	0.971176	-5.895294	-1.113113
C	-2.600983	0.392136	-0.947433
C	-1.393921	1.116364	-0.926102
C	-0.177734	0.386444	-1.197861
C	-0.284973	-0.779007	-1.994034
C	1.144409	0.783386	-0.787567
C	2.222168	0.437408	-1.628510
C	1.963348	-0.329773	-2.799271
C	0.752060	-0.948151	-2.953369
C	-3.767471	0.989456	-0.392014
C	-3.728668	2.255722	0.126938
C	-2.572372	3.060623	-0.036270
C	-1.446060	2.536423	-0.705566
C	1.432480	1.422455	0.472855
C	2.758179	1.841751	0.750443
C	3.802017	1.583450	-0.193237

C	3.547180	0.879486	-1.329468
C	-2.562576	4.406158	0.453903
C	-1.525146	5.237656	0.173248
C	-0.485870	4.814774	-0.717422
C	-0.472794	3.483337	-1.204330
C	0.476791	5.744965	-1.175064
C	1.379120	5.394394	-2.156326
C	1.329514	4.105957	-2.719986
C	0.423950	3.174026	-2.255371
C	0.459793	1.571533	1.493057
C	0.772461	2.169052	2.695190
C	2.077072	2.641113	2.938705
C	3.054489	2.473053	1.983017
H	-4.798508	-3.617126	-1.360306
H	-4.815170	-1.128967	-1.399918
H	-1.382843	-6.644623	-0.103439
H	-3.572464	-5.507782	-0.588913
H	0.509933	-1.456940	-3.896088
H	2.744751	-4.356232	-3.557678
H	3.006836	-6.120285	-1.804550
H	1.008270	-6.758575	-0.431839
H	2.751709	-0.425354	-3.559800
H	4.083328	2.817215	2.166763
H	-4.705215	0.419128	-0.326492
H	-4.603485	2.681381	0.641418
H	4.815186	1.945557	0.038040
H	4.349915	0.632950	-2.040634
H	-3.413330	4.738632	1.067627
H	-1.481674	6.259109	0.579926
H	0.479630	6.758575	-0.747025
H	2.126160	6.116913	-2.515320
H	2.017181	3.847305	-3.538620
H	0.382889	2.178177	-2.724823
H	-0.560074	1.192154	1.322739
H	0.004532	2.278030	3.475189
H	2.306946	3.130692	3.896088
H	0.638535	-3.121094	-3.760254