

SUPPORTING INFORMATION

Triphasic circularly polarized luminescence switch quantum simulation of topologically chiral catenane

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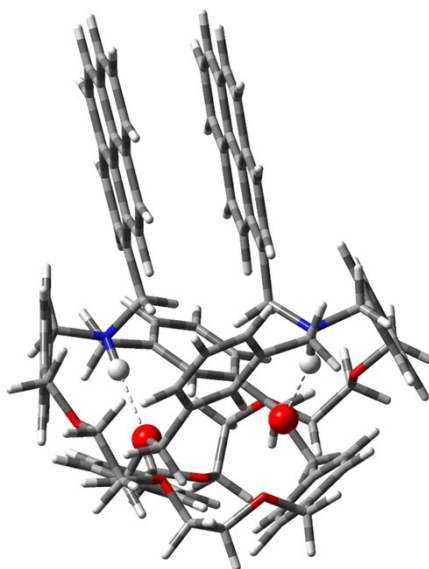


Fig. S1. Zoom of the optimized (LC-wHPBE/6-311G(d,p) level in gas phase) biprotonated form, ball and stick display format are related to the atoms involved in the hydrogen bonds.

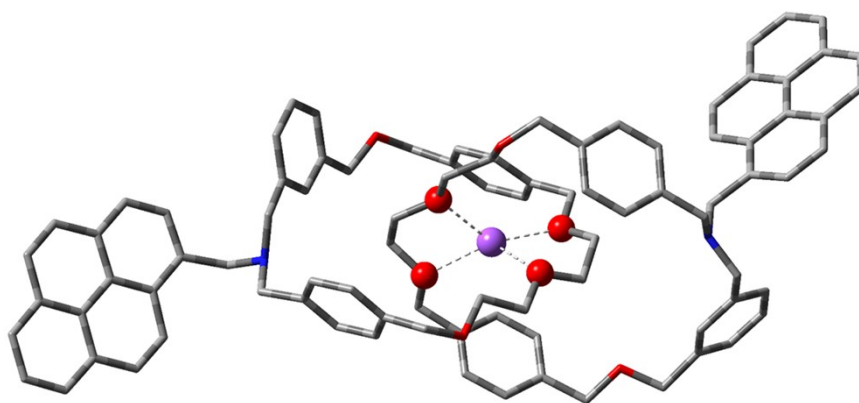


Fig. S2. Zoom of the optimized (LC-wHPBE/6-311G(d,p) level in gas phase) open form, ball and stick display format are related to the atoms involved in the cation entrapping. Hydrogens were omitted for clarity.

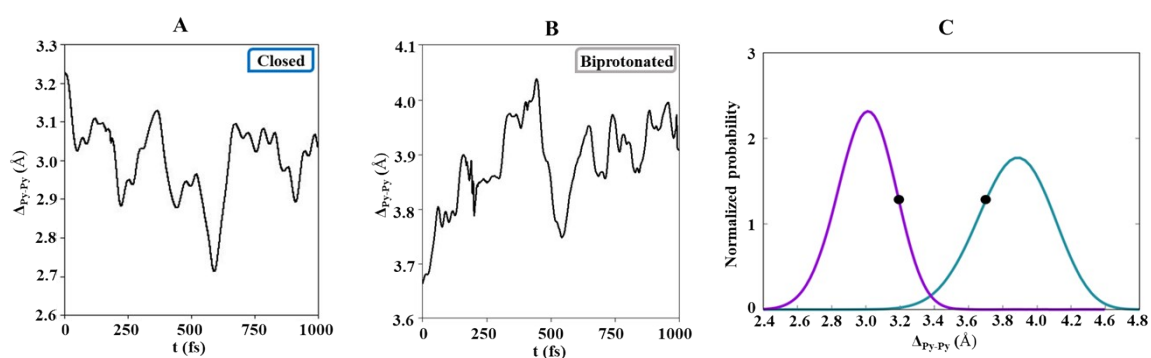


Fig. S3. (A,B) Pyrene-pyrene distance evolution plots of BOMD trajectories (S1) computed at LC-wHPBE/6-311G(d,p) level in solvent phase (CH_2Cl_2) for closed and biprotonated forms, respectively. (C) Distribution functions of pyrene-pyrene distance as obtained from the first excited state molecular dynamics in dichloromethane for closed (blue) and biprotonated (grey) forms. Black circles indicate the relative values for the S0 optimization.

Table S1. Computed rotational strengths for closed, biprotonated and open forms as function of time.

Rlength (cgs units)			Time (fs)
Closed	Biprotonated	Open	
69.8294	110.2536	0.0020	0
25.3668	40.0516	0.0001	40
28.2560	44.6134	0.0000	80
31.2453	90.3578	0.0000	120
30.6880	77.5576	0.0000	160
57.2283	50.9693	0.0001	200
32.2815	95.9564	0.0000	240
28.0978	60.0022	0.0000	300
60.7742	53.1071	0.0000	340
33.6355	81.1875	0.0006	380
51.4203	186.9978	0.0007	420
118.4355	186.7043	0.0006	460
118.2496	170.3444	0.0000	500
99.4434	157.0112	0.0001	540
110.0286	173.7242	0.0000	580
81.1655	128.1522	0.0000	620
126.1472	199.1738	0.0000	660
92.5392	178.5544	0.0000	700
97.0314	146.1101	0.0000	740
157.8443	153.2029	0.0000	780
175.9086	249.2204	0.0001	820
156.9492	261.0988	0.0001	880
170.9513	277.7421	0.0001	920
122.3531	247.8071	0.0000	960
111.0034	269.9150	0.0000	1000

Computational notes

For BOMD jobs all the initial structures (closed, biprotonated and open forms, see manuscript) were extracted as the minima of the optimization process (LC-wHPBE/6-311G(d,p) level), and placed into a unit cubic box (35 Å for edge, 42875 Å³). The effect of solvent has been taken into account by using the integral equation formalism for the polarizable continuum model (IEF-PCM, referred to simply as PCM), the default parameters of *Gaussian16* have been used for the construction of the cavity, built as the envelope of interlocked spheres centered on each atom of the solute (dichloromethane: $\epsilon=8.93$). The excited state (S1) BOMD simulation consisted of an initial equilibration part followed by the accumulation run in the NVT ensemble, particularly, the first part subsisted in a first energy minimization (100 steps) processed by a Hessian-based algorithm that incorporates a predictor step on the local quadratic surface followed by a corrector step. The latter uses a fifth-order polynomial fitted to the energy, gradient, and Hessian at the beginning and end points of each step. The equations of motion have been integrated using a time step of 2fs in a time-width of 1ps, the isothermal conditions were set at 298K. After the production dynamics, 25 snapshots (for each compound) were captured for the TD-DFT processing, checking that the main structural features of the starting conformation were preserved along the trajectories.

Cartesian coordinates in gas phase LC-wHPBE/6-311G(d,p)

CLOSED

Symbol	X	Y	Z
O	4.2465720	3.7503170	-3.6367370
O	3.5793960	5.7224550	-1.4693910
O	1.9089560	6.4406640	0.7299110
C	4.9266930	3.9607160	-2.4234030
C	4.8436990	5.4033880	-2.0023470
C	3.5864740	6.9882420	-0.8642650
C	2.2260320	7.3202960	-0.3170970
C	4.6617040	2.5707820	-4.3025070
C	4.5373560	1.3321920	-3.4529360
C	3.2906180	0.9085610	-3.0200790
C	5.6605930	0.6532740	-2.9979360
C	3.1700060	-0.1186350	-2.1007020
C	5.5391170	-0.3774980	-2.0829020
C	4.2926310	-0.7472840	-1.5922420
C	0.6956780	6.7687400	1.3693620

C	0.2426060	5.5997210	2.1960410
C	1.1589890	4.8621050	2.9382050
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H	6.6468570	0.9575440	-3.3381820
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H	-2.5264310	3.7652250	2.8529030
H	2.1985140	5.1701220	2.9529370
H	-1.8182940	5.7757660	1.6335720
H	0.8358790	7.6645580	1.9927030
H	-0.0751680	7.0033470	0.6239720
H	1.4755540	7.2489180	-1.1164180
H	2.2420130	8.3599110	0.0420230
H	3.8670450	7.7623440	-1.5937860
H	4.3192590	7.0140030	-0.0452220
H	5.6139900	5.5766460	-1.2366090
H	5.0683710	6.0469950	-2.8638640
H	5.9924790	3.7158440	-2.5451050
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C	-0.5997670	-2.8234430	3.5806550
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H	3.7170940	-2.6821840	1.7617930
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H	-1.4474290	-2.8545620	4.2591810
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H	0.4088320	0.5339210	-0.8665510
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H	-8.0625538	-0.0742758	-2.7189499
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H	-6.4997853	-5.5485793	1.6443491
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BIPROTONATED

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C	0.8699210	-6.4911020	-3.4915130
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C	-1.9072400	-4.9369960	-1.4101360
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N	0.8095910	-0.0724590	2.5461780
C	-3.7642400	-0.9847760	-0.4785300
C	-0.4709320	0.3873980	3.1789400
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C	3.8888940	1.3014450	0.1210660
C	1.6826980	4.3047420	2.1631820
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C	-1.9838350	-2.5361740	4.2759870
C	-2.9639980	-3.3549580	2.2636410
C	-1.8495500	-3.2294740	3.0810600
C	-6.8098870	1.8474290	-2.5452530
C	-5.4357930	1.5503430	-3.0683020
C	-5.1693210	0.3347220	-3.6870650
C	-4.3968140	2.4461220	-2.8710220
C	-3.8759860	-0.0023460	-4.0393810
C	-3.1027580	2.1175470	-3.2353290

C	-2.8259020	0.8731680	-3.7822850
H	-3.2600760	-1.3590590	5.5315590
H	-1.1490870	-2.4907450	4.9711570
H	-5.0362000	-2.8647780	1.9642620
H	-2.8862580	-3.9312090	1.3485260
H	-3.6849410	-0.9519250	-4.5310340
H	-2.3032890	2.8346330	-3.0833480
H	-5.9831010	-0.3555750	-3.8834950
H	-4.5969880	3.4122550	-2.4202630
H	-7.5784600	1.5076410	-3.2516600
H	-6.9387150	2.9272700	-2.4014700
H	-8.2151230	2.5310610	-0.4280370
H	-9.0071030	1.2222500	-1.3386750
H	-9.3091970	0.7858270	0.9775150
H	-8.1578000	-0.4115560	0.3419610
H	-8.6515210	1.1690480	3.1187360
H	-6.9242350	1.2775000	3.4765280
H	-8.0042350	-0.8696130	4.2046670
H	-8.3740810	-1.2473400	2.5250340
H	-5.3247900	-0.2457180	4.3488090
H	-6.0284220	-1.7595080	4.9440700
C	-0.5497270	-3.8374440	2.6510770
C	-1.4137890	0.4626340	-4.0736040
O	0.0901210	-3.0109110	1.6693360
N	-0.7829510	-0.2374000	-2.8975040
C	0.9763060	-3.7828360	0.8604650
C	0.3756610	-1.0675990	-3.3639190
C	1.5409120	-2.9930890	-0.2855230
C	2.9076020	-3.0353660	-0.5267550
C	1.2339900	-1.6849710	-2.2920360
C	2.6069640	-1.7186370	-2.5079280
C	0.7059600	-2.3295770	-1.1784560

C	3.4357550	-2.3998320	-1.6369520
H	-0.7353730	-4.8204980	2.2063100
H	0.1218000	-3.9868400	3.5041560
H	1.7942190	-4.1802240	1.4685100
H	0.4148580	-4.6323890	0.4554700
H	-0.3667630	-2.3522510	-1.0051140
H	3.0308860	-1.2371090	-3.3843110
H	4.5001100	-2.4526390	-1.8341180
H	3.5578310	-3.6053390	0.1289470
H	0.9721070	-0.4433640	-4.0273180
H	-0.0649730	-1.8566120	-3.9741520
H	-0.7737560	1.3151310	-4.3047160
H	-1.3755740	-0.2389130	-4.9080750
C	-0.5254720	0.6716660	-1.7291250
H	-1.5180280	0.9230930	-1.3691130
H	-0.0739680	0.0162860	-0.9887810
C	0.3055730	1.9109300	-1.9364660
C	-0.1059130	3.1324490	-1.3674750
C	1.5446190	1.8468390	-2.5659830
C	0.7260710	4.2728240	-1.5050580
C	-1.3240380	3.2899580	-0.6060950
C	2.3482190	2.9570080	-2.7082040
H	1.9241920	0.9020510	-2.9278630
C	0.3376080	5.5290250	-0.9433850
C	1.9553370	4.1842200	-2.1918560
C	-1.6829510	4.4742840	-0.0812050
H	-1.9770500	2.4452260	-0.4257060
H	3.3072220	2.8712110	-3.2067330
C	-0.8729720	5.6475040	-0.2341640
C	1.1672990	6.6606970	-1.0905870
C	2.7864040	5.3511120	-2.3229840
H	-2.6058330	4.5544510	0.4843690

C	-1.2412680	6.8762150	0.3054860
C	0.7679400	7.8741810	-0.5401080
C	2.4097130	6.5286020	-1.8029850
H	3.7277120	5.2536020	-2.8524750
C	-0.4262750	7.9820180	0.1505540
H	-2.1779570	6.9611310	0.8466300
H	1.4048020	8.7440150	-0.6613800
H	3.0392120	7.4055410	-1.9079220
H	-0.7239620	8.9369980	0.5681210
H	-1.4877940	-0.8893270	-2.5109550

OPEN

Symbol	X	Y	Z
O	-1.7991910	-0.6893990	-0.9528220
O	-1.0847090	0.7472390	1.2709970
O	0.8381350	0.8897740	4.2743560
N	6.6105920	-2.0862050	1.3715160
C	6.0081410	-3.9819790	-1.2056070
H	5.1911030	-4.3101650	-0.5693470
C	5.9054180	-4.1423310	-2.5822780
C	6.9556740	-3.7315890	-3.3887500
H	6.8860770	-3.8499660	-4.4654070
C	8.0991260	-3.1876800	-2.8269610
H	8.9208000	-2.8769780	-3.4623500
C	8.1959940	-3.0496220	-1.4547790
H	9.0958000	-2.6318140	-1.0134200
C	7.1472050	-3.4402130	-0.6288230
C	7.2618010	-3.2917430	0.8676660
H	6.7698080	-4.1440850	1.3444620
H	8.3249970	-3.3579710	1.1356400
C	6.5090400	-2.0301510	2.8263570
H	7.4325060	-1.6800550	3.3059340

H	6.3423790	-3.0511180	3.1777000
C	5.3688530	-1.1650020	3.3027630
C	4.1151180	-1.7117870	3.5508130
H	3.9649730	-2.7793660	3.4190870
C	3.0664030	-0.9238880	3.9896750
H	2.0976480	-1.3657220	4.1973580
C	3.2423800	0.4406800	4.1793990
C	4.4908420	0.9921830	3.9331200
H	4.6507760	2.0556240	4.0852310
C	5.5455680	0.1961700	3.5156460
H	6.5239390	0.6404460	3.3555770
C	2.1163780	1.2955750	4.7087920
H	2.0859580	1.2325190	5.7982850
H	2.2909650	2.3466700	4.4425570
C	0.6173810	1.0898610	2.9035700
H	1.2071610	0.3812870	2.3055960
H	0.9014710	2.1102400	2.6114270
C	-0.8567800	0.8608090	2.6647830
H	-1.1603200	-0.0612390	3.1733740
H	-1.4455370	1.6869450	3.0770980
C	-2.4589460	0.5418300	0.9741430
H	-3.0445660	1.4097920	1.2963950
H	-2.8204450	-0.3481450	1.5016540
C	-2.6350420	0.3669420	-0.5080430
H	-3.6871810	0.1348170	-0.7007660
H	-2.3681730	1.2888320	-1.0370010
C	-2.0709610	-1.1168940	-2.2833250
H	-2.0970420	-0.2453520	-2.9490240
H	-3.0487170	-1.6075230	-2.3170840
C	-0.9695040	-2.0534690	-2.6772900
C	0.2538290	-1.5388850	-3.0935400
H	0.3670520	-0.4667910	-3.2361790

C	1.3277370	-2.3755660	-3.3306360
H	2.2869810	-1.9691910	-3.6290610
C	1.1970580	-3.7486700	-3.1637490
C	-0.0311600	-4.2660580	-2.7806570
H	-0.1491150	-5.3375270	-2.6527800
C	-1.1057140	-3.4258390	-2.5372050
H	-2.0557110	-3.8451540	-2.2224900
C	2.3740030	-4.6481650	-3.4097270
H	2.2043230	-5.6294060	-2.9467370
H	2.4949410	-4.8135030	-4.4903680
C	4.6957420	-4.7949060	-3.1848130
H	4.8162770	-4.8748140	-4.2725320
H	4.5845780	-5.8142470	-2.7891590
O	-2.1521200	4.7017310	-2.6039800
O	2.5301450	-0.0978060	-0.7711330
O	1.4635400	-2.0229500	0.8441080
O	-1.3169120	-4.0105830	1.9058280
N	-6.4794550	0.4791000	-0.2164040
C	-4.7492190	2.7247500	-0.9578770
H	-4.7919850	1.8414260	-1.5869520
C	-3.9861800	3.8197380	-1.3483010
C	-3.9547560	4.9479960	-0.5452910
H	-3.3592650	5.8007670	-0.8470210
C	-4.6810110	4.9702140	0.6353240
H	-4.6668730	5.8579260	1.2582590
C	-5.4163800	3.8671150	1.0282140
H	-5.9684230	3.8896510	1.9632540
C	-5.4474600	2.7207340	0.2400610
C	-6.1461140	1.4901690	0.7704620
H	-5.4676630	1.0197630	1.4895610
H	-7.0283160	1.7990260	1.3519310
C	-6.8412130	-0.7749780	0.4434860

H	-7.2939020	-1.4247170	-0.3061390
H	-7.6080390	-0.6145030	1.2163330
C	-5.6684040	-1.5137800	1.0444550
C	-4.8146930	-2.2523840	0.2298490
H	-4.9967850	-2.2691340	-0.8409390
C	-3.7704520	-2.9855850	0.7616880
H	-3.1210430	-3.5692530	0.1183300
C	-3.5418810	-2.9979480	2.1330460
C	-4.3824370	-2.2573730	2.9501480
H	-4.2267430	-2.2566250	4.0251250
C	-5.4377030	-1.5324690	2.4128160
H	-6.1013800	-0.9837100	3.0744060
C	-2.4536980	-3.8642080	2.7259130
H	-2.1640440	-3.4743170	3.7109510
H	-2.8381570	-4.8754310	2.8741770
C	-0.5268600	-2.8526890	1.8277120
H	-0.2920300	-2.4749650	2.8321700
H	-1.0520690	-2.0613890	1.2772490
C	0.7496090	-3.2199790	1.1038210
H	1.3535530	-3.8952000	1.7195510
H	0.5058970	-3.7300790	0.1650640
C	2.7263080	-2.2447110	0.2306780
H	2.5951170	-2.7784640	-0.7167550
H	3.3687450	-2.8406830	0.8869490
C	3.3998330	-0.9194330	-0.0032580
H	3.6295260	-0.4283260	0.9500230
H	4.3347950	-1.1005490	-0.5424820
C	3.1107360	1.1193850	-1.2187080
H	3.8940400	0.9052010	-1.9540540
H	3.5698160	1.6377850	-0.3677100
C	2.0219600	1.9607240	-1.8230090
C	1.0998980	2.5994810	-1.0013070

H	1.2036780	2.5301130	0.0780590
C	0.0706490	3.3571170	-1.5354270
H	-0.6338820	3.8662860	-0.8870700
C	-0.0548590	3.5005840	-2.9104120
C	0.8573460	2.8536880	-3.7349350
H	0.7758030	2.9552570	-4.8131910
C	1.8834040	2.0927380	-3.1987230
H	2.5915380	1.6030170	-3.8601620
C	-1.1052930	4.4211560	-3.4954620
H	-0.6350260	5.3794330	-3.7296180
H	-1.4872740	4.0104090	-4.4387050
C	-3.1967490	3.7553110	-2.6288400
H	-2.7904640	2.7424790	-2.7514640
H	-3.8506650	3.9507690	-3.4896650
O	3.5332630	-4.0458350	-2.8849610
C	6.9417310	-0.8379510	0.7154960
H	6.1818490	-0.1111280	1.0156570
H	6.8009910	-0.9883540	-0.3589890
C	-7.5031670	0.9147920	-1.1789180
H	-7.5648310	0.1504990	-1.9546440
H	-7.1250800	1.8146280	-1.6682050
C	-8.8701310	1.2356840	-0.6081970
C	-9.9340050	0.3205880	-0.5761420
C	-9.0672310	2.5107660	-0.0874230
C	-11.1536880	0.6931070	0.0417970
C	-9.8665190	-0.9916790	-1.1754930
C	-10.2546770	2.8818480	0.5081280
H	-8.2635070	3.2376030	-0.1638420
C	-12.2451170	-0.2292150	0.1071880
C	-11.3074100	1.9798250	0.5986700
C	-10.8951870	-1.8527930	-1.1207990
H	-8.9712820	-1.2864480	-1.7073330

H	-10.3753940	3.8840410	0.9059520
C	-12.1255580	-1.5126270	-0.4616660
C	-13.4518080	0.1402710	0.7389000
C	-12.5514390	2.3326590	1.2312610
H	-10.8170800	-2.8281840	-1.5900450
C	-13.1936280	-2.4006500	-0.3874610
C	-14.4984380	-0.7744260	0.7970010
C	-13.5673250	1.4593970	1.3022640
H	-12.6470320	3.3281440	1.6519090
C	-14.3698520	-2.0337780	0.2398820
H	-13.0956290	-3.3864160	-0.8302420
H	-15.4241480	-0.4872200	1.2846870
H	-14.5005450	1.7337260	1.7827670
H	-15.1959010	-2.7340120	0.2921960
C	8.3060840	-0.1989370	0.9250270
C	8.5605880	1.0590170	0.3502510
C	9.3156510	-0.8073630	1.6552800
C	9.8174690	1.6768440	0.5319460
C	7.5762290	1.7598620	-0.4388100
C	10.5505310	-0.2086200	1.8343950
H	9.1477750	-1.7755990	2.1060740
C	10.0852070	2.9579080	-0.0434480
C	10.8235510	1.0340540	1.2848450
C	7.8292680	2.9634890	-0.9805370
H	6.6096920	1.3012570	-0.6061760
H	11.3158380	-0.7144920	2.4138390
C	9.0966840	3.6151630	-0.8021250
C	11.3423710	3.5717460	0.1446070
C	12.0975920	1.6829660	1.4596840
H	7.0728390	3.4689390	-1.5726410
C	9.3718510	4.8626280	-1.3557050
C	11.5813040	4.8182640	-0.4225760

C	12.3439210	2.8859220	0.9202870
H	12.8569480	1.1717850	2.0420540
C	10.6042230	5.4578010	-1.1659330
H	8.6075260	5.3644700	-1.9401040
H	12.5481200	5.2886250	-0.2768190
H	13.3063440	3.3674020	1.0575050
H	10.8082500	6.4294660	-1.6015160
Na	0.3366050	-0.3149660	-0.2572940