Supporting Information

Dendritic Molecular Switch: Chiral Folding and Helicity Inversion

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Table S1. Computed energies of (M)-$(S,S)_3$-**2** and (P)-$(S,S)_3$-**2**.

	(M)-$(S,S)_3$-**2**	(P)-$(S,S)_3$-**2**
G_{gas}/eV	–107829.122	–107828.597
G_{solv}/kcal mol^{-1}	–24.43	–24.70
G_{sol}/kcal mol^{-1}	–2486622.459	–2486610.622

Table S2. Comparison of calculated excitation energy, wavelength, and rotationals strength of (M)-$(S,S)_3$-**2**.

	BP86/TZP			LB94/TZP		
	eV	λ/nm	R_{vel}	eV	λ/nm	R_{vel}
1	2.4667	503	46.026	2.4667	503	46.423
2	2.5012	496	-15.31	2.5012	496	-15.3
3	2.5065	495	-16.485	2.5065	495	-16.529
4	2.7279	455	26.452	2.7279	455	26.194
5	2.7324	454	16.096	2.7324	454	15.91
6	2.7515	451	10.909	2.7544	450	14.234
7	2.7544	450	14.234	2.8335	438	18.089
8	2.8335	438	17.445	2.8836	430	30.426
9	2.8836	430	31.048	2.9955	414	11.605
10	2.9955	414	11.457	2.9995	414	14.139
11	2.9995	414	13.985	3.1906	389	15.079
12	3.1906	389	15.048	3.2324	384	11.55
13	3.2324	384	10.636	3.2639	380	-15.884
14	3.2639	380	-15.878	3.2644	380	-14.18
15	3.2644	380	-14.178	3.2754	379	11.5
16	3.2754	379	11.878	3.301	376	-60.376
17	3.301	376	-59.421	3.3051	375	-70.77
18	3.3051	375	-69.803	3.3111	375	11.067
19	3.312	375	73.449	3.312	375	75.277
20	3.4377	361	11.245	3.4377	361	12.151
21	3.4418	360	16.879	3.4418	360	16.935
22	3.5657	348	45.622	3.5657	348	45.231
23	3.5692	348	30.909	3.5692	348	30.518
24	3.6272	342	153.98	3.6272	342	153.13
25	3.6448	340	12.155	3.6448	340	11.86
26	3.646	340	-37.278	3.646	340	-37.637
27	3.6538	340	-62.111	3.6538	340	-62.138
28	3.6746	338	25.249	3.6746	338	25.591
29	3.6853	337	11.443	3.6853	337	11.232
30	3.6999	335	-13.078	3.6999	335	-13.098

Table S3. Cartesian coordinates of atoms in (M)-$(S,S)_3$-**2**.

Number	Atom	x	y	z
1	C	-0.091	-1.463	0.494
2	C	1.313	0.653	0.494
3	C	-1.222	0.81	0.494
4	C	0.086	1.437	0.468
5	C	-1.287	-0.644	0.468
6	C	1.201	-0.792	0.468
7	O	-0.178	-2.725	0.52
8	O	2.449	1.209	0.52
9	O	-2.271	1.517	0.52
10	C	-2.554	-1.201	0.361
11	H	-3.386	-0.521	0.258
12	C	0.237	2.813	0.361
13	H	1.242	3.193	0.258
14	C	2.318	-1.611	0.361
15	H	2.144	-2.672	0.258
16	N	-2.822	-2.505	0.352
17	N	3.581	-1.191	0.352
18	N	-0.759	3.696	0.352
19	H	-1.695	3.27	0.364
20	H	-1.985	-3.103	0.364
21	H	3.679	-0.167	0.364
22	C	-4.071	-3.118	0.168
23	C	-6.484	-4.479	-0.29
24	C	-5.297	-2.528	0.56
25	C	-4.061	-4.409	-0.417
26	C	-5.276	-5.073	-0.641
27	C	-6.491	-3.225	0.308
28	H	-5.25	-6.055	-1.1
29	H	-7.424	-2.76	0.606
30	H	-7.42	-4.997	-0.476
31	C	-5.356	-1.273	1.237
32	C	-5.389	-0.204	1.808
33	C	-2.822	-5.012	-0.779
34	C	-1.739	-5.476	-1.063
35	C	4.736	-1.967	0.168
36	C	7.121	-3.376	-0.29
37	C	5.849	-1.313	-0.417
38	C	4.838	-3.323	0.56
39	C	6.039	-4.009	0.308
40	C	7.031	-2.033	-0.641
41	H	6.102	-5.05	0.606
42	H	7.869	-1.519	-1.1
43	H	8.037	-3.928	-0.476
44	C	5.752	0.062	-0.779
45	C	5.612	1.232	-1.063
46	C	3.78	-4.002	1.237
47	C	2.871	-4.565	1.808
48	C	-0.665	5.085	0.168
49	C	-0.637	7.855	-0.29
50	C	-1.788	5.722	-0.417

Table S3. Cartesian coordinates of atoms in (M)-$(S,S)_3$-**2** (cont'd).

Number	Atom	x	y	z
51	C	0.459	5.851	0.56
52	C	0.453	7.234	0.308
53	C	-1.755	7.106	-0.641
54	H	1.322	7.809	0.606
55	H	-2.619	7.574	-1.1
56	H	-0.617	8.924	-0.476
57	C	-2.929	4.95	-0.779
58	C	-3.873	4.244	-1.063
59	C	1.576	5.275	1.237
60	C	2.518	4.769	1.808
61	C	-0.413	-6.035	-1.395
62	C	1.709	-5.153	2.495
63	H	1.527	-4.556	3.401
64	C	3.608	4.057	2.495
65	H	3.182	3.6	3.401
66	C	-5.02	3.375	-1.395
67	H	-4.629	2.348	-1.482
68	C	5.433	2.66	-1.395
69	H	4.348	2.835	-1.482
70	C	-5.317	1.096	2.495
71	H	-4.709	0.956	3.401
72	O	0.544	-5.121	1.665
73	H	0.396	-4.21	1.331
74	O	4.163	3.032	1.665
75	H	3.448	2.448	1.331
76	O	0.022	-6.942	-0.401
77	H	0.13	-6.425	0.424
78	O	-4.707	2.089	1.665
79	H	-3.844	1.762	1.331
80	O	-6.023	3.452	-0.401
81	H	-5.629	3.1	0.424
82	O	6.001	3.49	-0.401
83	H	5.499	3.325	0.424
84	C	-6.686	1.597	2.921
85	C	-9.185	2.583	3.705
86	C	-6.971	1.802	4.271
87	C	-7.664	1.882	1.961
88	C	-8.904	2.379	2.353
89	C	-8.217	2.292	4.665
90	H	-6.213	1.587	5.02
91	H	-7.443	1.747	0.906
92	H	-9.652	2.613	1.6
93	H	-8.426	2.453	5.719
94	H	-10.153	2.973	4.008
95	C	-5.606	3.783	-2.738
96	C	-6.624	4.602	-5.214
97	C	-5.147	3.197	-3.918
98	C	-6.582	4.78	-2.801
99	C	-7.09	5.186	-4.034
100	C	-5.651	3.604	-5.153

Table S3. Cartesian coordinates of atoms in (M)-$(S,S)_3$-**2** (cont'd).

Number	Atom	x	y	z
101	H	-4.389	2.418	-3.874
102	H	-6.942	5.221	-1.877
103	H	-7.85	5.961	-4.076
104	H	-5.288	3.14	-6.066
105	H	-7.02	4.921	-6.174
106	C	6.079	2.964	-2.738
107	C	7.297	3.436	-5.214
108	C	7.431	3.311	-2.801
109	C	5.342	2.859	-3.918
110	C	5.947	3.092	-5.153
111	C	8.036	3.547	-4.034
112	H	7.992	3.401	-1.877
113	H	4.288	2.592	-3.874
114	H	5.364	3.01	-6.066
115	H	9.088	3.818	-4.076
116	H	7.772	3.619	-6.174
117	C	1.96	-6.589	2.921
118	C	2.355	-9.246	3.705
119	C	2.202	-7.578	1.961
120	C	1.925	-6.938	4.271
121	C	2.124	-8.262	4.665
122	C	2.392	-8.901	2.353
123	H	2.208	-7.319	0.906
124	H	1.731	-6.174	5.02
125	H	2.088	-8.524	5.719
126	H	2.563	-9.665	1.6
127	H	2.501	-10.279	4.008
128	C	4.726	4.992	2.921
129	C	6.829	6.663	3.705
130	C	5.046	5.136	4.271
131	C	5.462	5.696	1.961
132	C	6.512	6.522	2.353
133	C	6.093	5.97	4.665
134	H	4.481	4.587	5.02
135	H	5.234	5.572	0.906
136	H	7.089	7.052	1.6
137	H	6.338	6.071	5.719
138	H	7.651	7.306	4.008
139	H	0.281	-5.183	-1.482
140	C	-0.473	-6.747	-2.738
141	C	-0.673	-8.038	-5.214
142	C	-0.195	-6.056	-3.918
143	C	-0.848	-8.091	-2.801
144	C	-0.946	-8.733	-4.034
145	C	-0.296	-6.696	-5.153
146	H	0.101	-5.01	-3.874
147	H	-1.05	-8.622	-1.877
148	H	-1.238	-9.779	-4.076
149	H	-0.075	-6.15	-6.066
150	H	-0.752	-8.54	-6.174

Table S4. Cartesian coordinates of atoms in (P)-$(S,S)_3$-**2**.

Number	Atom	x	y	z
1	O	-0.447	-2.693	0.416
2	C	-0.243	-1.441	0.442
3	C	1.117	-0.923	0.446
4	C	2.236	-1.769	0.389
5	N	2.156	-3.096	0.313
6	C	3.141	-4.082	0.111
7	C	2.663	-5.305	-0.442
8	C	4.514	-3.957	0.433
9	H	3.227	-1.333	0.394
10	H	1.176	-3.419	0.294
11	C	1.306	-5.427	-0.857
12	C	0.158	-5.458	-1.241
13	C	-1.236	-5.351	-1.695
14	O	-2.003	-4.577	-0.778
15	H	-1.441	-3.862	-0.401
16	H	-1.692	-6.35	-1.701
17	C	3.537	-6.384	-0.624
18	H	3.143	-7.303	-1.043
19	C	4.882	-6.266	-0.291
20	H	5.558	-7.103	-0.435
21	C	5.358	-5.066	0.218
22	H	6.406	-4.952	0.472
23	C	5.144	-2.792	0.966
24	C	5.877	-1.926	1.4
25	C	6.745	-0.841	1.893
26	O	7.067	0.084	0.873
27	H	6.26	0.263	0.345
28	H	7.695	-1.297	2.202
29	O	-2.109	1.733	0.416
30	C	-1.127	0.931	0.442
31	C	-1.358	-0.506	0.446
32	C	-2.65	-1.052	0.389
33	N	-3.76	-0.319	0.313
34	C	-5.106	-0.679	0.111
35	C	-5.926	0.346	-0.442
36	C	-5.684	-1.931	0.433
37	H	-2.768	-2.128	0.394
38	H	-3.549	0.691	0.294
39	C	-5.353	1.583	-0.857
40	C	-4.806	2.592	-1.241
41	C	-4.016	3.747	-1.695
42	O	-2.962	4.023	-0.778
43	H	-2.624	3.179	-0.401
44	H	-4.653	4.64	-1.701
45	C	-7.297	0.128	-0.624
46	H	-7.896	0.93	-1.043
47	C	-7.867	-1.095	-0.291
48	H	-8.93	-1.261	-0.435
49	C	-7.066	-2.107	0.218
50	H	-7.491	-3.072	0.472

Table S4. Cartesian coordinates of atoms in (P)-$(S,S)_3$-**2** (cont'd).

Number	Atom	x	y	z
51	C	-4.989	-3.059	0.966
52	C	-4.606	-4.126	1.4
53	C	-4.101	-5.421	1.893
54	O	-3.46	-6.162	0.873
55	H	-2.903	-5.553	0.345
56	H	-4.971	-6.015	2.202
57	O	2.556	0.96	0.416
58	C	1.37	0.51	0.442
59	C	0.241	1.429	0.446
60	C	0.414	2.821	0.389
61	N	1.603	3.416	0.313
62	C	1.964	4.761	0.111
63	C	3.262	4.959	-0.442
64	C	1.169	5.888	0.433
65	H	-0.459	3.461	0.394
66	H	2.373	2.728	0.294
67	C	4.047	3.844	-0.857
68	C	4.648	2.866	-1.241
69	C	5.253	1.605	-1.695
70	O	4.965	0.554	-0.778
71	H	4.065	0.683	-0.401
72	H	6.345	1.71	-1.701
73	C	3.76	6.255	-0.624
74	H	4.753	6.373	-1.043
75	C	2.985	7.361	-0.291
76	H	3.373	8.365	-0.435
77	C	1.709	7.173	0.218
78	H	1.086	8.023	0.472
79	C	-0.154	5.85	0.966
80	C	-1.27	6.052	1.4
81	C	-2.644	6.262	1.893
82	O	-3.606	6.078	0.873
83	H	-3.358	5.29	0.345
84	H	-2.724	7.313	2.202
85	C	-2.896	5.404	3.131
86	C	-3.048	4.018	3.017
87	H	-2.984	3.539	2.044
88	C	-3.281	3.241	4.148
89	H	-3.399	2.165	4.047
90	C	-3.359	3.838	5.408
91	H	-3.541	3.23	6.29
92	C	-3.208	5.218	5.529
93	H	-3.271	5.692	6.505
94	C	-2.978	5.995	4.392
95	H	-2.86	7.072	4.488
96	C	-3.232	-5.21	3.131
97	C	-3.703	-5.576	4.392
98	H	-4.695	-6.013	4.488
99	C	-2.915	-5.387	5.529
100	H	-3.294	-5.678	6.505

Table S4. Cartesian coordinates of atoms in (P)-$(S,S)_3$-**2** (cont'd).

Number	Atom	x	y	z
101	C	-1.644	-4.829	5.408
102	H	-1.027	-4.682	6.29
103	C	-1.166	-4.462	4.148
104	H	-0.175	-4.026	4.047
105	C	-1.955	-4.648	3.017
106	H	-1.572	-4.354	2.044
107	C	6.128	-0.194	3.131
108	C	5.003	0.631	3.017
109	H	4.557	0.815	2.044
110	C	4.447	1.221	4.148
111	H	3.574	1.861	4.047
112	C	5.004	0.99	5.408
113	H	4.568	1.451	6.29
114	C	6.123	0.169	5.529
115	H	6.565	-0.013	6.505
116	C	6.681	-0.419	4.392
117	H	7.555	-1.059	4.488
118	C	-3.502	3.519	-3.12
119	C	-2.142	3.354	-3.377
120	H	-1.435	3.404	-2.556
121	C	-1.691	3.151	-4.682
122	H	-0.628	3.026	-4.87
123	C	-2.597	3.119	-5.739
124	H	-2.246	2.967	-6.756
125	C	-3.96	3.288	-5.488
126	H	-4.673	3.269	-6.309
127	C	-4.409	3.486	-4.184
128	H	-5.472	3.617	-3.992
129	C	4.799	1.274	-3.12
130	C	3.976	0.179	-3.377
131	H	3.666	-0.459	-2.556
132	C	3.575	-0.111	-4.682
133	H	2.935	-0.969	-4.87
134	C	4	0.69	-5.739
135	H	3.692	0.462	-6.756
136	C	4.828	1.786	-5.488
137	H	5.167	2.412	-6.309
138	C	5.223	2.076	-4.184
139	H	5.868	2.93	-3.992
140	C	-1.296	-4.793	-3.12
141	C	-0.814	-5.561	-4.184
142	H	-0.397	-6.547	-3.992
143	C	-0.867	-5.074	-5.488
144	H	-0.495	-5.681	-6.309
145	C	-1.403	-3.809	-5.739
146	H	-1.446	-3.428	-6.756
147	C	-1.884	-3.04	-4.682
148	H	-2.307	-2.057	-4.87
149	C	-1.833	-3.532	-3.377
150	H	-2.23	-2.945	-2.556

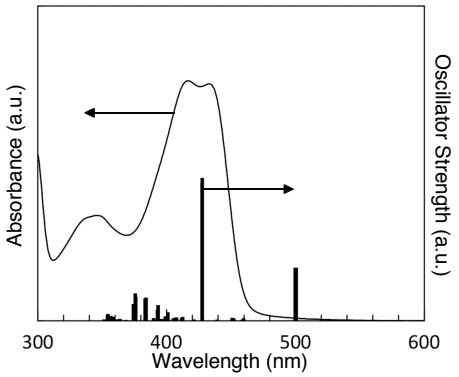

Figure S1. UV-vis spectrum of $(S,S)_3$-**3** ($CHCl_3$, 298 K) overlaid on the calculated plot of oscillator strength vs wavelength of DFT model $(S,S)_3$-**2**.

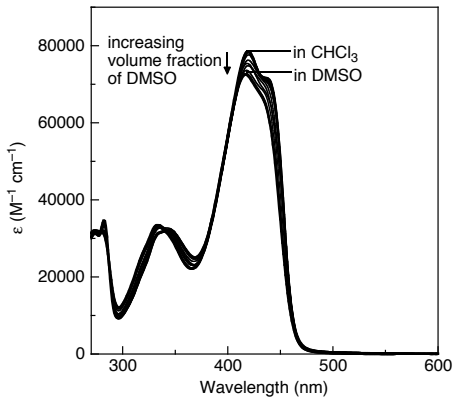

Figure S2. UV-vis spectra of $(S)_3$-**6** measured in $CHCl_3$-DMSO mixed solvents at 298 K; $CHCl_3$:DMSO (v/v) = 100:0, 90:10, 80:20, 70:30, 60:40, 40:60, 20:80, and 0:100 from top to bottom trace.

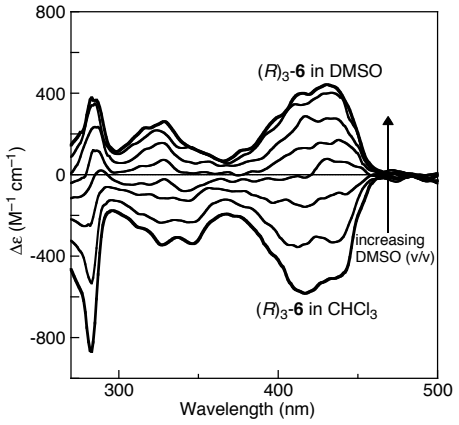

Figure S3. Changes in the CD spectrum of $(R)_3$-**6** with increasing volume fraction of DMSO in $CHCl_3$-DMSO mixed solvents at 298 K; $CHCl_3$:DMSO (v/v) = 100:0, 90:10, 80:20, 70:30, 60:40, 40:60, 20:80, and 0:100 from bottom to top trace.