Supporting Information:

Solvation Effects on the Thermal Helix Inversion of Molecular Motors from QM/MM Calculations

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Cartesian coordinates and dipole moments of the motors 1-5 in the S_0 state in gas phase.

Table S1: Coordinates of optimized **1a** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	-2.309526	4.175942	1.85388
C	-1.298093	4.214603	0.88896
C	-0.838611	3.016062	0.33952
C	-1.394517	1.767907	0.73099
C	-2.372819	1.743111	1.73511
C	-2.832216	2.946019	2.28107
C	0.236509	2.758058	-0.61817
C	0.379692	1.351449	-0.76059
C	-0.646956	0.676255	0.06827
C	1.286976	0.848727	-1.70293
C	1.022912	3.642279	-1.35952
C	1.954227	3.124995	-2.26521
C	2.074206	1.738224	-2.44066
H	2.790543	1.344337	-3.16514
H	1.384441	-0.223429	-1.86684
H	0.900861	4.721745	-1.24392
H	2.579488	3.802965	-2.85051
H	-0.861602	5.167511	0.58092
H	-2.680917	5.105203	2.29155
H	-3.602444	2.924919	3.05534
H	-2.771149	0.798675	2.10673
C	-0.896456	-0.675708	0.16607
C	-2.294759	-1.293743	0.34706
C	0.049673	-1.786571	0.00886
C	-2.130602	-2.728591	-0.23612
C	-0.650460	-2.969404	-0.24238
C	-3.445328	-0.562935	-0.35560
H	-2.514927	-1.388002	1.42736
C	1.472210	-1.844260	0.23652
C	0.006618	-4.197187	-0.45438
C	1.382991	-4.246243	-0.37564
C	2.138564	-3.096601	-0.00515
H	-0.572542	-5.095613	-0.68029
H	1.913824	-5.184753	-0.55484
H	-2.531810	-2.757577	-1.26515
H	-2.676604	-3.493712	0.33807
H	-3.211347	-0.433212	-1.42477
H	-3.652480	0.429383	0.06005
H	-4.367459	-1.162364	-0.27853
C	3.546411	-3.184015	0.18051
C	4.271306	-2.103508	0.63662
C	3.605197	-0.894579	0.94815
C	2.243685	-0.768936	0.75256
H	4.042298	-4.135893	-0.02665
H	5.350970	-2.184871	0.78017
H	4.170888	-0.051837	1.35140
H	1.749135	0.165177	1.00723

Table S2: Coordinates of optimized **1b** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	-2.912728	4.383407	0.32485
C	-1.514907	4.380350	0.35943
C	-0.839991	3.159646	0.40082
C	-1.541646	1.923432	0.40783
C	-2.942664	1.945620	0.35330
C	-3.616771	3.172342	0.32043
C	0.594785	2.879494	0.44679
C	0.777924	1.471943	0.44595
C	-0.552893	0.811518	0.38992
C	2.068128	0.956617	0.62778
C	1.679029	3.753062	0.54798
C	2.966186	3.222557	0.67739
C	3.152558	1.834416	0.73350
H	4.157461	1.427231	0.86550
H	2.239976	-0.114756	0.69866
H	1.521350	4.833994	0.54528
H	3.826311	3.891231	0.75658
H	-0.957392	5.319686	0.35121
H	-3.456449	5.330216	0.29483
H	-4.708541	3.180504	0.28604
H	-3.526689	1.028946	0.32735
C	-0.831801	-0.530009	0.38380
C	-2.151836	-1.146856	0.85233
C	0.064244	-1.677580	0.14875
C	-1.652455	-2.393071	1.64072
C	-0.382255	-2.756894	0.91372
C	-3.056741	-1.569474	-0.31862
H	-2.692855	-0.459354	1.51544
C	1.131750	-1.859030	-0.79059
C	0.298258	-3.990529	0.91814
C	1.403543	-4.152430	0.10592
C	1.825837	-3.118820	-0.77874
H	-0.052473	-4.808697	1.55164
H	1.948718	-5.099806	0.09941
H	-2.384732	-3.215863	1.65188
H	-1.441869	-2.120455	2.68977
H	-2.548325	-2.320005	-0.94523
H	-3.310852	-0.715250	-0.96408
H	-3.994088	-2.012197	0.05609
C	2.900719	-3.323387	-1.68905
C	3.251981	-2.351738	-2.60196
C	2.527683	-1.135036	-2.65295
C	1.494676	-0.894949	-1.76992
H	3.434237	-4.277130	-1.66300
H	4.075637	-2.523750	-3.29838
H	2.787690	-0.380887	-3.39894
H	0.941752	0.041837	-1.81815

Table S3: Coordinates of optimized transition state between **1a** and **1b** configurations in the S_0 state at B3LYP/cc-pVDZ level.

C	-4.926138	-0.939191	1.09448
C	-4.231275	0.266704	1.24359
C	-2.999065	0.424334	0.61241
C	-2.391739	-0.632811	-0.12439
C	-3.141054	-1.801017	-0.32678
C	-4.395576	-1.947341	0.28554
C	-2.209721	1.639113	0.40967
C	-1.107460	1.309203	-0.42535
C	-1.004747	-0.181275	-0.51617
C	-0.534414	2.345591	-1.16844
C	-2.532322	2.963599	0.70674
C	-1.822689	3.992251	0.07808
C	-0.870577	3.679149	-0.89793
H	-0.402417	4.476884	-1.47850
H	0.114090	2.132873	-2.01531
H	-3.368922	3.192541	1.37088
H	-2.066092	5.035562	0.29096
H	-4.662843	1.087799	1.82004
H	-5.897998	-1.074919	1.57366
H	-4.969036	-2.859597	0.10728
H	-2.805047	-2.585342	-1.00071
C	0.073064	-1.051470	-0.49448
C	-0.212384	-2.555479	-0.62927
C	1.529699	-0.952614	-0.12678
C	0.922647	-3.283230	0.09898
C	1.945035	-2.216102	0.31838
C	-0.307466	-2.944502	-2.11415
H	-1.155712	-2.806866	-0.13811
C	2.502043	0.118027	-0.03380
C	3.176574	-2.450249	0.96627
C	4.045513	-1.409189	1.17618
C	3.742044	-0.117348	0.66565
H	3.411440	-3.459040	1.31507
H	4.989329	-1.562113	1.70543
H	1.335902	-4.122005	-0.48654
H	0.586887	-3.704834	1.06172
H	0.647658	-2.746260	-2.62797
H	-1.090251	-2.365283	-2.62841
H	-0.538203	-4.017854	-2.22123
C	4.686882	0.936659	0.80260
C	4.472374	2.173433	0.23273
C	3.300968	2.384064	-0.52657
C	2.360432	1.380553	-0.64989
H	5.606537	0.736547	1.35818
H	5.210380	2.971284	0.34328
H	3.135899	3.340402	-1.02738
H	1.491352	1.546103	-1.26153

Table S4: Coordinates of optimized **2a** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	-5.095025	-0.733878	1.23501
C	-4.445754	0.440013	0.83865
C	-3.122257	0.369159	0.39918
C	-2.439371	-0.876201	0.33073
C	-3.087435	-2.035172	0.77949
C	-4.414075	-1.960030	1.21729
C	-2.191563	1.423235	0.00061
C	-0.922305	0.830264	-0.25064
C	-1.034066	-0.637732	-0.06823
C	0.120641	1.615728	-0.73912
C	-2.380904	2.789232	-0.18784
C	-1.320704	3.586209	-0.63864
C	-0.076873	2.994547	-0.92211
H	1.097990	1.205132	-0.98418
H	-3.355981	3.244602	-0.00004
H	-1.478171	4.654586	-0.77927
H	-4.961270	1.402025	0.88785
H	-6.130971	-0.693190	1.57912
H	-4.920826	-2.866461	1.55596
H	-2.567121	-2.993039	0.80555
C	-0.059354	-1.588019	-0.28076
C	-0.322130	-3.001212	-0.83218
C	1.395220	-1.438984	-0.15212
C	1.039660	-3.389877	-1.48096
C	2.037307	-2.461015	-0.85581
C	-1.453247	-3.120626	-1.86063
H	-0.507658	-3.693455	0.01095
C	2.175822	-0.556953	0.67881
C	3.441112	-2.556134	-0.92197
C	4.210724	-1.634959	-0.24204
C	3.609054	-0.644491	0.58657
H	3.908514	-3.350476	-1.50868
H	5.301562	-1.679005	-0.29545
H	0.988993	-3.225211	-2.57231
H	1.302569	-4.449144	-1.33226
H	-1.293291	-2.402202	-2.68099
H	-2.447605	-2.928873	-1.44255
H	-1.456378	-4.135438	-2.29169
C	4.412262	0.231594	1.36850
C	3.839343	1.124898	2.24857
C	2.432508	1.157434	2.39683
C	1.623780	0.339569	1.63233
H	5.499326	0.168609	1.27245
H	4.467071	1.789031	2.84675
H	1.979390	1.832916	3.12575
H	0.545598	0.372104	1.76835
O	1.015118	3.674337	-1.38648
C	0.900131	5.071081	-1.59602
H	0.661579	5.609486	-0.65998
H	1.880390	5.404768	-1.96211
H	0.130345	5.312468	-2.35240

Table S5: Coordinates of optimized **2b** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	5.310499	-0.790058	0.65680
C	4.605839	0.405910	0.48621
C	3.236829	0.355952	0.21952
C	2.547411	-0.883874	0.11847
C	3.266468	-2.071639	0.31196
C	4.641695	-2.017634	0.57133
C	2.280073	1.438048	-0.00108
C	0.993377	0.868520	-0.20507
C	1.101446	-0.612171	-0.10754
C	-0.067929	1.693228	-0.57337
C	2.470155	2.813253	-0.09570
C	1.391245	3.647193	-0.41650
C	0.130151	3.081759	-0.66932
H	-1.060165	1.312163	-0.79895
H	3.459765	3.248151	0.06156
H	1.548793	4.722577	-0.48579
H	5.118392	1.367587	0.56327
H	6.382856	-0.766856	0.86351
H	5.195591	-2.948344	0.71312
H	2.780902	-3.043771	0.27441
C	0.106564	-1.542094	-0.25570
C	0.331059	-2.997367	-0.67300
C	-1.357217	-1.361823	-0.26871
C	-0.844166	-3.221962	-1.66926
C	-1.916264	-2.310237	-1.12733
C	0.236121	-3.974971	0.51170
H	1.297594	-3.115344	-1.17998
C	-2.208230	-0.527212	0.52722
C	-3.303356	-2.360783	-1.36882
C	-4.135309	-1.484200	-0.70017
C	-3.622805	-0.578512	0.27254
H	-3.712024	-3.090927	-2.07144
H	-5.213523	-1.502762	-0.87882
H	-1.168435	-4.273467	-1.72083
H	-0.543978	-2.915853	-2.68679
H	-0.760774	-3.917391	0.97792
H	0.980125	-3.744075	1.28893
H	0.398230	-5.011428	0.17317
C	-4.491915	0.252089	1.03442
C	-4.000633	1.065313	2.03335
C	-2.614032	1.068236	2.32436
C	-1.740574	0.292176	1.59025
H	-5.564019	0.220557	0.82335
H	-4.679229	1.694662	2.61339
H	-2.232935	1.688964	3.13821
H	-0.676868	0.298054	1.82265
O	-0.981684	3.794860	-1.02274
C	-0.866997	5.201441	-1.15011
H	-1.863039	5.562289	-1.43979
H	-0.573209	5.678492	-0.19663
H	-0.137608	5.486364	-1.93100

Table S6: Coordinates of optimized transition state between **2a** and **2b** configurations in the S_0 state at B3LYP/cc-pVDZ level.

C	4.738677	-1.944209	-1.09743
C	4.154228	-0.700177	-1.36244
C	2.952553	-0.365224	-0.74076
C	2.266171	-1.284650	0.10549
C	2.907626	-2.491779	0.41642
C	4.132837	-2.814706	-0.18799
C	2.274367	0.928109	-0.66427
C	1.165136	0.784899	0.21710
C	0.931270	-0.672271	0.46074
C	0.684833	1.927042	0.84522
C	2.690426	2.184333	-1.09026
C	2.068863	3.336862	-0.58589
C	1.099734	3.202544	0.41743
H	0.032255	1.892253	1.71342
H	3.532953	2.284584	-1.77811
H	2.394732	4.317724	-0.92913
H	4.648397	0.015255	-2.02385
H	5.685656	-2.215807	-1.56905
H	4.622429	-3.755179	0.07456
H	2.511155	-3.171741	1.16698
C	-0.224217	-1.432416	0.53544
C	-0.077047	-2.934993	0.82287
C	-1.670505	-1.233840	0.16687
C	-1.294396	-3.623267	0.19533
C	-2.211396	-2.491595	-0.13682
C	0.022906	-3.176303	2.33808
H	0.826359	-3.322428	0.34398
C	-2.536166	-0.089552	-0.04345
C	-3.467146	-2.672553	-0.75505
C	-4.231187	-1.580372	-1.08249
C	-3.797308	-0.275982	-0.71935
H	-3.803404	-3.685411	-0.98975
H	-5.189593	-1.697468	-1.59437
H	-1.775344	-4.342776	0.87954
H	-1.023570	-4.186138	-0.71438
H	-0.896045	-2.837751	2.84528
H	0.868593	-2.622973	2.77525
H	0.157159	-4.249722	2.55317
C	-4.630101	0.847308	-0.98018
C	-4.287013	2.113070	-0.55351
C	-3.098862	2.287398	0.18920
C	-2.268363	1.211723	0.43292
H	-5.568527	0.680298	-1.51539
H	-4.939633	2.963869	-0.76129
H	-2.827035	3.270146	0.58147
H	-1.389836	1.353950	1.03479
O	0.495401	4.242757	1.06968
C	0.901663	5.562513	0.74495
H	0.690107	5.807549	-0.31209
H	0.316025	6.228840	1.39226
H	1.978453	5.719389	0.94027

Table S7: Coordinates of optimized **3a** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	-4.788078	1.885124	0.46213
C	-4.683285	0.494116	0.35596
C	-3.441485	-0.069779	0.06193
C	-2.291542	0.740395	-0.13687
C	-2.404888	2.130239	0.00605
C	-3.654742	2.691742	0.29454
C	-3.050044	-1.472492	-0.08459
C	-1.653639	-1.526201	-0.33768
C	-1.118841	-0.140355	-0.37242
C	-1.063996	-2.760966	-0.63757
C	-3.826972	-2.631791	-0.06194
C	-3.214349	-3.863165	-0.31600
C	-1.846416	-3.921032	-0.61580
H	-1.380691	-4.883306	-0.83975
H	-0.009775	-2.831665	-0.89550
H	-4.900085	-2.575211	0.13423
H	-3.807273	-4.780451	-0.29989
H	-5.558200	-0.141904	0.50859
H	-5.753263	2.343059	0.68991
H	-3.740848	3.775583	0.39945
H	-1.538846	2.784075	-0.07307
C	0.158025	0.271035	-0.64924
C	1.418047	-0.490451	-0.65376
C	1.647603	1.273031	-2.24180
C	2.280328	0.066690	-1.59938
C	0.967511	2.684175	-0.22946
C	1.888821	-1.520584	0.22566
C	3.562036	-0.467446	-1.83602
C	3.996214	-1.536205	-1.07680
C	3.197237	-2.064047	-0.02200
H	4.204780	-0.031819	-2.60448
H	4.985924	-1.967454	-1.24754
H	2.359607	2.097564	-2.39411
H	1.214410	1.015117	-3.22420
C	3.688961	-3.094182	0.82774
C	2.949927	-3.540966	1.90278
C	1.688222	-2.960891	2.18238
C	1.170530	-1.977018	1.36412
H	4.677030	-3.514405	0.62274
H	3.342148	-4.328098	2.55048
H	1.120003	-3.293643	3.05371
H	0.199693	-1.537562	1.58767
C	0.502619	1.639609	-1.23988
C	1.080553	4.022614	-0.64149
C	1.512285	5.013036	0.24273
C	1.840635	4.679613	1.56139
C	1.727548	3.352625	1.98273
C	1.292158	2.362856	1.09534
H	-0.357088	2.048533	-1.78874
H	0.819927	4.290025	-1.66976
H	1.588717	6.048853	-0.09667
H	1.196263	1.332795	1.44196
H	2.176566	5.452054	2.25685
H	1.975102	3.081879	3.01184

Table S8: Coordinates of optimized **3b** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	3.765972	2.468619	-1.76357
C	2.864277	3.087558	-0.89141
C	1.772847	2.357627	-0.41839
C	1.576659	1.002649	-0.79559
C	2.460599	0.412488	-1.70691
C	3.556379	1.144401	-2.17492
C	0.662692	2.757953	0.44695
C	-0.240249	1.665582	0.55262
C	0.307536	0.515840	-0.21123
C	-1.336836	1.768674	1.41876
C	0.441749	3.947391	1.14350
C	-0.681725	4.050979	1.97001
C	-1.554984	2.963307	2.11328
H	-2.418214	3.045332	2.77751
H	-2.018711	0.932136	1.56022
H	1.145645	4.778231	1.05606
H	-0.870575	4.976097	2.51931
H	3.004657	4.129641	-0.59521
H	4.627946	3.024197	-2.13979
H	4.254701	0.676801	-2.87249
H	2.306936	-0.605109	-2.05965
C	-0.196810	-0.762272	-0.27605
C	0.644827	-2.046585	-0.40056
C	-1.591583	-1.198884	-0.12379
C	-0.237002	-3.103097	0.34388
C	-1.626124	-2.543636	0.25121
C	2.056380	-2.046948	0.15702
H	0.682685	-2.343350	-1.46453
C	-2.819621	-0.523011	-0.45082
C	-2.837519	-3.223042	0.48425
C	-4.030089	-2.553816	0.29770
C	-4.053755	-1.217027	-0.19398
H	-2.826869	-4.266428	0.80781
H	-4.981439	-3.057813	0.48634
H	0.091013	-3.174061	1.39502
H	-0.146290	-4.110276	-0.09055
C	-5.287879	-0.569491	-0.48138
C	-5.315570	0.688940	-1.04373
C	-4.100933	1.342989	-1.36144
C	-2.886515	0.753213	-1.07178
H	-6.218880	-1.099547	-0.26421
H	-6.269518	1.173076	-1.26396
H	-4.122712	2.322805	-1.84342
H	-1.962857	1.267019	-1.32885
C	2.366965	-1.412063	1.36960
C	3.658582	-1.471902	1.89490
C	4.663455	-2.175742	1.22224
C	4.362378	-2.823317	0.02184
C	3.067634	-2.758496	-0.50216
H	2.840917	-3.260730	-1.44720
H	5.137582	-3.376888	-0.51334
H	5.675397	-2.216562	1.63148
H	3.883884	-0.959605	2.83320
H	1.594279	-0.848241	1.89578

Table S9: Coordinates of optimized transition state between **3a** and **3b** configurations in the S_0 state at B3LYP/cc-pVDZ level.

C	0.800975	-3.802230	1.93182
C	0.205254	-4.793136	1.14485
C	-0.724500	-4.430847	0.16316
H	-1.298635	-5.195150	-0.36529
H	0.404290	-5.847594	1.34818
H	1.430331	-4.083455	2.77891
C	0.569905	-2.444567	1.66936
H	0.946536	-1.706377	2.37461
C	-0.216861	-2.060934	0.57959
C	-0.969287	-3.077841	-0.06961
C	-2.116962	-2.441479	-0.71903
C	-3.209902	-3.024397	-1.35729
H	-3.209848	-4.093001	-1.58390
C	-4.323002	-2.232303	-1.66351
H	-5.192060	-2.675942	-2.15415
C	-4.340366	-0.886441	-1.28783
H	-5.237939	-0.286840	-1.45552
C	-3.228383	-0.290459	-0.67235
H	-3.314588	0.737052	-0.32688
C	-2.073371	-1.047346	-0.43474
C	-0.693691	-0.728490	0.08833
C	-0.035660	0.434417	-0.27402
C	-0.891293	1.616904	-0.76187
C	-1.422749	2.479945	0.37692
C	-0.806483	2.532277	1.63517
C	-1.296992	3.376652	2.63619
C	-2.414716	4.180904	2.39833
C	-3.038953	4.136839	1.14754
C	-2.544096	3.295395	0.14856
H	-3.036387	3.267524	-0.82815
H	-3.916287	4.757414	0.94969
H	-2.799898	4.835694	3.18322
H	-0.802011	3.402700	3.60999
H	0.063065	1.904711	1.83679
H	-1.751211	1.246666	-1.32758
C	-0.003912	2.424473	-1.72737
H	-0.070344	3.509932	-1.55456
H	-0.289869	2.246755	-2.77852
C	1.368399	1.902210	-1.46119
C	2.516716	2.405282	-2.10811
C	3.743761	1.847492	-1.85142
H	4.642078	2.205280	-2.36043
H	2.408728	3.225444	-2.82182
C	1.390206	0.829948	-0.55792
C	2.696575	0.315703	-0.19635
C	3.864142	0.812698	-0.88444
C	5.148099	0.292003	-0.56408
H	6.011401	0.672877	-1.11585
C	5.315765	-0.651218	0.42729
H	6.309382	-1.038415	0.66283
C	4.187242	-1.087533	1.15451
H	4.303573	-1.803544	1.97143
C	2.929683	-0.608792	0.84452
H	2.086426	-0.932509	1.42684

Table S10: Coordinates of optimized **4a** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	-4.812101	-0.454717	-1.79913
C	-4.247638	-1.378944	-0.91567
C	-2.952966	-1.159898	-0.43951
C	-2.208343	-0.013315	-0.83075
C	-2.776385	0.884173	-1.74589
C	-4.074490	0.664586	-2.21548
C	-2.122268	-1.960133	0.45811
C	-0.846548	-1.339752	0.55516
C	-0.849789	-0.100097	-0.25002
C	0.086691	-1.837131	1.47728
C	-2.428763	-3.098377	1.20725
C	-1.467133	-3.615281	2.08082
C	-0.225119	-2.977148	2.22315
H	0.508524	-3.371752	2.92965
H	1.047771	-1.343961	1.61681
H	-3.413816	-3.564046	1.12750
H	-1.691321	-4.505680	2.67248
H	-4.806608	-2.265890	-0.60842
H	-5.824860	-0.609688	-2.17760
H	-4.517229	1.372607	-2.91974
H	-2.218605	1.749585	-2.10296
C	0.157821	0.844645	-0.35145
C	-0.103450	2.365294	-0.30305
C	1.605477	0.636474	-0.37524
C	1.276237	2.996580	-0.60123
C	2.253907	1.878748	-0.39516
C	-0.667079	2.844055	1.10424
H	-0.843530	2.681799	-1.04844
C	2.405352	-0.554701	-0.55985
C	3.654271	1.999340	-0.31971
C	4.427379	0.857899	-0.28043
C	3.834873	-0.427399	-0.44324
H	4.115032	2.989491	-0.29001
H	5.514140	0.926247	-0.18683
H	1.502916	3.877786	0.01260
H	1.343247	3.328768	-1.65252
C	0.301568	2.479822	2.24484
C	-2.041745	2.229702	1.42406
C	-0.864158	4.374622	1.05106
C	4.652305	-1.585087	-0.56453
C	4.105012	-2.813987	-0.86816
C	2.712894	-2.919801	-1.09083
C	1.887825	-1.821442	-0.93825
H	5.733032	-1.475158	-0.44266
H	4.744464	-3.693597	-0.96928
H	2.281743	-3.876842	-1.39245
H	0.824265	-1.924770	-1.13244
H	0.078311	4.926067	0.91639
H	-1.541942	4.656704	0.22787
H	-1.316084	4.729566	1.99122
H	-2.430713	2.676478	2.35388
H	-2.771708	2.422474	0.62401
H	-1.989541	1.144552	1.57991
H	1.303260	2.914989	2.10452
H	-0.090233	2.853579	3.20492
H	0.417652	1.388315	2.33163

Table S11: Coordinates of optimized **4b** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	-1.966018	-4.237854	-0.57549
C	-2.911548	-3.268484	-0.22836
C	-2.516467	-1.931009	-0.16584
C	-1.174828	-1.541190	-0.40981
C	-0.253983	-2.518163	-0.81137
C	-0.653430	-3.857367	-0.88461
C	-3.317427	-0.726112	0.04123
C	-2.474550	0.410574	-0.09712
C	-1.070162	-0.058267	-0.29732
C	-3.061916	1.681325	-0.01446
C	-4.685591	-0.600939	0.28708
C	-5.247095	0.675422	0.37894
C	-4.436805	1.805878	0.21795
H	-4.878653	2.803261	0.27364
H	-2.476167	2.587978	-0.13340
H	-5.309031	-1.491088	0.39683
H	-6.316638	0.791431	0.56735
H	-3.948688	-3.549234	-0.03167
H	-2.256648	-5.289376	-0.63050
H	0.072557	-4.613228	-1.19220
H	0.764441	-2.254153	-1.08286
C	0.066564	0.702769	-0.37139
C	0.125766	2.202401	-0.66588
C	1.470223	0.248825	-0.49092
C	1.201190	2.217554	-1.79779
C	2.121415	1.093101	-1.38865
C	0.494210	3.131604	0.56052
H	-0.830473	2.553952	-1.06740
C	2.210028	-0.729537	0.24308
C	3.472001	0.894593	-1.73707
C	4.183474	-0.117109	-1.12153
C	3.591749	-0.922365	-0.10599
H	3.952832	1.547795	-2.46913
H	5.233154	-0.285785	-1.37543
H	1.724963	3.178811	-1.90354
H	0.714143	2.001777	-2.76460
C	-0.336551	2.753157	1.80232
C	0.161839	4.580605	0.15588
C	1.980420	3.060242	0.97007
C	4.351776	-1.892560	0.60611
C	3.792912	-2.610679	1.64208
C	2.446455	-2.379309	2.02007
C	1.673956	-1.462997	1.33675
H	5.397299	-2.046954	0.32681
H	4.389720	-3.347758	2.18387
H	2.017303	-2.931305	2.85908
H	0.638308	-1.290817	1.62799
H	2.261348	2.059232	1.32690
H	2.662387	3.328489	0.14959
H	2.163230	3.771773	1.79228
H	0.399977	5.278279	0.97522
H	0.736313	4.899151	-0.72920
H	-0.909380	4.694762	-0.08030
H	-0.149137	1.711056	2.10403
H	-0.062659	3.404334	2.64863
H	-1.416142	2.862960	1.63741

Table S12: Coordinates of optimized transition state between **4a** and **4b** configurations in the S_0 state at B3LYP/cc-pVDZ level.

C	-2.357926	1.621585	0.71060
C	-2.441510	0.562794	-0.22277
C	-3.613777	0.539906	-1.06539
C	-4.542297	1.616014	-1.01120
C	-4.381324	2.660717	-0.12649
C	-3.285776	2.642692	0.76445
C	-3.870900	-0.574013	-1.91058
C	-3.027699	-1.657976	-1.89538
C	-1.862721	-1.626234	-1.10180
C	-1.488798	-0.521972	-0.32311
C	-0.860580	-2.736070	-1.05702
C	0.144277	-2.270851	0.00669
C	-0.063483	-0.757631	0.10125
C	1.029252	0.080703	0.24822
C	2.390330	-0.228055	-0.33445
C	2.957501	1.010987	-0.76165
C	2.184570	2.105874	-0.17723
C	1.108983	1.535082	0.55031
C	3.138730	-1.391323	-0.57188
C	4.340547	-1.328412	-1.29196
C	4.830071	-0.114020	-1.78049
C	4.140632	1.068712	-1.49681
C	0.533391	2.299085	1.57022
C	0.851990	3.657011	1.69488
C	1.787504	4.251496	0.83890
C	2.492184	3.463421	-0.07800
C	0.001386	-2.986041	1.40617
H	0.386159	4.247627	2.48673
H	-0.104722	1.832682	2.31903
H	3.310892	3.890875	-0.66115
H	2.019732	5.314168	0.93769
H	4.534053	2.033622	-1.82461
H	5.763177	-0.084818	-2.34704
H	4.908262	-2.247729	-1.45256
H	2.849013	-2.356119	-0.16365
H	1.150325	-2.501787	-0.33894
H	-3.233574	-2.540390	-2.50612
H	-4.763499	-0.565355	-2.54090
H	-1.337573	-3.702448	-0.83577
H	-0.365389	-2.847428	-2.03718
C	-1.419166	-2.855360	1.98425
C	1.002594	-2.389034	2.41305
C	0.345067	-4.477139	1.21950
H	-5.407423	1.585499	-1.67866
H	-5.106155	3.477014	-0.09423
H	-3.170752	3.434912	1.50778
H	-1.550486	1.608576	1.42293
H	-2.183624	-3.269481	1.30833
H	-1.489267	-3.401289	2.93962
H	-1.681040	-1.803834	2.17657
H	2.036811	-2.438262	2.03717
H	0.781968	-1.334878	2.63340
H	0.963065	-2.950176	3.36106
H	-0.351203	-4.983651	0.53324
H	1.364869	-4.603071	0.81825
H	0.298081	-5.005953	2.18536

Table S13: Coordinates of optimized **5a** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	0.294815	-2.387029	2.38785
C	-0.503057	-3.393545	1.85164
C	-1.401013	-3.101509	0.82452
H	-2.034855	-3.904320	0.43876
H	-0.444274	-4.412356	2.24583
H	0.983224	-2.604311	3.20941
C	0.209569	-1.099173	1.87201
H	0.823706	-0.292886	2.28851
C	-0.656947	-0.808784	0.81230
C	-1.502334	-1.810474	0.30314
C	-2.451326	-1.414952	-0.81951
C	-3.529379	-2.469718	-1.03337
H	-3.074598	-3.437043	-1.29748
H	-4.187908	-2.201926	-1.87376
H	-4.152253	-2.614129	-0.13514
C	-1.664904	-1.284387	-2.13909
H	-1.189349	-2.245849	-2.39939
H	-0.877073	-0.516698	-2.08466
H	-2.347969	-1.001311	-2.95760
C	-3.035997	-0.046923	-0.46128
C	-4.375722	0.252930	-0.71018
H	-5.030533	-0.503703	-1.14874
C	-4.917219	1.500351	-0.40975
H	-5.972916	1.701806	-0.61205
C	-4.106916	2.469576	0.16333
H	-4.513866	3.448001	0.43428
C	-2.765187	2.194056	0.41026
H	-2.172965	2.964211	0.90002
C	-2.192155	0.952861	0.09324
C	-0.767186	0.568984	0.30120
C	0.316859	1.374769	0.05453
C	0.219913	2.895628	0.12812
C	0.142390	3.295888	1.60594
H	-0.006274	4.382961	1.72004
H	1.089022	3.032024	2.10956
H	-0.658913	2.773231	2.15077
H	-0.657314	3.279806	-0.41851
C	1.526747	3.425770	-0.44595
H	1.883421	4.334219	0.07002
H	1.436438	3.690365	-1.51661
C	2.449559	2.261920	-0.31078
C	3.852870	2.327268	-0.37549
C	4.579564	1.165092	-0.33460
H	5.674308	1.182081	-0.34095
H	4.346736	3.302091	-0.44108
C	1.748904	1.060797	-0.16628
C	2.488238	-0.165553	-0.35083
C	3.921432	-0.092073	-0.36034
C	4.688598	-1.279721	-0.46767
H	5.780173	-1.192743	-0.43834
C	4.089389	-2.503693	-0.64223
H	4.693803	-3.410856	-0.73072
C	2.686815	-2.569156	-0.75128
H	2.194762	-3.525361	-0.95468
C	1.916293	-1.436232	-0.61019
H	0.839795	-1.525127	-0.73297

Table S14: Coordinates of optimized **5b** minimum in the S_0 state at B3LYP/cc-pVDZ level.

C	0.354469	-2.666790	-2.16899
C	-0.478367	-3.596263	-1.54316
C	-1.399193	-3.175700	-0.57661
H	-2.048631	-3.919667	-0.11559
H	-0.424440	-4.653378	-1.81338
H	1.064941	-2.987227	-2.93393
C	0.275448	-1.321375	-1.80973
H	0.923129	-0.583354	-2.28537
C	-0.626171	-0.898293	-0.82404
C	-1.496858	-1.827652	-0.21093
C	-2.489531	-1.298505	0.84127
C	-1.731162	-0.997968	2.16514
H	-2.435119	-0.623454	2.92540
H	-0.950065	-0.238248	2.02537
H	-1.256195	-1.915128	2.54902
C	-3.585447	-2.327771	1.15752
H	-3.144150	-3.246872	1.56981
H	-4.170056	-2.593193	0.26386
H	-4.274415	-1.942225	1.92289
C	-3.070957	0.014695	0.28500
C	-4.430615	0.338857	0.36696
H	-5.124314	-0.335380	0.86842
C	-4.933643	1.513549	-0.20145
H	-5.999688	1.739456	-0.12578
C	-4.077064	2.370635	-0.89251
H	-4.465112	3.266907	-1.38163
C	-2.716963	2.066359	-0.97389
H	-2.058181	2.708301	-1.55912
C	-2.190431	0.921319	-0.35622
C	-0.751849	0.528300	-0.43368
C	0.289524	1.346956	-0.11544
C	0.174404	2.843978	0.19524
C	0.142958	3.081315	1.71453
H	0.107414	4.160057	1.93941
H	1.036878	2.657168	2.20045
H	-0.746379	2.607857	2.15977
H	-0.720683	3.296248	-0.23780
C	1.455457	3.416604	-0.46221
H	1.831736	4.321101	0.04256
H	1.261142	3.684926	-1.51646
C	2.422854	2.263505	-0.36855
C	3.825045	2.317977	-0.51026
C	4.566274	1.170768	-0.32402
H	5.652771	1.187192	-0.44251
H	4.311594	3.263005	-0.76398
C	1.753685	1.071896	-0.08512
C	2.514208	-0.098353	0.25452
C	3.943504	-0.042354	0.08799
C	4.725241	-1.191633	0.39423
H	5.806749	-1.141915	0.24242
C	4.143176	-2.335508	0.89695
H	4.756373	-3.208033	1.13339
C	2.747737	-2.365365	1.13373
H	2.288477	-3.256117	1.56793
C	1.958244	-1.278089	0.82093
H	0.892369	-1.318579	1.02179

Table S15: Coordinates of optimized transition state between **5a** and **5b** configurations in the S_0 state at B3LYP/cc-pVDZ level.

C	0.009863	3.582432	-1.14023
C	0.522536	4.049352	0.06885
C	1.150898	3.156358	0.94397
H	1.631466	3.553801	1.83753
H	0.491422	5.114306	0.30985
H	-0.399488	4.277260	-1.87673
C	0.035851	2.213016	-1.41296
H	-0.303855	1.854412	-2.38435
C	0.531588	1.294028	-0.48089
C	1.212352	1.786619	0.66299
C	2.127593	0.813693	1.43674
C	1.288660	-0.116838	2.35394
H	0.803787	0.483562	3.14008
H	1.940180	-0.861776	2.83844
H	0.501822	-0.646609	1.80579
C	3.117772	1.564820	2.34248
H	2.581993	2.145867	3.10710
H	3.762084	2.250043	1.77187
H	3.759337	0.852820	2.88251
C	2.876436	0.012864	0.34223
C	4.250903	-0.246079	0.36766
H	4.855244	0.062574	1.22069
C	4.885390	-0.888592	-0.70439
H	5.961516	-1.071645	-0.66142
C	4.154129	-1.262850	-1.83312
H	4.652304	-1.733735	-2.68358
C	2.775558	-1.035347	-1.86383
H	2.179701	-1.340085	-2.72690
C	2.134906	-0.438976	-0.77379
C	0.665867	-0.180140	-0.72819
C	-0.239114	-1.201121	-0.62743
C	0.192268	-2.707060	-0.60529
C	1.448770	-3.129692	0.18515
H	1.465551	-4.231114	0.23609
H	1.404238	-2.750984	1.21751
H	2.397334	-2.811206	-0.25282
H	0.322451	-3.024854	-1.65381
C	-1.011690	-3.462725	0.01457
H	-0.727435	-3.967154	0.95319
H	-1.401602	-4.250893	-0.65219
C	-2.052061	-2.420255	0.25657
C	-3.259190	-2.638420	0.95655
C	-4.150465	-1.603307	1.11180
H	-5.068079	-1.734905	1.69064
H	-3.458603	-3.621578	1.38992
C	-1.693453	-1.179591	-0.26931
C	-2.719345	-0.163189	-0.31463
C	-3.924476	-0.363278	0.45078
C	-4.919513	0.653032	0.46701
H	-5.808504	0.498796	1.08424
C	-4.796724	1.786889	-0.30840
H	-5.574247	2.553853	-0.29381
C	-3.681525	1.920061	-1.16637
H	-3.611639	2.773815	-1.84421
C	-2.682326	0.967384	-1.16400
H	-1.865735	1.046906	-1.86625

Table S16: Dipole moments of motors **1-5** calculated at B3LYP/cc-pVDZ level in the unit of Debye for **a** and **b** configurations respectively.

motors	**a**	**b**
1	1.892	1.673
2	1.459	1.377
3	1.654	1.650
4	1.914	1.583
5	0.550	0.401