

Supporting Information for

Identification of the Specific, Shutter-like Conformational Reorientation in a Chiroptical Switching Polycarbodiimide by VCD Spectroscopy

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1. Views of the calculated helical model structures

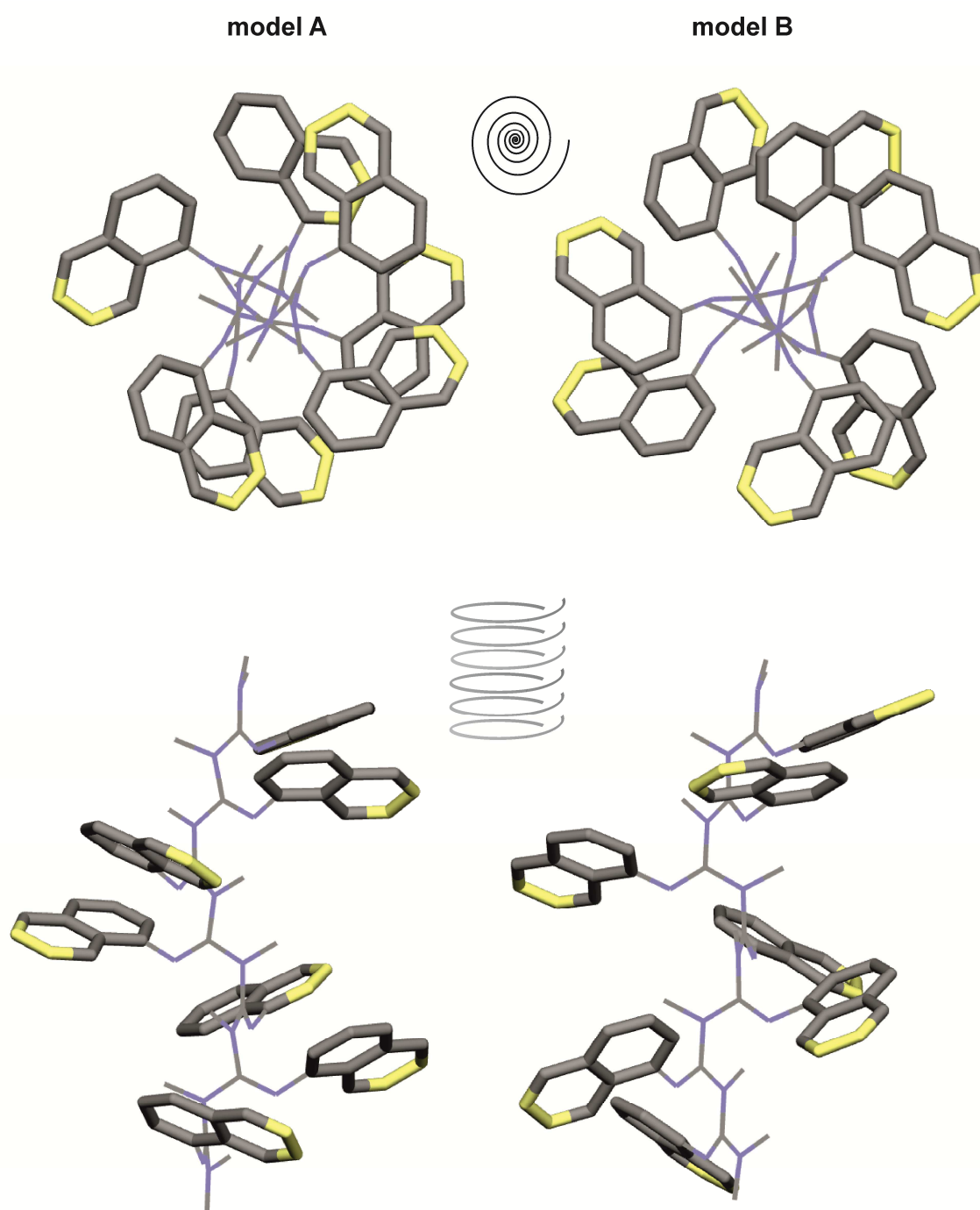


Figure S1. Top and side view of the helical model structures. Carbons C₇ and C₈ of each naphthyl pendant group are highlighted in yellow for easier recognition of the naphthyl orientation.

2. Cartesian coordinates of the optimized geometries of the PNOC-7mer

Model A

C	5.60457500	4.54588800	-28.43461400
C	5.69634400	6.68628500	-27.24150100
C	6.97943600	2.50942200	-28.31798400
N	6.93705900	1.13518600	-28.48333700
N	5.72684800	3.12234800	-28.31715600
N	5.79672100	5.26095000	-27.26996600
N	6.64673700	7.38338600	-27.94776900
N	4.85453800	7.32476200	-26.50906800
N	5.22428200	5.14193800	-29.49925200
N	8.00774400	3.25791600	-28.09463900
C	4.49145100	2.42289700	-27.94956000
H	3.88090400	3.07246200	-27.31663300
H	3.89437800	2.14698900	-28.82409700
H	4.74195500	1.52348600	-27.38617100
C	6.00682700	4.59328100	-25.97941200
H	5.11047600	4.07145200	-25.63348200
H	6.84696700	3.90355500	-26.06419900
H	6.25363900	5.35728500	-25.24357200
C	7.84429900	6.77776700	-28.54064000
H	8.73484200	7.29819600	-28.18443100
H	7.91498100	5.73120300	-28.25136600
H	7.79689700	6.84836900	-29.63176000
C	6.57645000	8.81369600	-28.02932200
C	6.19192400	0.52740600	-29.58068700
H	6.88777600	0.06399100	-30.29182100
H	5.50440800	-0.24584300	-29.21637700
H	5.62208700	1.28401200	-30.11900900
C	7.93906600	0.27522000	-27.87427900
H	7.45294800	-0.65606000	-27.56023800
H	8.75528700	0.02508600	-28.56300700
H	8.36270500	0.75736100	-26.99430100
N	7.46636400	9.60733100	-27.55256500
C	9.34884300	2.88806800	-28.27567700
C	9.88418200	2.41184700	-29.52330400
C	10.21700400	3.09504600	-27.21498900
C	9.09416800	2.24836900	-30.69050800
C	11.28385800	2.10599900	-29.60581800
C	11.58914700	2.79380800	-27.30866200
H	9.81014700	3.49109800	-26.29067200
C	9.63788900	1.78177700	-31.86492500
H	8.04760900	2.51876300	-30.66157000
C	11.80936100	1.62033500	-30.83246200
C	12.11677100	2.29787200	-28.47564300
H	12.22677500	2.95768700	-26.44563500
C	11.01018300	1.45491200	-31.93672400
H	9.00890200	1.67107500	-32.74264900
H	12.86904600	1.38659800	-30.88078100
H	13.17301400	2.06062700	-28.55453300
H	11.43071800	1.08431200	-32.86603500
C	5.14047700	4.49891000	-30.74871300
C	3.86630500	4.11646300	-31.28164100
C	6.27288600	4.35451700	-31.52842500
C	2.65927700	4.26780400	-30.55214700
C	3.80508900	3.56484600	-32.60269900
C	6.20062300	3.81320700	-32.83010500
H	7.22593600	4.68416200	-31.13179000
C	1.45191300	3.88781500	-31.08966300
H	2.70449500	4.69443500	-29.55799300
C	2.54228700	3.17967400	-33.12339000
C	4.99603700	3.42078400	-33.35901600
H	7.11290600	3.71829100	-33.41046500
C	1.39196400	3.33487700	-32.38852700
H	0.53879200	4.01831500	-30.51779900
H	2.50284200	2.75994500	-34.12429800

H	4.93551000	3.00743600	-34.36092400
H	0.43446800	3.03801400	-32.80423000
C	3.72024500	6.71618500	-25.95479800
C	3.44995900	6.90225800	-24.55834200
C	2.80523600	6.02707400	-26.73395900
C	4.31889600	7.63565000	-23.71121800
C	2.26512400	6.32696200	-23.99683800
C	1.63479900	5.47489200	-26.17237500
H	2.98626800	5.94857600	-27.79971500
C	4.04045900	7.78876900	-22.37313700
H	5.19975800	8.09287700	-24.14442100
C	2.01367800	6.49862600	-22.61071200
C	1.37093700	5.60855500	-24.83101300
H	0.93800200	4.94630200	-26.81590100
C	2.87917800	7.20935300	-21.81475300
H	4.71319200	8.36058500	-21.74206400
H	1.11431100	6.05852100	-22.18985200
H	0.47211500	5.18370200	-24.39522900
H	2.66984200	7.33403200	-20.75717400
C	8.42360800	9.23751800	-26.60281800
C	9.77067000	9.70735600	-26.77759000
C	8.10227100	8.52746700	-25.45648600
C	10.16756100	10.46532900	-27.90839400
C	10.75056900	9.39948200	-25.78011100
C	9.07463200	8.23897600	-24.47720900
H	7.07624200	8.21368600	-25.30844700
C	11.46580000	10.89582300	-28.05369800
H	9.42269200	10.71294500	-28.65387200
C	12.08174100	9.85477100	-25.96546000
C	10.37355200	8.65637500	-24.63261000
H	8.78187100	7.68505000	-23.59040500
C	12.43526300	10.58407900	-27.07481800
H	11.74798800	11.47998500	-28.92372100
H	12.81983500	9.61647100	-25.20508000
H	11.12373800	8.43574300	-23.87955500
H	13.45756000	10.92671400	-27.19946900
C	5.41714300	10.76237500	-28.89188200
C	4.68765300	12.84368300	-27.87592100
C	5.70300900	15.04780700	-27.73255500
C	4.61717300	8.55363100	-29.58984000
H	4.60851200	8.94294200	-30.61042600
H	4.92776100	7.51140300	-29.61870000
H	3.60672000	8.61505700	-29.17280600
C	4.41011700	10.78147600	-26.58470900
H	3.34036000	10.97674400	-26.47033500
H	4.56880500	9.70663300	-26.63188400
H	4.93971400	11.18083600	-25.71450800
C	7.10466200	13.04754300	-27.33377500
H	7.07957100	12.69052400	-26.30073900
H	7.38756400	12.22566300	-27.98827400
H	7.85492900	13.83444800	-27.40396300
N	5.63553600	11.41481100	-29.97746500
C	6.27397700	10.88779300	-31.10546500
C	5.71374800	11.19419600	-32.39393200
C	7.46160100	10.17580800	-31.04239300
C	4.52271800	11.95021200	-32.53970700
C	6.37385600	10.72102100	-33.57311600
C	8.10834300	9.72599500	-32.21232600
H	7.90814200	9.98338600	-30.07527000
C	4.00081700	12.21920600	-33.78373300
H	4.03688200	12.32513500	-31.64788400
C	5.80410800	11.01254000	-34.83980900
C	7.57752100	9.98075000	-33.45269800
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C	4.64458300	11.74168800	-34.94688000
H	3.08973700	12.80227000	-33.87346600
H	6.30887500	10.64650900	-35.72933200
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H	4.22328300	11.95640400	-35.92395400
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N	6.01512200	15.77413400	-26.71475800
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N	5.81848500	13.61799300	-27.75204300
N	5.32078600	15.63469700	-28.89785400
C	5.30529300	14.97353600	-30.18897800
H	4.28942500	14.96766100	-30.60227400
H	5.95689000	15.51002400	-30.89097000
H	5.65067100	13.94547400	-30.10579500
C	5.02095800	17.05457300	-28.90558800
H	5.89813800	17.65320200	-29.18702700
H	4.22292000	17.24549100	-29.63048200
H	4.70115500	17.36518900	-27.91223100
C	2.33399200	12.71907100	-28.17266300
C	1.19341100	13.09613200	-27.38173500
C	2.16870300	11.78744600	-29.18650400
C	1.27440200	14.08590200	-26.36996700
C	-0.06480200	12.45717400	-27.61949900
C	0.91761700	11.18038700	-29.42395600
H	3.01136900	11.54149200	-29.81962200
C	0.17397000	14.41748200	-25.61431700
H	2.21964700	14.59289600	-26.22114000
C	-1.17703300	12.81748200	-26.81496400
C	-0.17514000	11.49193700	-28.65298100
H	0.82853600	10.45876600	-30.23050900
C	-1.06324000	13.77098300	-25.83226800
H	0.25426000	15.18191400	-24.84790400
H	-2.12777300	12.32421600	-26.99661100
H	-1.13608500	11.01881100	-28.83094200
H	-1.92460700	14.03596200	-25.22710400
C	6.15648200	15.28146800	-25.41930400
C	7.30015900	15.70895600	-24.66040600
C	5.20478200	14.48311500	-24.80076000
C	8.29639800	16.54482100	-25.22366500
C	7.44638200	15.27750700	-23.30417300
C	5.35617400	14.07041200	-23.46005600
H	4.32248600	14.18926100	-25.35726700
C	9.39216100	16.93440600	-24.48927100
H	8.16235100	16.87682300	-26.24637000
C	8.59089000	15.69616600	-22.57655100
C	6.45237900	14.44896900	-22.72330100
H	4.58642800	13.44924700	-23.01137400
C	9.54312200	16.50276800	-23.15213600
H	10.14436000	17.57777600	-24.93497100
H	8.69989700	15.36450300	-21.54766700
H	6.56844000	14.13030600	-21.69189600
H	10.41191000	16.81341200	-22.57996600

Model B

C	-5.39322500	4.24936200	-17.05904600
C	-5.80844600	6.44616200	-16.17411800
C	-4.27854500	2.13268700	-16.75976600
N	-4.41423000	0.77240300	-16.94974300
N	-5.47393600	2.84884700	-16.80451200
N	-5.56784700	5.05756600	-15.95318000
N	-4.72635400	7.26499600	-15.93973300
N	-6.91809300	6.94550700	-16.56937800
N	-5.18327300	4.77974600	-18.20450600
N	-3.20386300	2.78334900	-16.44687500
C	-6.74466000	2.29181800	-16.33859300
H	-7.36826600	3.10280100	-15.95794200
H	-7.29706000	1.80207100	-17.14795700
H	-6.57164400	1.56548400	-15.54091200
C	-5.31011300	4.58978800	-14.58918800
H	-6.17247700	4.04783600	-14.18599500
H	-4.42706000	3.94935700	-14.57265100
H	-5.13774600	5.45908100	-13.95218400

C	-3.34659400	6.77648600	-15.87043300
H	-3.05776700	6.55469200	-14.83741800
H	-3.22811100	5.87756300	-16.47500400
H	-2.67826100	7.55411200	-16.24603100
C	-4.96171100	8.67313200	-15.87754100
C	-5.20304300	0.22747300	-18.04655800
H	-4.54417900	-0.29136600	-18.75631100
H	-5.94732600	-0.49286800	-17.68419800
H	-5.70638900	1.02782200	-18.58723100
C	-3.48311200	-0.16053400	-16.33846900
H	-4.03354000	-1.06445700	-16.05290200
H	-2.66731000	-0.44491500	-17.01473000
H	-3.04849200	0.28071900	-15.44176400
N	-5.47260600	9.28640700	-14.87878400
C	-1.92101800	2.34172600	-16.78503400
C	-0.88053800	2.43069700	-15.79818100
C	-1.59435000	1.92027200	-18.06563200
C	-1.13873100	2.85906700	-14.47201200
C	0.45759200	2.06815700	-16.15445300
C	-0.27144100	1.56798500	-18.40571000
H	-2.36694000	1.89584200	-18.82595600
C	-0.13041000	2.93116300	-13.53887800
H	-2.15358400	3.13330800	-14.21040400
C	1.47328200	2.15316900	-15.16694200
C	0.73709900	1.63421000	-17.47572100
H	-0.05769200	1.24993300	-19.42155100
C	1.19063000	2.57367300	-13.88951800
H	-0.34752200	3.26474700	-12.52900700
H	2.48701300	1.87703100	-15.44306600
H	1.75581300	1.36508600	-17.73745700
H	1.98068600	2.63300600	-13.14749100
C	-5.27761600	4.05908100	-19.40006300
C	-4.16504900	4.07156200	-20.30487100
C	-6.45657200	3.44054900	-19.78611800
C	-2.94427000	4.71823300	-19.98602500
C	-4.28675400	3.41035500	-21.56886300
C	-6.56793300	2.80052600	-21.03925100
H	-7.31946100	3.49443300	-19.13179200
C	-1.88953700	4.71199000	-20.86846900
H	-2.86177700	5.22017800	-19.02999900
C	-3.17550400	3.41794700	-22.45161100
C	-5.50728100	2.77372700	-21.91145100
H	-7.51036600	2.33444700	-21.30997300
C	-2.00430300	4.05201100	-22.11268000
H	-0.96248000	5.21265200	-20.60853600
H	-3.27128800	2.91263600	-23.40847600
H	-5.59180000	2.28222000	-22.87584500
H	-1.16483300	4.05035500	-22.80087900
C	-8.10215900	6.19992300	-16.61547900
C	-8.80718100	6.10115400	-17.86069700
C	-8.66483800	5.65218400	-15.47368000
C	-8.29841200	6.66283400	-19.05868300
C	-10.06042800	5.41023000	-17.89998200
C	-9.90438900	4.97805100	-15.52364700
H	-8.16297800	5.78643700	-14.52226400
C	-8.99041100	6.55155400	-20.24160400
H	-7.34985600	7.18329700	-19.02026000
C	-10.74476200	5.30982500	-19.13976700
C	-10.58760600	4.84943300	-16.70829000
H	-10.31775000	4.56800800	-14.60727000
C	-10.22562800	5.86636800	-20.28380000
H	-8.58578200	6.98723100	-21.14938500
H	-11.69530400	4.78451700	-19.16505100
H	-11.54169400	4.33269200	-16.74725900
H	-10.76313600	5.78227300	-21.22310400
C	-5.66101400	8.66564300	-13.63682000
C	-6.98897700	8.56753000	-13.10451900
C	-4.58856000	8.24944600	-12.86510200
C	-8.12541200	8.99688500	-13.83538900
C	-7.17630200	8.01199500	-11.79832900

C	-4.78559700	7.70726400	-11.57631000
H	-3.58226500	8.38765600	-13.24355700
C	-9.38941400	8.88618900	-13.30539500
H	-7.97434900	9.41038400	-14.82459100
C	-8.49569700	7.90901900	-11.28491500
C	-6.04870200	7.58263500	-11.05184700
H	-3.92029300	7.39676000	-10.99878800
C	-9.57741500	8.33510800	-12.01757800
H	-10.24874600	9.21790300	-13.87905400
H	-8.63358500	7.48675100	-10.29361200
H	-6.20131500	7.16840600	-10.05987700
H	-10.57960500	8.25042600	-11.60910400
C	-4.56296200	10.79228900	-16.93008000
C	-5.53572600	12.84972500	-17.69716300
C	-6.37324300	15.00255800	-16.99748600
C	-4.38856400	8.72491300	-18.31129500
H	-3.33500500	8.46042600	-18.45201900
H	-4.99703400	7.82538300	-18.40136900
H	-4.66632200	9.42811000	-19.09901800
C	-6.89837500	10.76901000	-17.82958200
H	-6.92795200	10.45395800	-18.87825400
H	-7.04480800	9.89901400	-17.18988800
H	-7.71571500	11.47525900	-17.66700700
C	-6.62484800	13.06636500	-15.45761200
H	-7.69552400	12.83357500	-15.45755300
H	-6.06654500	12.16495800	-15.20881400
H	-6.43722900	13.81967400	-14.68859000
N	-3.63887500	11.46671900	-16.35580300
C	-2.44067300	10.87779300	-15.93068600
C	-2.07783200	10.96960800	-14.54592700
C	-1.55134600	10.30720900	-16.82671500
C	-2.93060500	11.56559400	-13.58278300
C	-0.81965200	10.43674200	-14.11847900
C	-0.31151000	9.78879500	-16.39389400
H	-1.79686400	10.30256100	-17.88241800
C	-2.56190700	11.63805200	-12.25994800
H	-3.88303000	11.96012300	-13.91365500
C	-0.47483800	10.52289600	-12.74404000
C	0.04864900	9.84211100	-15.06968300
H	0.36046900	9.35196400	-17.12606400
C	-1.32200700	11.10950500	-11.83497900
H	-3.22712300	12.09753100	-11.53598300
H	0.48037000	10.11634300	-12.42390800
H	1.00184000	9.44406800	-14.73557200
H	-1.04133400	11.16907500	-10.78796600
N	-4.89526200	13.41772600	-18.64477500
N	-7.26395000	15.48998000	-17.77746800
N	-4.60331200	9.36614300	-17.01124800
N	-5.63037800	11.43170000	-17.51414900
N	-6.19829100	13.59683600	-16.75261100
N	-5.55465500	15.82113600	-16.26461000
C	-4.20486100	15.42205500	-15.88593400
H	-3.46561500	15.82059300	-16.59434700
H	-3.97251800	15.81572200	-14.89077900
H	-4.10763700	14.33787900	-15.86850500
C	-5.77019400	17.25536200	-16.36826700
H	-5.29824700	17.74364300	-15.51064400
H	-5.34059000	17.66788500	-17.29157400
H	-6.83930300	17.46588700	-16.37146800
C	-4.37859200	12.69741300	-19.72965600
C	-2.96059300	12.68382400	-19.94148100
C	-5.20855900	12.09262800	-20.65886900
C	-2.06210000	13.30882400	-19.04048700
C	-2.43411400	12.01484300	-21.09238600
C	-4.67800600	11.43911600	-21.79265000
H	-6.28246200	12.16431400	-20.52924200
C	-0.70504500	13.27726000	-19.26104200
H	-2.47238000	13.80751000	-18.17137300
C	-1.02771300	11.99760200	-21.28497900
C	-3.32195600	11.39140200	-22.00646400

H	-5.35939100	10.97845100	-22.50119400
C	-0.18181900	12.61308700	-20.39363100
H	-0.03054500	13.76024600	-18.56136100
H	-0.63111900	11.48752300	-22.15834600
H	-2.91318100	10.88967200	-22.87822500
H	0.89112700	12.59173000	-20.55756400
C	-8.26733600	14.71008600	-18.36103100
C	-8.31495300	14.60973500	-19.79166600
C	-9.27700500	14.12884900	-17.61163900
C	-7.32585700	15.20574800	-20.61399100
C	-9.38471700	13.88495900	-20.40681100
C	-10.33130500	13.42004600	-18.22872000
H	-9.27203900	14.25610400	-16.53439500
C	-7.38642600	15.09231600	-21.98305100
H	-6.52036300	15.74793100	-20.13468400
C	-9.41212300	13.78424700	-21.82254600
C	-10.38556700	13.29088400	-19.59494000
H	-11.10521300	12.97934900	-17.60761100
C	-8.43871500	14.37296500	-22.59378800
H	-6.62114000	15.55288800	-22.59936100
H	-10.22431000	13.23206400	-22.28687700
H	-11.19482900	12.74552300	-20.07064400
H	-8.47589700	14.28797700	-23.67540700