

Supporting Information

Theoretical Studies on the Structure and Thermochemistry of Cyclicparaphenylenediazenes

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Table S1: Optimized geometries of cis-cyclic [n_c]paraphenylenediazenes obtained using the B3LYP/6-31+G(d,p).

[2_c]CPPD				[3_c]CPPD			
C	0.69896900	1.52210100	1.20412600	C	-2.78468100	0.01946600	0.05090700
C	-0.69896900	1.52210100	1.20412600	C	-2.73588700	-0.85784800	1.13884700
C	-1.37768300	1.30109500	0.00000000	C	-2.01883600	-2.05080500	1.03563400
C	-0.69896900	1.52210100	-1.20412600	C	-1.37423100	-2.37944000	-0.16333700
C	0.69896900	1.52210100	-1.20412600	C	-1.56812800	-1.57967900	-1.29461500
C	1.37768300	1.30109500	0.00000000	C	-2.25762000	-0.37450500	-1.18400100
H	1.23777600	1.49815100	2.14621700	H	-3.21734200	-0.58636800	2.07339300
H	-1.23777600	1.49815100	2.14621700	H	-1.93705000	-2.71715600	1.88866100
H	-1.23777600	1.49815100	-2.14621700	H	-1.16551000	-1.88452900	-2.25355400
H	1.23777600	1.49815100	-2.14621700	H	-2.36894500	0.26936100	-2.05022900
H	-1.23777600	-1.49815100	2.14621700	H	-1.24924500	3.44110100	-1.74930400
C	-0.69896900	-1.52210100	1.20412600	C	-0.69823900	2.98309500	-0.93372400
C	0.69896900	-1.52210100	1.20412600	C	0.69824200	2.98309400	-0.93372400
C	-1.37768300	-1.30109500	0.00000000	C	-1.39643600	2.35732900	0.10593800
H	1.23777600	-1.49815100	2.14621700	C	1.39643900	2.35732700	0.10593700
C	-0.69896900	-1.52210100	-1.20412600	H	1.24924800	3.44110000	-1.74930500
C	0.69896900	-1.52210100	-1.20412600	C	-0.69471200	1.85677500	1.21127600
H	-1.23777600	-1.49815100	-2.14621700	C	0.69471500	1.85677500	1.21127500
H	1.23777600	-1.49815100	-2.14621700	H	-1.23442600	1.45733400	2.06196700
C	1.37768300	-1.30109500	0.00000000	H	1.23442900	1.45733300	2.06196600
N	2.67926300	-0.63108500	0.00000000	H	2.36894100	0.26936000	-2.05022900
N	2.67926300	0.63108500	0.00000000	C	2.25761700	-0.37450600	-1.18400100
N	-2.67926300	-0.63108500	0.00000000	C	2.78468100	0.01946300	0.05090600
N	-2.67926300	0.63108500	0.00000000	C	1.56812400	-1.57967900	-1.29461500
				C	2.73588800	-0.85785200	1.13884500
				C	1.37422900	-2.37944100	-0.16333700
				H	1.16550300	-1.88452800	-2.25355300
				C	2.01883600	-2.05080800	1.03563300
				H	3.21734600	-0.58637300	2.07339000
				H	1.93705100	-2.71716000	1.88865900
				N	3.47776900	1.28348500	0.15726400
				N	2.83841100	2.35757800	0.09929700
				N	-2.83840800	2.35758100	0.09929800
				N	-3.47776700	1.28348900	0.15726500
				N	-0.62497200	-3.61621100	-0.22405700

	N	0.62496800	-3.61621200	-0.22405600
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[4_c]CPPD				[5_c]CPPD			
C	0.69589600	2.75334400	0.82092700	C	-3.65998000	-2.65033900	0.04569800
C	1.40192900	3.43903300	-0.18298700	C	-4.21868000	-1.70391200	-0.80369600
C	0.69431400	4.16029600	-1.15888900	C	-4.34753800	-0.36589900	-0.39482700
C	-0.69432300	4.16029800	-1.15888600	C	-4.02259700	-0.00952700	0.92588400
C	-1.40193700	3.43903600	-0.18298200	C	-3.53817000	-0.97535000	1.80234900
C	-0.69590200	2.75334400	0.82092800	C	-3.29146900	-2.28011500	1.34995300
H	1.23433000	2.24979300	1.61651700	H	-3.53239400	-3.67540500	-0.28535500
H	1.25100700	4.74359400	-1.88558500	H	-4.55632700	-1.97954200	-1.79770500
H	-1.25101700	4.74359800	-1.88558000	H	-4.18745700	1.00196400	1.27762400
H	-1.23433300	2.24979400	1.61652000	H	-3.32675900	-0.72728000	2.83782700
C	3.43903400	1.40193100	0.18297700	H	0.82504200	-6.05052100	-0.94424900
C	2.75335800	0.69589600	-0.82094400	C	0.46472200	-5.11980500	-0.51757600
C	4.16028600	0.69431700	1.15888800	C	0.97691100	-3.90814900	-1.00527000
C	2.75335900	-0.69590200	-0.82094400	C	-0.46547000	-5.11974200	0.51757100
H	2.24981800	1.23432800	-1.61654200	C	0.48412900	-2.69227200	-0.49632400
C	4.16028700	-0.69432000	1.15888900	C	-0.97748300	-3.90801500	1.00527400
H	4.74357300	1.25101200	1.88559200	H	-0.82592800	-6.05040800	0.94423500
C	3.43903600	-1.40193500	0.18297800	C	-0.48452200	-2.69220600	0.49634000
H	2.24981900	-1.23433500	-1.61654000	H	0.84860000	-1.74893300	-0.88330600
H	4.74357600	-1.25101300	1.88559200	H	-0.84885500	-1.74881600	0.88333000
C	-4.16030500	0.69432100	1.15888500	C	-3.64357500	2.39463800	-0.91188500
C	-4.16030400	-0.69431600	1.15888600	C	-2.33253000	2.09189700	-1.32017700
C	-3.43903400	1.40193600	0.18298900	C	-3.88955000	3.57104300	-0.18652600
C	-3.43903200	-1.40193000	0.18299000	C	-1.27709700	2.94291700	-0.99228700
H	-4.74361000	-1.25101000	1.88557500	H	-2.15051500	1.21381200	-1.93220000
C	-2.75333300	0.69590200	-0.82091600	C	-2.83645400	4.40952600	0.14516900
C	-2.75333200	-0.69589600	-0.82091600	H	-4.91068200	3.83340400	0.07244100
H	-2.24977600	1.23433400	-1.61650200	C	-1.51447100	4.11044000	-0.24246600
H	-2.24977500	-1.23432800	-1.61650200	H	-0.28048300	2.71636300	-1.35435100
C	-1.40193200	-3.43903400	-0.18297900	H	-3.01443800	5.34561500	0.66478700
C	-0.69431900	-4.16029200	-1.15888700	H	0.28088500	2.71631800	1.35431800
C	-0.69589600	-2.75335000	0.82093600	C	1.27753300	2.94272700	0.99226200
C	0.69431800	-4.16029300	-1.15888900	C	2.33284000	2.09155500	1.32016000
H	-1.25101400	-4.74358500	-1.88558500	C	1.51508500	4.11021700	0.24244500
C	0.69590200	-2.75335200	0.82093400	C	3.64393300	2.39410600	0.91188200
H	-1.23432700	-2.24980500	1.61653100	H	2.15069300	1.21349400	1.93218200
C	1.40193400	-3.43903500	-0.18298400	C	2.83711400	4.40911000	-0.14517900

H	1.25101000	-4.74358700	-1.88558900	C	3.89008500	3.57047400	0.18652600
H	1.23433600	-2.24980600	1.61652700	H	3.01523900	5.34517500	-0.66479400
H	-4.74361200	1.25101500	1.88557300	H	4.91125800	3.83268900	-0.07243200
N	-2.81142000	3.67457800	-0.13165700	H	4.18757200	1.00137600	-1.27759400
N	-3.67457800	2.81141900	0.13166100	C	4.02257400	-0.01009700	-0.92586300
N	-3.67457400	-2.81141400	0.13166300	C	4.34748000	-0.36652700	0.39484100
N	-2.81141600	-3.67457300	-0.13165800	C	3.53800200	-0.97584300	-1.80233300
N	2.81141800	-3.67457600	-0.13166700	C	4.21843400	-1.70452500	0.80370000
N	3.67457500	-2.81141900	0.13166300	C	3.29112300	-2.28057800	-1.34994800
N	3.67457100	2.81141600	0.13166000	H	3.32661800	-0.72773400	-2.83780600
N	2.81141400	3.67457300	-0.13166800	C	3.65959300	-2.65086500	-0.04569800
[6_c]CPPD₁				H	4.55605100	-1.98021300	1.79770300
C	-2.11281900	2.08765500	2.27444800	H	3.53186600	-3.67591700	0.28534600
C	-2.93921600	0.95334500	2.32429800	N	1.87018800	-4.00678900	-2.11951400
C	-4.15026500	0.94185100	1.64197400	N	2.83289600	-3.23218800	-2.31479300
C	-4.58320800	2.09328300	0.96370600	N	5.02755100	0.49406300	1.31086400
C	-3.82219600	3.26998500	1.03811500	N	4.77653400	1.70720100	1.45583900
C	-2.57495900	3.26146100	1.65730500	N	0.62426500	5.20771800	0.04636400
H	-2.60615800	0.08325000	2.88154500	N	-0.62349000	5.20781000	-0.04638600
H	-4.76874200	0.05092600	1.65012200	N	-4.77628200	1.70789800	-1.45583000
H	-4.20822300	4.17702400	0.58330800	N	-5.02747700	0.49479600	-1.31085200
H	-1.96923800	4.16164900	1.67995200	N	-2.83338000	-3.23179700	2.31479300
H	0.09483100	1.92438100	-2.04621800	N	-1.87078000	-4.00653300	2.11951300
C	0.57288400	2.29447400	-1.14408200	[7_c]CPPD₁			
C	1.78920000	2.98377900	-1.24317100	C	5.48876700	-1.61052300	1.32390500
C	-0.00498800	2.06164700	0.10136600	C	4.38723200	-1.74374100	2.15906200
C	2.40004600	3.49223600	-0.08869900	C	3.45067500	-2.76825800	1.94620100
C	0.60165100	2.56820900	1.26791200	C	3.69122300	-3.72997300	0.95001500
H	-0.91657000	1.48169900	0.15923300	C	4.83256400	-3.63872300	0.16442400
C	1.81292500	3.27012600	1.15175900	C	5.71069900	-2.55166900	0.30373400
H	3.32882400	4.04727900	-0.16605300	H	6.19783600	-0.80558500	1.48476400
H	2.28842100	3.62352900	2.06146500	H	4.22713500	-1.05496800	2.98287800
C	-5.48583400	0.28399700	-1.02903000	H	3.00627900	-4.56124700	0.82115900
C	-6.10488500	-0.96161500	-1.21476400	H	5.05918600	-4.39957900	-0.57618200
C	-4.20031000	0.49995600	-1.55007500	H	8.75921100	0.59085600	-0.68700400
C	-5.41484400	-2.00916700	-1.82113900	C	7.72594600	0.77883500	-0.96197400
H	-7.12848200	-1.09370500	-0.87844600	C	6.85672500	-0.31428900	-1.10956100
C	-3.50670500	-0.54609300	-2.14683300	C	7.27106900	2.07143400	-1.18624200

H	-3.74583100	1.48223600	-1.48984700	C	5.54278700	-0.09703000	-1.55706100
C	-4.09286500	-1.81744800	-2.24077200	C	5.93500300	2.29288300	-1.55256900
H	-5.88994000	-2.97422600	-1.96691300	H	7.93789200	2.92276200	-1.08962500
H	-2.51661100	-0.37775600	-2.55611900	C	5.08457600	1.19646600	-1.77231800
C	-1.78920000	-2.98378700	-1.24315600	H	4.88839200	-0.94090000	-1.74737400
C	-0.57288300	-2.29448100	-1.14407100	H	4.07370700	1.35764700	-2.13060900
C	-2.40004500	-3.49223700	-0.08868200	H	1.62762600	-1.37664000	0.59105600
C	0.00498800	-2.06164600	0.10137500	C	0.90252700	-2.15736500	0.38940000
H	-0.09483100	-1.92439300	-2.04621000	C	0.21257400	-2.17092000	-0.81638200
C	-1.81292500	-3.27011900	1.15177600	C	0.65841400	-3.15724100	1.34690900
H	-3.32882300	-4.04728100	-0.16603200	C	-0.76554200	-3.14695500	-1.06635900
C	-0.60165100	-2.56820000	1.26792500	H	0.41394000	-1.42266700	-1.57768400
H	0.91657000	-1.48169700	0.15923900	C	-0.32708100	-4.12511700	1.09791900
H	-2.28842100	-3.62351600	2.06148300	C	-1.02169200	-4.13763000	-0.10544000
C	2.11281800	-2.08764000	2.27445900	H	-0.53261400	-4.86582200	1.86500700
C	2.93921500	-0.95333000	2.32430100	H	-1.76476300	-4.90351000	-0.30371400
C	2.57495900	-3.26145000	1.65732500	H	5.02789800	3.34525000	0.98228200
C	4.15026400	-0.94184100	1.64197800	C	3.98790500	3.23279100	0.69450400
H	2.60615700	-0.08323000	2.88154100	C	3.58278600	3.55208800	-0.61031800
C	3.82219600	-3.26997900	1.03813600	C	3.05124300	2.75749000	1.59973600
H	1.96923800	-4.16163800	1.67997900	C	2.22968500	3.44983000	-0.96649300
C	4.58320800	-2.09327700	0.96371900	C	1.69899000	2.60887500	1.24341300
H	4.76874100	-0.05091500	1.65012000	H	3.34173000	2.46933400	2.60523800
H	4.20822300	-4.17702200	0.58333700	C	1.29539400	2.96091500	-0.06111500
H	7.12848400	1.09369700	-0.87845300	H	1.92549300	3.73942500	-1.96802600
C	6.10488600	0.96160600	-1.21477000	H	0.26780500	2.85007400	-0.37779500
C	5.48583500	-0.28400500	-1.02902700	C	-1.24400200	2.55017000	1.48849000
C	5.41484600	2.00915400	-1.82115000	C	-2.01397900	1.74642500	0.63307800
C	4.20031000	-0.49996600	-1.55006900	C	-1.55251900	3.91089200	1.63006600
C	4.09286600	1.81743400	-2.24078000	C	-3.07590800	2.29087200	-0.07669800
H	5.88994100	2.97421300	-1.96693100	H	-1.76160400	0.69475900	0.52996100
C	3.50670500	0.54608000	-2.14683300	C	-2.61189600	4.45375400	0.91015000
H	3.74583000	-1.48224500	-1.48983500	H	-0.96170500	4.53129900	2.29689500
H	2.51661000	0.37774000	-2.55611600	C	-3.40923000	3.64830500	0.08317500
N	0.23004100	2.31984400	2.63220200	H	-3.64129300	1.66173700	-0.75332000
N	-0.91492700	2.04476800	3.05158700	H	-2.84773500	5.51120000	0.98431700
N	-5.86731800	2.18240700	0.33413800	C	-3.59921400	-3.00788900	-1.70100600
N	-6.29552400	1.33236600	-0.47885500	C	-4.82301600	-3.61733400	-2.02333600

N	-3.41238800	-2.87198300	-2.94209100	C	-3.55069500	-2.09167500	-0.63348800
N	-2.32289800	-3.32424300	-2.53504700	C	-5.96261900	-3.35783500	-1.27250200
N	-0.23004200	-2.31982600	2.63221300	H	-4.85381400	-4.29829400	-2.86830700
N	0.91492500	-2.04474700	3.05159700	C	-4.70260500	-1.78203700	0.07529900
N	5.86731800	-2.18240600	0.33415300	H	-2.62048900	-1.60104300	-0.37510700
N	6.29552400	-1.33237000	-0.47884600	C	-5.92381500	-2.39711000	-0.25221800
N	3.41238800	2.87196400	-2.94210500	H	-6.90134600	-3.85808100	-1.48993100
N	2.32289900	3.32422700	-2.53506400	H	-4.65840100	-1.06353400	0.88612100
[8_c]CPPD₁ (at B3LYP/6-31G(d))							
C	6.46662400	-1.43182500	1.89264300	C	-7.00750800	0.13354800	0.37156000
C	6.02117200	-0.16046100	1.49060300	C	-6.89583700	0.40596900	-1.00061700
C	7.30146300	-2.17068600	1.03849100	C	-6.72153200	1.13895300	1.30583300
C	6.32554200	0.31515700	0.22148100	C	-6.43160500	1.64588400	-1.42392000
H	5.44482000	0.45777700	2.16922400	H	-7.18448300	-0.34583600	-1.72779700
C	7.61655100	-1.69251500	-0.22637800	C	-6.17695200	2.34681400	0.88540100
H	7.69748200	-3.11736800	1.39268700	H	-6.88771100	0.94173300	2.36056800
C	7.09115900	-0.46608300	-0.65964800	C	-5.99458500	2.59063900	-0.48475200
H	5.98562000	1.29853300	-0.08761600	H	-6.36170700	1.88042700	-2.48176700
H	8.26950200	-2.25246700	-0.88878000	H	-5.89963400	3.10538900	1.61031700
H	-1.60626800	-3.19235600	-1.61449500	N	-1.32417300	-3.19999800	-2.37985600
C	-1.42478200	-2.97671200	-0.56826400	N	-2.54664700	-3.24342000	-2.63966700
C	-1.59900000	-3.97797500	0.40065500	N	-7.11625500	-2.21508300	0.52057500
C	-1.04233000	-1.69893700	-0.18476300	N	-7.54781000	-1.09461100	0.87264700
C	-1.29617800	-3.70573600	1.74112700	N	-5.52537100	3.85127300	-0.97484000
C	-0.77590900	-1.41577800	1.16287300	N	-4.41915900	4.34470500	-0.65737100
H	-0.94769100	-0.90940900	-0.92500100	N	-0.30456400	1.91358200	2.35444800
C	-0.90548000	-2.42702800	2.12764300	N	0.94002100	1.98322600	2.28301800
H	-1.39705400	-4.49845400	2.47661500	N	4.48401400	4.15414900	-1.54256300
H	-0.71336200	-2.20635100	3.17283000	N	5.57155200	3.63832500	-1.87868100
H	-5.11350100	-3.02585300	-3.81727600	N	7.44993800	-1.61166500	-1.01037500
C	-4.95802500	-3.28123700	-2.77373700	N	6.90359300	-2.60479700	-0.48155800
C	-5.65339400	-2.54965000	-1.79739400	N	2.41505700	-2.90052600	2.92258300
C	-4.07666300	-4.29238300	-2.40825200	N	1.22172600	-3.16762900	2.66110400
C	-5.55300700	-2.93548900	-0.45006400	[6_c]CPPD₂			
C	-3.86999000	-4.56606300	-1.05161900	C	-5.88050300	1.63695600	-0.43792400
H	-3.51873200	-4.84549400	-3.15793500	C	-4.58384400	1.99384100	-0.83900300
C	-4.65816800	-3.93092800	-0.07998100	C	-3.49161100	1.21450000	-0.41282400
H	-6.15368800	-2.44605100	0.30773600	C	-3.69541900	0.11545300	0.41145900
				C	-4.99451700	-0.22124700	0.83688800

H	-4.55339000	-4.20970300	0.96378700	C	-6.07723600	0.57607900	0.43497300
C	5.36826300	0.35659200	-2.80321500	H	-6.71770500	2.22314100	-0.80388100
C	4.64816000	1.42153400	-3.36925300	H	-2.48791900	1.46560600	-0.73830800
C	4.70382900	-0.84756100	-2.51067300	H	-2.84827300	-0.47801600	0.73782900
C	3.27639000	1.32783600	-3.56227500	H	-7.06904900	0.32864800	0.80039500
H	5.18779700	2.31808600	-3.65854900	C	-2.85726900	4.14747300	0.51526200
C	3.34592500	-0.96630200	-2.77500800	C	-1.83893300	4.53418800	1.37485500
H	5.25874600	-1.69942500	-2.13433600	C	-0.57873600	4.91080300	0.87763800
C	2.60940600	0.12648600	-3.26120200	C	-0.39258700	5.02404400	-0.51144600
H	2.73364400	2.16110800	-3.99356900	C	-1.42813400	4.68568400	-1.37093200
H	2.83184600	-1.91050600	-2.62236200	C	-2.64319200	4.18185600	-0.87397500
C	0.35624600	1.88561500	-2.87665900	H	-3.81815200	3.84464600	0.91525900
C	0.69782100	1.94905800	-1.51732400	H	-1.99178700	4.54423100	2.44950900
C	-0.14740100	3.02455100	-3.52305900	H	0.54383100	5.39603500	-0.91112600
C	0.53414800	3.13461700	-0.81163500	H	-1.31727100	4.79356300	-2.44536000
H	1.06465700	1.06364200	-1.00877400	C	2.30614600	4.43362500	0.83862400
C	-0.21970400	4.23294100	-2.84131900	C	3.53776100	4.97286600	0.43629800
H	-0.44423800	2.95422700	-4.56513100	C	4.35724200	4.27291200	-0.43817600
C	0.07888000	4.28716800	-1.47191500	C	4.01774700	2.97185900	-0.84002000
H	0.77730700	3.16726400	0.24426000	C	2.79725500	2.41514000	-0.41293900
H	-0.53791800	5.13899700	-3.34814300	C	1.94781200	3.14068400	0.41222900
H	-4.11037100	-0.37702700	-1.03987200	H	3.81967100	5.95523600	0.80224200
C	-4.79264400	0.07699300	-0.32931200	H	5.28304800	4.70533800	-0.80471400
C	-6.18062100	0.03338000	-0.55920700	H	2.51229000	1.42074300	-0.73906600
C	-4.28558900	0.69957800	0.80637500	H	1.01035100	2.70365100	0.73863900
C	-7.04633300	0.65990100	0.35013700	C	-3.96553000	-2.95858400	0.87498300
C	-5.16342600	1.27709700	1.74381400	C	-4.15391900	-2.85135200	-0.51430700
H	-3.21346400	0.72059800	0.98000100	C	-3.34153800	-3.57745400	-1.37359300
C	-6.54782900	1.22372000	1.51608400	C	-2.29889200	-4.37903800	-0.87601600
H	-8.11158600	0.65940600	0.14026100	C	-2.16539000	-4.55049000	0.51315200
H	-7.21536100	1.64408400	2.26210600	C	-3.01101600	-3.86338600	1.37239000
C	-3.01766000	3.23365100	2.39876100	H	-4.94300600	-2.22508700	-0.91446300
C	-1.79248300	3.64578200	2.95243000	H	-3.48819000	-3.53318200	-2.44823900
C	-3.38525100	3.71022900	1.12751200	H	-1.42386500	-5.23247200	0.91318800
C	-0.92426000	4.46273600	2.24337100	H	-2.94573400	-4.00304300	2.44690000
H	-1.55528600	3.31793700	3.95918900	C	0.69368400	-3.62959000	-0.41000400
C	-2.50538100	4.50399300	0.40119000	C	1.74676600	-3.25640700	0.41493500
H	-4.35351400	3.47108600	0.70570000	C	2.68829500	-4.21275000	0.84023500

C	-1.25924900	4.85842100	0.94276300	C	2.54038400	-5.54881300	0.43713700
H	0.01279900	4.79515700	2.67958700	C	1.52422800	-5.90878900	-0.43694600
H	-2.78761900	4.87185700	-0.58033500	C	0.56615100	-4.96478900	-0.83768800
C	1.51591400	-0.34339400	2.59453200	H	-0.02571700	-2.88592800	-0.73528200
C	2.12407500	0.09856100	3.78060600	H	1.83644800	-2.22608600	0.74174200
C	2.16804400	-1.31060900	1.80547500	H	3.25114200	-6.28373200	0.80206300
C	3.33460500	-0.43877400	4.19759000	H	1.43648500	-6.92656100	-0.80422400
H	1.62242100	0.86423700	4.36434500	C	4.76713400	-1.10592300	-1.37378600
C	3.40833900	-1.80039600	2.18868000	C	4.94207800	0.19797400	-0.87743800
H	1.72550500	-1.65286400	0.87807700	C	5.02430700	0.40066900	0.51150600
C	4.01245900	-1.34944400	3.37475900	C	4.85205500	-0.67440600	1.37177900
H	3.79250000	-0.13053900	5.13235200	C	4.54478600	-1.95375800	0.87570100
H	3.91875800	-2.52874100	1.56749900	C	4.54409700	-2.17150300	-0.51344600
N	0.09135200	5.57816900	-0.85013500	H	4.80104400	-1.25606900	-2.44833100
N	-0.41501600	5.80017500	0.26926600	H	5.24512800	1.38410200	0.91040000
N	-3.82325100	2.49634000	3.32018100	H	4.94124100	-0.54720800	2.44611200
N	-4.77672900	1.73622900	3.03908600	H	4.39502600	-3.16813900	-0.91268000
N	-6.80701000	-0.46832800	-1.74419500	N	-5.30682600	-1.22344300	1.80606500
N	-6.53492200	-1.54952400	-2.31501800	N	-4.80149000	-2.36686800	1.86915600
N	-2.93193500	-5.58739000	-0.67860300	N	-1.58286900	-5.11112500	-1.87031400
N	-1.94880500	-5.32696600	0.05103100	N	-0.37424200	-5.43047800	-1.80716200
N	-0.58019200	-0.04116100	1.50675100	N	3.71231500	-3.98159700	1.80924600
N	0.35869700	0.40004900	2.20608500	N	4.45009400	-2.97229100	1.87118000
N	5.23821900	-1.88796200	3.87260400	N	4.89055600	2.38981900	-1.80988500
N	6.28520000	-1.99559200	3.19531100	N	5.21779400	1.18326500	-1.87267800
N	7.54679300	0.04626600	-1.91328100	N	0.35169700	5.33799000	1.87220300
N	6.79196700	0.50005500	-2.79932400	N	1.59463900	5.20438600	1.80856900
N	1.26259400	-0.16494700	-3.64757600	N	-4.51628300	3.04255300	-1.80695500
N	0.30934200	0.64185300	-3.58057100	N	-3.63495600	3.92930700	-1.86886600
[7_c]CPPD₂				[8_c]CPPD₂			
C	-5.60965400	2.63577700	-0.75134400	C	-2.84732400	-4.91259000	-1.02814700
C	-6.99050300	2.41563400	-0.89708000	C	-2.60107900	-4.16807600	0.13774000
C	-7.58142000	1.25077100	-0.42870800	C	-1.97387900	-2.91085000	0.02309300
C	-6.78733600	0.23654100	0.12620900	C	-1.60970500	-2.42345800	-1.22436400
C	-5.40255200	0.44302400	0.26804200	C	-1.85121700	-3.17933600	-2.38524100
C	-4.81864600	1.62640800	-0.16328800	C	-2.43518200	-4.44948500	-2.27069400
H	-7.58030200	3.19244000	-1.37298300	H	-3.35991200	-5.86422100	-0.92832300
H	-8.65400700	1.09833700	-0.49637700	H	-1.80346300	-2.29696800	0.89727000

H	-4.78564200	-0.32194300	0.72615800	H	-1.14235900	-1.44795400	-1.30833400
H	-3.74997800	1.74784900	-0.05635400	H	-2.58512900	-5.04285400	-3.16727900
C	5.52092900	-2.66251400	0.54993800	C	-1.64539300	-3.76628500	2.84354800
C	4.33946600	-2.23873400	-0.08421100	C	-0.35590000	-4.27606500	2.61558900
C	3.15884800	-2.12458400	0.63661800	C	-1.81047400	-2.59659700	3.59875800
C	3.14192300	-2.40832400	2.01535800	C	0.75979100	-3.56732200	3.04284500
C	4.32871900	-2.81817700	2.64518200	H	-0.23741900	-5.22470500	2.10115600
C	5.49349900	-2.99778200	1.91110500	C	-0.69338600	-1.88854300	4.02217700
H	4.34706600	-2.01128600	-1.14428400	H	-2.80982100	-2.24318300	3.83270300
H	2.25917300	-1.79415100	0.13194300	C	0.60099300	-2.33333600	3.70023100
H	4.30771000	-2.99989500	3.71519500	H	1.74869200	-3.97315200	2.86394500
H	6.40138200	-3.36191600	2.38205200	H	-0.81194900	-0.97134800	4.59046700
C	-0.62652800	-1.98335100	0.70502000	H	-3.96845200	-1.76963600	-2.85823200
C	-1.30798200	-2.51923700	-0.37942600	C	-3.56248200	-0.78180400	-3.04260700
C	-1.09633300	-3.85900500	-0.74931900	C	-2.32763000	-0.62686400	-3.69923800
C	-0.14420900	-4.62231400	-0.05602200	C	-4.27208500	0.33639900	-2.62340600
C	0.54170400	-4.08739400	1.02803400	C	-1.88274800	0.66553600	-4.02891500
C	0.31301500	-2.75523900	1.40769100	C	-3.76227300	1.62453100	-2.85879200
H	-0.80708900	-0.96019000	1.02237700	H	-5.22151000	0.22090600	-2.10973300
H	-2.00762800	-1.90489500	-0.93518900	C	-2.59164700	1.78512200	-3.61354200
H	0.03882900	-5.64275100	-0.37943100	H	-0.96491600	0.78070900	-4.59685800
H	1.25487200	-4.69200200	1.57924600	H	-2.23839100	2.78306000	-3.85366800
C	-5.20626700	-3.51101300	0.51964000	C	-4.16880500	2.59872400	-0.16011100
C	-6.00386200	-2.53677100	-0.10210000	C	-2.91145300	1.97296700	-0.03915800
C	-5.78709300	-2.22202400	-1.45408000	C	-4.91510500	2.85296700	1.00290000
C	-4.74520500	-2.82964900	-2.14361100	C	-2.42546900	1.61831300	1.21160300
C	-3.86385700	-3.69810200	-1.47966500	H	-2.29636900	1.79644600	-0.91126400
C	-4.12066700	-4.06194400	-0.14714800	C	-4.45351700	2.45003300	2.24901500
H	-5.44057500	-3.80328300	1.53853500	H	-5.86688500	3.36428200	0.89808400
H	-6.44579700	-1.52725200	-1.96425200	C	-3.18307600	1.86791000	2.36963300
H	-4.58411800	-2.62634000	-3.19788100	H	-1.44974500	1.15230100	1.30027600
H	-3.48526600	-4.78721700	0.34973100	H	-5.04819800	2.60615900	3.14367600
N	2.05785100	-2.14532100	2.90908900	C	-0.63201100	2.35501900	3.68409400
N	0.84523300	-2.20196800	2.61145500	C	0.65964500	1.91226300	4.01953300
N	-1.66665000	-4.47468200	-1.90825400	C	-0.78531700	3.58498200	3.01784900
N	-2.85433700	-4.32489600	-2.27434100	C	1.78023300	2.61756900	3.60080800
N	-7.49580900	-0.87132300	0.68860600	H	0.77341300	0.99882000	4.59481500
N	-7.10976100	-2.06065300	0.66549600	C	0.33390100	4.29080900	2.59502200

N	-4.10133000	4.45213100	-1.14636600	H	-1.77263200	3.98998800	2.82867000
N	-5.19301600	3.87351300	-1.33861500	C	1.62141900	3.78230500	2.83666700
C	-3.10305700	4.06720000	-0.20676300	H	2.77761700	2.26589100	3.84552100
C	-3.29754000	4.19045900	1.17763300	H	0.21973500	5.23616300	2.07360200
C	-2.25238900	3.88602600	2.03870000	C	2.59926200	4.16900000	0.13660200
C	-0.99160300	3.49067600	1.55402600	C	2.85423600	4.90752100	-1.03120900
C	-0.79396200	3.41849600	0.15968200	C	1.97414100	2.91057900	0.02347000
C	-1.83742400	3.72080700	-0.70572100	C	2.45243200	4.43750100	-2.27453200
H	-4.26601100	4.49204400	1.56409400	H	3.36520600	5.86012600	-0.93235900
H	-2.38839000	3.92440300	3.11506400	C	1.62060400	2.41617100	-1.22431400
H	0.15609400	3.11701700	-0.25705500	H	1.79704300	2.30106000	0.89941100
H	-1.69095200	3.67240700	-1.78060100	C	1.87074200	3.16611500	-2.38721200
C	2.35733800	2.02690900	0.58226800	H	2.60913000	5.02628000	-3.17299000
C	3.29508900	2.19948600	-0.42787800	H	1.15492300	1.43975000	-1.30675000
C	3.86761000	3.46621400	-0.65444100	C	3.16227400	-1.85623300	2.40304100
C	3.41934700	4.55572400	0.11066700	C	4.43409000	-2.43806300	2.29618400
C	2.48009100	4.39028300	1.12129000	C	2.41393600	-1.61444800	1.23736500
C	1.93438900	3.12069200	1.35692600	C	4.90620400	-2.84789700	1.05625900
H	1.93804300	1.04433300	0.77873800	H	5.02182300	-2.58793800	3.19648900
H	3.57781100	1.34960100	-1.03590700	C	2.91031000	-1.97619800	-0.00727100
H	3.83180200	5.53569600	-0.10925600	H	1.43731400	-1.14838100	1.31519700
H	2.16135200	5.23346400	1.72619800	C	4.16927800	-2.60128200	-0.11436900
C	6.68976900	0.10387700	-0.22808300	H	5.85941300	-3.35863700	0.96220100
C	6.75407200	-0.85532600	-1.25176200	H	2.30208500	-1.80503000	-0.88527100
C	6.51823300	-0.47235000	-2.57926900	C	2.35968600	0.60690500	-3.68497900
C	6.11047300	0.82483400	-2.86329700	C	1.91891600	-0.68714000	-4.01387200
C	5.95089100	1.76234000	-1.83012800	C	3.58793500	0.76524300	-3.01683800
C	6.30244000	1.40728300	-0.51693600	C	2.62435400	-1.80459200	-3.58708200
H	6.94647900	-0.17347600	0.78938200	H	1.00694500	-0.80518400	-4.59061900
H	6.64587100	-1.20385500	-3.37150000	C	4.29386800	-0.35083100	-2.58591500
H	5.91227700	1.13621500	-3.88426000	H	3.99137300	1.75407800	-2.83224200
H	6.25721100	2.14684200	0.27587600	C	3.78725200	-1.64020600	-2.82131300
N	-0.10644200	3.10151300	2.60813800	H	2.27418400	-2.80371500	-3.82681900
N	1.12176700	2.89841700	2.50850000	H	5.23792900	-0.23273700	-2.06305200
N	4.78083700	3.83887000	-1.69040300	N	-1.36094500	-2.80430900	-3.67315200
N	5.62327700	3.09150400	-2.23955300	N	-1.50113600	-1.67716200	-4.20295100
N	6.72784700	-2.94897600	-0.16472000	N	-4.51389200	2.78729400	-2.51284900
N	7.22071100	-2.19012500	-1.02785500	N	-4.74486500	3.16365500	-1.34294900

	N	-2.80954600	1.38791500	3.66187400
	N	-1.68318500	1.53237800	4.19222400
	N	2.78520100	4.53054700	2.48692100
	N	3.16301200	4.75333100	1.31590500
	N	1.39166500	2.78407200	-3.67732400
	N	1.53717800	1.65453400	-4.20057000
	N	4.53578400	-2.80116800	-2.46294200
	N	4.75620000	-3.17177900	-1.28917800
	N	2.77870200	-1.36702900	3.68884300
	N	1.64816500	-1.50747700	4.21130300
	N	-2.80625900	-4.51656200	2.48847100
	N	-3.17461700	-4.74570700	1.31564300

Table S2: Optimized geometries of tran-cyclic [n_t]paraphenylenediazenes obtained using the B3LYP/6-31+G(d,p).

[2_t]CPPD				[3_t]CPPD			
C	-1.39335500	1.35069800	0.25092300	C	2.53770200	-1.47719500	-0.01963500
C	-2.46738800	0.67977700	-0.52195000	C	1.71380300	-1.37101900	1.18483400
C	-1.01511900	0.66949200	1.50500000	C	2.26365400	-2.61353800	-0.90427300
C	-2.46767700	-0.67879500	-0.52201600	C	0.54008000	-2.02433400	1.26167800
H	-3.08399400	1.25212600	-1.20766300	H	2.07454400	-0.75109500	1.99870000
C	-1.01543000	-0.66929600	1.50496100	C	1.07061300	-3.25680500	-0.83750500
H	-0.65817900	1.26558800	2.33859900	H	2.98518400	-2.83578000	-1.68423200
C	-1.39397100	-1.35025400	0.25084500	C	0.06127600	-2.83090800	0.13353200
H	-3.08452100	-1.25081800	-1.20778600	H	-0.09150500	-1.95645100	2.13952300
H	-0.65875100	-1.26560400	2.33852100	H	0.79412300	-4.01553200	-1.56295600
C	1.39331900	-1.35068900	-0.25087600	C	-2.62335900	-1.34342300	0.37401000
C	2.46722800	-0.67976900	0.52217200	C	-2.81743600	-0.97255900	-1.03251100
C	1.01533200	-0.66951700	-1.50504700	C	-2.95045600	-0.32896400	1.37992200
C	2.46754200	0.67880300	0.52218700	C	-2.95055400	0.32769100	-1.37987500
H	3.08372500	-1.25211300	1.20798900	H	-2.83788600	-1.76761800	-1.77034900
C	1.01565900	0.66926900	-1.50504500	C	-2.81797300	0.97135400	1.03256300
H	0.65856300	-1.26563200	-2.33870600	H	-3.07829000	-0.64349000	2.41104600
C	1.39397300	1.35025300	-0.25087200	C	-2.62402000	1.34231800	-0.37394900
H	3.08429600	1.25084000	1.20802700	H	-3.07849600	0.64215300	-2.41100500
H	0.65916700	1.26555900	-2.33869800	H	-2.83884700	1.76640300	1.77039900
N	0.63226100	2.24963000	0.30582300	H	-0.09285600	1.95563800	-2.13923100
N	-0.63136100	2.24978900	-0.30586300	C	0.53886700	2.02412100	-1.26153000
N	-0.63230800	-2.24956800	-0.30600400	C	0.05993200	2.83091700	-0.13360000
N	0.63126800	-2.24982000	0.30576300	C	1.71287400	1.37131900	-1.18465000
[4_t]CPPD				C	1.06926100	3.25760800	0.83709200
C	-3.92218900	0.37558100	-0.21851600	C	2.53694100	1.47829500	0.01963500
C	-3.93363200	-0.18471400	1.13295100	H	2.07371900	0.75121900	-1.99833700
C	-3.92294900	-0.56579000	-1.33118900	C	2.26257700	2.61485600	0.90389500
C	-3.66942600	-1.49824100	1.33119400	H	0.79256500	4.01646800	1.56232700
H	-4.13206300	0.48587200	1.96029200	H	2.98413700	2.83766800	1.68366400
C	-3.48575300	-1.83228900	-1.13294700	N	3.40615100	0.57008300	0.37378100
H	-4.11967400	-0.17694600	-2.32558700	N	3.40650400	-0.56850800	-0.37358600
C	-3.19218100	-2.30966400	0.21851700	N	-1.21013800	-3.07001300	-0.07617700
H	-3.64218000	-1.93315700	2.32559600	N	-1.99411900	-2.39319900	0.82048500
H	-3.31737000	-2.51104400	-1.96028900	N	-1.99529200	2.39241100	-0.82039000

C	-0.37558000	-3.92218500	-0.21851900	N	-1.21154800	3.06951400	0.07626700
C	0.56579200	-3.92293900	-1.33119100	[5_t]CPPD			
C	0.18471400	-3.93363100	1.13294800	C	3.46389200	-3.67956700	-0.18581900
C	1.83229100	-3.48574200	-1.13294700	C	3.83622900	-3.28692400	1.11848300
H	0.17695000	-4.11966100	-2.32559000	C	4.54992900	-2.11248900	1.29549900
C	1.49824100	-3.66942500	1.33119400	C	4.88295500	-1.30191100	0.18569300
H	-0.48587300	-4.13206500	1.96028800	C	4.71412200	-1.81601400	-1.11861000
C	2.30966400	-3.19217600	0.21851900	C	4.01923700	-3.00167800	-1.29562400
H	2.51104500	-3.31735400	-1.96028700	H	3.44862900	-3.83309900	1.97042200
H	1.93315500	-3.64218100	2.32559600	H	4.73738700	-1.72189300	2.29097300
C	3.92219100	-0.37558200	-0.21851800	H	5.01084800	-1.21560300	-1.97055000
C	3.93363900	0.18471500	1.13294800	H	3.76444600	-3.35208600	-2.29109800
C	3.92294500	0.56578900	-1.33119100	C	4.56990100	2.15730300	-0.18578300
C	3.66943100	1.49824100	1.33119200	C	4.31151700	2.63270400	1.11853400
H	4.13207500	-0.48587100	1.96029000	C	4.09679500	2.89497800	-1.29556700
C	3.48574700	1.83228700	-1.13294900	C	3.41508600	3.67436800	1.29558000
H	4.11966700	0.17694400	-2.32559000	H	4.71118900	2.09527500	1.97045600
C	3.19218000	2.30966200	0.21851600	C	3.18388300	3.92223000	-1.11852200
H	3.64218800	1.93315800	2.32559300	H	4.35133100	2.54441300	-2.29105100
H	3.31736000	2.51104100	-1.96029000	C	2.74709700	4.24161000	0.18578900
H	0.48587100	4.13207000	1.96028800	H	3.10151900	3.97330900	2.29106100
C	-0.18471600	3.93363400	1.13294800	H	2.70455800	4.39000000	-1.97044800
C	0.37558000	3.92218500	-0.21851900	C	-0.63954400	5.01286200	-0.18570000
C	-1.49824200	3.66942800	1.33119300	C	-1.48728400	4.79084100	-1.29549900
C	-0.56579200	3.92293700	-1.33119200	C	-1.17155300	4.91405700	1.11860700
C	-2.30966500	3.19217700	0.21851800	C	-2.74636600	4.24004800	-1.11847500
H	-1.93315800	3.64218500	2.32559400	H	-1.07519400	4.92456500	-2.29097500
C	-1.83229000	3.48574100	-1.13294800	C	-2.43925400	4.38340100	1.29563300
H	-0.17694800	4.11965800	-2.32559100	H	-0.53693700	5.12810200	1.97053900
H	-2.51104400	3.31735300	-1.96028900	C	-3.18512800	3.92337100	0.18583200
N	-3.30491600	2.38949300	0.52837900	H	-3.33933400	3.92869800	-1.97040800
N	-3.73387800	1.64024200	-0.52837900	H	-2.82048700	4.17757900	2.29110800
N	-2.38949500	-3.30491700	0.52837400	C	-4.96517200	0.94082400	-0.18571000
N	-1.64024200	-3.73387600	-0.52838300	C	-5.03562100	0.40429300	1.11858500
N	3.30491600	-2.38949100	0.52838000	C	-5.01598600	0.06599100	-1.29553000
N	3.73388100	-1.64024300	-0.52837800	C	-4.92267600	-0.96534700	1.29558200
N	2.38949200	3.30491300	0.52837600	H	-5.04311300	1.07397300	1.97053100
N	1.64024200	3.73387600	-0.52838100	C	-4.88122100	-1.30167400	-1.11853300

[6_t]CPPD							
C	1.89241600	5.75289500	0.18530100	H	-5.01582100	0.49925800	-2.29099600
C	2.39337100	5.56040100	-1.11792300	C	-4.71561900	-1.81684400	0.18576500
C	3.57159100	4.84958400	-1.29468200	H	-4.84475100	-1.39154600	2.29104900
C	4.25571500	4.30893000	-0.18540500	H	-4.76835100	-1.96181700	-1.97047800
C	3.85584400	4.66687000	1.11781700	H	-2.57980600	-4.46430700	1.97045900
C	2.68569100	5.39089300	1.29457500	C	-1.94059200	-4.66416600	1.11851900
H	1.79748000	5.86892300	-1.96879600	C	-2.42909400	-4.43140600	-0.18578300
H	3.92168100	4.59237000	-2.28960800	C	-0.60308900	-4.97999600	1.29552800
H	4.40230100	4.27744200	1.96869200	C	-1.61277500	-4.75009300	-1.29559200
H	2.29707400	5.58505000	2.28950100	C	0.27071900	-5.04623800	0.18571500
H	-3.68830200	4.78189600	2.28951300	H	-0.17367100	-5.03756100	2.29099700
C	-3.32584900	5.02134000	1.29457900	C	-0.27040400	-5.04455700	-1.11858400
C	-4.03602400	4.51535700	0.18531900	H	-2.02477800	-4.61606700	-2.29106300
C	-2.11372300	5.67265300	1.11779800	H	0.39231200	-5.14122300	-1.97052600
C	-3.61884300	4.85291800	-1.11791400	N	5.04459900	0.06125000	0.49834100
C	-1.60381300	5.83994300	-0.18543200	N	4.97361400	0.84530600	-0.49845600
H	-1.50322100	5.95117500	1.96866100	N	1.50059900	4.81656300	0.49845000
C	-2.41411900	5.51782300	-1.29469500	N	0.73299800	4.99138300	-0.49835200
H	-4.18400000	4.49113300	-1.96877700	N	-4.11713800	2.91555300	0.49847800
H	-2.01632700	5.69237700	-2.28962800	N	-4.52060300	2.23955800	-0.49833500
C	5.92845800	1.23760000	0.18537100	N	-4.04512900	-3.01467100	0.49839400
C	6.01225600	0.70750900	-1.11785100	N	-3.52688000	-3.60726600	-0.49841900
C	6.01152900	0.36960000	1.29464800	N	1.61711000	-4.77871200	0.49835000
C	5.98574200	-0.66826800	-1.29460900	N	2.34084800	-4.46894200	-0.49846300
H	5.98154500	1.37782600	-1.96872600	[7_t]CPPD			
C	5.96954400	-1.00579100	1.11789000	C	6.89045500	0.86249300	-0.71832600
H	5.98534500	0.80323300	2.28957300	C	6.57729300	2.20870000	-0.71059400
C	5.85952400	-1.53105700	-0.18533500	C	6.36841000	2.88019100	0.51842900
H	5.93805400	-1.10006100	-2.28953500	C	6.64054000	2.21355800	1.72589100
H	5.90546700	-1.67375000	1.96876300	C	6.95453600	0.85871700	1.71814000
C	4.03602500	-4.51535300	0.18539700	C	7.00201700	0.15393200	0.50265800
C	3.32585100	-5.02131600	1.29466600	H	6.95662500	0.31393300	-1.65082300
C	3.61884200	-4.85293700	-1.11783000	H	6.39227000	2.74025400	-1.63688100
C	2.11372500	-5.67263300	1.11789700	H	6.49537900	2.74864800	2.65883500
H	3.68830500	-4.78185600	2.28959500	H	7.06172200	0.30419700	2.64486900
C	2.41411800	-5.51784400	-1.29459800	H	6.45367500	-3.38645800	-2.51566200
H	4.18399900	-4.49116700	-1.96870000	C	6.04182700	-3.82059000	-1.61026600
				C	6.28558200	-3.17795500	-0.38409400

C	1.60381300	-5.83994500	-0.18532900	C	5.17909000	-4.91041200	-1.66618500
H	1.50322300	-5.95113900	1.96876700	C	5.77936200	-3.74360600	0.81149500
H	2.01632400	-5.69241500	-2.28952700	C	4.54523200	-5.36681500	-0.49749800
C	-1.89241700	-5.75289100	0.18540600	H	4.89764800	-5.35269900	-2.61641000
C	-2.39337200	-5.56042100	-1.11782200	C	4.91920300	-4.82379900	0.75556500
C	-2.68569200	-5.39086800	1.29467300	H	5.99803400	-3.25719800	1.75510800
C	-3.57159300	-4.84960800	-1.29459300	H	4.44767700	-5.20407100	1.65428800
H	-1.79748200	-5.86895800	-1.96869000	H	4.02276300	5.54162600	1.82713700
C	-3.85584500	-4.66685100	1.11790300	C	3.58304300	5.86921200	0.89219100
H	-2.29707300	-5.58500700	2.28960300	C	2.33722500	6.46731100	0.86798500
C	-4.25571600	-4.30893500	-0.18532600	C	4.24467500	5.56144400	-0.32131400
H	-3.92168500	-4.59241300	-2.28952300	C	1.72162700	6.77231600	-0.37026400
H	-4.40230300	-4.27740800	1.96877100	H	1.77739200	6.61962000	1.78351900
H	-5.98154400	-1.37786200	-1.96869900	C	3.70384100	6.01296500	-1.53785300
C	-6.01225600	-0.70753000	-1.11783500	C	2.44993000	6.61418000	-1.56225200
C	-5.92845800	-1.23759800	0.18539500	H	4.23361100	5.78680600	-2.45762300
C	-5.98574000	0.66824400	-1.29461800	H	1.97127700	6.87149800	-2.50165500
C	-6.01152900	-0.36957800	1.29465800	H	1.41049800	-6.86280900	-2.05338600
C	-5.85952200	1.53105300	-0.18536000	C	0.78975400	-6.90597300	-1.16622800
H	-5.93805100	1.10001900	-2.28955300	C	1.39515300	-6.82354800	0.10486200
C	-5.96954300	1.00581100	1.11787400	C	-0.59333600	-6.90736600	-1.26304200
H	-5.98534500	-0.80319300	2.28959000	C	0.59335100	-6.90736500	1.26304200
H	-5.90546500	1.67378400	1.96873500	C	-1.39513800	-6.82355100	-0.10486200
N	-0.24018600	6.04206700	-0.49777100	H	-1.08368000	-6.86881200	-2.23089500
N	0.54053500	6.02263200	0.49763200	C	-0.78973900	-6.90597400	1.16622800
N	5.11259900	3.22907000	-0.49772400	H	1.08369400	-6.86881000	2.23089500
N	5.48612000	2.54323800	0.49768700	H	-1.41048300	-6.86281200	2.05338600
N	5.35277100	-2.81306400	-0.49766900	C	-4.54522100	-5.36682500	0.49749800
N	4.94557800	-3.47947100	0.49773200	C	-4.91919300	-4.82381000	-0.75556500
N	0.24018500	-6.04207300	-0.49766300	C	-5.17907900	-4.91042300	1.66618500
N	-0.54053500	-6.02261900	0.49774000	C	-5.77935400	-3.74361800	-0.81149500
N	-5.11260300	-3.22908100	-0.49766400	H	-4.44766500	-5.20408100	-1.65428800
N	-5.48612200	-2.54323000	0.49773500	C	-6.04181900	-3.82060300	1.61026600
N	-5.35276700	2.81305300	-0.49771600	H	-4.89763600	-5.35271000	2.61641000
N	-4.94557600	3.47947900	0.49767300	C	-6.28557500	-3.17796800	0.38409400
[8_t]CPPD (at B3LYP/6-31G (d))				H	-5.99802700	-3.25721100	-1.75510800
C	6.63523900	-4.56533400	0.18581400	H	-6.45366800	-3.38647200	2.51566200
C	6.31665800	-4.99352400	-1.11808900	C	-1.72164100	6.77231300	0.37026400

C	6.08430400	-5.23933700	1.29499400	C	-2.33723900	6.46730600	-0.86798500
C	5.35778300	-5.98024900	-1.29495600	C	-2.44994400	6.61417500	1.56225200
H	6.76099000	-4.48804900	-1.96729100	C	-3.58305600	5.86920500	-0.89219100
C	5.11659100	-6.21739700	1.11812700	H	-1.77740600	6.61961600	-1.78351900
H	6.36842400	-4.90931200	2.28942300	C	-3.70385400	6.01295800	1.53785300
C	4.69473200	-6.54431600	-0.18577600	H	-1.97129200	6.87149400	2.50165500
H	5.03339300	-6.27078900	-2.28938500	C	-4.24468700	5.56143500	0.32131400
H	4.61994300	-6.67157300	1.96732900	H	-4.02277500	5.54161800	-1.82713700
H	4.48805500	6.76098300	-1.96730700	H	-4.23362400	5.78679700	2.45762300
C	4.99352800	6.31665300	-1.11810200	C	-6.36841600	2.88017800	-0.51842900
C	4.56533500	6.63523700	0.18579900	C	-6.57729800	2.20868600	0.71059400
C	5.98025500	5.35777900	-1.29496500	C	-6.64054500	2.21354400	-1.72589100
C	5.23933600	6.08430500	1.29498200	C	-6.89045700	0.86247800	0.71832600
C	6.54432000	4.69473100	-0.18578200	H	-6.39227600	2.74024000	1.63688100
H	6.27079800	5.03338800	-2.28939200	C	-6.95453800	0.85870200	-1.71814000
C	6.21739700	5.11659300	1.11812000	H	-6.49538500	2.74863400	-2.65883500
H	4.90930700	6.36842700	2.28940900	C	-7.00201700	0.15391700	-0.50265800
H	6.67157200	4.61994700	1.96732400	H	-6.95662600	0.31391800	1.65082300
H	-1.03176100	7.97456000	2.28939400	H	-7.06172300	0.30418200	-2.64486900
C	-0.59748900	8.00702600	1.29496700	N	3.40091100	-6.16468800	-0.70810100
C	-1.46364700	7.92001700	0.18578400	N	2.72361300	-6.40878800	0.33288900
C	0.77838100	8.01433600	1.11810600	N	-2.72359900	-6.40879400	-0.33288900
C	-0.93559500	7.99753000	-1.11811700	N	-3.40089700	-6.16469500	0.70810100
C	1.30785200	7.94721200	-0.18579600	N	-6.80956000	-1.87247600	0.48082700
H	1.45071300	7.98428900	1.96731000	N	-6.90460000	-1.24805500	-0.61609500
C	0.44015300	8.01722000	-1.29497900	N	-5.66457000	4.09509200	-0.64888700
H	-1.60720800	7.95430600	-1.96732100	N	-5.28366600	4.61551900	0.44035000
H	0.87497900	7.99329300	-2.28940500	N	-0.33805800	6.98857200	0.53504600
C	1.46364500	-7.92001700	0.18581200	N	0.33804300	6.98857300	-0.53504600
C	0.93560200	-7.99753400	-1.11809200	N	5.28365500	4.61553100	-0.44035000
C	0.59748000	-8.00702300	1.29499100	N	5.66456100	4.09510400	0.64888700
C	-0.44014500	-8.01722500	-1.29496200	N	6.90460300	-1.24804000	0.61609500
H	1.60722000	-7.95431200	-1.96729200	N	6.80956400	-1.87246200	-0.48082700
C	-0.77838900	-8.01433300	1.11812100				
H	1.03174600	-7.97455400	2.28942000				
C	-1.30785100	-7.94721300	-0.18578500				
H	-0.87496400	-7.99330100	-2.28939100				
H	-1.45072600	-7.98428400	1.96732000				

C	-4.56533600	-6.63523600	0.18578800
C	-5.23934400	-6.08430200	1.29496500
C	-4.99352100	-6.31665500	-1.11811700
C	-6.21740500	-5.11659100	1.11809500
H	-4.90932100	-6.36842200	2.28939500
C	-5.98024700	-5.35778100	-1.29498800
H	-4.48804200	-6.76098600	-1.96731800
C	-6.54432000	-4.69473200	-0.18581000
H	-6.67158500	-4.61994400	1.96729500
H	-6.27078400	-5.03339200	-2.28941700
H	-4.61995500	6.67158000	1.96728500
C	-5.11659800	6.21740200	1.11808100
C	-4.69473200	6.54431700	-0.18582000
C	-6.08431100	5.23934200	1.29494500
C	-5.35777600	5.98024700	-1.29500300
C	-6.63524000	4.56533500	0.18576500
H	-6.36843800	4.90931900	2.28937400
C	-6.31665200	4.99352200	-1.11813900
H	-5.03338100	6.27078500	-2.28943000
H	-6.76097900	4.48804400	-1.96734200
C	-7.94721500	1.30785100	-0.18581800
C	-8.01722100	0.44014600	-1.29499700
C	-8.01434100	0.77838700	1.11808600
C	-7.99753200	-0.93560100	-1.11812900
H	-7.99329100	0.87496700	-2.28942600
C	-8.00703300	-0.59748200	1.29495400
H	-7.98429600	1.45072300	1.96728600
C	-7.92002200	-1.46364600	0.18577500
H	-7.95430700	-1.60721800	-1.96732900
H	-7.97456800	-1.03174900	2.28938300
C	7.92002000	1.46364600	0.18581900
C	7.99753800	0.93559800	-1.11808400
C	8.00702600	0.59748500	1.29500000
C	8.01722900	-0.44015000	-1.29494900
H	7.95431600	1.60721400	-1.96728600
C	8.01433700	-0.77838500	1.11813500
H	7.97455600	1.03175400	2.28942800
C	7.94721800	-1.30785200	-0.18576900

H	7.99330600	-0.87497200	-2.28937700
H	7.98428800	-1.45071900	1.96733700
N	-7.24267100	-3.50683400	-0.49788500
N	-7.54774400	-2.79037400	0.49785000
N	-7.60105000	2.64163000	-0.49789500
N	-7.31013300	3.36395400	0.49783900
N	-3.50683100	7.24266700	-0.49788900
N	-2.79037600	7.54773800	0.49785100
N	2.64163200	7.60104900	-0.49786700
N	3.36395100	7.31012800	0.49787000
N	7.24267200	3.50683200	-0.49785100
N	7.54774000	2.79037400	0.49788800
N	7.60105700	-2.64163200	-0.49784500
N	7.31013100	-3.36395300	0.49789000
N	3.50683200	-7.24266600	-0.49784900
N	2.79037300	-7.54773700	0.49788700
N	-2.64163000	-7.60105100	-0.49786500
N	-3.36395400	-7.31012500	0.49786700

Table S3: Vibrational frequencies cis-cyclic [n]paraphenylenediazenes ([n_c]CPPDs) obtained using the B3LYP/6-31+G(d,p).

[2 _c]CPPD	[3 _c]CPPD	[4 _c]CPPD	[5 _c]CPPD	[6 _c]CPPD ₁	[7 _c]CPPD ₁	[8 _c]CPPD ₁
83.34	17.87	10.11	12.77	13.93	11.73	10.29
150.32	59.96	52.3	26.15	15.89	13.14	12.32
159.3	86.83	55.57	30.39	19.72	16.44	15.33
176.86	98.35	59.56	38.72	24.84	19.4	17.72
276.67	99.48	67.52	44.14	29.53	25.39	19.45
306.52	105.11	67.52	52.99	37.63	30.6	20.88
308.87	113.78	68.74	62.36	40.53	32	29.23
341.25	182.43	119.45	63.57	45.41	34.71	33.96
385.14	206.78	135.42	73.15	61.53	47.62	35.13
441.28	208.89	135.42	83.13	64.83	54.78	37.16
450.47	268.18	158	103.92	66.89	57.61	52.29
463.7	302.42	158	114.31	74.8	60.15	54.69
503.74	327.1	179.12	120.87	78.29	65.97	57.39
575.95	343.03	218.2	142.42	99.2	72.3	62.36
595.15	346.15	222.3	144.63	106.23	76.23	65.42
605.15	399.86	235.26	170.31	108.42	86.75	67.74
609.6	406.9	269.69	179.23	118.8	90.07	70.45
631.37	415.79	269.69	187.91	139.53	106.44	78.98
635.63	425.99	309.17	208.56	150.59	115.2	81.89
635.78	450.26	309.17	211.74	155.11	118.92	90.76
670.7	452.44	339.71	242.67	181.57	133.76	94.8
701.96	481.13	372.75	257.03	186.42	138.66	109.11
706.73	490.05	398.49	265.01	195.89	140.41	120.77
773.85	567.02	406.24	288.46	205.41	165.69	126.14
791.82	597	410.89	295.73	222.64	172.12	129.13
800.51	604.63	410.89	333.03	228.55	178.1	142.98
802.97	610.76	415.63	336.01	246.89	186.13	149.08
840.97	614.03	418.89	350.95	261.1	210.47	155.29
859.83	639.48	430.18	354.84	264.84	212.99	171.18
937.68	642.13	430.18	392.31	299.67	220.33	180.19
942.12	656.97	495.59	397.86	319.75	232.74	182.94
955.73	658.66	513.16	407.41	320.75	242.52	191.27
957.3	673.99	513.16	411.77	341.43	265.19	211.39
966.43	686.62	529.76	414.12	351.18	273.38	215.66
1023.62	705.67	566.37	417.48	358.98	277.25	219.6
1025.31	715.62	592.09	423.44	359.08	296.88	236.82
1113.88	776.89	592.09	430.53	397.55	307.69	238.92
1116.5	777.09	616.13	442.88	404.29	315.38	257.81
1132.13	807.87	619.6	455.84	408.14	327.1	265.01
1132.32	819.02	634.3	485.01	408.9	333.38	279.4
1151.94	822.08	642.61	490.5	413.16	339.63	283.93

1152.19	829.24	642.61	504.93	414.34	356.22	294.27
1186.46	830.95	661.26	532.14	416.36	363.79	304.23
1191.86	839.84	661.26	534.1	417.38	392.17	312.7
1303.14	865.4	673.78	565.43	426.78	401.65	320.46
1303.28	868.75	690.21	585.83	430.16	409.72	331.31
1305.65	920.56	703.37	591.16	453.39	411.16	333.8
1315.46	920.6	711.73	608.24	455.08	412.14	339.3
1394.16	955.85	711.73	615.97	473.99	414.89	358.77
1419.9	961.52	736.1	623.16	484.15	416.26	363.57
1487.5	961.57	752.35	626.7	503.84	417.7	393.32
1497.73	966.89	798.43	635.44	523.24	422.19	401.74
1523.98	972.21	798.43	638.97	528.82	425.27	403.85
1533.34	972.58	811.29	646.33	538.21	432.78	408.62
1573.6	1030.11	833.19	658.23	581.06	434.55	412.44
1599.06	1031.19	833.19	661.88	585.4	454.13	413.23
1607.46	1031.38	833.68	673.38	596.71	460.89	415.61
1616.67	1128.36	837.23	676.07	606.43	480.97	416.83
3192.32	1128.88	837.77	688.74	608.17	484.21	418.45
3194.24	1129.94	837.77	698.03	618.56	506.43	419.52
3194.74	1149.77	840.91	708.15	623.12	511.61	425.06
3196.94	1156.01	856.18	716.02	626.82	518.58	426.4
3206.74	1156.84	868.86	726.94	630.11	530.94	438.82
3207.52	1178.36	888.77	751.71	635.76	539.05	440.82
3209.44	1179	888.77	752.23	642.56	574.19	445.82
3210.51	1183.02	896.15	782.3	644.19	581.6	468.96
	1198.88	964.98	796.2	648.4	590.54	487.87
	1202.59	966.38	802.04	661.07	598.93	492.51
	1206.52	966.7	810.75	666.35	611.22	502.95
	1312.06	966.7	826.42	669.56	613.19	508.99
	1318.46	980.99	831.08	676.06	621.19	517.97
	1320.62	981.66	834.31	688.96	626.34	525.17
	1326.45	981.66	835.6	694.82	628.23	529.69
	1330.4	982.18	837.89	700.68	630.07	535.76
	1335.28	1025.55	839.19	708.04	633.78	570.49
	1429.23	1025.78	839.9	721.62	634.82	580.81
	1436.59	1025.81	841.19	733.13	648.29	584.75
	1439.11	1025.81	842.56	748.22	649.02	597.49
	1514.54	1126.24	850.64	759.63	656.93	598.76
	1514.66	1127.79	869.72	770.39	658.95	612.93
	1514.69	1131.68	879.7	792.41	666.08	614.39
	1593.24	1131.68	883.4	795.03	671.96	619.95
	1599.44	1136.04	897.96	808.51	676.77	625.67
	1600.8	1138	902.94	813.29	681.9	626.36
	1601.75	1138	966.38	823.15	687.91	630.29

	1608.37	1163.17	968.15	826.6	700.21	636.47
	1616.22	1163.84	968.32	831.82	705.16	639.5
	1638.67	1183.57	970.47	833.17	713.15	643.11
	1638.91	1183.57	976.81	835.13	724.91	644.2
	1645.38	1192.52	980.78	836.67	728.02	647.41
	3194.22	1208.83	980.88	837.58	746.44	658.06
	3194.47	1208.83	984.58	838.38	752.22	659.39
	3196.46	1209.15	984.59	839.77	770.91	661.88
	3201.76	1209.46	985.94	842.85	775.24	667.54
	3204.29	1322.67	1024.84	846.69	790.28	677.44
	3208.62	1324.15	1025.37	857.3	793.05	679.83
	3209.03	1324.15	1025.49	870.12	798.17	682.62
	3210.26	1326.21	1025.68	874.75	809.68	686.27
	3213.73	1328.33	1025.69	897.52	816.12	701.76
	3216.84	1336.76	1112.58	898.3	825.8	703.68
	3224.91	1336.76	1128.52	908.32	825.94	712.02
	3227.71	1345.36	1130.12	908.93	836.98	714.78
		1438.78	1132.89	964.07	837.96	725.31
		1442.46	1134.26	964.42	839.63	738.15
		1442.46	1134.38	966.03	840.82	744.16
		1447.82	1137.56	966.06	841.76	755.85
		1509.43	1138.3	969.93	841.87	769.87
		1511.61	1151.47	971.55	843.22	775.55
		1511.62	1154.58	978.24	843.74	782.04
		1513.26	1170.8	978.27	847.53	793.52
		1583.64	1171.83	980.39	849.15	796.03
		1591.85	1183.67	980.61	856.87	807.23
		1593.59	1189.13	981.75	863.99	811.38
		1593.59	1193.46	982.14	875.16	816.1
		1598.64	1206.73	1026.76	880.37	823.52
		1598.64	1208.63	1026.83	885.7	825.37
		1603.81	1209.42	1027.38	889.93	833.82
		1614.45	1209.57	1027.61	894.86	836.45
		1633.94	1215.61	1029.24	901.57	836.69
		1647.6	1321.32	1029.49	907.33	837.41
		1647.6	1322.98	1125.62	962.17	839.99
		1655.91	1324.11	1126.28	963.39	841.18
		3199.78	1324.61	1130.16	965.78	843.22
		3199.83	1325.57	1130.85	966.81	843.89
		3199.83	1328.23	1132.06	967.48	845.01
		3199.87	1328.38	1132.25	968.73	850.5
		3204.41	1335.52	1135.43	969.43	853.28
		3204.74	1338.83	1135.76	971.84	854.88
		3204.77	1348.88	1143.01	972.34	857.59

		3204.77	1439.73	1144.89	972.66	867.68
		3213.78	1439.81	1156.84	974.31	871.2
		3213.8	1443.75	1160.46	977.37	881.23
		3213.8	1444.67	1171.77	981.18	886.82
		3213.86	1448.6	1177.08	981.33	890.84
		3218.17	1506.99	1180.49	1028.04	894.91
		3218.17	1511.04	1185.81	1028.7	899.64
		3218.3	1513.05	1189.39	1029.35	903.8
		3218.44	1513.99	1191.31	1029.89	908.68
			1516.38	1205.29	1030.17	956.67
			1575.31	1205.72	1030.62	964.12
			1581.06	1206.65	1031.02	965.41
			1584.98	1207.48	1130.23	966
			1590.54	1207.85	1132.62	967.2
			1590.64	1210.02	1134.32	970.93
			1598.54	1319.88	1135.69	972.32
			1599	1321.6	1137.24	973.07
			1606.36	1322.23	1137.64	974.27
			1610.54	1322.56	1139.55	975.45
			1611.55	1323.22	1140.84	976.2
			1634.16	1323.38	1141.79	976.51
			1642.04	1327.87	1144.95	976.54
			1648.35	1329.04	1148.15	978.99
			1650.93	1331.38	1151.7	980.74
			1654.72	1335.24	1159.98	986.12
			3197	1338.87	1162.92	1028.55
			3197.24	1340.97	1174.19	1028.72
			3199.26	1435.86	1176.06	1029.08
			3199.3	1438.27	1185.2	1029.15
			3202.53	1439.18	1187.86	1029.55
			3202.56	1442.39	1193.26	1029.73
			3202.63	1444.3	1195.81	1030.01
			3204.55	1445.09	1197.68	1030.89
			3204.57	1510.32	1212.07	1127.85
			3214.83	1510.42	1214.79	1133.04
			3214.84	1513.76	1215.3	1134.3
			3215.51	1513.96	1216.3	1135.89
			3217.74	1515.14	1217.29	1136.87
			3217.98	1515.3	1220.07	1137.09
			3217.99	1580.45	1221.61	1138.49
			3219.31	1580.77	1324.79	1139.63
			3223.89	1588.1	1330	1140.93
			3228.47	1588.17	1330.08	1141.54
			3228.48	1594.35	1331.17	1142.95

			3237.07	1595.14	1331.65	1144.47
				1601.5	1332.45	1149.22
				1602.71	1333.54	1156.55
				1607.89	1335.77	1160.44
				1608.31	1336.5	1168.1
				1615.09	1337.57	1170.05
				1616.24	1340.43	1179.58
				1635.46	1344.13	1181.35
				1637.88	1349.27	1187.91
				1643.01	1350.54	1188.82
				1646.27	1447.2	1193.4
				1649.38	1449.03	1194.77
				1651.33	1450.41	1196.49
				3194.7	1452.76	1213.7
				3194.95	1454.27	1214.83
				3198.57	1456.64	1216.01
				3198.58	1457.47	1216.87
				3199.64	1519.87	1217.16
				3199.65	1520.5	1217.46
				3202.36	1522.55	1217.67
				3202.39	1522.85	1220.8
				3202.84	1524.91	1327.65
				3202.84	1525.68	1329.71
				3207.25	1526.57	1330.54
				3207.25	1583.04	1331.13
				3212.41	1585.19	1331.69
				3212.42	1589.06	1332.06
				3213.62	1591.59	1333.5
				3213.63	1594.81	1333.81
				3216.67	1599.95	1335.61
				3216.68	1600.83	1336.43
				3216.92	1604.38	1336.65
				3216.93	1605.47	1339.36
				3222.64	1607.29	1342.32
				3222.64	1609.69	1345.5
				3241.67	1612.13	1347.12
				3242.5	1613.02	1350.57
					1616.64	1447.15
					1645.75	1448.76
					1647.27	1450.3
					1651.49	1452.52
					1652.76	1452.95
					1656.33	1454.84
					1658.12	1455.98

					1663.53	1457.72
					3198.35	1520.36
					3201.73	1521.1
					3205.3	1521.75
					3206.2	1522.74
					3206.49	1523.27
					3207.71	1525.06
					3208.01	1525.34
					3208.15	1525.97
					3208.77	1581.28
					3208.94	1582.92
					3210.76	1586.09
					3212.14	1591.81
					3215.44	1594.72
					3218.9	1600.13
					3220.27	1601.04
					3221.09	1601.78
					3221.94	1603.19
					3222.02	1604.91
					3222.24	1606.14
					3222.57	1608.82
					3224.98	1611.23
					3225.63	1612.69
					3225.83	1614.21
					3227.74	1616.18
					3229.32	1643.52
					3239.23	1647.09
					3241.82	1648.35
					3267.09	1652.1
						1653.67
						1656.97
						1658.78
						1660.12
						3202.81
						3203.03
						3205.19
						3205.22
						3205.22
						3206.31
						3206.84
						3208.2
						3208.74
						3209.31
						3210.14

						3210.95
						3211.62
						3212.63
						3215.4
						3217.7
						3218.89
						3219.41
						3219.76
						3221.53
						3222.32
						3222.48
						3222.62
						3225.95
						3231.65
						3232.44
						3233.42
						3234.46
						3234.49
						3237.57
						3240.89
						3244.82

[6_c]CPPD₂	[7_c]CPPD₂	[8_c]CPPD₂
15.3	8.1	21.3
16.3	13.0	21.4
23.0	15.2	26.0
23.7	19.6	26.4
26.2	23.7	31.4
34.3	24.9	33.4
36.6	29.2	33.4
49.6	33.2	35.4
51.4	37.9	39.1
63.1	51.4	40.0
73.2	55.1	48.9
73.5	60.9	55.2
90.2	65.3	55.2
97.5	71.2	66.3
98.0	76.2	70.0
142.1	84.3	75.6
144.7	89.3	75.6
145.0	100.3	84.5
154.0	114.6	96.5
154.1	123.6	96.6
190.8	128.5	97.8
192.4	142.7	105.0
192.6	152.8	128.7
199.0	156.9	134.3

219.1	170.5	134.3
252.2	186.0	147.6
252.6	190.3	154.4
256.6	203.8	168.4
281.1	212.7	174.4
281.3	220.5	174.4
313.4	240.9	193.3
319.9	250.1	193.3
320.0	256.4	202.7
328.7	275.6	210.2
329.0	284.2	233.5
368.5	296.3	239.0
399.9	305.3	244.3
400.1	312.1	244.4
402.8	325.1	276.0
411.6	327.5	280.0
412.8	336.6	280.0
413.5	350.2	288.5
426.3	358.3	312.3
426.9	396.1	315.3
427.7	405.5	319.8
451.5	408.8	319.8
454.1	411.0	340.6
454.3	414.0	342.9
472.8	415.1	342.9
496.7	417.1	370.4
497.1	421.9	395.4
519.6	423.5	398.0
519.8	424.8	410.9
524.6	429.5	410.9
567.8	438.6	413.6
568.0	448.2	415.5
593.9	462.4	415.6
598.7	483.4	417.1
616.0	486.8	421.1
616.2	508.2	424.4
624.2	509.4	425.9
626.3	518.7	425.9
626.4	526.3	438.0
643.9	533.0	438.0
644.2	574.6	445.0
644.3	581.1	462.2
660.6	597.0	492.8
665.9	598.6	506.3
666.1	604.9	506.9
683.4	616.2	507.0
683.5	620.1	523.1
686.3	623.1	524.9
704.6	625.4	524.9
704.7	631.7	528.6
712.9	632.5	580.5
728.8	635.7	582.8

745.7	645.5	582.8
746.0	650.4	591.6
778.0	658.3	603.1
778.3	660.5	613.7
786.2	666.8	613.7
799.6	670.4	618.6
799.7	679.0	621.0
814.6	682.2	626.5
822.8	683.5	626.5
832.3	701.0	639.9
832.8	705.0	640.5
842.3	717.5	645.3
844.0	722.3	645.3
844.2	739.9	646.5
844.7	745.1	658.7
845.5	753.1	664.1
845.8	772.3	667.0
852.9	778.6	667.0
856.8	788.4	674.4
857.0	793.5	674.5
876.6	794.5	676.8
876.8	808.6	684.9
883.0	813.1	705.1
892.4	822.5	712.7
898.1	826.3	712.7
898.3	834.4	718.7
974.3	837.9	730.1
975.0	841.2	741.8
976.3	842.1	741.8
979.3	843.0	753.3
979.8	843.6	777.1
980.7	845.6	779.9
986.8	847.3	780.2
987.6	848.9	780.2
987.8	849.8	805.9
989.5	857.2	810.4
990.0	863.0	810.4
990.7	877.3	814.5
1025.0	881.1	826.6
1025.1	886.3	830.1
1025.3	887.6	830.1
1025.7	888.8	832.8
1025.7	901.1	838.3
1026.1	901.3	841.3
1122.1	961.4	841.3
1127.1	963.3	843.3
1127.2	967.4	844.8
1131.8	970.4	845.3
1131.8	971.1	845.3
1133.4	971.6	847.3
1137.3	972.6	854.9
1138.6	973.2	857.2

1138.7	974.7	857.2
1146.2	975.2	859.6
1146.3	976.9	880.3
1161.2	982.4	885.5
1161.7	984.0	885.5
1176.1	990.5	889.8
1176.4	1027.1	898.2
1188.6	1027.9	899.0
1188.8	1028.7	899.0
1193.9	1029.1	903.5
1211.6	1029.2	963.0
1211.7	1029.6	966.0
1211.7	1030.3	966.0
1214.0	1124.3	966.3
1214.1	1129.8	967.2
1214.3	1133.9	967.8
1324.7	1134.7	967.9
1324.8	1136.0	970.8
1325.5	1136.4	984.5
1326.0	1140.4	984.6
1327.0	1140.9	984.6
1327.2	1142.3	984.7
1331.5	1144.1	988.5
1331.7	1145.2	988.6
1338.2	1149.3	992.9
1343.1	1157.6	993.0
1349.0	1161.6	1028.7
1349.1	1171.6	1028.7
1445.2	1175.9	1028.8
1445.3	1185.7	1029.1
1448.9	1187.3	1029.3
1448.9	1193.0	1029.3
1452.1	1195.8	1029.5
1452.1	1197.7	1029.9
1510.5	1213.3	1126.1
1511.4	1215.1	1130.9
1511.7	1215.4	1130.9
1514.8	1215.8	1136.7
1515.1	1221.7	1139.1
1516.7	1222.6	1139.6
1566.8	1224.9	1139.6
1572.5	1324.8	1142.0
1572.6	1329.5	1145.1
1589.2	1330.5	1145.2
1589.3	1331.2	1145.4
1596.1	1331.7	1148.0
1596.1	1332.2	1149.5
1596.6	1332.9	1155.8
1597.7	1336.1	1155.8
1601.4	1336.6	1164.5
1602.4	1338.5	1174.5
1602.5	1339.7	1180.5

1638.9	1342.4	1180.5
1643.5	1349.5	1185.3
1643.7	1351.0	1195.7
1651.4	1448.6	1197.0
1651.6	1449.2	1197.0
1654.4	1451.6	1199.9
3200.4	1452.5	1219.6
3200.5	1454.3	1219.6
3200.7	1456.2	1221.0
3203.8	1457.4	1221.2
3203.9	1517.8	1221.3
3204.0	1520.3	1222.4
3204.1	1521.2	1222.4
3204.2	1522.4	1224.8
3204.3	1524.1	1328.9
3205.9	1526.0	1329.5
3205.9	1527.0	1329.5
3206.0	1580.5	1331.5
3213.8	1582.1	1334.9
3213.8	1588.1	1334.9
3214.1	1591.3	1335.9
3217.7	1594.9	1336.3
3217.9	1597.7	1337.9
3218.2	1599.8	1337.9
3222.4	1603.1	1339.0
3222.6	1605.0	1340.3
3222.8	1606.7	1344.4
3223.3	1608.2	1346.7
3223.8	1609.7	1346.8
3223.8	1611.6	1348.9
	1614.6	1450.3
	1645.9	1450.3
	1647.8	1450.4
	1651.9	1452.4
	1654.0	1453.8
	1658.4	1455.5
	1658.7	1455.5
	1662.7	1457.2
	3200.8	1520.0
	3200.8	1520.0
	3205.6	1520.3
	3206.6	1522.5
	3207.1	1524.6
	3208.1	1525.7
	3208.5	1525.7
	3209.2	1526.8
	3210.0	1574.0
	3210.0	1577.3
	3212.0	1577.3
	3213.3	1581.5
	3220.2	1598.1
	3220.5	1598.8

	3221.2	1598.9
	3221.9	1598.9
	3222.3	1602.2
	3223.6	1602.2
	3223.8	1603.2
	3224.5	1604.4
	3224.9	1605.1
	3226.5	1607.6
	3226.7	1607.7
	3227.1	1609.7
	3239.4	1645.5
	3244.1	1648.3
	3266.4	1648.3
	3273.1	1651.0
		1655.0
		1657.6
		1657.6
		1658.4
		3209.5
		3209.5
		3209.6

Table S4: Vibrational frequencies trans-cyclic [n]paraphenylenediazenes ([n]CPPDs) obtained using the B3LYP/6-31+G(d,p).

[2 _t]CPPD	[3 _t]CPPD	[4 _t]CPPD	[5 _t]CPPD	[6 _t]CPPD	[7 _t]CPPD	[8 _t]CPPD
123.4	52.2	23.97	27.51	19.53	14.66	12.49
159.9	62.3	37.45	27.54	19.55	14.81	12.51
181.0	87.7	56.63	33.66	25.09	19.97	19.11
216.6	99.7	71.1	33.66	25.11	20.1	19.13
250.0	114.3	85.2	73.3	39.39	37.63	31.35
282.5	139.0	85.2	73.36	44.37	37.7	31.35
358.1	198.4	119.73	85.38	61.27	40.11	39.74
401.1	216.3	119.73	85.39	77.98	40.21	39.74
401.8	230.1	122.22	89.17	78	67.57	47.05
408.1	259.9	144.92	89.18	78.95	68.16	49.13
425.9	269.0	195.71	92.34	79.04	68.48	63.86
486.6	282.3	207.57	120.84	79.08	70.31	65.2
534.0	328.4	218.51	120.85	88.96	71.12	65.2
543.9	345.5	228.11	145.93	92.38	75.2	69.26
557.0	369.6	228.11	168.08	92.42	76.49	70.44
557.1	390.3	249.25	195.56	121.89	80.11	70.46
575.6	417.5	249.25	195.57	121.91	82.22	81.45
596.8	422.1	321.57	225.15	135.51	109.42	81.45
624.2	427.5	326.66	225.15	144.64	109.74	87.44
642.1	438.9	330.34	228.87	178.51	118.35	87.44
708.6	461.5	341.44	228.89	197.95	133.19	95.56
712.7	494.9	341.44	237.66	197.97	139.96	106.83
745.5	495.7	395.74	237.67	203.79	145.16	106.85
751.8	499.4	395.74	239.63	203.79	156.85	110.04
773.6	563.6	421.95	316.83	219.61	163.44	121.27
784.0	579.4	424.96	316.83	231.38	205.6	121.27
786.6	583.4	428.55	336.28	231.39	209.99	127.44
797.6	586.4	434.38	358.88	231.81	224.26	153.84
822.6	598.8	434.38	382.44	231.82	230.6	153.84
855.2	607.1	466.22	382.45	245.5	232.11	169.5
934.1	631.5	481.01	390.7	315.24	237.77	188.92
951.3	642.0	497.29	390.72	315.24	247.09	188.92
952.8	645.3	497.29	417.34	339.41	248.2	200.53
957.7	723.7	513.87	417.34	342.08	254.13	212.29
963.8	733.3	529.86	417.56	342.08	254.29	212.29
965.2	747.1	533.29	417.57	356.65	258.03	214.78
978.9	763.7	569.05	424.33	377.24	279.39	214.78
979.0	770.5	569.05	426.81	377.26	281.59	220.69
1090.9	780.9	586.74	426.82	416.25	304.12	220.69
1092.3	786.6	592.13	484.75	416.26	317.41	239.48
1162.4	793.3	607.37	502.85	418.93	335.9	239.48

1163.9	798.9	607.37	502.85	419.01	347.71	251.83
1241.0	804.8	614.2	517.79	419.03	361.27	298.85
1245.8	806.5	614.2	517.79	419.93	364.54	298.86
1279.0	818.3	630.06	549.36	419.94	388.59	322.96
1287.9	843.6	675.69	549.37	424.35	389.56	322.96
1360.7	857.3	737.06	558.14	426.97	393.45	341.93
1375.6	863.6	739.61	558.15	445.54	400.43	355.93
1395.9	961.8	740.15	558.98	472.78	415.63	356.83
1401.4	961.9	740.15	558.99	485.39	419.27	356.83
1540.6	962.3	773.28	570.69	512.9	421.83	370.43
1541.7	981.5	782.61	625.98	512.9	430.88	370.43
1580.7	986.6	782.61	633.58	525.9	431.67	400.85
1583.1	988.1	787.1	633.58	525.91	435.75	400.86
1584.6	989.4	805.78	648.77	530.06	437.88	418.96
1586.6	1004.2	807.98	648.78	546.47	453.67	423.39
1682.4	1004.7	807.98	650.83	546.47	456.58	423.39
1684.3	1037.7	813.08	650.83	556.09	481.45	423.48
3204.2	1043.2	833.45	707.29	567.38	490.61	423.49
3204.2	1052.6	835.21	715.68	567.39	496.18	424.03
3204.9	1109.0	835.21	730.5	583.01	511.2	424.03
3205.0	1116.4	842.57	730.51	583.01	511.74	425.05
3220.2	1117.3	855.19	751.03	583.33	530.6	425.17
3220.4	1170.2	866.96	751.06	629.9	531.73	434.56
3221.6	1178.1	866.96	799.67	635.03	539.35	434.56
3221.7	1180.0	876	816.24	635.04	539.6	452.89
	1269.3	965.36	816.26	647.42	544.26	477.26
	1279.7	966.43	821.07	647.42	545.06	487.28
	1279.9	966.43	821.07	654.73	551	505.46
	1314.4	967.29	824.19	665.73	552.02	505.46
	1329.2	990.58	830.04	665.73	568.21	520.34
	1329.2	991.29	830.04	709.17	569.39	520.34
	1382.4	991.29	861.54	718.15	578.11	525.71
	1394.0	992.78	861.54	727.19	607.53	532.5
	1399.0	994.56	863.26	727.2	608.9	532.5
	1428.5	995.4	863.26	747.09	630.96	552.93
	1437.9	995.4	872.86	747.11	635.08	552.93
	1439.5	995.84	872.86	756.76	635.19	557.34
	1534.3	1074.51	879.24	794.88	644.25	557.35
	1539.4	1075.55	915.19	821.86	644.68	558.13
	1563.9	1075.55	915.19	821.86	652.34	558.13
	1595.4	1082.99	936.16	824.75	652.86	558.98
	1597.9	1120.14	936.16	826.49	676.62	581.35
	1601.3	1120.19	947.13	826.5	678.58	581.35
	1607.1	1120.19	981.9	830.03	712.73	590.98

	1609.1	1121.9	984.11	830.04	714.66	624.57
	1615.6	1169.34	984.12	831.75	725.47	624.57
	1663.8	1170.51	985.64	852.98	726.31	634.77
	1686.4	1170.51	985.65	852.98	742.97	637.57
	1687.6	1172.1	989.91	863.48	742.97	637.57
	3201.9	1278.26	990.22	867.01	755.8	645.24
	3201.9	1282.82	990.23	868.71	755.91	645.25
	3204.4	1282.82	990.26	868.72	796.77	654.27
	3205.2	1289.08	990.26	877.96	816.17	654.27
	3210.0	1329.42	1009.56	877.97	816.64	658.48
	3210.0	1331.22	1009.56	883.02	831.46	685.12
	3217.7	1331.22	1009.59	914.02	831.81	685.12
	3217.8	1332.83	1009.6	924.97	833.12	719.72
	3222.1	1380.12	1009.95	924.98	833.15	721.09
	3223.2	1391.5	1056.48	941.94	834.74	731.75
	3229.7	1391.5	1123.55	941.94	835.06	731.75
	3229.7	1410.8	1123.55	949.8	836.2	746.91
		1424.31	1124.69	983.32	846.37	746.91
		1444.22	1124.69	984.89	846.64	760.74
		1444.22	1129.12	984.89	863.73	760.74
		1446.49	1133.79	986.41	863.85	766.34
		1491.38	1133.8	986.42	867.62	792.55
		1492.7	1160.13	986.94	867.84	812.28
		1492.7	1160.13	992.53	874.49	812.28
		1537.95	1191.62	992.54	874.59	838.91
		1548.18	1191.63	992.56	882.45	838.91
		1583.6	1202.65	992.57	882.45	844.33
		1583.61	1202.65	992.57	886.36	844.9
		1595.37	1208.78	992.58	922.78	844.9
		1598.13	1245.71	1013.74	926.77	847.24
		1598.13	1262.42	1013.74	928.3	847.24
		1598.61	1262.42	1013.74	929.29	848.46
		1600.24	1280.71	1013.75	930.81	848.46
		1657.97	1280.71	1013.75	931.66	849.09
		1664.89	1310.93	1013.78	939.8	859.55
		1664.89	1312.99	1118.52	980.29	859.55
		1672.82	1313	1122.82	980.6	867.6
		3203.7	1314.79	1122.83	980.73	872.67
		3203.7	1314.79	1122.92	981.02	875.45
		3203.71	1354.06	1123.66	981.24	875.45
		3203.73	1361.2	1123.67	981.4	882
		3204.86	1361.2	1127.97	988.62	882
		3204.87	1374.26	1131.19	996.11	888.21
		3204.87	1374.26	1131.2	1003.56	888.21

		3204.94	1403.69	1153.2	1003.78	891.15
		3234.72	1430.53	1153.21	1004.04	917.75
		3234.94	1430.53	1163.54	1004.36	924.54
		3234.94	1436.65	1184.37	1004.61	924.54
		3235.26	1436.65	1190.54	1004.83	937.64
		3235.64	1449.58	1190.54	1013.85	937.64
		3235.8	1464.18	1200.83	1013.86	948.76
		3235.8	1464.18	1200.83	1013.97	948.76
		3235.89	1480.51	1209.68	1014.03	953.24
			1480.51	1238.06	1014.11	992.66
			1516.39	1251.75	1014.19	992.66
			1516.4	1251.75	1014.22	992.69
			1516.85	1268.45	1099.97	992.69
			1522.82	1268.45	1119.13	992.7
			1522.83	1275.88	1121.01	992.7
			1582.83	1313.88	1124.27	992.71
			1582.84	1314.78	1124.98	992.78
			1590.3	1314.79	1126.49	996.12
			1590.3	1316.54	1126.74	997.09
			1594	1316.55	1127.56	997.09
			1630.53	1317.42	1129.35	998.36
			1632.58	1354.8	1129.97	998.36
			1632.59	1359.99	1149.35	999.19
			1632.83	1359.99	1149.38	999.19
			1632.83	1370.07	1161.07	999.46
			3202.46	1370.07	1161.32	1019.74
			3202.49	1374.76	1192.75	1019.97
			3202.49	1439.24	1193.37	1019.97
			3202.55	1439.24	1198.42	1020.24
			3202.55	1439.69	1198.64	1020.25
			3204.5	1439.7	1206.64	1020.58
			3204.5	1440.97	1207.23	1020.58
			3204.52	1446.78	1212.35	1020.74
			3204.53	1456.83	1246.39	1122.86
			3204.59	1472.04	1255.18	1125.53
			3229.61	1472.04	1255.99	1126.11
			3229.61	1488.43	1267.05	1126.11
			3229.75	1488.43	1268.36	1127.24
			3229.75	1489.77	1274.79	1127.24
			3229.88	1519.94	1276.96	1127.44
			3230.19	1521.28	1313.96	1127.45
			3230.2	1521.28	1314.08	1131.28
			3230.21	1532.26	1315.48	1134.17
			3230.23	1532.26	1315.73	1134.17

			3230.23	1542.3	1318.2	1150.21
				1592.2	1318.81	1150.21
				1596.58	1320.22	1163.36
				1596.58	1364.5	1163.36
				1603.09	1369.49	1168.72
				1603.09	1370.38	1190.1
				1605.78	1372.21	1193.65
				1635.65	1373.33	1193.65
				1636.87	1373.55	1200.83
				1636.87	1375.84	1200.83
				1639	1413.99	1208.81
				1639.01	1423.96	1208.81
				1640.85	1429.09	1214.54
				3202.66	1439.72	1243.53
				3202.69	1445.68	1252.89
				3202.69	1448.5	1252.89
				3202.74	1451.11	1266.17
				3202.74	1474.62	1266.17
				3202.76	1482.36	1277.2
				3204.74	1483.11	1277.2
				3204.75	1486.62	1281.5
				3204.75	1487.61	1321.76
				3204.79	1492.17	1322.33
				3204.79	1493.88	1322.33
				3204.85	1517.59	1323.88
				3229.98	1519.8	1323.88
				3230.02	1521.78	1325.2
				3230.03	1526.72	1325.2
				3230.14	1528.36	1325.56
				3230.15	1533	1357.59
				3230.23	1535.73	1360.56
				3230.56	1596.14	1360.56
				3230.57	1598.82	1367.22
				3230.57	1600.61	1367.22
				3230.59	1601.5	1373.51
				3230.59	1604.28	1373.51
				3230.6	1604.6	1375.92
					1605.94	1448.18
					1638.7	1448.19
					1638.91	1448.98
					1640.24	1448.98
					1640.47	1449.7
					1641.61	1450.21
					1641.68	1450.22

					1642.06	1454.67
					3202.24	1473.31
					3203.22	1484.62
					3203.23	1484.62
					3203.25	1500.89
					3203.26	1500.89
					3203.26	1505.46
					3203.27	1505.46
					3204.29	1505.51
					3217	1531.6
					3217	1532.49
					3217.02	1532.49
					3217.05	1538.64
					3217.08	1538.64
					3217.14	1551.91
					3218.74	1551.91
					3218.75	1559.05
					3218.81	1602.04
					3218.87	1605.19
					3219.16	1605.19
					3219.16	1610.79
					3230.2	1610.79
					3230.67	1615.05
					3231.38	1615.05
					3231.39	1616.59
					3231.46	1645.79
					3231.54	1646.66
					3231.83	1646.66
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						1648.59
						1650.31
						1650.31
						1651.15
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						3212.11
						3212.13
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						3214.15

						3214.18
						3214.18
						3214.24
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						3214.3
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						3241.26
						3241.69
						3241.7
						3241.7
						3241.7
						3241.7
						3241.7
						3241.71
						3241.73

Table S5: Optimized geometries of all cis-[n_c]CPPDs (n = 2 to 8) and all trans-[n_t]CPPDs (n = 2 to 8) comparing to strain free molecules.

[n]CPPDs	distance (Å)		Angle (deg)		Point Group
	d (C-N)	d (N=N)	∠CNN	∠CNNC	
[2 _c]CPPD	1.464	1.262	117.2	0.0	D _{2h}
[2 _t]CPPD	1.303	1.403	109.9	85.6	C _{2h}
[3 _c]CPPD	1.446	1.251	120.2	8.3	C _s
[3 _t]CPPD	1.303	1.370	116.8	104.9	C ₂
[4 _c]CPPD	1.430	1.249	125.1	12.3	D _{2d}
[4 _t]CPPD	1.316	1.365	112.9	134.9	D ₄
[5 _c]CPPD	1.427	1.251	129.3	10.9	C ₁
[5 _t]CPPD	1.408	1.270	114.6	154.4	D ₅
[6 _c]CPPD ₁	1.433	1.252	123.3	10.3	C ₂
[6 _c]CPPD ₂	1.428	1.251	125.9	-9.8	C ₁
[6 _t]CPPD	1.412	1.265	114.8	158.8	D ₆
[7 _c]CPPD ₁	1.430	1.249	123.4	11.1	C ₁
[7 _c]CPPD ₂	1.430	1.249	126.4	5.9	C ₁
[7 _t]CPPD	1.410	1.266	115.1	160.6	D ₇
^c [8 _c]CPPD ₁	1.433	1.248	124.2	11.1	C ₁
^c [8 _c]CPPD ₂	1.427	1.251	124.7	8.1	C ₁
^c [8 _t]CPPD	1.413	1.264	114.9	164.1	D ₈
^{a,b} trans-DB	1.431	1.251	115.1	^e 180.0	C _{2h}
^{a,b} cis-DB	1.432	1.245	120.2	^e 2.4	C ₂
^b trans AB	1.420	1.258	115.3	179.9	C _{2h}
^d trans AB	1.430	1.250	114.1	180.0	C _{2h}
^b trans AB	1.440	1.249	124.0	-9.5	C ₂
^d cis AB	1.450	1.250	121.9	0.0	C _{2h}

^{a,b}1,4-bis(diazenyl)benzene(bDB) ^bcalculated at B3LYP/6-31+G(d,p); ^ccalculated at B3LYP/6-31G(d), ^e∠CNNH; ^dexperimentally determined value of cis –trans azobenzene (AB);

Table S6: Zero point energy (kJ mol⁻¹), entropy (cal mol⁻¹ K⁻¹) and thermal correction (kJ mol⁻¹).

[n]CPPDs	ZPE	S	H _T
[2 _c]CPPD	462.7	97.73	493.7
[2 _t]CPPD	462.5	99.39	493.4
[3 _c]CPPD	702.6	134.49	784.1
[3 _t]CPPD	702.4	130.31	749.9
[4 _c]CPPD	937.7	166.16	1003.0
[4 _t]CPPD	937.4	162.00	1053.7
[5 _c]CPPD	1172.9	198.89	1255.5
[5 _t]CPPD	1173.0	194.53	1255.0
[6 _c]CPPD ₁	1407.8	232.35	1507.7
[6 _c]CPPD ₂	1409.5	232.211	1509.1
[6 _t]CPPD	1409.8	229.28	1509.6
[7 _c]CPPD ₁	1648.3	264.28	1765.1
[7 _c]CPPD ₂	1648.5	266.82	1765.5
[7 _t]CPPD	1646.6	262.27	1763.6
^c [8 _c]CPPD ₁	1884.4	295.87	2018.3
^c [8 _c]CPPD ₂	1887.1	286.57	2020.0
^c [8 _t]CPPD	1888.7	295.48	2023.6

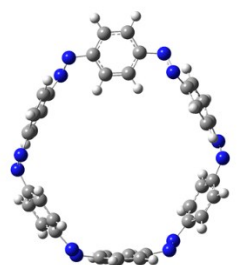
^cCalculated using B3LYP/6-31G(d) level

Table 7: Ring diameter (r_d) (nm) and HOMO-LUMO (H-L) gap (eV) for cis and trans isomer of CPPDs, CPPAs, and CPPs.

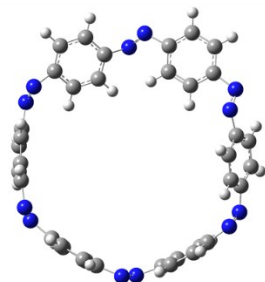
[n]CPPDs/ [n]CPPAs/ [n]CPPs	^a CPPD _s H-L	^b CPPD _s H-L	^c CPPA _s H-L	^d CPP _s H-L	^a CPPD _s r_d	^c CPPA _s r_d	^d CPP _s r_d
[4]	2.00	2.49	2.99	2.51	0.75	0.83	-
[5]	2.36	2.57	3.51	2.71	0.97	1.09	0.67
[6]	1.98	^e 2.85 ^f 2.63	3.02	3.14	1.18	1.30	0.79
[7]	2.22	^e 2.67 ^f 2.58	3.32	3.17	1.39	1.53	0.95
[8]	2.12	^e 2.39 ^f 2.74	3.05	3.41	1.58	1.73	1.1

^atrans isomer; ^bcis isomer; ^cvalues taken from Ali and Krishnan²⁰; ^dvalues taken from Iwamoto et al.; ^econformation 1 and ^fconformation 2

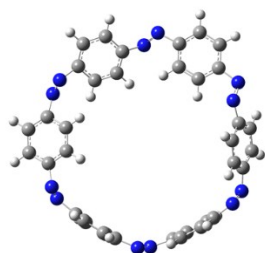
Starting unoptimized structure



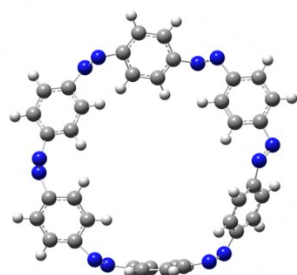
Final optimized structure



Starting unoptimized structure



Final optimized structure



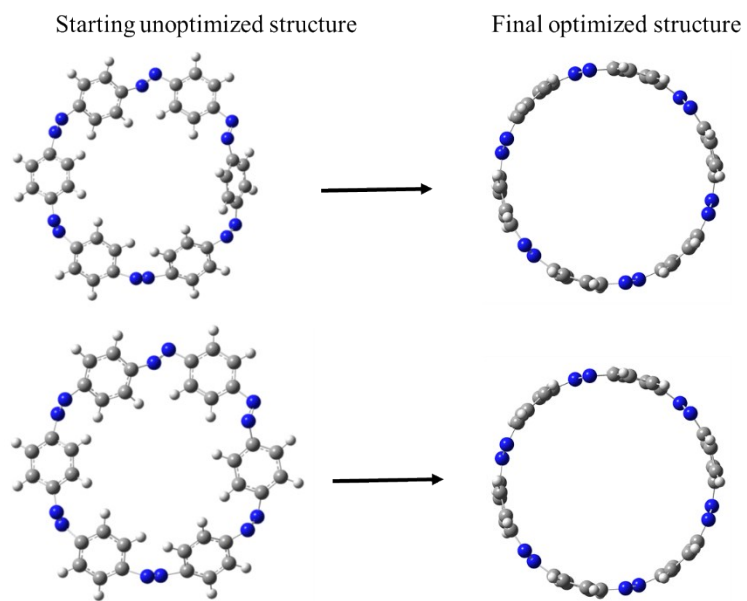


Figure S1: Different initial guess of [6_t]CPPD.

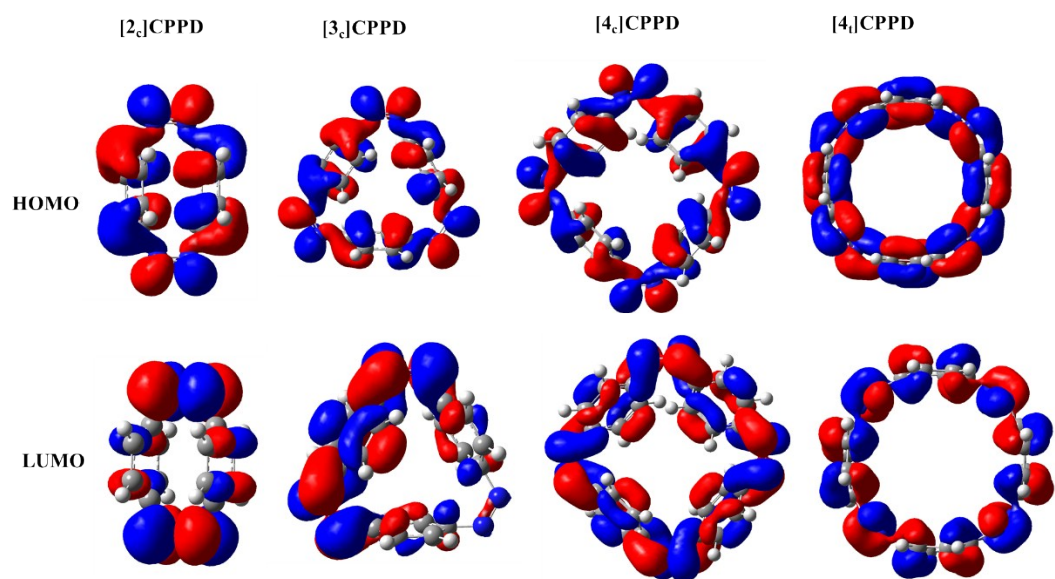


Figure S2a: HOMO and LUMO spatial diagram for [n]CPPDs (n = 2 to 4) obtained using B3LYP/6-31+G(d,p) level of theory .

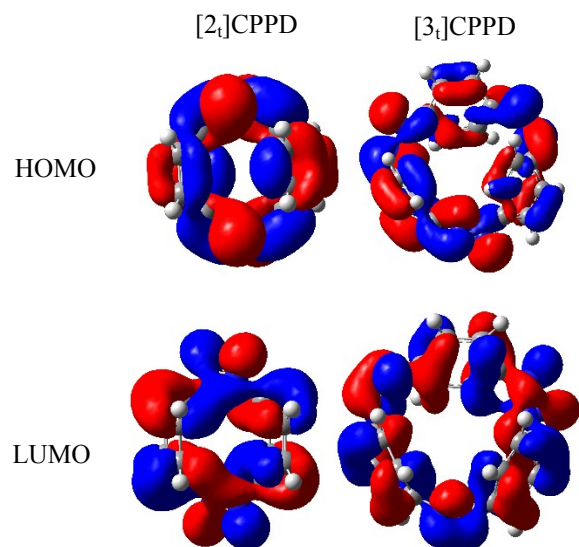


Figure S2b: HOMO and LUMO spatial diagram for trans [n]CPPDs (n = 2 to 3) obtained using B3LYP/6-31+G(d,p) level of theory.

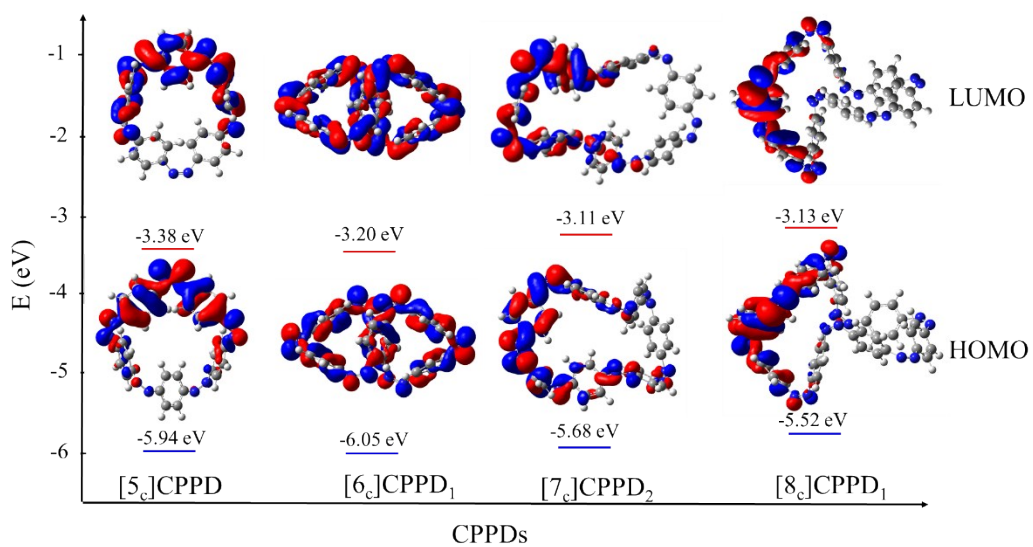


Figure S2c. Spatial distribution (0.02 au) and energy level diagram of HOMO and LUMO orbitals for cis isomer of [n]CPPD (n = 5 to 8).

Full Reference of Gaussian 09

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