

Supporting Information

Novel Photoresponsive Cyclicparaphenylenediazenes: Structure, Strain Energy, Cis-Trans Isomerization, and Electronic Properties

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Table S1: Optimized geometries of cis-trans-[n]CPPDs) (n =3 to 6) obtained using at the B3LYP/6-31+G(d,p). *Page 2-34*

Table S2: Zero point energy (kJ mol⁻¹), entropy (cal mol⁻¹ K⁻¹) and thermal correction (kJ mol⁻¹). *Page 35.*

Table S3: SE (kJ mol⁻¹) and SE/n (kJ mol⁻¹) calculated based on homodesmotic Scheme 1 using at B3LYP/6-31+G(d,p) level. A: HN=NH; B: HN=N-Ph-N=NH; Ph: Phenyl ring. *Page 36.*

Table S4: $\Delta_f H_{298}^\circ$ (kJ mol⁻¹), $\Delta_f H_{298}^\circ /n$ (kJ mol⁻¹) and molar enthalpies of combustion (kJ mol⁻¹) for [n]CPPDs (n = 3 to 6). *Page 37.*

Table S5: HOMO, LUMO and HOMO-LUMO (H-L) gap (eV) for cis-trans isomer of CPPDs. *Page 38-39.*

Figure S1: Optimized structure of all-cis, cis-trans, and all-trans isomer of [n]CPPDs (n=3 to 6) obtained at B3LYP/6-31+G(d,p) level. The $\angle C-N=N-C$ - (sp^2 - sp^2 - sp^2 - sp^2) angle is shown on the structure. The 6-ccttttc-anti is the most stable structure. *Page 40-43.*

Full Reference of Gaussian 09. *Page 44.*

Table S1: Optimized geometries of cis-tran-CPPDs obtained using the B3LYP/6-31+G(d,p).

3-cct (2)				3-ctt-syn (3)			
C	-3.19535800	-0.05915100	0.03488000	C	3.03753300	-1.37239500	-0.06380300
C	-2.59445500	-0.47708600	1.23646500	C	3.15176900	-0.68729500	1.18245200
C	-1.82761300	-1.62611600	1.24662600	C	3.15177700	0.68736100	1.18241500
C	-1.60140200	-2.33040300	0.03961900	C	3.03755300	1.37239200	-0.06387800
C	-2.43685200	-2.06096200	-1.06410400	C	3.43556100	0.69951400	-1.23386900
C	-3.26816300	-0.94093200	-1.05221600	C	3.43555100	-0.69959000	-1.23383100
H	-2.64976200	0.15726700	2.11551100	H	3.00843800	-1.23082600	2.10993500
H	-1.23662500	-1.87717600	2.11953000	H	3.00845100	1.23094400	2.10986800
H	-2.30712500	-2.63578900	-1.97622700	H	3.43609500	1.23641800	-2.17726900
H	-3.83064000	-0.65983700	-1.93728300	H	3.43607600	-1.23654400	-2.17720200
H	-1.36215700	0.86102000	-1.78908700	H	0.04001900	-2.41012200	-1.88341600
C	-0.79715100	1.40828100	-1.04494000	C	-0.64167200	-2.26513200	-1.05287300
C	0.59181700	1.42989700	-1.13275100	C	-1.90055200	-1.71630000	-1.27095000
C	-1.46255300	2.10251700	-0.01953700	C	-0.17710800	-2.47479000	0.26431000
C	1.35810400	2.14600400	-0.19820900	C	-2.71128500	-1.37100800	-0.17846200
H	1.07769600	0.90307300	-1.94488700	H	-2.22344700	-1.47497200	-2.27891600
C	-0.69982100	2.89207700	0.85975200	C	-1.08268100	-2.31265400	1.33175000
C	0.69148900	2.91475300	0.77176700	C	-2.34802600	-1.77272500	1.11305900
H	-1.20945700	3.49261800	1.60699500	H	-0.73315200	-2.49490000	2.34319200
H	1.27149100	3.53332000	1.44973700	H	-3.01209000	-1.57616700	1.94857600
H	3.29590800	-0.67847000	-2.18645600	H	-2.22324800	1.47423600	-2.27896700
C	2.98118000	-0.91525500	-1.17429000	C	-1.90043400	1.71588200	-1.27105200
C	3.15137300	0.03729200	-0.15231600	C	-2.71128400	1.37099700	-0.17852300
C	2.24764000	-2.06548100	-0.91282300	C	-0.64156100	2.26475100	-1.05304700
C	2.91041400	-0.31570400	1.17988200	C	-2.34811400	1.77312200	1.11289600
C	1.75853800	-2.29440200	0.39187700	C	-0.17708500	2.47480400	0.26410500
H	1.93257700	-2.70963100	-1.72651300	H	0.04020500	2.40945200	-1.88357800
C	2.24158700	-1.50478600	1.45307100	C	-1.08274900	2.31303700	1.33152600
H	3.15150400	0.37819500	1.97840800	H	-3.01226300	1.57687500	1.94842000
H	1.90649700	-1.72881600	2.46045300	H	-0.73330200	2.49558500	2.34294200
N	3.58936100	1.37202800	-0.45119300	N	-3.93461600	0.62657900	-0.38436100
N	2.78186100	2.32482600	-0.36738200	N	-3.93460700	-0.62659700	-0.38439300
N	-2.89895800	2.24481000	0.01285900	N	1.18495100	-2.39228300	0.62655800
N	-3.69272000	1.27696300	-0.07343500	N	2.02142500	-2.32620900	-0.32895100
N	-0.31493200	-2.83324400	-0.26273000	N	2.02146100	2.32619800	-0.32909300
N	0.48787900	-2.82524700	0.72092400	N	1.18496400	2.39234000	0.62639400

	3-ctt-anti (3_a)		
C	0.79141400	1.11993100	3.04479400
C	1.40076400	-0.12889800	3.29132800
C	0.59533100	-1.25958300	3.30457900
C	-0.79141400	-1.11993100	3.04479400
C	-1.40076400	0.12889800	3.29132800
C	-0.59533100	1.25958300	3.30457900
H	2.47630100	-0.23659500	3.20588600
H	1.04325700	-2.24629800	3.23416400
H	-2.47630100	0.23659500	3.20588600
H	-1.04325700	2.24629800	3.23416400
H	-0.07078800	2.71706500	0.00240200
C	0.59533100	2.18140200	-0.66439800
C	0.16267800	1.80738600	-1.92983500
C	1.82776100	1.70640200	-0.16440600
C	0.96559400	0.97477000	-2.72589600
H	-0.82765100	2.09006800	-2.27115300
C	2.69855900	1.03351200	-1.04502300
C	2.28029400	0.69336800	-2.33040000
H	3.65824000	0.68864400	-0.67244600
H	2.92677100	0.11784300	-2.98566900
H	-2.92677100	-0.11784300	-2.98566900
C	-2.28029400	-0.69336800	-2.33040000
C	-0.96559400	-0.97477000	-2.72589600
C	-2.69855900	-1.03351200	-1.04502300
C	-0.16267800	-1.80738600	-1.92983500
C	-1.82776100	-1.70640200	-0.16440600
H	-3.65824000	-0.68864400	-0.67244600
C	-0.59533100	-2.18140200	-0.66439800
H	0.82765100	-2.09006800	-2.27115300
H	0.07078800	-2.71706500	0.00240200
N	-2.02072500	-1.46570700	1.21531700
N	-1.18775400	-2.00856100	2.00423100
N	2.02072500	1.46570700	1.21531700
N	1.18775400	2.00856100	2.00423100
N	-0.45864800	-0.42784500	-3.96206800
N	0.45864800	0.42784500	-3.96206800

4-ccct (6)				4-ctct-syn (8 _s)			
C	1.57671500	1.96318000	-0.72437800	C	2.69130700	2.51884900	-1.19778300
C	1.50577700	3.00025400	0.22449800	C	1.75945500	2.43595500	-0.15000900
C	2.57905000	3.17706800	1.12131600	C	2.16724900	1.92162000	1.09558800
C	3.68025700	2.33445000	1.08653500	C	3.43078400	1.36697500	1.23702300
C	3.74528400	1.28553000	0.15203300	C	4.30472900	1.32881100	0.13824700
C	2.68555300	1.11944000	-0.76170100	C	3.97564000	1.99717600	-1.04572000
H	0.78938200	1.84505000	-1.46151000	H	2.37349800	2.93768600	-2.14769000
H	2.54864400	4.02091100	1.80333200	H	1.45091300	1.87989400	1.90812600
H	4.52472500	2.49874600	1.74855800	H	3.72389500	0.90442600	2.17346900
H	2.73961000	0.35322600	-1.52633800	H	4.68443400	2.02095800	-1.86741300
C	-1.50536500	3.00042900	-0.22450800	C	-1.75956400	2.43592200	0.15018200
C	-1.57671300	1.96382800	0.72485500	C	-2.69119400	2.51824200	1.19818800
C	-2.57835300	3.17695100	-1.12172100	C	-2.16752700	1.92213300	-1.09557000
C	-2.68565800	1.12023300	0.76224100	C	-3.97549400	1.99646200	1.04618000
H	-0.78960800	1.84594700	1.46226800	H	-2.37319900	2.93668900	2.14820200
C	-3.67965400	2.33445700	-1.08689100	C	-3.43106600	1.36746900	-1.23700500
H	-2.54763200	4.02045100	-1.80414700	H	-1.45136300	1.88084900	-1.90828100
C	-3.74507000	1.28596700	-0.15193700	C	-4.30477600	1.32869100	-0.13806200
H	-2.74001700	0.35438400	1.52721600	H	-4.68411500	2.01977700	1.86803600
H	-4.52388200	2.49850300	-1.74928200	H	-3.72437100	0.90538500	-2.17362400
C	3.80250600	-2.28809900	-1.27437600	C	3.73713300	-1.40299600	-1.21955200
C	2.60823400	-3.00009600	-1.33359000	C	2.46909000	-1.95200200	-1.38874600
C	4.06789000	-1.49544100	-0.14874700	C	4.29293300	-1.34320000	0.06306500
C	1.72506400	-2.98946900	-0.23873700	C	1.74487400	-2.41739500	-0.28165000
H	2.30559100	-3.50492500	-2.24587200	H	1.98361200	-1.93927200	-2.35927600
C	3.27748700	-1.61613700	1.00868300	C	3.65936500	-1.98700900	1.13753100
C	2.11997300	-2.37120100	0.96736500	C	2.37498400	-2.49606500	0.97484100
H	3.54407500	-1.06134700	1.90235400	H	4.14241500	-2.00735500	2.10978000
H	1.44556500	-2.40029000	1.81551100	H	1.82863000	-2.89759600	1.82075500
C	-1.72547900	-2.98938800	0.23882000	C	-1.74477400	-2.41734900	0.28134800
C	-2.60858300	-2.99972600	1.33373000	C	-2.46911100	-1.95244200	1.38857400
C	-2.12041600	-2.37133600	-0.96738300	C	-2.37474800	-2.49547900	-0.97523700
C	-3.80277900	-2.28760700	1.27446400	C	-3.73718800	-1.40348200	1.21950400
H	-2.30592000	-3.50439100	2.24609600	H	-1.98372100	-1.94009200	2.35915500
C	-3.27785700	-1.61616700	-1.00876900	C	-3.65912700	-1.98638300	-1.13784400
H	-1.44606300	-2.40064900	-1.81556500	H	-1.82827600	-2.89660300	-1.82126600

C	-4.06814000	-1.49512300	0.14870900	C	-4.29287900	-1.34318300	-0.06314300
H	-4.47348000	-2.24496100	2.12675100	H	-4.26640900	-0.97080400	2.06149100
H	-3.54443400	-1.06150300	-1.90252000	H	-4.14205400	-2.00631300	-2.11016400
H	4.47329100	-2.24572200	-2.12661200	H	4.26622200	-0.96989000	-2.06140400
N	5.01855900	0.62597800	0.04894100	N	5.55303700	0.60880400	0.24586600
N	5.17010200	-0.59529200	-0.18354900	N	5.54120900	-0.64336500	0.26977600
N	0.38077900	-3.31018900	-0.50451900	N	0.35693900	-2.58538100	-0.51956800
N	-0.38119600	-3.31012000	0.50460200	N	-0.35684800	-2.58545900	0.51927800
N	-5.17016100	-0.59473700	0.18348400	N	-5.54125100	-0.64344300	-0.26967600
N	-5.01841600	0.62650100	-0.04907200	N	-5.55309500	0.60872500	-0.24580900
N	-0.60371300	4.10285200	-0.15848200	N	-0.40186400	2.65542500	0.48601700
N	0.60430500	4.10280400	0.15812100	N	0.40177300	2.65531400	-0.48582700
4-cttc-anti (8a)				4-cctt-syn (7s)			
C	-2.24408300	1.97197600	0.97170800	C	-2.62185100	-0.66325500	-0.41192100
C	-1.74682500	2.43785300	-0.26097900	C	-3.56869800	-1.35027600	0.37043400
C	-2.60187100	2.48305900	-1.37462500	C	-4.47745600	-0.60851000	1.14672800
C	-3.89462500	1.96638600	-1.29534900	C	-4.43629600	0.77950500	1.15009500
C	-4.30713300	1.33781900	-0.11551500	C	-3.48513100	1.46998300	0.37725500
C	-3.51463400	1.42137300	1.04271300	C	-2.58055100	0.73185000	-0.40859200
H	-1.58969400	1.96594900	1.83580100	H	-1.94209900	-1.21062900	-1.05496300
H	-2.21615400	2.86859300	-2.31339300	H	-5.24516400	-1.14075800	1.69951900
H	-4.54421900	1.95861300	-2.16499100	H	-5.17133900	1.35357000	1.70543100
H	-3.87507200	0.99621600	1.97318600	H	-1.86987100	1.24081300	-1.04974700
C	1.74682600	2.43785300	0.26097800	C	-1.65997900	-3.53545100	0.22999200
C	2.24408500	1.97197700	-0.97170900	C	-1.09437200	-3.12834600	1.44646000
C	2.60187100	2.48305900	1.37462500	C	-0.83294400	-3.97134600	-0.82292000
C	3.51463600	1.42137300	-1.04271300	C	0.28756500	-3.02835700	1.55194300
H	1.58969700	1.96595000	-1.83580200	H	-1.73397500	-2.86064700	2.28098100
C	3.89462600	1.96638400	1.29535000	C	0.54514900	-3.82265100	-0.73323700
H	2.21615400	2.86859200	2.31339300	H	-1.29245700	-4.36154500	-1.72607700
C	4.30713400	1.33781800	0.11551600	C	1.11464200	-3.30067400	0.44648100
H	3.87507400	0.99621700	-1.97318600	H	0.74955600	-2.64495100	2.45597700
H	4.54421900	1.95861000	2.16499300	H	1.18433200	-4.05074700	-1.57888700
C	-3.89462500	-1.96638200	1.29535100	C	-0.60040600	3.93339400	-0.80222000
C	-2.60187100	-2.48305700	1.37462700	C	0.76654200	3.70379900	-0.71286400
C	-4.30713400	-1.33781800	0.11551600	C	-1.45217300	3.54132600	0.24820500
C	-1.74682600	-2.43785300	0.26097900	C	1.30370000	3.14300800	0.46420100
H	-2.21615200	-2.86858800	2.31339500	H	1.41853700	3.89829200	-1.55712600

C	-3.51463700	-1.42137500	-1.04271300	C	-0.91215600	3.09532700	1.46266600
C	-2.24408600	-1.97197900	-0.97170900	C	0.46147900	2.91389900	1.56800900
H	-3.87507500	-0.99622100	-1.97318600	H	-1.56681600	2.86104300	2.29556100
H	-1.58969800	-1.96595400	-1.83580200	H	0.89952300	2.49941700	2.47025400
C	1.74682500	-2.43785200	-0.26097900	C	4.05091900	1.21827000	-0.43002600
C	2.60187000	-2.48305800	-1.37462600	C	4.32634300	0.51813100	0.77288700
C	2.24408400	-1.97197800	0.97170800	C	4.14716500	0.54097800	-1.65447900
C	3.89462500	-1.96638500	-1.29535000	C	4.28568200	-0.85921500	0.76891500
H	2.21615300	-2.86859000	-2.31339500	H	4.38346100	1.06261900	1.70865200
C	3.51463500	-1.42137400	1.04271400	C	4.10623300	-0.85748600	-1.65852600
H	1.58969500	-1.96595100	1.83580100	H	4.00642400	1.09578600	-2.57652400
C	4.30713300	-1.33781900	-0.11551500	C	3.97010900	-1.53504900	-0.43800000
H	4.54421900	-1.95861100	-2.16499200	H	4.31051600	-1.41144200	1.70153600
H	3.87507200	-0.99621900	1.97318700	H	3.93348000	-1.39771900	-2.58377400
H	-4.54421700	-1.95860700	2.16499400	H	-1.03580400	4.35447000	-1.70345600
N	-5.55861600	0.62072100	-0.08582600	N	-3.72339600	2.88342400	0.25697600
N	-5.55861700	-0.62071900	0.08582500	N	-2.85312800	3.76597700	0.10197800
N	-0.37007500	-2.65134100	0.51076900	N	2.55173800	2.49705300	0.57507200
N	0.37007300	-2.65133900	-0.51076900	N	3.22395200	2.37182300	-0.49186000
N	5.55861600	-0.62072100	-0.08582500	N	3.07664800	-2.63764100	-0.50630500
N	5.55861700	0.62071900	0.08582500	N	2.39820900	-2.72915200	0.56007500
N	0.37007500	2.65134200	0.51076800	N	-3.07178500	-3.67767300	0.08403000
N	-0.37007400	2.65134000	-0.51076900	N	-3.88923100	-2.74674900	0.24396800
4-cctt-anti (7a)				4-cttt-syn (9_s)			
C	-2.59512500	-0.55342000	-0.82731100	C	2.08184000	-2.02825500	1.46441500
C	-3.55538500	-1.30040500	-0.12065700	C	1.44023600	-2.80079600	0.47729800
C	-4.45484500	-0.63029800	0.72641100	C	2.11739600	-3.07154200	-0.73242000
C	-4.38561800	0.74882300	0.87230500	C	3.36129300	-2.49951600	-0.97161300
C	-3.42442900	1.50333300	0.17315900	C	3.90751100	-1.58782000	-0.04806500
C	-2.52993400	0.83359100	-0.68390800	C	3.29672300	-1.41138800	1.20421000
H	-1.92472900	-1.04734600	-1.52219000	H	1.56112300	-1.85663800	2.40090400
H	-5.23393700	-1.20080600	1.22226200	H	1.63676200	-3.68715900	-1.48462600
H	-5.10935300	1.27769700	1.48437000	H	3.88712900	-2.68757700	-1.90297300
H	-1.80753000	1.38948000	-1.26977600	H	3.75663000	-0.76836600	1.94620500
C	-1.67947200	-3.49320700	-0.24273400	C	-1.99907200	-3.22879100	-0.01901000
C	-1.26290000	-3.17440800	1.05726300	C	-2.75288900	-3.11388400	-1.20058700
C	-0.73520300	-3.87469900	-1.21471600	C	-2.55159600	-2.75022900	1.19984200
C	0.09673400	-3.10586000	1.33539300	C	-3.84237600	-2.24600500	-1.23668800

H	-1.99632200	-2.95135000	1.82487400	H	-2.36110300	-3.54540900	-2.11615300
C	0.62296400	-3.75528100	-0.95002900	C	-3.63395300	-1.90038800	1.16798300
H	-1.08553700	-4.19916500	-2.18994200	H	-2.02821200	-2.94009200	2.12969400
C	1.04845400	-3.31914300	0.32152100	C	-4.17387800	-1.49876800	-0.08678800
H	0.44901700	-2.79037300	2.31213700	H	-4.30060700	-1.97779200	-2.18330700
H	1.35814400	-3.93926100	-1.72540900	H	-3.96523200	-1.40030100	2.07098100
C	-0.70173600	4.13666200	-1.11068900	C	4.05836300	2.13120800	0.79123300
C	0.66977400	3.93179000	-1.21259900	C	2.90826300	2.90698200	0.90961100
C	-1.40420000	3.62380900	-0.00682900	C	4.13676400	1.15646500	-0.21596200
C	1.37248100	3.29749500	-0.17036600	C	1.86814100	2.79384300	-0.03416600
H	1.20782600	4.21877400	-2.11080100	H	2.78080400	3.58205100	1.75030300
C	-0.69983700	3.07379400	1.07825800	C	3.14889100	1.10707600	-1.21842400
C	0.67703600	2.92805800	1.00246400	C	2.03791000	1.92866100	-1.13812800
H	-1.24162200	2.73178800	1.95451800	H	3.24670700	0.40021400	-2.03526500
H	1.22450500	2.43886400	1.80009900	H	1.24354100	1.85599100	-1.87179700
C	4.10108700	1.19951300	0.21702800	C	-1.57684200	3.32011100	-0.28050100
C	4.31059700	0.37140300	1.34329300	C	-2.45482300	2.98135000	-1.33935100
C	4.24380700	0.65159900	-1.07397100	C	-2.03934000	3.21616000	1.05122300
C	4.24628800	-1.00677500	1.19942300	C	-3.60607500	2.25816300	-1.08440800
H	4.29581300	0.82347800	2.33043000	H	-2.11772500	3.14243700	-2.35896200
C	4.21404300	-0.72873700	-1.21981800	C	-3.20304300	2.51135300	1.30916600
H	4.16576800	1.29387200	-1.94377900	H	-1.39789700	3.53563900	1.86478400
C	4.00361500	-1.53798600	-0.08210100	C	-3.89556300	1.87363400	0.24750600
H	4.17687200	-1.64573300	2.07222900	H	-4.17474300	1.82691400	-1.90017900
H	4.11837900	-1.17679400	-2.20404900	H	-3.48333500	2.26429300	2.32859300
H	-1.25247500	4.62557300	-1.90807000	H	4.85944300	2.21168100	1.51938200
N	-3.65842900	2.92159100	0.22719100	N	5.15658900	-0.94866700	-0.33595000
N	-2.81286400	3.82523400	0.05154300	N	5.27921500	0.29678200	-0.28690200
N	2.63771100	2.75745300	-0.46876900	N	0.61633100	3.34564500	0.29391700
N	3.30017100	2.32771500	0.52128900	N	-0.22505900	3.35754700	-0.65725100
N	3.10956400	-2.61263300	-0.34348000	N	-4.40685600	0.61899200	0.61140300
N	2.31305500	-2.77510300	0.62795400	N	-4.58337600	-0.18476500	-0.36518300
N	-3.06463100	-3.59893400	-0.56932700	N	-0.62461400	-3.48607000	-0.21119000
N	-3.88372000	-2.66912700	-0.41663900	N	0.08111600	-3.03398400	0.74317500
				4-cttt-anti (9_a)			
				C	2.55792100	-2.89873400	1.37079700
				C	1.64491000	-2.87118700	0.29498400
				C	2.00087300	-2.17738300	-0.88583900

5-cccc (12)							
C	4.16606500	-2.38039600	-0.62560900	C	3.16020000	-1.42528500	-0.93174000
C	2.91979800	-2.78066400	-1.09240300	C	4.01840400	-1.37832400	0.18712300
C	1.94221600	-3.24852900	-0.19844300	C	3.75912800	-2.20311500	1.29602700
C	2.27545900	-3.44988100	1.15582100	H	2.28847400	-3.44505600	2.26947200
C	3.53164900	-3.08164700	1.61821300	H	1.30779500	-2.17621400	-1.71920200
C	4.43762800	-2.45199000	0.74859800	H	3.39991500	-0.84576900	-1.81657700
H	4.90051600	-1.96401100	-1.30633100	H	4.46398400	-2.21926500	2.12139500
H	2.65614300	-2.67204800	-2.13976600	C	-1.76356200	-3.26928900	-0.29776100
H	1.52521700	-3.84306400	1.83208500	C	-2.53582400	-3.14977600	-1.47531600
H	3.79896700	-3.19677500	2.66430900	C	-2.33215000	-2.85341700	0.93893100
H	5.59117000	2.59644700	-1.94397000	C	-3.67383800	-2.35748800	-1.47839600
C	5.12515000	1.99835500	-1.16782800	H	-2.12781800	-3.53381300	-2.40511800
C	3.76232200	2.22261900	-0.89731500	C	-3.45975900	-2.06555300	0.93884000
C	5.84686200	1.03308500	-0.47583000	H	-1.78174700	-3.02990900	1.85642000
C	3.13454800	1.46203100	0.11136200	C	-4.04070500	-1.66111300	-0.30051700
C	5.19379800	0.22091000	0.45996100	H	-4.16485500	-2.09930600	-2.41139500
H	6.90077100	0.86976800	-0.67687900	H	-3.80509300	-1.60101600	1.85559600
C	3.84691400	0.47449200	0.78188700	C	3.16020000	1.42528200	0.93173900
H	2.09363600	1.61293500	0.36039600	C	2.00087300	2.17738100	0.88583900
H	3.35109600	-0.11573600	1.54395100	C	4.01840500	1.37832300	-0.18712300
C	-1.58061300	-3.50250400	-0.30734800	C	1.64491100	2.87118600	-0.29498300
C	-1.93872500	-2.62419900	-1.35097500	H	1.30779600	2.17621100	1.71920200
C	-2.58253800	-4.06003100	0.50402000	C	3.75913000	2.20311600	-1.29602600
C	-3.25786900	-2.23075200	-1.50387400	C	2.55792200	2.89873500	-1.37079500
H	-1.15981400	-2.21757200	-1.98562400	H	4.46398600	2.21926600	-2.12139400
C	-3.91545000	-3.70303500	0.32146900	H	2.28847500	3.44505900	-2.26947000
H	-2.29253500	-4.74941600	1.29092100	C	-1.76356100	3.26928900	0.29776100
C	-4.24125000	-2.71983500	-0.62330300	C	-2.33214900	2.85341600	-0.93893100
H	-3.53563900	-1.51548700	-2.27155800	C	-2.53582400	3.14977700	1.47531600
H	-4.69759800	-4.12053800	0.94746500	C	-3.45975800	2.06555300	-0.93884000
H	-3.81068500	-1.11970000	1.22177200	H	-1.78174500	3.02990800	-1.85642000
C	-4.13688700	-0.15622300	0.85274400	C	-3.67383800	2.35749000	1.47839500
C	-3.53885500	0.99193700	1.36256200	H	-2.12781900	3.53381400	2.40511700
C	-5.17449900	-0.05821900	-0.09589300	C	-4.04070400	1.66111400	0.30051600
C	-3.95783000	2.26361000	0.93434100	H	-3.80509100	1.60101500	-1.85559600
H	-2.76259200	0.90912300	2.11686000	H	-4.16485600	2.09930800	2.41139400
				H	3.39991500	0.84576500	1.81657500
				N	5.21612300	-0.60751700	0.15578100

C	-5.62004600	1.21992100	-0.47986100	N	5.21612300	0.60751500	-0.15578200
C	-5.02276600	2.36948600	0.02367900	N	0.34037800	3.31792600	-0.53321000
H	-6.46154700	1.28696700	-1.16233500	N	-0.39200900	3.43405700	0.50337400
H	-5.38951200	3.35196900	-0.25627000	N	-4.53510200	0.37855600	0.51764200
H	-2.28515400	2.54012900	-0.84817900	N	-4.53510200	-0.37855500	-0.51764200
C	-1.35749700	2.95389800	-0.47567500	N	-0.39201000	-3.43405700	-0.50337300
C	-1.30396200	3.60167700	0.77556800	N	0.34037700	-3.31792500	0.53321100
C	-0.22590100	2.90595800	-1.28167900	5-ccctt-syn (13_s)			
C	-0.08506600	4.16965000	1.19300700	C	-4.77836600	0.47379900	-0.61841800
C	0.99737100	3.44471100	-0.84036500	C	-4.07226600	1.52222500	-1.19537600
H	-0.28113200	2.47424200	-2.27612400	C	-3.60807100	2.59295000	-0.40656400
C	1.06163600	4.07826100	0.41341600	C	-3.99866300	2.67544800	0.94671400
H	-0.07279700	4.70821800	2.13531800	C	-4.72912400	1.64382800	1.51593700
H	1.98886200	4.53709400	0.74190300	C	-5.02735900	0.49224900	0.76451100
N	3.19511400	3.17265300	-1.80459200	H	-5.08204600	-0.37688100	-1.21852900
N	2.02741000	3.61374100	-1.80967600	H	-3.79243600	1.49043300	-2.24380600
N	-2.39508300	3.94602300	1.63247700	H	-3.66014700	3.51376500	1.54419800
N	-3.53433100	3.43403800	1.63188600	H	-5.01121000	1.66921400	2.56403500
N	-5.98398100	-1.13010000	-0.59799000	H	-3.58145000	-4.93313700	-1.37152800
N	-5.60061300	-2.31234600	-0.75290800	C	-3.40264000	-4.05415200	-0.76080100
N	-0.24708700	-3.73994400	0.08704200	C	-2.10443400	-3.51022700	-0.75127100
N	0.62992100	-3.31834600	-0.71605400	C	-4.42566400	-3.47208800	-0.02701800
N	5.63994600	-1.93527600	1.32692600	C	-1.85487300	-2.35167300	0.01396700
N	6.00194000	-0.75169200	1.14154100	C	-4.19988600	-2.26617800	0.65458300
5-cctet-syn(14_s)				H	-5.41971500	-3.90706400	-0.00687600
C	2.32111900	-2.92738100	-0.86453800	C	-2.89654400	-1.73050500	0.69958000
C	0.93978800	-2.83751800	-0.75590500	H	-0.86451800	-1.91272100	0.04299100
C	0.29736800	-3.24171600	0.42981200	H	-2.70012800	-0.82399300	1.26125600
C	1.05587500	-3.77072100	1.48688400	C	-0.75944400	4.61263300	-0.50976300
C	2.43081100	-3.92734400	1.35269000	C	-0.01197800	4.06675000	-1.58087500
C	3.07561700	-3.45697000	0.19845500	C	-0.08714400	5.22939100	0.56182300
H	2.82343100	-2.59640700	-1.76785600	C	1.35229200	3.90325400	-1.44241500
H	0.34372900	-2.42733000	-1.56348600	H	-0.53455500	3.64840200	-2.43336400
H	0.54525200	-4.07261100	2.39596100	C	1.28311500	5.04616100	0.71025100
H	3.02107700	-4.38195300	2.14207800	H	-0.67519900	5.68833500	1.35009200
H	6.50731800	1.20472400	-1.90087200	C	1.98730200	4.27194400	-0.22974400
C	5.89108800	0.65034900	-1.20007400	H	1.92170100	3.35266000	-2.18360500
C	5.15517700	1.36070500	-0.23606800	H	1.78981700	5.35659400	1.61867500

C	5.86494100	-0.73780200	-1.21894200	H	2.98183200	1.65342600	1.69997900
C	4.42409000	0.65211300	0.73432900	C	3.76801300	1.12353500	1.17453400
C	5.10337800	-1.44816600	-0.27476900	C	4.11352900	-0.16729700	1.53688700
H	6.46099400	-1.29562100	-1.93429500	C	4.35174700	1.72804100	0.04093300
C	4.39766600	-0.73968400	0.71487400	C	5.08441200	-0.86166400	0.79728500
H	3.90296900	1.18568200	1.52138800	H	3.61654400	-0.65964600	2.36657100
H	3.85676000	-1.27307800	1.48792600	C	5.37851200	1.05513900	-0.64661100
C	-3.12892700	-2.52358200	-0.11965000	C	5.78379500	-0.21071900	-0.23257200
C	-3.52922900	-1.88574400	1.06870900	H	5.83337200	1.52642600	-1.51257400
C	-4.03299300	-2.62848800	-1.18828800	H	6.58006000	-0.73561100	-0.75129300
C	-4.76729300	-1.26475500	1.13748000	H	3.95436300	-1.97884600	-1.24843000
H	-2.83319400	-1.82984500	1.89783900	C	3.16013800	-2.54261100	-0.77596500
C	-5.29664000	-2.04571500	-1.10386800	C	3.33843300	-3.08525700	0.51217000
H	-3.71680300	-3.14166200	-2.09120800	C	2.00261300	-2.81274100	-1.49004700
C	-5.62331800	-1.28555800	0.02379600	C	2.30862100	-3.86316300	1.07032900
H	-5.05893100	-0.72138200	2.02980000	C	0.95437200	-3.55748400	-0.91662500
H	-5.99287100	-2.10489600	-1.93453000	H	1.90502200	-2.48483600	-2.52018000
H	-5.37030200	0.80730700	-2.18766000	C	1.10960700	-4.06377700	0.38831300
C	-4.90773400	1.32542500	-1.35516100	H	2.47197800	-4.32827000	2.03778800
C	-3.64055100	1.88187700	-1.48581800	H	0.33092800	-4.67820800	0.82914200
C	-5.55851400	1.38402900	-0.11672900	N	-1.25774600	-4.12603500	-1.72236800
C	-3.01289200	2.48737500	-0.38677900	N	-0.01816900	-4.04205600	-1.83791800
H	-3.08942400	1.79973100	-2.41710200	N	4.61217100	-3.13280400	1.17139000
C	-5.00974000	2.13202500	0.93681100	N	5.43563300	-2.18991300	1.18254800
C	-3.72828500	2.65769800	0.81474500	N	3.73513700	2.84911800	-0.54778300
H	-5.56280400	2.23072700	1.86606000	N	3.10914200	3.58504700	0.26933000
H	-3.25377100	3.16305700	1.64821000	N	-2.09893600	4.27166200	-0.22572600
H	0.51935200	2.32881500	-1.65239100	N	-2.55766500	3.34902300	-0.96232500
C	1.07893000	2.78236000	-0.84267700	N	-5.65545100	-0.56613700	1.48324200
C	0.37920600	3.29333400	0.26896300	N	-5.33047100	-1.77032200	1.38288700
C	2.46374400	2.83681700	-0.87915300	5-ccctt-anti (13_a)			
C	1.09021200	3.89449800	1.31942900	C	5.53644600	0.34858700	0.08783900
C	3.17348700	3.42409200	0.18643800	C	4.93864200	1.59840500	0.21541700
H	3.00430000	2.43415800	-1.72939500	C	3.93148600	1.98018100	-0.69087100
C	2.47650600	3.99778500	1.26020400	C	3.59962200	1.13477000	-1.76265800
H	0.53606900	4.28695400	2.16622300	C	4.13968200	-0.14124700	-1.84591200
H	3.03454600	4.49741600	2.04573000	C	5.06606900	-0.55676000	-0.88067300
N	5.42300100	2.76537000	-0.16210300	H	6.31593200	0.03457000	0.77573800

N	4.58239400	3.64254700	0.12890400	H	5.21535800	2.26731200	1.02321300
N	-1.02075200	3.17925100	0.44264600	H	2.84674300	1.47087100	-2.46797100
N	-1.64515600	2.78431300	-0.57869400	H	3.83661100	-0.82348400	-2.63306100
N	-6.82218000	0.71126400	0.06243900	H	0.78368400	-4.78455400	-0.52327900
N	-6.85879300	-0.54039800	0.05974000	C	1.48264300	-4.05547700	-0.12548900
N	-1.08138000	-3.05439100	0.67028800	C	1.21201600	-3.41805100	1.10034200
N	-1.80137000	-2.95327800	-0.35939600	C	2.69774900	-3.82992900	-0.77111600
N	4.47231200	-3.71900700	0.06206100	C	2.15519100	-2.51639000	1.62601900
N	5.32692000	-2.86279100	-0.24783100	C	3.62206300	-2.90162100	-0.26340000
5-cctet-anti (14_a)				H	2.95208700	-4.38863800	-1.66677100
C	-2.55591600	-2.76982000	1.11288100	C	3.32431000	-2.22802500	0.93653000
C	-1.18413300	-2.61167100	1.26863600	H	1.97313700	-2.07809700	2.60224800
C	-0.29208200	-3.07700900	0.28838700	H	4.04174800	-1.54375300	1.37162700
C	-0.78761100	-3.76920900	-0.83401300	C	1.68680500	4.29892500	0.67125900
C	-2.15481700	-3.96647100	-0.96951300	C	0.94802700	4.08924500	1.85230200
C	-3.04848100	-3.42075700	-0.02855000	C	1.07918200	4.91528200	-0.43536900
H	-3.24122500	-2.39761300	1.86638100	C	-0.43719300	4.18625400	1.82087300
H	-0.77599600	-2.10453600	2.13706800	H	1.45731100	3.68535800	2.72176000
H	-0.09213900	-4.14470500	-1.57587600	C	-0.30154000	5.05908700	-0.44908400
H	-2.55670100	-4.52403200	-1.81011900	H	1.66828100	5.13976100	-1.31709100
H	-6.69433900	1.12081300	1.63356200	C	-1.07108600	4.54798900	0.61600800
C	-6.02369600	0.58342800	0.97050900	H	-1.03327900	3.85207700	2.66218200
C	-5.19998500	1.32168900	0.10290200	H	-0.81558300	5.40267000	-1.34129100
C	-6.00944500	-0.80540600	0.94566600	H	-3.77618600	3.28175000	-1.63965300
C	-4.39404100	0.63936300	-0.82671500	C	-4.08661200	2.41890000	-1.06225300
C	-5.16638700	-1.48619700	0.05225500	C	-4.69228600	1.33244600	-1.67497300
H	-6.66696900	-1.38010400	1.59037700	C	-3.78598500	2.36724500	0.31469300
C	-4.37805100	-0.75214800	-0.85126400	C	-4.94910900	0.16054500	-0.94001900
H	-3.80223900	1.19040000	-1.54807100	H	-4.90425200	1.33668400	-2.73978100
H	-3.77309300	-1.26798100	-1.58890900	C	-4.21846600	1.26475000	1.07524800
C	3.18787500	-2.57907600	-0.17771200	C	-4.79491000	0.16149500	0.45603500
C	3.61620400	-1.98836500	1.02651000	H	-4.01003000	1.25554500	2.14057900
C	4.06653400	-2.63731800	-1.27029800	H	-5.07055100	-0.71045700	1.03881300
C	4.84176400	-1.34613500	1.08208100	H	-2.48038600	-1.00390400	-1.34514300
H	2.95624200	-1.99715300	1.88559100	C	-2.64744000	-1.89641400	-0.75209100
C	5.31032500	-2.00785300	-1.20983700	C	-3.91433100	-2.51320200	-0.74616000
H	3.73879700	-3.13614500	-2.17695500	C	-1.60657600	-2.41721900	0.01423000
C	5.65455900	-1.28323500	-0.06463600	C	-4.10176100	-3.69847500	-0.01861200

H	5.16069100	-0.85573800	1.99512300	C	-1.82523700	-3.55127100	0.82316000
H	5.97967400	-2.01261200	-2.06437800	H	-0.64568200	-1.91602400	0.01502500
H	5.10525700	0.98036000	-1.90143400	C	-3.08583100	-4.17666900	0.79590100
C	4.75526700	1.43827600	-0.98257000	H	-5.06416800	-4.19778700	-0.06658100
C	3.49425500	2.01139800	-0.92276600	H	-3.24319900	-5.03474200	1.44138200
C	5.56187400	1.39731500	0.16823800	N	0.23481600	-3.89904600	2.02159600
C	3.01861200	2.53815800	0.29259700	N	-0.99255400	-4.05663700	1.86794300
H	2.83921800	2.00349000	-1.78638800	N	-5.02649200	-2.11872000	-1.56085000
C	5.15670500	2.05254400	1.33618100	N	-5.44070400	-0.94586800	-1.69461200
C	3.87000300	2.58391300	1.40783300	N	-2.83631600	3.20181800	0.94443200
H	5.81485000	2.06897600	2.19930300	N	-2.35739300	4.11790300	0.21573700
H	3.49644100	3.01361100	2.33218000	N	3.03364300	3.05929700	-0.56006900
H	-0.51358800	2.37536800	1.62106600	N	2.89369900	3.54691100	0.59745800
C	-1.08325900	2.78601500	0.79489100	N	5.62928500	-1.86737800	-0.99220100
C	-0.39959500	3.21748200	-0.35809200	N	4.93958900	-2.89903700	-0.83586200
C	-2.46915500	2.85144500	0.84785000	5-ccttt-syn (15_s)			
C	-1.12403800	3.74989800	-1.43716100	C	2.43167900	-3.04426400	-1.13881800
C	-3.18960600	3.37951600	-0.23972600	C	1.05660700	-3.12196300	-1.32193800
H	-3.00212600	2.49994600	1.72554900	C	0.23793800	-3.76904700	-0.37809200
C	-2.50634300	3.87792700	-1.35943800	C	0.82719600	-4.40724700	0.73243800
H	-0.58171900	4.07479000	-2.31957700	C	2.20429000	-4.37095100	0.89177500
H	-3.07190000	4.33138600	-2.16736300	C	3.01062200	-3.64253800	-0.00729000
N	-5.44953700	2.73225700	0.08587600	H	3.05556900	-2.53205500	-1.86341200
N	-4.59647100	3.61019300	-0.16277900	H	0.58068100	-2.65342100	-2.17749700
N	0.99084300	3.06293800	-0.54930500	H	0.19448400	-4.91646200	1.45048100
N	1.67128000	2.91918500	0.50222600	H	2.68317300	-4.88326800	1.72067600
N	6.83264200	0.71875400	0.13650600	H	6.70064800	1.29460200	-1.13342000
N	6.87575200	-0.51997200	-0.04530400	C	5.92772000	0.71349800	-0.64038600
N	1.87155900	-3.05432300	-0.39982100	C	4.97454600	1.38786800	0.14585300
N	1.06090900	-2.74802600	0.51687400	C	5.91963100	-0.67010300	-0.72266300
N	-4.43296000	-3.73306500	-0.18669000	C	4.01736100	0.63743300	0.85618300
N	-5.35589600	-2.90289900	-0.04585200	C	4.96086100	-1.42529600	-0.02033000
5-ccttt				H	6.68590000	-1.19773000	-1.28174800
C	-2.25062100	3.16757300	-1.11785200	C	4.01064600	-0.75442600	0.77436300
C	-0.87156700	3.20815700	-1.27875200	H	3.30804900	1.13687900	1.50750000
C	-0.04832700	3.80496400	-0.30596000	H	3.29488200	-1.31871500	1.36212500
C	-0.63432600	4.43144300	0.81313700	C	-3.23280900	-3.54499700	0.17159300
C	-2.01415300	4.43403100	0.95043900	C	-3.74551000	-3.02276900	-1.04054200

C	-2.82831400	3.75549500	0.01982900	C	-3.94658800	-3.34981200	1.36523000
H	-2.87775200	2.69463500	-1.86570400	C	-4.77496500	-2.10610900	-1.00532300
H	-0.39662900	2.74853300	-2.13961600	H	-3.24352400	-3.25542400	-1.97255600
H	0.00259900	4.90158500	1.55374800	C	-4.96880400	-2.40346000	1.40550600
H	-2.49065200	4.93957300	1.78483700	H	-3.57984800	-3.81032900	2.27693800
H	-6.55332000	-0.97130800	-1.58784200	C	-5.29102700	-1.67486700	0.24490300
C	-5.81642500	-0.44579300	-0.98871500	H	-5.08356300	-1.59139300	-1.90791000
C	-4.98540400	-1.19933100	-0.13633800	H	-5.40045200	-2.09588600	2.35270400
C	-5.75079300	0.93818400	-1.00007200	H	-5.44631400	1.79153800	1.86758600
C	-4.07810800	-0.52337300	0.70347800	C	-4.98040700	2.23662400	0.99598500
C	-4.84713300	1.61668800	-0.16024800	C	-3.96062600	3.16625100	1.13942900
H	-6.43428000	1.52127700	-1.60921700	C	-5.26500000	1.72001500	-0.28692300
C	-4.01001000	0.86942400	0.69103200	C	-3.19737300	3.55026100	0.01693800
H	-3.46102600	-1.07821000	1.40139400	H	-3.63056000	3.48164500	2.12441500
H	-3.34181100	1.37661700	1.37889700	C	-4.70791300	2.34933400	-1.42387700
C	3.40388100	3.44641800	0.27422700	C	-3.66070900	3.24568400	-1.27729900
C	3.90916000	2.95144300	-0.95282800	H	-4.99008100	1.98270700	-2.40596800
C	4.09385600	3.17326500	1.46720100	H	-3.11599900	3.60808900	-2.14123600
C	4.89206400	1.98527100	-0.94271800	H	0.76715600	2.86599000	-2.14656500
H	3.43093800	3.24469200	-1.88018100	C	1.18353500	3.24131000	-1.21719600
C	5.06790900	2.17753300	1.48140600	C	0.30418600	3.80161500	-0.27319000
H	3.73725400	3.61439800	2.39239300	C	2.54182900	3.12813100	-0.94603900
C	5.36738700	1.47748100	0.29590200	C	0.81562200	4.31996000	0.93389100
H	5.18702500	1.49072500	-1.86119000	C	3.04175200	3.60616900	0.27649700
H	5.47147100	1.81257400	2.42060900	H	3.21270500	2.68271400	-1.67263000
H	4.98766100	-1.90049000	1.75022500	C	2.17770900	4.25229700	1.18463900
C	4.62657400	-2.33880100	0.82683200	H	0.13586900	4.76382000	1.65226100
C	3.53779200	-3.18537200	0.83280700	H	2.59971800	4.67621100	2.09074600
C	5.14818300	-1.87008700	-0.40826900	N	5.26358600	2.76816000	0.38400400
C	2.95377000	-3.58817500	-0.39454900	N	4.43372300	3.68487600	0.55859300
H	3.03861200	-3.43819800	1.76129900	N	-1.88442000	3.98373000	0.31203900
C	4.74000300	-2.49193700	-1.60538100	N	-1.06096700	3.67507700	-0.59864000
C	3.64089300	-3.34396600	-1.59694100	N	-5.67263700	0.39590300	-0.54619000
H	5.17454800	-2.15659200	-2.54168800	N	-5.71543600	-0.35124900	0.47985700
H	3.20973900	-3.70391000	-2.52576300	N	-1.91160400	-4.02059600	0.32525100
H	-0.48451500	-3.12069100	-1.60962000	N	-1.14349400	-3.60236300	-0.59136500
C	-1.09335700	-3.39799300	-0.75644400	N	4.41749600	-3.75338000	0.16493100
C	-0.46059200	-3.93138900	0.38684100	N	5.24511100	-2.82603400	0.03803500

C	-2.46409500	-3.18395300	-0.76232000		
C	-1.23785100	-4.28598700	1.50483600		
C	-3.23583700	-3.53839000	0.36182600		
H	-2.94832300	-2.75414600	-1.63343100		
C	-2.61842300	-4.14199100	1.47195600		
H	-0.73887000	-4.68608400	2.38187000		
H	-3.23379800	-4.46220100	2.30672300		
N	-5.37993900	-2.56750000	-0.00347100		
N	-4.65607900	-3.52819200	0.33240000		
N	0.93619100	-3.97805900	0.53761600		
N	1.60167300	-3.95577900	-0.53948100		
N	5.66832100	-0.57561700	-0.58144400		
N	5.70712400	0.12535100	0.47877300		
N	2.09976600	3.96434000	0.43174700		
N	1.32922600	3.60129400	-0.50673200		
N	-4.23315900	3.90878700	0.17461000		
N	-5.08679400	3.01998000	-0.02743500		
5-ctttt-syn (17s)					
C	4.50120700	1.42625700	1.26747800		
C	3.32081500	2.14914800	1.39062100		
C	2.87207500	2.97381100	0.34567100		
C	3.68095300	3.14991800	-0.79500900		
C	4.88490800	2.46252200	-0.89964300		
C	5.26225700	1.54292000	0.09551300		
H	4.82358500	0.76231200	2.06163100		
H	2.69503800	2.04721800	2.27134800		
H	3.34356600	3.80502400	-1.59039800		
H	5.52272500	2.59117700	-1.76903900		
H	3.99546100	-3.63457900	2.02625200		
C	4.16500200	-2.97536900	1.18051800		
C	3.21480400	-2.94150400	0.14533900		
C	5.29655400	-2.16516400	1.12461200		
C	3.42623800	-2.09273200	-0.95921400		
C	5.43667100	-1.23998800	0.08026600		
H	6.04348300	-2.19847100	1.91163100		
C	4.51847200	-1.23792300	-0.98427400		
H	2.69031700	-2.07446400	-1.75491400		
H	4.65559800	-0.55246200	-1.81378800		
				5-ccttt-anti (15a)	
C	-2.25062100	3.16757300	-1.11785200		
C	-0.87156700	3.20815700	-1.27875200		
C	-0.04832700	3.80496400	-0.30596000		
C	-0.63432600	4.43144300	0.81313700		
C	-2.01415300	4.43403100	0.95043900		
C	-2.82831400	3.75549500	0.01982900		
H	-2.87775200	2.69463500	-1.86570400		
H	-0.39662900	2.74853300	-2.13961600		
H	0.00259900	4.90158500	1.55374800		
H	-2.49065200	4.93957300	1.78483700		
H	-6.55332000	-0.97130800	-1.58784200		
C	-5.81642500	-0.44579300	-0.98871500		
C	-4.98540400	-1.19933100	-0.13633800		
C	-5.75079300	0.93818400	-1.00007200		
C	-4.07810800	-0.52337300	0.70347800		
C	-4.84713300	1.61668800	-0.16024800		
H	-6.43428000	1.52127700	-1.60921700		
C	-4.01001000	0.86942400	0.69103200		
H	-3.46102600	-1.07821000	1.40139400		
H	-3.34181100	1.37661700	1.37889700		
C	3.40388100	3.44641800	0.27422700		
C	3.90916000	2.95144300	-0.95282800		
C	4.09385600	3.17326500	1.46720100		
C	4.89206400	1.98527100	-0.94271800		
H	3.43093800	3.24469200	-1.88018100		
C	5.06790900	2.17753300	1.48140600		
H	3.73725400	3.61439800	2.39239300		
C	5.36738700	1.47748100	0.29590200		
H	5.18702500	1.49072500	-1.86119000		
H	5.47147100	1.81257400	2.42060900		
H	4.98766100	-1.90049000	1.75022500		
C	4.62657400	-2.33880100	0.82683200		
C	3.53779200	-3.18537200	0.83280700		
C	5.14818300	-1.87008700	-0.40826900		
C	2.95377000	-3.58817500	-0.39454900		

C	-0.37035600	4.20612500	-0.33678700	H	3.03861200	-3.43819800	1.76129900
C	-1.06121300	4.07447800	0.89006700	C	4.74000300	-2.49193700	-1.60538100
C	-1.09777400	4.31027300	-1.53304800	C	3.64089300	-3.34396600	-1.59694100
C	-2.42233800	3.83781300	0.89068000	H	5.17454800	-2.15659200	-2.54168800
H	-0.49658800	4.05770900	1.81496100	H	3.20973900	-3.70391000	-2.52576300
C	-2.46609700	4.04982700	-1.53556200	H	-0.48451500	-3.12069100	-1.60962000
H	-0.55709300	4.45827800	-2.46232700	C	-1.09335700	-3.39799300	-0.75644400
C	-3.12033800	3.71201200	-0.33653100	C	-0.46059200	-3.93138900	0.38684100
H	-2.94416500	3.61873500	1.81529100	C	-2.46409500	-3.18395300	-0.76232000
H	-3.01546400	3.97498700	-2.46867600	C	-1.23785100	-4.28598700	1.50483600
H	-5.47867600	1.08143900	-1.70021400	C	-3.23583700	-3.53839000	0.36182600
C	-5.51883600	0.52929800	-0.76818500	H	-2.94832300	-2.75414600	-1.63343100
C	-5.45854600	-0.84852300	-0.76833400	C	-2.61842300	-4.14199100	1.47195600
C	-5.42144200	1.23553300	0.45912400	H	-0.73887000	-4.68608400	2.38187000
C	-5.29699400	-1.54530200	0.45816900	H	-3.23379800	-4.46220100	2.30672300
H	-5.37043500	-1.39452600	-1.70062000	N	-5.37993900	-2.56750000	-0.00347100
C	-5.57470800	0.53196500	1.66803100	N	-4.65607900	-3.52819200	0.33240000
C	-5.51011100	-0.85919400	1.66782600	N	0.93619100	-3.97805900	0.53761600
H	-5.55005800	1.08622700	2.60086300	N	1.60167300	-3.95577900	-0.53948100
H	-5.43450600	-1.40901200	2.60059300	N	5.66832100	-0.57561700	-0.58144400
H	-2.58046100	-3.72971700	1.74934000	N	5.70712400	0.12535100	0.47877300
C	-2.07992800	-3.91501200	0.80574700	N	2.09976600	3.96434000	0.43174700
C	-2.83009800	-3.84056500	-0.39453500	N	1.32922600	3.60129400	-0.50673200
C	-0.70486500	-4.05408200	0.75440000	N	-4.23315900	3.90878700	0.17461000
C	-2.19518200	-4.11439800	-1.62092700	N	-5.08679400	3.01998000	-0.02743500
C	-0.04926200	-4.12674500	-0.49714800	5-cttct-syn (16_s)			
H	-0.10809400	-3.99187500	1.65753800	C	-2.38459300	-2.06818900	-0.73988300
C	-0.81274200	-4.25246700	-1.67092000	C	-3.73118900	-1.73026500	-0.76555500
H	-2.78391000	-4.07474100	-2.53182400	C	-4.67190400	-2.52980100	-0.08716400
H	-0.29488000	-4.33598600	-2.62115500	C	-4.24613700	-3.73245500	0.50433600
N	1.99668300	-3.62869600	0.34851000	C	-2.89768100	-4.08380200	0.51256500
N	1.31364100	-3.81723600	-0.69729500	C	-1.95503600	-3.22331400	-0.06609200
N	-4.05647500	-3.15627700	-0.50467300	H	-1.65253400	-1.44246800	-1.23813700
N	-4.54791500	-2.73359600	0.58566400	H	-4.04049300	-0.84690300	-1.30811400
N	-4.77916300	2.48434800	0.59569900	H	-4.99152500	-4.37531500	0.96148600
N	-4.28489400	2.93286600	-0.48311800	H	-2.56237700	-5.00152700	0.98506300
N	1.02635700	4.01715100	-0.48545900	H	4.14200800	-4.31338500	-1.37260500
N	1.55358100	3.44907200	0.51258100	C	3.61019200	-3.64106000	-0.70621100

N	6.51156700	0.84946100	-0.04199100	C	4.34838700	-2.72324000	0.05974800
N	6.59658600	-0.39492900	0.05005500	C	2.21794200	-3.65540800	-0.64299600
5-ctttt-anti (17_a)				C	3.68363000	-1.89780200	0.98447700
C	4.50120700	1.42625700	1.26747800	C	1.55337300	-2.76155500	0.21357600
C	3.32081500	2.14914800	1.39062100	H	1.63853700	-4.32777400	-1.26680000
C	2.87207500	2.97381100	0.34567100	C	2.29715900	-1.90037400	1.03615300
C	3.68095300	3.14991800	-0.79500900	H	4.24342500	-1.23449200	1.63132500
C	4.88490800	2.46252200	-0.89964300	H	1.76600600	-1.22706800	1.70154300
C	5.26225700	1.54292000	0.09551300	C	-5.90937700	0.03246200	0.05470700
H	4.82358500	0.76231200	2.06163100	C	-6.03436800	0.96325700	-0.98658100
H	2.69503800	2.04721800	2.27134800	C	-5.11963900	0.33453300	1.17990100
H	3.34356600	3.80502400	-1.59039800	C	-5.19509100	2.07368500	-1.01175100
H	5.52272500	2.59117700	-1.76903900	H	-6.70964200	0.75367700	-1.81002600
H	3.99546100	-3.63457900	2.02625200	C	-4.31843300	1.46515000	1.17302800
C	4.16500200	-2.97536900	1.18051800	H	-5.08636000	-0.35788000	2.01513300
C	3.21480400	-2.94150400	0.14533900	C	-4.28677200	2.30259900	0.03690500
C	5.29655400	-2.16516400	1.12461200	H	-5.18251000	2.74198200	-1.86723800
C	3.42623800	-2.09273200	-0.95921400	H	-3.63748300	1.66496600	1.99233100
C	5.43667100	-1.23998800	0.08026600	H	-0.54621600	3.81831800	2.39664000
H	6.04348300	-2.19847100	1.91163100	C	-0.19617900	3.89564400	1.37176300
C	4.51847200	-1.23792300	-0.98427400	C	1.15926300	3.86474600	1.08003900
H	2.69031700	-2.07446400	-1.75491400	C	-1.15096100	3.86536100	0.33433200
H	4.65559800	-0.55246200	-1.81378800	C	1.57687300	3.80158900	-0.26537400
C	-0.37035600	4.20612500	-0.33678700	H	1.89495200	3.75733500	1.86874800
C	-1.06121300	4.07447800	0.89006700	C	-0.72705400	4.00548700	-1.00340400
C	-1.09777400	4.31027300	-1.53304800	C	0.62770900	3.97166600	-1.29529400
C	-2.42233800	3.83781300	0.89068000	H	-1.46624700	4.00939800	-1.79594500
H	-0.49658800	4.05770900	1.81496100	H	0.97413400	3.95168100	-2.32417100
C	-2.46609700	4.04982700	-1.53556200	H	3.73597800	1.41665500	-1.98399300
H	-0.55709300	4.45827800	-2.46232700	C	4.44713100	1.14977000	-1.21069200
C	-3.12033800	3.71201200	-0.33653100	C	4.57992100	1.99175900	-0.08581800
H	-2.94416500	3.61873500	1.81529100	C	5.11374600	-0.06359900	-1.25158800
H	-3.01546400	3.97498700	-2.46867600	C	5.53159900	1.67627600	0.90039800
H	-5.47867600	1.08143900	-1.70021400	C	5.93910800	-0.44126500	-0.17709000
C	-5.51883600	0.52929800	-0.76818500	H	4.94502500	-0.75584100	-2.07022600
C	-5.45854600	-0.84852300	-0.76833400	C	6.24339700	0.48074600	0.83385100
C	-5.42144200	1.23553300	0.45912400	H	5.64979500	2.34615600	1.74659100
C	-5.29699400	-1.54530200	0.45816900	H	6.94654500	0.20538700	1.61364200

H	-5.37043500	-1.39452600	-1.70062000	N	5.77994800	-2.77787500	-0.07038500
C	-5.57470800	0.53196500	1.66803100	N	6.50373200	-1.75499100	-0.10280400
C	-5.51011100	-0.85919400	1.66782600	N	3.62718600	2.98081200	0.24257800
H	-5.55005800	1.08622700	2.60086300	N	2.81254600	3.26330400	-0.68155800
H	-5.43450600	-1.40901200	2.60059300	N	-3.23682300	3.20450000	-0.23622100
H	-2.58046100	-3.72971700	1.74934000	N	-2.42566800	3.39211700	0.71483500
C	-2.07992800	-3.91501200	0.80574700	N	-6.64303500	-1.18933600	-0.04133800
C	-2.83009800	-3.84056500	-0.39453500	N	-6.09338100	-2.31591700	-0.04538900
C	-0.70486500	-4.05408200	0.75440000	N	-0.57501900	-3.56652100	0.01080000
C	-2.19518200	-4.11439800	-1.62092700	N	0.15178100	-2.56730600	0.24420100
C	-0.04926200	-4.12674500	-0.49714800	5-ettet-anti (16_a)			
H	-0.10809400	-3.99187500	1.65753800	C	-2.36613200	-1.98230200	-0.82758000
C	-0.81274200	-4.25246700	-1.67092000	C	-3.70569400	-1.62228300	-0.87482900
H	-2.78391000	-4.07474100	-2.53182400	C	-4.68519100	-2.47633000	-0.33314100
H	-0.29488000	-4.33598600	-2.62115500	C	-4.30372200	-3.74513100	0.13569200
N	1.99668300	-3.62869600	0.34851000	C	-2.95989800	-4.11515600	0.16789800
N	1.31364100	-3.81723600	-0.69729500	C	-1.98078700	-3.21087500	-0.26597100
N	-4.05647500	-3.15627700	-0.50467300	H	-1.60522700	-1.31712200	-1.21999000
N	-4.54791500	-2.73359600	0.58566400	H	-3.98178400	-0.67871000	-1.32655700
N	-4.77916300	2.48434800	0.59569900	H	-5.07563600	-4.42419500	0.48360200
N	-4.28489400	2.93286600	-0.48311800	H	-2.65740700	-5.08460600	0.55087800
N	1.02635700	4.01715100	-0.48545900	H	4.15980800	-4.29873900	-1.35848500
N	1.55358100	3.44907200	0.51258100	C	3.60428200	-3.65147400	-0.68658700
N	6.51156700	0.84946100	-0.04199100	C	4.31304600	-2.76137000	0.13772400
N	6.59658600	-0.39492900	0.05005500	C	2.21082500	-3.66710500	-0.67393400
				C	3.61588000	-1.97084300	1.06843700
				C	1.51472600	-2.80569600	0.19157900
				H	1.65471500	-4.31466600	-1.34349600
				C	2.22855500	-1.97691000	1.07221600
				H	4.15294800	-1.33142400	1.75751100
				H	1.67257400	-1.32920200	1.74270600
				C	-5.83415100	0.04795900	0.19831600
				C	-5.82154500	1.15153400	-0.67482300
				C	-5.13770700	0.10363200	1.41273300
				C	-4.93012400	2.19370500	-0.45531200
				H	-6.44303800	1.12819500	-1.56490800
				C	-4.28078300	1.17196100	1.65350600
				H	-5.21028600	-0.71674200	2.11902000

	C	-4.09747400	2.17153100	0.68231200
	H	-4.82051100	2.99199100	-1.18061800
	H	-3.66071400	1.19674000	2.54388200
	H	-0.82049900	3.69551600	1.99494900
	C	-0.36282200	3.85507200	1.02555400
	C	1.00977300	3.79428600	0.87415300
	C	-1.18893600	3.98190700	-0.11472600
	C	1.58239400	3.84799500	-0.41952500
	H	1.65213800	3.58564900	1.72240800
	C	-0.60949500	4.25077400	-1.36555600
	C	0.77156300	4.16814500	-1.52097200
	H	-1.26090500	4.38267900	-2.22344700
	H	1.22684000	4.23161700	-2.50428900
	H	3.76567100	1.38474900	-1.93670700
	C	4.43833300	1.11953700	-1.12898200
	C	4.51743600	1.96554000	-0.00267500
	C	5.10727900	-0.09382900	-1.13490900
	C	5.41359400	1.64911300	1.03392100
	C	5.88433900	-0.46602000	-0.02389000
	H	4.97877500	-0.78784300	-1.95926500
	C	6.13217300	0.45658200	1.00226300
	H	5.48875700	2.31972000	1.88448600
	H	6.79811600	0.18467300	1.81526000
	N	5.74867800	-2.80464600	0.06424900
	N	6.46143100	-1.77386200	0.06940100
	N	3.55313700	2.96209000	0.26102500
	N	2.84530500	3.30018100	-0.72944800
	N	-2.54723000	3.58543200	-0.16518300
	N	-2.92102300	2.93318100	0.85143000
	N	-6.61422300	-1.09534300	-0.16435900
	N	-6.10191800	-2.22573700	-0.34061600
	N	-0.60906000	-3.57753300	-0.15972000
	N	0.11451000	-2.60690200	0.18260800

6-ccccct				6-cctcct-syn (21 _s)			
C	4.56870400	3.70590300	-0.17965800	C	-1.25118100	-3.94198000	4.08010800
C	5.12741100	2.54262500	-0.73460700	C	-0.17208500	-4.55944300	3.43007100
C	4.31388800	1.63019200	-1.42495500	C	0.80186600	-3.77123400	2.78288100
C	2.94048000	1.82661000	-1.45195900	C	0.68525200	-2.38901700	2.77443100
C	2.36413600	2.93616800	-0.81411000	C	-0.41673800	-1.76973600	3.39804000
C	3.19083100	3.89380000	-0.19692500	C	-1.38835100	-2.55956000	4.03409500
H	5.22155800	4.42992500	0.29848300	H	-1.96376700	-4.55779200	4.61958600
H	4.75525500	0.76736800	-1.91066400	H	1.65866700	-4.24796600	2.31841000
H	2.28631200	1.12333300	-1.95651500	H	1.43983500	-1.77071800	2.30205700
H	2.73938300	4.75702500	0.27967500	H	-2.22296200	-2.06329300	4.51890400
C	5.63146100	0.64951200	1.58941200	C	-0.66477200	-5.92839100	0.69574400
C	4.98316600	-0.36131400	2.29240700	C	-0.66477200	-5.92839100	-0.69574400
C	4.97952200	-1.67202500	1.79418200	C	0.37439300	-6.56062000	-1.40186600
C	5.76024400	-1.99243400	0.67235100	C	1.38611500	-7.23154500	-0.69397700
C	6.47543800	-0.99234900	0.01612500	C	1.38611500	-7.23154500	0.69397700
C	6.35300400	0.34196600	0.42555200	C	0.37439300	-6.56062000	1.40186600
H	5.59520800	1.67117600	1.95184100	H	-1.48536400	-5.46553900	1.23277400
H	4.44737000	-0.13919000	3.21000200	H	-1.48536400	-5.46553900	-1.23277400
H	5.81066000	-3.01938500	0.32483700	H	2.14206100	-7.77509700	-1.25184600
H	7.09909900	-1.23157100	-0.83981900	H	2.14206100	-7.77509700	1.25184600
C	2.63679300	-3.16553300	0.95159700	C	-0.17208500	-4.55944300	-3.43007100
C	1.92809400	-4.30216500	0.52426700	C	0.80186600	-3.77123400	-2.78288100
C	1.11951000	-4.26623400	-0.60802900	C	0.68525200	-2.38901700	-2.77443100
C	0.97706500	-3.06300300	-1.31520200	C	-0.41673800	-1.76973600	-3.39804000
C	1.66596500	-1.91790500	-0.88568800	C	-1.38835100	-2.55956000	-4.03409500
C	2.47004400	-1.95635800	0.24639100	C	-1.25118100	-3.94198000	-4.08010800
H	2.02877900	-5.21469300	1.10363400	H	1.65866700	-4.24796600	-2.31841000
H	0.59884200	-5.15767400	-0.94249200	H	1.43983500	-1.77071800	-2.30205700
H	1.55044700	-0.99411700	-1.44258600	H	-2.22296200	-2.06329300	-4.51890400
H	2.95428400	-1.04677800	0.57329600	H	-1.96376700	-4.55779200	-4.61958600
C	-1.00140000	3.93148100	-0.31283600	C	0.10157200	1.73249400	3.11745100
C	-1.78539200	5.05004600	-0.62603000	C	1.10202600	2.54058400	2.55368600
C	-3.16257600	4.99346400	-0.44436500	C	1.03383700	3.92667500	2.64996100
C	-3.78019400	3.83978300	0.07476700	C	-0.03852900	4.52097900	3.33445200
C	-2.97725300	2.73824500	0.43977200	C	-1.01675800	3.71183300	3.94300400
C	-1.60476900	2.78471000	0.23579400	C	-0.96893700	2.33260700	3.81054700

H	-1.30525900	5.94222400	-1.01469300	H	1.93163900	2.05769700	2.04692300
H	-3.79521500	5.84235000	-0.68149900	H	1.81433900	4.54451900	2.21952900
H	-3.40905100	1.85705100	0.89118300	H	-1.80574700	4.18870900	4.51670400
H	-0.97811000	1.94571300	0.51594000	H	-1.72661300	1.70252900	4.26123600
C	-5.63547100	0.89719500	-0.39010100	C	-0.81124000	5.88992300	-0.69527400
C	-5.59984900	-0.48464400	-0.21978400	C	-0.81124000	5.88992300	0.69527400
C	-5.73805800	-1.04296300	1.06415400	C	0.14188900	6.64522600	1.40075100
C	-5.96338400	-0.19293700	2.16065600	C	1.04816100	7.45274400	0.69470000
C	-5.97966400	1.18653200	1.99764000	C	1.04816100	7.45274400	-0.69470000
C	-5.78653500	1.74308400	0.72242700	C	0.14188900	6.64522600	-1.40075100
H	-5.55391100	1.32492400	-1.38446800	H	-1.56259000	5.32173300	-1.23232000
H	-5.49200500	-1.12437200	-1.08817900	H	-1.56259000	5.32173300	1.23232000
H	-6.14041000	-0.63879900	3.13441700	H	1.72808700	8.08918000	1.25222600
H	-6.16481800	1.84264000	2.84213200	H	1.72808700	8.08918000	-1.25222600
C	-3.07628600	-3.86512000	-2.16229500	C	1.10202600	2.54058400	-2.55368600
C	-1.90483800	-3.18908300	-1.77883300	C	0.10157200	1.73249400	-3.11745100
C	-1.87898800	-2.49885500	-0.55130300	C	-0.96893700	2.33260700	-3.81054700
C	-3.00505200	-2.48507400	0.26402400	C	-1.01675800	3.71183300	-3.94300400
C	-4.16517000	-3.18228900	-0.11680400	C	-0.03852900	4.52097900	-3.33445200
C	-4.17704400	-3.91086700	-1.31617500	C	1.03383700	3.92667500	-2.64996100
H	-3.09255100	-4.36209900	-3.12708100	H	1.93163900	2.05769700	-2.04692300
H	-0.99846100	-1.95078900	-0.24335000	H	-1.72661300	1.70252900	-4.26123600
H	-2.98643900	-1.94290700	1.20354500	H	-1.80574700	4.18870900	-4.51670400
H	-5.06256800	-4.47936200	-1.58211800	H	1.81433900	4.54451900	-2.21952900
N	0.95292300	2.93972200	-0.77568400	N	-0.61787500	-0.37461200	3.48830800
N	0.40057800	4.03560200	-0.49321300	N	0.28951300	0.33823400	2.97832300
N	-5.19118000	4.02050100	0.24935400	N	-0.07619400	5.91452500	-3.64576700
N	-6.02215700	3.14337900	0.56651600	N	0.10644900	6.83239100	-2.81830600
N	-5.88175000	-2.43655200	1.35136800	N	0.10644900	6.83239100	2.81830600
N	-5.26955900	-3.35841200	0.77072200	N	-0.07619400	5.91452500	3.64576700
N	0.32829400	-3.02338700	-2.58807300	N	-0.61787500	-0.37461200	-3.48830800
N	-0.89631900	-3.15437200	-2.79113500	N	0.28951300	0.33823400	-2.97832300
N	4.32861300	-2.68553800	2.56944400	N	0.34797200	-6.79423300	-2.81155500
N	3.35655300	-3.36699400	2.17364100	N	0.00346400	-5.95533200	-3.67016700
N	6.55236700	2.38236300	-0.71805300	N	0.00346400	-5.95533200	3.67016700
N	7.10000800	1.34612100	-0.28155400	N	0.34797200	-6.79423300	2.81155500

6-ccccctt (22)				6-cctcct-anti (21 _a)			
C	-6.22711100	2.21363100	0.15409900	C	-3.40841400	4.08258700	1.03554600
C	-6.23662400	0.97955600	0.82711100	C	-4.09729600	2.90082700	1.36853900
C	-5.20845800	0.65448500	1.72217400	C	-3.43531200	1.66356900	1.28383700
C	-4.12129900	1.50934500	1.84811600	C	-2.12270800	1.61511600	0.83062400
C	-4.02969400	2.66714200	1.05864000	C	-1.44410300	2.79142400	0.47747200
C	-5.11107500	3.03845200	0.23594200	C	-2.10030600	4.03334100	0.57256700
H	-7.07105800	2.48252100	-0.47418200	H	-3.92205400	5.03200900	1.15282100
H	-5.25666000	-0.26832700	2.29017000	H	-3.93153600	0.74972700	1.58183900
H	-3.29291000	1.26692400	2.50597100	H	-1.59415500	0.66988300	0.76015300
H	-5.04959600	3.95159200	-0.34563500	H	-1.56822400	4.93816300	0.30180300
C	-5.47315700	-0.85915600	-1.45165900	C	-6.37643900	1.46669300	-0.49023100
C	-4.42486200	-1.43984400	-2.15604500	C	-6.52312200	0.40589500	-1.38268300
C	-3.87098400	-2.65716200	-1.73033900	C	-6.55893400	-0.90748500	-0.90273100
C	-4.44891600	-3.33745400	-0.64458600	C	-6.57712200	-1.14997400	0.47805400
C	-5.55282900	-2.79242800	0.00907900	C	-6.52119100	-0.08288400	1.37076800
C	-6.04095400	-1.52895100	-0.35471400	C	-6.35345000	1.22132500	0.89014600
H	-5.88273900	0.08837300	-1.78172800	H	-6.30130700	2.48451000	-0.85941300
H	-4.02391700	-0.95760600	-3.04205000	H	-6.58000600	0.59113000	-2.45097200
H	-4.06096500	-4.30558600	-0.34428000	H	-6.66618300	-2.16658400	0.84686200
H	-6.03799700	-3.33671700	0.81358700	H	-6.57221100	-0.25619800	2.44135500
C	-1.10887500	-3.43822900	-1.04299100	C	-4.56231500	-2.74617700	-1.47570400
C	-0.07729200	-4.35634900	-0.77597500	C	-4.03927400	-3.75506500	-0.64917200
C	0.75139400	-4.20602600	0.32981900	C	-2.70540100	-3.71631100	-0.26153900
C	0.58094200	-3.09693200	1.17428300	C	-1.85916400	-2.70570600	-0.75872800
C	-0.44600400	-2.17279400	0.91399700	C	-2.37260800	-1.74121500	-1.63877700
C	-1.27043600	-2.32463000	-0.19544800	C	-3.72060600	-1.74351100	-1.97994600
H	0.05934100	-5.18567000	-1.46307800	H	-4.68835300	-4.55906400	-0.31572300
H	1.52912800	-4.93323300	0.53921400	H	-2.29499600	-4.47512300	0.39517600
H	-0.58092500	-1.33105800	1.58637800	H	-1.69918000	-0.98915100	-2.03729800
H	-2.02869000	-1.57923600	-0.39813300	H	-4.11509800	-0.99391100	-2.65644400
C	-1.12810600	4.43371600	0.10726200	C	1.94461800	3.44208100	-0.34701100
C	-0.63617300	4.79662000	-1.15447500	C	2.86459000	4.44084900	0.00639100
C	0.73649400	4.76087200	-1.39552800	C	4.20494900	4.31276300	-0.34288300
C	1.61940900	4.39346200	-0.36839800	C	4.64494000	3.16856800	-1.02590500
C	1.12904600	4.22362100	0.94736700	C	3.71055300	2.19996400	-1.44447600
C	-0.23207900	4.23790500	1.18191500	C	2.37313000	2.33277800	-1.10331500

H	-1.34129900	4.98404900	-1.95780600	H	2.50859800	5.30539900	0.55754200
H	1.13250400	4.91561900	-2.39413500	H	4.92650300	5.08267500	-0.08914900
H	1.82676000	3.98779400	1.74230700	H	4.04050300	1.35162400	-2.03451100
H	-0.62797000	4.01616900	2.16607500	H	1.64612300	1.58862900	-1.40748600
C	5.37987900	2.02354900	0.74589200	C	5.80520300	0.79021000	0.49631300
C	6.21634600	0.95148100	0.45853100	C	5.71518900	-0.45898700	1.10325600
C	6.39187200	0.55963600	-0.87637800	C	6.32168100	-1.57928800	0.50870500
C	5.87263700	1.34646400	-1.91937400	C	7.07542300	-1.42130800	-0.66497400
C	5.00582900	2.39147100	-1.62965000	C	7.15480300	-0.17552100	-1.27373100
C	4.70627700	2.69879200	-0.28646900	C	6.49438300	0.93670700	-0.72191800
H	5.16517700	2.30153500	1.77287300	H	5.35256900	1.64858100	0.97858200
H	6.68223300	0.38697800	1.25892400	H	5.19395600	-0.56560100	2.04910900
H	6.09250000	1.07190000	-2.94666300	H	7.60383400	-2.27623100	-1.07498900
H	4.50875500	2.93869900	-2.42232700	H	7.74564800	-0.03152100	-2.17274800
C	4.78026900	-3.11329200	1.93693600	C	1.78974000	-3.63543500	1.97205400
C	3.48262700	-2.71394600	1.56983600	C	1.33185200	-3.21382900	0.71399400
C	3.30276400	-1.98423300	0.37835500	C	2.26012300	-2.84226400	-0.27777000
C	4.40263400	-1.62859100	-0.39462100	C	3.62050700	-2.86339800	-0.00390300
C	5.69946100	-2.00988400	-0.00491400	C	4.07901000	-3.26019500	1.26897600
C	5.87282900	-2.81296900	1.13124100	C	3.15301900	-3.67186700	2.24172600
H	4.90773700	-3.65390900	2.86942000	H	1.06281300	-3.94947800	2.71419400
H	2.31783800	-1.65498400	0.07319200	H	1.89727300	-2.55983900	-1.25934400
H	4.25540200	-1.04138500	-1.29370100	H	4.32815300	-2.60639100	-0.78310800
H	6.87100900	-3.14588000	1.39746500	H	3.52603700	-4.03384100	3.19441800
N	-2.75881100	3.27543100	1.08873400	N	-0.10892900	2.61079700	0.05162000
N	-2.50199500	4.08667700	0.15547800	N	0.61481400	3.64232600	0.09013900
N	2.90518200	3.97783900	-0.78432900	N	6.01185300	3.16253800	-1.43570000
N	3.61786300	3.49029900	0.13737300	N	6.77671300	2.17371600	-1.38302300
N	7.14867700	-0.60017900	-1.23631700	N	6.41836500	-2.83499900	1.18379300
N	6.87349600	-1.73498300	-0.78635300	N	5.44938800	-3.50572100	1.59725200
N	1.26510000	-2.99824200	2.42217800	N	-0.47617000	-2.60582900	-0.48669800
N	2.50142600	-2.93854300	2.58790100	N	-0.06853300	-3.26182600	0.50941000
N	-2.91700900	-3.27523400	-2.60005400	N	-6.77105400	-2.00392800	-1.81427800
N	-1.77758800	-3.67901000	-2.28400500	N	-5.89884500	-2.87862900	-1.98597500
N	-7.36687100	0.10672800	0.70690400	N	-5.38394200	3.08556700	1.97170800
N	-7.24780200	-1.05971900	0.27162800	N	-6.34857300	2.30383500	1.83402300

6-ctctccc-anti (23 _a)				6-ctctccc-syn (23 _s)			
C	5.32599800	1.32194100	1.33937900	C	0.83923300	5.45461900	-0.85126400
C	6.34162400	1.00569900	0.42347400	C	1.86748000	4.63659900	-1.35379200
C	6.30785800	1.52575600	-0.87657600	C	1.57386200	3.34957700	-1.82860500
C	5.18235800	2.22543800	-1.30412900	C	0.27428800	2.86635800	-1.73376600
C	4.14128900	2.50688400	-0.40572400	C	-0.73377100	3.63840000	-1.13382200
C	4.23988200	2.08562100	0.93111000	C	-0.44616100	4.94879900	-0.70511000
H	5.38356800	0.94941400	2.35674400	H	1.07278400	6.47272900	-0.55457500
H	7.12645300	1.32005600	-1.55927600	H	2.35764500	2.74317300	-2.26995200
H	5.09383500	2.56140600	-2.33265100	H	0.01967200	1.87397000	-2.09206600
H	3.43331400	2.31702500	1.61813900	H	-1.23705400	5.55184800	-0.27343000
C	5.42753200	-2.28764400	2.01601600	C	3.41745900	3.57011800	0.97807300
C	4.20931200	-2.92964400	1.79460200	C	3.61621200	2.58465800	1.93568500
C	3.66684100	-3.00117400	0.50204000	C	4.56787200	1.57130300	1.73183600
C	4.38947600	-2.47025200	-0.58369900	C	5.40049900	1.62040300	0.59967300
C	5.58224000	-1.80322900	-0.36158400	C	5.25077600	2.65262500	-0.32191800
C	6.07894000	-1.66141700	0.94764300	C	4.22655600	3.60233600	-0.17143200
H	5.85140200	-2.22608100	3.01336500	H	2.67033500	4.33701500	1.14384500
H	3.65311500	-3.36695900	2.61784500	H	3.04015900	2.58269900	2.85551700
H	3.98279000	-2.55976000	-1.58373300	H	6.18170500	0.87970700	0.46508700
H	6.13012200	-1.37604100	-1.19372600	H	5.92019800	2.73489700	-1.17258600
C	0.57748100	-3.98312500	-0.94311100	C	4.76411400	-1.37591900	1.64166900
C	-0.28062800	-4.38679400	0.10039200	C	5.51803100	-2.56134600	1.67062700
C	-1.61454400	-4.66209200	-0.16694900	C	5.34490300	-3.53176600	0.69256600
C	-2.10835100	-4.54558100	-1.48235800	C	4.33609400	-3.38756100	-0.27291600
C	-1.23363000	-4.24339200	-2.53552000	C	3.57164700	-2.20482500	-0.30341700
C	0.09270300	-3.93306000	-2.26032900	C	3.78707700	-1.20628800	0.64004000
H	0.10886400	-4.45288600	1.11006900	H	6.24123800	-2.69413200	2.46889400
H	-2.28267500	-4.95609400	0.63603400	H	5.95733000	-4.42763200	0.67745300
H	-1.61652600	-4.22527500	-3.55081500	H	2.81052300	-2.06628700	-1.06254700
H	0.77644500	-3.64405200	-3.05200500	H	3.17875300	-0.31047000	0.61265000
C	1.01912400	4.17434100	-0.54183500	C	-4.02743600	2.81916400	-0.10476800
C	0.49162400	5.37169200	-0.03275100	C	-4.42409700	1.78681800	-0.97554700
C	-0.79861000	5.76672100	-0.37126800	C	-5.54935500	1.03215700	-0.68637600
C	-1.61415900	4.90601100	-1.12165000	C	-6.29552300	1.29540700	0.47810500
C	-1.08896800	3.71126500	-1.64101700	C	-5.97951500	2.40281500	1.27472200
C	0.22827300	3.35935000	-1.37035000	C	-4.83764000	3.15115000	0.99181700

H	1.11324700	5.98930100	0.60812400	H	-3.82480600	1.57352900	-1.85267700
H	-1.20105000	6.71212600	-0.02083300	H	-5.84724800	0.22861000	-1.34994800
H	-1.71615400	3.06840300	-2.25063100	H	-6.60518500	2.63993500	2.12939900
H	0.64838500	2.43740500	-1.75775400	H	-4.54119700	3.97875700	1.62844600
C	-5.05790200	2.70701900	-0.47842900	C	-6.01846500	-2.40896400	-0.17500800
C	-5.29920000	1.68132500	0.42988700	C	-4.79679300	-3.05476200	-0.31750900
C	-4.55851700	1.62209700	1.62433900	C	-3.75443100	-2.78850000	0.59133900
C	-3.60409100	2.61711400	1.89511400	C	-3.98396300	-1.93588300	1.68175800
C	-3.31466000	3.59793100	0.95591500	C	-5.18383800	-1.24060100	1.78897800
C	-4.03585400	3.64612200	-0.25132300	C	-6.18072200	-1.43307800	0.82242200
H	-5.66016000	2.80271800	-1.37647700	H	-6.83452300	-2.60419500	-0.86428500
H	-6.08367300	0.95738100	0.23683000	H	-4.62781100	-3.75212100	-1.13012500
H	-3.10116200	2.60751700	2.85685100	H	-3.18449400	-1.78164900	2.39931800
H	-2.57058100	4.35002100	1.18371800	H	-5.33994300	-0.53389800	2.59684000
C	-5.55492000	-3.44572200	0.58108400	C	1.00462300	-4.41624800	-2.45446100
C	-4.49755400	-3.36335500	-0.33887100	C	1.92197200	-4.55997100	-1.40270300
C	-3.66758500	-2.22438800	-0.33686600	C	1.46449700	-4.55481500	-0.06892000
C	-3.87090000	-1.21057800	0.59237600	C	0.12767300	-4.30129200	0.20471500
C	-4.90315500	-1.31846800	1.54537500	C	-0.77323400	-4.05293400	-0.85031200
C	-5.72205800	-2.46015100	1.54485700	C	-0.33132000	-4.14657600	-2.17880500
H	-6.21335500	-4.30743600	0.54003600	H	1.36241100	-4.49901700	-3.47565700
H	-2.86743600	-2.12637600	-1.06022700	H	2.15793300	-4.74217100	0.74386700
H	-3.21346500	-0.34965900	0.58941100	H	-0.23329200	-4.27402900	1.22658300
H	-6.48919400	-2.54649300	2.30763000	H	-1.04915300	-3.99022000	-2.97754300
N	2.96621400	3.10092100	-0.92665600	N	-1.98074100	2.99085700	-1.00646000
N	2.30686400	3.78679300	-0.10194600	N	-2.81702000	3.54365900	-0.24088800
N	-2.92689900	5.34329400	-1.48790400	N	-7.46261700	0.52902800	0.81486300
N	-3.97397800	4.73171600	-1.18460800	N	-7.42503800	-0.71968800	0.89312400
N	-4.87042500	0.76592300	2.72280700	N	-2.43114000	-3.27127200	0.46743900
N	-5.10705800	-0.45999400	2.66957700	N	-2.12493700	-3.66817800	-0.68968800
N	-3.44633400	-4.87676200	-1.85150600	N	4.29325300	-4.42444200	-1.25706600
N	-4.47376500	-4.41970500	-1.30463300	N	3.25817700	-4.87298400	-1.79747800
N	2.37017300	-3.56101200	0.38752100	N	4.78278400	0.69694200	2.83938500
N	1.91286800	-3.55791000	-0.78812200	N	4.95843100	-0.53918200	2.78445500
N	7.46896100	0.21926800	0.85199200	N	3.16412500	5.20997200	-1.54207900
N	7.32342000	-0.97956400	1.17744200	N	4.21363700	4.68915800	-1.10474100

6-cttct-syn (25 _s)				6-cccttt (24)			
C	1.88457200	-4.54764400	0.99495100	C	2.84043200	-2.44239000	0.30153000
C	2.85304600	-4.02175800	0.11331400	C	2.99093600	-2.88599700	1.62871800
C	2.46104900	-3.10577000	-0.87868700	C	4.27924600	-3.16110100	2.12151300
C	1.12094300	-2.74101000	-0.98564400	C	5.39566200	-3.01428100	1.30898600
C	0.15757300	-3.26781800	-0.10827700	C	5.24987200	-2.46735800	0.02549300
C	0.55889700	-4.15727700	0.90921400	C	3.96565500	-2.21620000	-0.48664800
H	2.19993100	-5.28797600	1.72392100	H	1.85891800	-2.22205400	-0.09906100
H	3.18900700	-2.71926000	-1.58373700	H	4.37942900	-3.47933200	3.15440100
H	0.79175200	-2.06172600	-1.76585700	H	6.38887800	-3.25527500	1.67438200
H	-0.18703000	-4.56256600	1.58262500	H	3.85095200	-1.83045800	-1.49395900
C	6.73304100	-2.55519400	-0.90064000	C	0.12022000	-4.88822900	0.96359200
C	7.36014700	-1.32083800	-0.82246000	C	-0.79739400	-5.39823100	0.04840600
C	6.86971300	-0.33324000	0.04845800	C	-1.76599700	-4.57430400	-0.54995000
C	5.75235900	-0.61615900	0.85617900	C	-1.71980500	-3.18645900	-0.29817900
C	5.12405900	-1.85753400	0.77894200	C	-0.81555900	-2.67385300	0.62380100
C	5.60307800	-2.83807400	-0.10969000	C	0.09834600	-3.52012900	1.27686000
H	7.13179400	-3.34307700	-1.53168500	H	0.82307500	-5.54714700	1.46327600
H	8.25969400	-1.11650800	-1.39456500	H	-0.80196500	-6.45507900	-0.19945900
H	5.39836800	0.11902600	1.57066900	H	-2.39287400	-2.50390000	-0.79872400
H	4.28898700	-2.07561300	1.43583500	H	-0.82721200	-1.61459300	0.86301400
C	5.98282800	2.39810500	0.15189300	C	-4.45259800	-3.75938300	-1.22594900
C	5.39662300	3.25212500	1.10487400	C	-4.81326200	-2.75330500	-2.14127800
C	4.11338800	3.74053300	0.90794100	C	-5.32177000	-1.54795800	-1.68054800
C	3.42819200	3.43522000	-0.28463800	C	-5.52749000	-1.35357100	-0.29796500
C	4.06185100	2.67107100	-1.27801800	C	-5.33517200	-2.43329200	0.58394300
C	5.32759500	2.13952800	-1.06168800	C	-4.80690000	-3.63616200	0.12668500
H	5.95483100	3.49519900	2.00386300	H	-4.60863900	-2.90475800	-3.19676200
H	3.62574000	4.35164700	1.65861900	H	-5.49915100	-0.72389800	-2.36177400
H	3.52359100	2.47569500	-2.20000800	H	-5.52783900	-2.28003600	1.64133800
H	5.80683300	1.53068500	-1.82051500	H	-4.59464000	-4.44402200	0.81926900
C	-3.38887900	-3.11307400	0.09308700	C	6.05044100	-0.02814000	-1.15765100
C	-4.35544900	-3.75659100	0.88392000	C	5.75884300	0.71813200	-2.30798600
C	-5.71028400	-3.48703300	0.70686300	C	5.03512600	1.90133400	-2.19544000
C	-6.11101000	-2.52194000	-0.22637000	C	4.65731600	2.38613400	-0.93184300
C	-5.14870600	-1.90748500	-1.05317900	C	5.07893100	1.70341300	0.22798200
C	-3.80228700	-2.20247000	-0.89882200	C	5.76233800	0.50245800	0.11598500

H	-4.02280900	-4.47501900	1.62639200	H	6.05367600	0.33104200	-3.27812500
H	-6.46255400	-3.99937200	1.29831600	H	4.72138800	2.45068000	-3.07730400
H	-5.46186400	-1.20356700	-1.81561300	H	4.81117000	2.09976900	1.20057100
H	-3.05666800	-1.73162600	-1.52889100	H	6.05522100	-0.03998700	1.00804100
C	-6.72611600	0.13192900	1.15807300	C	1.57558700	5.15092800	-0.98736200
C	-5.91236300	1.22804200	1.41958500	C	0.24856200	5.55020600	-0.93930300
C	-5.61823300	2.14905800	0.40192600	C	-0.49065600	5.43399100	0.25753500
C	-6.29152000	2.06599200	-0.83288400	C	0.17723500	5.12004700	1.45848000
C	-7.15191500	1.00314600	-1.07554600	C	1.51086500	4.74056800	1.41366100
C	-7.27990700	-0.01929800	-0.11978100	C	2.18533200	4.64822300	0.17893800
H	-6.89304400	-0.62595700	1.91577200	H	2.11449100	5.12106400	-1.92698400
H	-5.41629500	1.33888300	2.37832400	H	-0.27960700	5.83632200	-1.84359500
H	-6.09221800	2.80697800	-1.59862200	H	-0.38570900	5.06386500	2.38271100
H	-7.66405300	0.90615700	-2.02812700	H	2.02135800	4.39349600	2.30672100
C	-0.76448800	4.44280000	1.29156500	C	-5.12615600	3.14471700	-0.88252500
C	0.05583200	4.40324200	0.14820300	C	-5.40403900	2.13854800	0.06753200
C	-0.52446700	4.35677800	-1.13208600	C	-5.05124800	2.34271100	1.41658400
C	-1.89840500	4.20076000	-1.24846300	C	-4.23931300	3.41725900	1.74888900
C	-2.69636900	4.05333300	-0.09826400	C	-3.75579800	4.28228600	0.74378100
C	-2.13395200	4.24873200	1.17658200	C	-4.29949800	4.20847200	-0.55524200
H	-0.29139000	4.53298700	2.26441300	H	-5.45760200	2.99270600	-1.90516100
H	0.11312900	4.37476700	-2.00797700	H	-5.30557400	1.59069200	2.15426200
H	-2.36924000	4.09180100	-2.22044500	H	-3.84503900	3.52514700	2.75465300
H	-2.76325500	4.17061500	2.05522600	H	-3.96192000	4.90261100	-1.31584000
N	-1.18163100	-2.88794000	-0.36090800	N	6.43734000	-2.32174700	-0.76432500
N	-2.04486800	-3.46667800	0.35589400	N	6.74858100	-1.26168200	-1.35023800
N	-7.52229600	-2.32231200	-0.41595500	N	3.72992400	3.45144100	-0.93966000
N	-8.04336400	-1.18516400	-0.45262100	N	3.34202300	3.83788000	0.19947600
N	-4.50997400	2.98032200	0.67585800	N	-1.88619000	5.33612800	0.06492800
N	-3.98132000	3.51139700	-0.33994600	N	-2.53040500	4.90507500	1.06636800
N	2.08449700	3.76687800	-0.55916700	N	-5.67351800	-0.08788000	0.30722100
N	1.44011900	4.26801200	0.40359900	N	-5.74489700	0.88813000	-0.49463100
N	7.72087400	0.80361900	0.23816200	N	-2.65429800	-5.28862000	-1.42062400
N	7.32455400	1.97825000	0.38881400	N	-3.80663000	-4.91925800	-1.74820600
N	4.10631200	-4.69906000	0.12671400	N	1.97595200	-2.87718000	2.63485300
N	5.23768700	-4.21779500	-0.08908900	N	0.75633000	-3.04819600	2.45454500

6-cttct-anti (25 _a)				6-cctttt-syn (26 _s)			
C	1.82105600	-4.64129100	0.76748400	C	-1.47807200	3.56339100	3.94404900
C	2.75857200	-4.05391700	-0.10844100	C	-0.34922300	4.40096600	3.81984600
C	2.33613600	-3.05926500	-1.00729900	C	0.91276600	3.93288100	4.24004300
C	0.99734800	-2.68162200	-1.03210200	C	1.05462500	2.60557400	4.62169200
C	0.06511900	-3.26839100	-0.16073900	C	-0.04313100	1.72503300	4.55433800
C	0.49852500	-4.23795300	0.76532900	C	-1.33095100	2.23090500	4.29678500
H	2.15991200	-5.43891800	1.42199600	H	-2.44479000	3.95785600	3.64700300
H	3.04077000	-2.62438200	-1.70846900	H	1.77485700	4.58548800	4.16487800
H	0.63986000	-1.94228100	-1.74238900	H	2.02891100	2.19906900	4.87499200
H	-0.22842500	-4.68916700	1.43083200	H	-2.17892800	1.55635600	4.29872300
C	6.58514000	-2.52547300	-1.19022300	C	1.52370500	7.03390800	0.69736200
C	7.23367600	-1.31256000	-1.03401900	C	1.52370500	7.03390800	-0.69736200
C	6.81676700	-0.40704400	-0.04267000	C	0.32256200	6.80777000	-1.38907700
C	5.74061100	-0.75206200	0.79594400	C	-0.90845500	6.89082200	-0.68943700
C	5.08964800	-1.97287100	0.63993500	C	-0.90845500	6.89082200	0.68943700
C	5.50296300	-2.87263600	-0.35928400	C	0.32256200	6.80777000	1.38907700
H	6.93162100	-3.25428900	-1.91637700	H	2.45679500	7.01979500	1.25135100
H	8.10115900	-1.06182200	-1.63683000	H	2.45679500	7.01979500	-1.25135100
H	5.44198500	-0.08425700	1.59691900	H	-1.83782600	6.80380300	-1.24023700
H	4.29158500	-2.24668900	1.32228400	H	-1.83782600	6.80380300	1.24023700
C	6.04341100	2.32110200	0.51203400	C	-0.34922300	4.40096600	-3.81984600
C	5.58333700	3.05173500	1.61803400	C	-1.47807200	3.56339100	-3.94404900
C	4.30911900	3.60220600	1.59676300	C	-1.33095100	2.23090500	-4.29678500
C	3.51640700	3.50997500	0.44134900	C	-0.04313100	1.72503300	-4.55433800
C	4.01877400	2.85002000	-0.69721300	C	1.05462500	2.60557400	-4.62169200
C	5.26455000	2.24738500	-0.65831100	C	0.91276600	3.93288100	-4.24004300
H	6.22130700	3.14341700	2.49160200	H	-2.44479000	3.95785600	-3.64700300
H	3.90318500	4.11402500	2.46384700	H	-2.17892800	1.55635600	-4.29872300
H	3.39482900	2.79248700	-1.58211200	H	2.02891100	2.19906900	-4.87499200
H	5.64807300	1.71861900	-1.52513400	H	1.77485700	4.58548800	-4.16487800
C	-3.45744600	-3.07699900	0.21717100	C	-0.26988700	-1.76815000	4.01497000
C	-4.39340900	-3.66835800	1.08057600	C	-1.18145400	-2.56315500	3.29932200
C	-5.74791300	-3.37200300	0.96754600	C	-0.94741700	-3.92130000	3.11029700
C	-6.17877700	-2.43444300	0.01973400	C	0.20443300	-4.50573300	3.66260300
C	-5.24940900	-1.87672000	-0.88081800	C	1.09372500	-3.71959300	4.42386700
C	-3.90528100	-2.19648500	-0.78548000	C	0.88123900	-2.35828300	4.57404200

H	-4.03370900	-4.36590100	1.83062500	H	-2.06797300	-2.08826000	2.89101300
H	-6.47889100	-3.83999200	1.61984600	H	-1.65991900	-4.52966300	2.56384000
H	-5.58907900	-1.19714300	-1.65414500	H	1.94412400	-4.20587900	4.89202600
H	-3.18079800	-1.77023300	-1.46999800	H	1.57413900	-1.74215300	5.13533800
C	-6.65209000	0.30881400	1.27510900	C	-0.70460800	-7.34393300	0.69285600
C	-5.79157300	1.38772300	1.42241600	C	-0.70460800	-7.34393300	-0.69285600
C	-5.52389700	2.23501700	0.33621600	C	0.08553700	-6.42389900	-1.40713300
C	-6.26617900	2.09895500	-0.85300700	C	0.87537800	-5.49994700	-0.69751500
C	-7.17068400	1.05523700	-0.98285900	C	0.87537800	-5.49994700	0.69751500
C	-7.28007300	0.09898900	0.04113400	C	0.08553700	-6.42389900	1.40713300
H	-6.79935500	-0.39850600	2.08456200	H	-1.26249600	-8.09122000	1.24828600
H	-5.23371600	1.53814900	2.34121300	H	-1.26249600	-8.09122000	-1.24828600
H	-6.07622700	2.78050900	-1.67473700	H	1.52642300	-4.81609700	-1.23170900
H	-7.73203000	0.91278200	-1.90179700	H	1.52642300	-4.81609700	1.23170900
C	-0.51630700	4.21411300	0.79105200	C	-1.18145400	-2.56315500	-3.29932200
C	0.18646100	4.27555600	-0.43309500	C	-0.26988700	-1.76815000	-4.01497000
C	-0.52377800	4.34451800	-1.64035700	C	0.88123900	-2.35828300	-4.57404200
C	-1.90914700	4.22629000	-1.63939500	C	1.09372500	-3.71959300	-4.42386700
C	-2.59159000	4.01597700	-0.43251600	C	0.20443300	-4.50573300	-3.66260300
C	-1.89005700	4.08340800	0.79164700	C	-0.94741700	-3.92130000	-3.11029700
H	0.05066500	4.18816100	1.71488400	H	-2.06797300	-2.08826000	-2.89101300
H	0.03646600	4.40933600	-2.56789300	H	1.57413900	-1.74215300	-5.13533800
H	-2.47306500	4.18914100	-2.56609600	H	1.94412400	-4.20587900	-4.89202600
H	-2.43837300	3.94257800	1.71598400	H	-1.65991900	-4.52966300	-2.56384000
N	-1.27751500	-2.86244600	-0.33246300	N	0.26943300	0.34808700	4.62728000
N	-2.10934900	-3.45148300	0.41736400	N	-0.59267300	-0.39541700	4.07908400
N	-7.59328600	-2.20948800	-0.09919300	N	0.40693600	-5.91376800	3.72744900
N	-8.08931600	-1.06225900	-0.17713000	N	0.23814000	-6.72735100	2.79650900
N	-4.37589600	3.03537700	0.50146600	N	0.23814000	-6.72735100	-2.79650900
N	-3.91353800	3.53170500	-0.56698000	N	0.40693600	-5.91376800	-3.72744900
N	2.19598900	3.98798500	0.54640700	N	0.26943300	0.34808700	-4.62728000
N	1.57925800	4.08920600	-0.55381500	N	-0.59267300	-0.39541700	-4.07908400
N	7.71471900	0.67925800	0.20557400	N	0.48154500	6.14377300	-2.62732700
N	7.37846100	1.82990600	0.55796000	N	-0.56022900	5.52001300	-2.98935200
N	4.00344700	-4.73800000	-0.20073600	N	-0.56022900	5.52001300	2.98935200
N	5.12733700	-4.24650200	-0.43252400	N	0.48154500	6.14377300	2.62732700

6-cttttc-syn (27 _s)				6-cctttt-anti (26 _a)			
C	0.45452700	3.76798600	-1.19654100	C	-3.04706300	-4.27402000	-1.50860700
C	1.31646400	3.68522700	-0.08688100	C	-3.92489100	-4.07530300	-0.42188600
C	0.78136600	3.67540200	1.21527000	C	-3.46473700	-4.29538900	0.89344700
C	-0.59338200	3.63848400	1.38647000	C	-2.11794400	-4.53497400	1.11046600
C	-1.45664400	3.61608600	0.27327800	C	-1.21279000	-4.57983200	0.03021700
C	-0.92405700	3.72654800	-1.02508300	C	-1.69884800	-4.52510500	-1.29013200
H	0.89301800	3.79411900	-2.18937800	H	-3.42653100	-4.11140800	-2.51266800
H	1.45221800	3.63519900	2.06484600	H	-4.14590500	-4.15486200	1.72423900
H	-1.03179400	3.56958000	2.37722900	H	-1.71863800	-4.60278000	2.11778700
H	-1.59415400	3.71617100	-1.87705400	H	-0.99881200	-4.57678200	-2.11661100
C	5.32691400	2.02670300	1.37951300	C	-6.81556700	-1.06707700	1.18826800
C	6.53917100	1.37862300	1.17560600	C	-6.93930500	0.31241000	1.11378800
C	7.14776400	1.43891700	-0.08514800	C	-6.83017800	0.94180700	-0.14300500
C	6.60374000	2.25085100	-1.09458300	C	-6.87973100	0.15734400	-1.31759600
C	5.36702300	2.85734900	-0.90438700	C	-6.72504100	-1.21840500	-1.24262500
C	4.69959100	2.71311500	0.32797100	C	-6.55047800	-1.81757200	0.02141100
H	4.81299500	1.96065400	2.33297800	H	-6.74379800	-1.56588900	2.14980700
H	6.99762800	0.80452300	1.97300800	H	-6.95853400	0.91453300	2.01478400
H	7.12819800	2.34629300	-2.04064300	H	-6.86567600	0.66503600	-2.27715700
H	4.89510000	3.41980400	-1.70215400	H	-6.58363900	-1.80844100	-2.14059100
C	7.24188900	-1.28005100	-0.14806100	C	-4.74638900	3.66556500	0.46202500
C	6.28467400	-1.24216000	-1.17781500	C	-4.07159300	3.73765600	-0.77946600
C	5.11140300	-1.96909200	-1.05968800	C	-2.76368600	4.17871200	-0.83012200
C	4.86834400	-2.73372400	0.09792100	C	-2.11150500	4.58478200	0.35388100
C	5.86534500	-2.83317400	1.08166000	C	-2.84240700	4.71142900	1.54499300
C	7.06799600	-2.14139500	0.94149400	C	-4.14755400	4.22664900	1.60520900
H	6.45472800	-0.61768600	-2.04802600	H	-4.55449100	3.33344200	-1.66154700
H	4.34505200	-1.91338400	-1.82372800	H	-2.20229200	4.14581500	-1.75671400
H	5.67209200	-3.43867500	1.96176300	H	-2.33977500	5.07352400	2.43614100
H	7.84070200	-2.20928400	1.70086000	H	-4.68067000	4.18292600	2.54972100
C	-4.86832700	2.73386900	-0.09770600	C	2.29717000	-4.16786900	-0.14051800
C	-5.86549200	2.83361500	-1.08124600	C	3.40301900	-4.75876000	-0.77360800
C	-7.06811400	2.14179600	-0.94106200	C	4.69388700	-4.40442200	-0.39273700
C	-7.24181600	1.28009200	0.14825000	C	4.89374500	-3.37448100	0.54129600
C	-6.28442400	1.24188000	1.17781700	C	3.78594800	-2.73874700	1.13048400
C	-5.11117600	1.96885700	1.05969500	C	2.50010900	-3.14925400	0.80903500

H	-5.67241000	3.43938300	-1.96120200	H	3.23392000	-5.52918500	-1.51935200
H	-7.84098000	2.20992600	-1.70024500	H	5.55540800	-4.91569400	-0.81078000
H	-6.45428800	0.61710500	2.04784900	H	3.93986700	-1.95760200	1.86667000
H	-4.34467600	1.91291500	1.82357000	H	1.63794300	-2.68639000	1.27530800
C	-6.53921900	-1.37878600	-1.17581400	C	6.32662200	-0.66783200	-0.70891300
C	-5.32698100	-2.02689600	-1.37972200	C	6.26901000	0.61167500	-1.25542900
C	-4.69967800	-2.71333300	-0.32818100	C	6.05360200	1.72512400	-0.43062200
C	-5.36711900	-2.85756400	0.90416800	C	5.93263400	1.54521200	0.95751400
C	-6.60382300	-2.25103500	1.09435900	C	6.09360100	0.27725300	1.51202000
C	-7.14780700	-1.43905200	0.08494400	C	6.27429200	-0.84038100	0.68479900
H	-6.99764200	-0.80464000	-1.97320100	H	6.49882600	-1.52468500	-1.35223600
H	-4.81304800	-1.96084700	-2.33317800	H	6.41011500	0.75657800	-2.32234700
H	-4.89519100	-3.42000400	1.70194300	H	5.79738200	2.40691500	1.60345600
H	-7.12828400	-2.34645100	2.04042100	H	6.09994600	0.15054400	2.59045500
C	0.59347200	-3.63838800	-1.38643000	C	1.90057300	2.98106200	-1.11331400
C	1.45667400	-3.61600000	-0.27318400	C	1.30463600	4.02006900	-0.37956900
C	0.92400600	-3.72650200	1.02513900	C	2.11403500	4.98620400	0.24932300
C	-0.45458800	-3.76797800	1.19650900	C	3.49347100	4.92038600	0.10308000
C	-1.31646700	-3.68524600	0.08680100	C	4.08948400	3.85732300	-0.60496500
C	-0.78128100	-3.67536400	-1.21531900	C	3.28250500	2.88086400	-1.21120200
H	1.03194400	-3.56940000	-2.37715700	H	1.25259700	2.26117900	-1.60273500
H	1.59404500	-3.71610100	1.87715700	H	1.64786900	5.79384800	0.80289800
H	-0.89313500	-3.79410300	2.18932100	H	4.13273400	5.69484900	0.51597400
H	-1.45208000	-3.63513600	-2.06493400	H	3.73146100	2.08336600	-1.79118300
N	-2.80247500	3.31735800	0.57538200	N	0.14505800	-4.46162100	0.39310500
N	-3.60809000	3.30769000	-0.39522000	N	0.99866600	-4.57470800	-0.52962000
N	-8.44480000	0.49874200	0.25592800	N	6.20416100	-3.18378100	1.07816800
N	-8.38964500	-0.75012300	0.31648100	N	6.73365300	-2.07180900	1.26625900
N	-3.37568100	-3.11567100	-0.60543900	N	6.28469100	3.03644500	-0.97048900
N	-2.68756600	-3.48120700	0.38686300	N	5.47662900	3.98369400	-0.92127600
N	3.60807000	-3.30746600	0.39544500	N	-0.70534300	4.74546700	0.43212900
N	2.80248000	-3.31713200	-0.57518900	N	-0.10489300	3.98958900	-0.38238000
N	8.38966900	0.75010500	-0.31665500	N	-6.28776600	2.22846600	-0.35378600
N	8.44489900	-0.49874100	-0.25585900	N	-5.81686200	2.77519000	0.68725700
N	2.68755000	3.48123700	-0.38700900	N	-5.09618700	-3.35127400	-0.73371800
N	3.37561300	3.11550700	0.60525200	N	-5.77911300	-2.97586300	0.26507100

6-cttttc-anti (27 _a)				6-ctttct (28)			
C	0.82900000	-3.59020600	1.13882300	C	-6.70580700	-1.09546100	1.37245700
C	1.39119200	-3.54436800	-0.15160700	C	-6.36556700	-1.87590200	0.25771000
C	0.55087300	-3.58463800	-1.28178000	C	-5.80060900	-1.27143300	-0.88033400
C	-0.82902800	-3.59033000	-1.13867200	C	-5.50477300	0.08244800	-0.86911700
C	-1.39122000	-3.54433900	0.15175200	C	-5.73942800	0.84899700	0.29024500
C	-0.55090200	-3.58448600	1.28193000	C	-6.34945200	0.24918200	1.40565400
H	1.48207700	-3.56180700	2.00318700	H	-7.19699500	-1.56406900	2.21940400
H	1.01019200	-3.55252100	-2.26493900	H	-5.58530200	-1.87025700	-1.75861400
H	-1.48210600	-3.56202500	-2.00304000	H	-5.03707200	0.55555100	-1.72477300
H	-1.01022000	-3.55225300	2.26508500	H	-6.52619200	0.85089800	2.29168900
C	5.17266900	-2.10216900	-0.86963400	C	-3.90529500	-4.51556500	-1.31494500
C	6.36959800	-1.40904900	-0.94808400	C	-2.51840300	-4.46776200	-1.41831300
C	7.22988400	-1.36211000	0.16513600	C	-1.74252200	-3.99245300	-0.34844100
C	6.94237900	-2.12007900	1.30673900	C	-2.37818400	-3.50908300	0.80975300
C	5.71763700	-2.77823500	1.40017200	C	-3.76555900	-3.48996900	0.88578000
C	4.81003800	-2.74888400	0.32860200	C	-4.53855600	-3.98930300	-0.17976300
H	4.47823600	-2.10632600	-1.70159500	H	-4.50805100	-4.94004100	-2.11175400
H	6.63125100	-0.87256200	-1.85354700	H	-2.01261800	-4.83240100	-2.30680400
H	7.64541500	-2.12900000	2.13374500	H	-1.77284500	-3.14244000	1.63132500
H	5.43291200	-3.29825300	2.30952500	H	-4.25631900	-3.10836100	1.77479800
C	7.22986800	1.36207300	-0.16521500	C	1.74330500	-3.99229400	0.34845100
C	6.36965000	1.40917100	0.94805200	C	2.37888200	-3.50850800	-0.80961600
C	5.17272200	2.10229100	0.86958400	C	3.76625400	-3.48918800	-0.88566300
C	4.81002500	2.74884700	-0.32871600	C	4.53933300	-3.98872600	0.17972300
C	5.71755200	2.77804000	-1.40035100	C	3.90616400	-4.51538000	1.31477500
C	6.94229500	2.11988700	-1.30690500	C	2.51926800	-4.46779300	1.41817900
H	6.63135800	0.87282100	1.85357800	H	1.77348000	-3.14171800	-1.63107500
H	4.47834400	2.10657400	1.70159100	H	4.25695000	-3.10726600	-1.77458200
H	5.43277400	3.29793700	-2.30975700	H	4.50899000	-4.94000200	2.11145300
H	7.64528100	2.12869000	-2.13395500	H	2.01354700	-4.83275100	2.30657500
C	-4.81005900	-2.74889300	-0.32857300	C	-4.02947200	3.83990700	-0.45477800
C	-5.17270300	-2.10203900	0.86958400	C	-3.46826100	4.23886000	0.78131900
C	-6.36963100	-1.40890400	0.94793900	C	-2.31540300	4.99998800	0.79857200
C	-7.22989700	-1.36208200	-0.16530000	C	-1.69807700	5.37415000	-0.42015300
C	-6.94237900	-2.12017900	-1.30681500	C	-2.36710000	5.14454700	-1.63488600
C	-5.71764200	-2.77835800	-1.40015300	C	-3.52864600	4.37939900	-1.65130800

H	-4.47828100	-2.10610400	1.70155500	H	-3.88915200	3.84790200	1.70065400
H	-6.63129200	-0.87230800	1.85333600	H	-1.80688800	5.21374800	1.73161300
H	-7.64540200	-2.12918600	-2.13383200	H	-1.89263700	5.45964100	-2.55867000
H	-5.43290700	-3.29847900	-2.30944500	H	-3.99200400	4.08650500	-2.58799900
C	-6.94229900	2.11979100	1.30682300	C	2.36617300	5.14480300	1.63491100
C	-5.71755000	2.77792100	1.40036300	C	3.52780400	4.37978500	1.65135100
C	-4.81000300	2.74883100	0.32874200	C	4.02871500	3.84035800	0.45482800
C	-5.17268400	2.10240500	-0.86963200	C	3.46748400	4.23925500	-0.78127800
C	-6.36961400	1.40930100	-0.94819500	C	2.31453700	5.00024800	-0.79854900
C	-7.22985600	1.36209700	0.16505000	C	1.69714600	5.37433600	0.42016600
H	-7.64530200	2.12851700	2.13385900	H	1.89165900	5.45984000	2.55868700
H	-5.43278600	3.29772200	2.30982800	H	3.99118000	4.08694200	2.58805000
H	-4.47829100	2.10677200	-1.70162700	H	3.88844000	3.84835400	-1.70060700
H	-6.63131100	0.87305300	-1.85378400	H	1.80601700	5.21395800	-1.73159900
C	0.55097000	3.58456600	1.28189900	C	5.80066100	-1.27076200	0.88024800
C	1.39122900	3.54441900	0.15167700	C	6.36589400	-1.87504000	-0.25776100
C	0.82896900	3.59039300	-1.13871700	C	6.70610000	-1.09446100	-1.37242200
C	-0.55094000	3.58470800	-1.28175200	C	6.34947000	0.25010900	-1.40557900
C	-1.39120000	3.54444200	-0.15153500	C	5.73919200	0.84973200	-0.29020500
C	-0.82893900	3.59027300	1.13886500	C	5.50455100	0.08306100	0.86908000
H	1.01033900	3.55232300	2.26503000	H	5.58537200	-1.86968600	1.75846300
H	1.48200000	3.56207000	-2.00311900	H	7.19749100	-1.56291300	-2.21933700
H	-1.01031000	3.55257400	-2.26488600	H	6.52619700	0.85191800	-2.29155300
H	-1.48197100	3.56186000	2.00326400	H	5.03665200	0.55601500	1.72471000
N	-3.51854200	-3.26686400	-0.58080300	N	-5.22597000	2.15185800	0.45786900
N	-2.75367400	-3.29062100	0.42283300	N	-4.89400900	2.73607700	-0.61228700
N	-8.45536700	-0.61484800	-0.11794700	N	-0.32323300	5.66153600	-0.54441200
N	-8.45535300	0.61491800	0.11748900	N	0.32226900	5.66157400	0.54440800
N	-3.51847400	3.26670400	0.58109500	N	4.89339200	2.73663800	0.61235000
N	-2.75366200	3.29072500	-0.42257600	N	5.22551200	2.15250900	-0.45780700
N	3.51849400	3.26675300	-0.58099300	N	5.95692000	-4.17081600	0.05341800
N	2.75369000	3.29066500	0.42268700	N	6.74813300	-3.25243600	-0.24825900
N	8.45536200	-0.61489500	0.11768800	N	0.33888900	-4.02458800	0.53161100
N	8.45535400	0.61487200	-0.11775000	N	-0.33809900	-4.02449000	-0.53159900
N	3.51852100	-3.26682100	0.58090700	N	-6.74750600	-3.25338400	0.24818500
N	2.75364700	-3.29069200	-0.42272100	N	-5.95612700	-4.17160100	-0.05356000

6-cttttt-anti (29 _a)				6-cttttt-syn (29 _s)			
C	-5.15930000	3.32452100	-0.79361800	C	0.62698200	4.66038900	-1.38746600
C	-4.75581700	3.87503400	0.44696600	C	1.52494800	4.52412100	-0.30897700
C	-5.40920200	3.47234700	1.62465900	C	1.07590200	4.76276400	1.00522300
C	-6.26847000	2.38102600	1.60152700	C	-0.27231700	4.99807600	1.23320800
C	-6.48996600	1.68929000	0.39687200	C	-1.19273600	5.00186000	0.16381100
C	-6.01858300	2.24757700	-0.81827700	C	-0.71880700	4.90257500	-1.16109700
H	-4.68153800	3.67684900	-1.70025600	H	1.00162300	4.49000900	-2.39213500
H	-5.11237800	3.93064700	2.56227200	H	1.77409100	4.66953200	1.82912000
H	-6.65834600	1.95769900	2.52143600	H	-0.65861000	5.08770000	2.24384400
H	-6.23056100	1.72633500	-1.74470700	H	-1.42833300	4.91656600	-1.97991100
C	-0.85685200	4.85384300	1.13126900	C	5.78506000	3.04641100	0.92396100
C	0.51045500	4.67185200	1.24777200	C	6.85380000	2.16593800	0.78052100
C	1.31395800	4.50470200	0.10263600	C	6.80621900	1.16962200	-0.20564200
C	0.74099400	4.64953400	-1.17607900	C	5.74760400	1.14938200	-1.13353900
C	-0.62713600	4.82729100	-1.29368700	C	4.71469000	2.06767800	-1.02698300
C	-1.44913000	4.86592000	-0.14791200	C	4.70507400	3.00498000	0.02575100
H	-1.49669000	4.88647800	2.00508000	H	5.76823200	3.77574000	1.72780700
H	0.98225400	4.57030800	2.21996600	H	7.70465000	2.20764800	1.45326600
H	1.37122200	4.53098000	-2.04964100	H	5.73790800	0.40669700	-1.92405500
H	-1.10782000	4.84632800	-2.26665000	H	3.88102600	2.04759800	-1.71931600
C	4.50435600	3.08416700	-0.43623900	C	6.57252600	-1.63245500	-0.15221800
C	5.43946900	3.02550500	-1.48258000	C	6.15052100	-2.61928600	-1.06288300
C	6.56662600	2.21996700	-1.37496000	C	4.97892600	-3.32881400	-0.83226400
C	6.72524000	1.39085900	-0.25465800	C	4.25056600	-3.10835500	0.35431100
C	5.81193700	1.47432600	0.81390600	C	4.74073600	-2.20281000	1.31011000
C	4.72151200	2.32246500	0.72891000	C	5.88542700	-1.45650000	1.05885400
H	5.25917600	3.62121100	-2.37153200	H	6.73536900	-2.78930400	-1.96182800
H	7.30858700	2.18578100	-2.16605200	H	4.61103000	-4.04742500	-1.55585700
H	5.96399500	0.86556000	1.69829900	H	4.17987500	-2.07035000	2.22969500
H	3.99599400	2.38374400	1.53157000	H	6.24312400	-0.73905400	1.78870300
C	-6.48997100	-1.68928500	-0.39684600	C	-4.56628000	4.05194200	-0.07035200
C	-6.26848600	-2.38101500	-1.60150700	C	-5.28385700	3.52529800	-1.16614500
C	-5.40922000	-3.47233700	-1.62465300	C	-6.15559000	2.46193300	-0.98714700
C	-4.75582400	-3.87503000	-0.44696800	C	-6.33146500	1.92448500	0.30557900
C	-5.15929400	-3.32452300	0.79362300	C	-5.80547500	2.61601200	1.42024600
C	-6.01857500	-2.24757700	0.81829500	C	-4.92128100	3.66769500	1.23967400

H	-6.65837100	-1.95768400	-2.52141000	H	-5.03075700	3.87433200	-2.16253800
H	-5.11240500	-3.93063300	-2.56227100	H	-6.59127500	1.95355100	-1.83931300
H	-4.68152400	-3.67685500	1.70025500	H	-5.99365700	2.21315100	2.41070400
H	-6.23054400	-1.72633900	1.74473000	H	-4.40210000	4.10692400	2.08335200
C	-0.85685900	-4.85382600	-1.13129300	C	-6.39870300	-2.25903700	-1.42665600
C	0.51044800	-4.67183400	-1.24779400	C	-5.59184700	-3.39409100	-1.41998900
C	1.31395200	-4.50470000	-0.10265700	C	-4.94239000	-3.78240600	-0.23597500
C	0.74098900	-4.64954900	1.17605600	C	-5.30584200	-3.16946100	0.98921300
C	-0.62714100	-4.82730700	1.29366300	C	-6.10823700	-2.04678000	0.98375700
C	-1.44913600	-4.86592200	0.14788900	C	-6.56198100	-1.50975000	-0.24790200
H	-1.49669800	-4.88644900	-2.00510400	H	-6.78214500	-1.85487800	-2.35805000
H	0.98224600	-4.57027600	-2.21998800	H	-5.33565000	-3.90015400	-2.34524800
H	1.37121800	-4.53100700	2.04961900	H	-4.84833400	-3.51697500	1.90813300
H	-1.10782400	-4.84635900	2.26662700	H	-6.28872400	-1.49313700	1.89788800
C	5.81194100	-1.47432700	-0.81389200	C	0.28450200	-5.00726100	-1.05383400
C	6.72523800	-1.39086600	0.25467800	C	1.10216800	-4.70384000	0.05238300
C	6.56661500	-2.21997800	1.37497700	C	0.54136100	-4.65827400	1.34336000
C	5.43945700	-3.02551500	1.48258500	C	-0.83249300	-4.76442300	1.49230100
C	4.50435000	-3.08417200	0.43623700	C	-1.66939100	-4.90641900	0.36541700
C	4.72151400	-2.32246400	-0.72890700	C	-1.09365200	-5.09513600	-0.90758200
H	5.96400600	-0.86555700	-1.69828100	H	0.74675900	-5.07666800	-2.03371900
H	7.30857100	-2.18579700	2.16607300	H	1.18213600	-4.46503600	2.19533700
H	5.25915700	-3.62122500	2.37153300	H	-1.29846100	-4.64939100	2.46602800
H	3.99600100	-2.38373800	-1.53157200	H	-1.73893500	-5.22065800	-1.76925500
N	-6.83356400	0.33308600	0.54128100	N	-2.54225200	4.83141900	0.53774700
N	-6.83356900	-0.33307900	-0.54124600	N	-3.35596300	4.68686700	-0.42157200
N	-2.81781500	-4.64210000	0.38845200	N	-6.67340200	0.58376000	0.57298600
N	-3.54724500	-4.57187900	-0.64823000	N	-6.84289600	-0.14294900	-0.45230700
N	2.61387800	-4.01968900	-0.35173900	N	-3.76762100	-4.54438500	-0.42114300
N	3.32840400	-3.82641100	0.67558000	N	-3.02198200	-4.58957800	0.60117300
N	7.91431100	0.60262400	-0.16798000	N	2.99322600	-3.66675400	0.66654600
N	7.91430900	-0.60263200	0.16800900	N	2.43076300	-4.32281400	-0.25482100
N	2.61388500	4.01969500	0.35172400	N	7.92657300	0.28780400	-0.33415500
N	3.32841200	3.82640600	-0.67559100	N	7.80504300	-0.95404600	-0.41727800
N	-3.54723500	4.57188300	0.64821400	N	2.77452700	3.95878600	-0.63926100
N	-2.81781000	4.64209500	-0.38847100	N	3.59729100	3.83434500	0.31082400

Table S2: Zero point energy (kJ mol⁻¹), entropy (cal mol⁻¹ K⁻¹) and thermal correction (kJ mol⁻¹) for cis, trans-[n]CPPDs (n = 3 to 6).

[n]CPPDs	ZPE	H _T	S
3-cct	700.9	748.7	131.0
3-ctt-syn	697.7	746.2	134.1
3-ctt-anti	698.5	746.5	130.2
4-ccct	938.0	1002.9	163.3
4-cctt-syn	936.8	1002.0	163.9
4-cctt-anti	936.5	1001.6	164.0
4-ctct-syn	939.2	1004.1	163.0
4-ctct-anti	939.5	1004.1	161.7
4-cttt-syn	936.8	1001.5	161.9
4-cttt-anti	935.8	1000.5	161.8
5-cccct	1174.2	1256.7	197.6
5-ccctt-syn	1172.5	1254.9	197.1
5-ccctt-anti	1172.4	1255.1	198.3
5-cctct-syn	1175.2	1257.5	195.9
5-cctct-anti	1175.0	1258.4	195.7
5-ccctt-syn	1172.7	1255.1	196.4
5-ccctt-anti	1172.5	1254.8	196.3
5-cttct-syn	1174.9	1257.0	195.3
5-cttct-anti	1175.2	1257.1	194.7
5-ctttt-syn	1173.8	1256.0	195.2
5-ctttt-anti	1173.5	1255.8	195.3
6-ccccct	1409.0	1509.1	237.8
6-cctcct-syn	1414.3	1514.0	229.1
6-cctcct-anti	1410.1	1510.2	231.8
6-cccctt	1409.2	1509.1	230.9
6-ctctcc-syn	1412.3	1511.5	227.4
6-ctctcc-anti	1410.0	1510.0	231.4
6-cccttt	1408.9	1508.8	231.1
6-cttctt-syn	1410.3	1510.2	231.4
6-cttctt-anti	1415.3	1515.3	230.5
6-cctttt-syn	1408.7	1508.8	231.4
6-cctttt-anti	1408.1	1508.3	231.7
6-cttttc-syn	1411.6	1511.5	230.0
6-cttttc-anti	1415.8	1515.4	228.4
6-ctttct	1409.4	1509.2	231.1
6-cttttt-syn	1410.3	1510.0	229.1
6-cttttt-anti	1413.6	1512.9	228.0

Table 3: SE (kJ mol⁻¹) and SE/n (kJ mol⁻¹) calculated based on homodesmotic Scheme 1 using at B3LYP/6-31+G(d,p) level. A: HN=NH; B: HN=N-Ph-N=NH; Ph: Phenyl ring.

Homodesmotic reaction scheme 1		
cis-trans-CPPDs	SE	SE/n
3-ctc + 3A → 3B	313.6	104.5
3-ctt-syn + 3A → 3B	384.9	128.3
3-ctt-anti + 3A → 3B	383.9	128.0
4-ccct + 4A → 4B	250.8	83.6
4-cctt-syn + 4A → 4B	299.2	99.7
4-cctt-anti + 4A → 4B	301.0	100.3
4-ctct-syn + 4A → 4B	205.4	68.5
4-ctct-anti + 4A → 4B	198.5	66.2
4-cttt-syn + 4A → 4B	289.7	96.6
4-cttt-anti + 4A → 4B	284.1	94.7
5-cccct + 5A → 5B	278.3	92.8
5-ccctt-syn + 5A → 5B	305.2	101.7
5-ccctt-anti + 5A → 5B	307.6	102.7
5-ectct-syn + 5A → 5B	201.1	67.0
5-ectct-anti + 5A → 5B	196.0	65.3
5-ecttt-syn + 5A → 5B	274.1	91.4
5-ecttt-anti + 5A → 5B	275.5	91.8
5-ettct-syn + 5A → 5B	214.6	71.5
5-ettct-anti + 5A → 5B	212.5	70.8
5-ctttt-syn + 5A → 5B	238.0	79.3
5-ctttt-anti + 5A → 5B	240.2	80.1
6-ccccct + 6A → 6B	326.3	108.8
6-ectcct-syn + 6A → 6B	231.5	77.2
6-ectcct-anti + 6A → 6B	246.0	82.0
6-cccctt + 6A → 6B	297.5	99.2
6-ctctcc-syn + 6A → 6B	222.9	74.3
6-ctctcc-anti + 6A → 6B	261.2	87.1
6-cccttt + 6A → 6B	302.1	100.7
6-cttcct-syn + 6A → 6B	212.6	70.9
6-cttcct-anti + 6A → 6B	186.3	62.1
6-cttttt-syn + 6A → 6B	254.4	84.8
6-cttttt-anti + 6A → 6B	273.7	91.2
6-ctttct + 6A → 6B	226.1	75.4
6-cttttc-syn + 6A → 6B	157.7	52.6
6-cttttc-anti + 6A → 6B	153.9	51.3
6-cttttt-syn + 6A → 6B	197.8	65.9
6-cttttt-anti + 6A → 6B	179.3	59.8

Table S4: $\Delta_f H_{298}^\circ$ (kJ mol⁻¹), $\Delta_f H_{298}^\circ / n$ (kJ mol⁻¹) and molar enthalpies of combustion (kJ mol⁻¹) for [n]CPPDs (n = 3 to 6).

[n]CPPDs	$\Delta_f H_{298}^\circ$	$\Delta_f H_{298}^\circ / n$	$\Delta_{comb} H_{298}^\circ$
3-ctc	1301.1	433.7	-31.5
3-ctt-syn	1373.2	457.7	-31.7
3-ctt-anti	1371.7	457.2	-31.7
4-ccct	1568.8	392.2	-31.1
4-cctt-syn	1617.4	404.4	-31.2
4-cctt-anti	1619.2	404.8	-31.2
4-ctct-syn	1523.4	380.9	-31.0
4-ctct-anti	1516.2	379.1	-31.0
4-cttt-syn	1607.5	401.9	-31.2
4-cttt-anti	1601.9	400.5	-31.2
5-cccct	1927.1	385.4	-31.0
5-ccctt-syn	1953.9	390.8	-31.1
5-ccctt-anti	1956.6	391.3	-31.1
5-cctct-syn	1844.6	368.9	-30.9
5-cctct-anti	1849.7	369.9	-30.9
5-ccttt-syn	1922.9	384.6	-31.0
5-ccttt-anti	1924.3	384.9	-31.0
5-ctctt-syn	1863.0	372.6	-30.9
5-ctctt-anti	1860.8	372.2	-30.9
5-ctttt-syn	1886.5	377.3	-31.0
5-ctttt-anti	1888.9	377.8	-31.0
6-ccccct	2306.1	384.3	-31.0
6-cctcct-syn	2207.0	367.8	-30.9
6-cctcct-anti	2206.5	367.7	-30.9
6-cccctt	2277.0	379.5	-31.0
6-ctctcc-syn	2202.0	367.0	-30.9
6-ctctcc-anti	2281.6	373.0	-30.9
6-cccctt	2281.6	380.3	-31.0
6-cttctt-syn	2192.1	365.4	-30.9
6-cttctt-anti	2166.0	361.0	-30.8
6-cctttt-syn	2234.1	372.3	-30.9
6-cctttt-anti	2253.5	375.6	-31.0
6-cttttc-syn	2137.2	356.2	-30.8
6-cttttc-anti	2133.2	355.5	-30.8
6-ctttct	2175.4	362.6	-30.8
6-cttttt-syn	2220.1	361.0	-30.9
6-cttttt-anti	2178.0	363.0	-30.9

Table S5: HOMO, LUMO and HOMO-LUMO (H-L) gap (eV) for cis-trans isomer of CPPDs

CPPDs	HOMO	LUMO	HOMO-LUMO
3-cct	-5.81	-3.05	2.76
3-ctt-syn	-5.49	-3.36	2.13
3-ctt-anti	-5.53	-3.36	2.13
4-ccct	-6.05	-3.28	2.77
4-cctt-syn	-5.82	-3.42	2.40
4-cctt-anti	-5.76	-3.49	2.27
4ctct-syn	-6.00	-3.08	2.92
4-ctct-anti	-5.95	-3.22	2.73
4-cttt-syn	-5.74	-3.54	2.21
4-cttt-anti	-5.95	-3.22	2.73
5cccct	-6.01	-3.42	2.59
5ccctt-syn	-5.90	-3.54	2.35
5-ccctt-anti	-6.01	-3.39	2.35
5cctct-syn	-5.99	-3.34	2.35
5cctct-anti	-5.99	-3.36	2.62
5-ccttt-syn	-5.85	-3.50	2.35
5-ccttt-anti	-5.90	-3.45	2.45
5-ctctt-syn	-5.87	-3.51	2.35
5ctctt-anti	-5.78	-3.58	2.20
5ctttt-syn	-5.69	-3.68	2.01
5-ctttt-anti	-5.70	-3.72	1.97
6-ccccct	-6.04	-3.42	2.62
6-cctcct-syn	-6.05	-3.38	2.67

6-cctcct-anti	-6.08	-3.42	2.66
6-cccctt	-5.96	-3.46	2.50
6-ctctcc-syn	-5.75	-3.04	2.71
6-ctctcc-anti	-6.08	-3.42	2.66
6-cccttt	-5.90	-3.58	2.31
6-cttcct-syn	-6.00	-3.40	2.61
6-cttcct-anti	-6.08	-3.42	2.66
6-cctttt-syn	-5.81	-3.65	2.16
6-cctttt-anti	-5.83	-3.64	2.19
6-cttttc-syn	-6.00	-3.44	2.56
6-ctttt-anti	-5.95	-3.53	2.43
6-ctttct	-5.85	-3.62	2.23
6-cttttt-syn	-5.88	-3.64	2.24
6-cttttt-anti	-5.51	-3.36	2.14

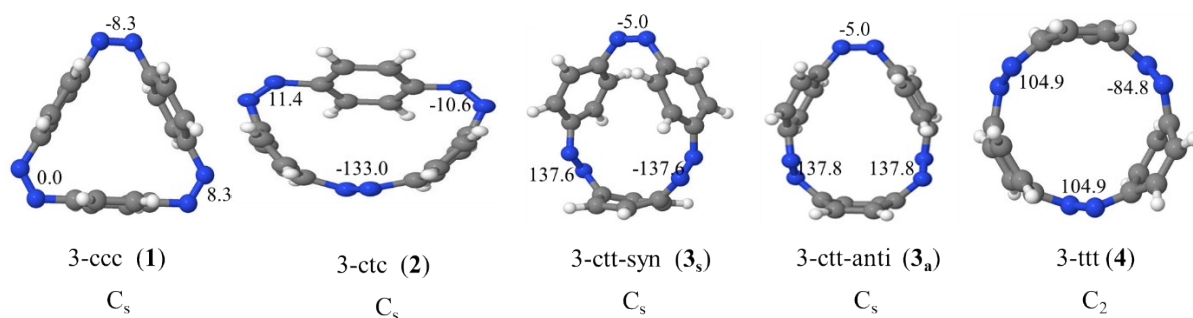


Figure S1 (a): Optimized structure of all-cis, cis-trans and all-trans isomer of [3]CPPD obtained at B3LYP/6-31+G(d,p) level. Bond angles $\angle C-N=N-C-$ ($sp^2-sp^2-sp^2-sp^2$) are shown in the structure. The structure of 3-ccc (1) and 3-ttt (4) was taken from our previous work (Ali and Alam, 2017) .

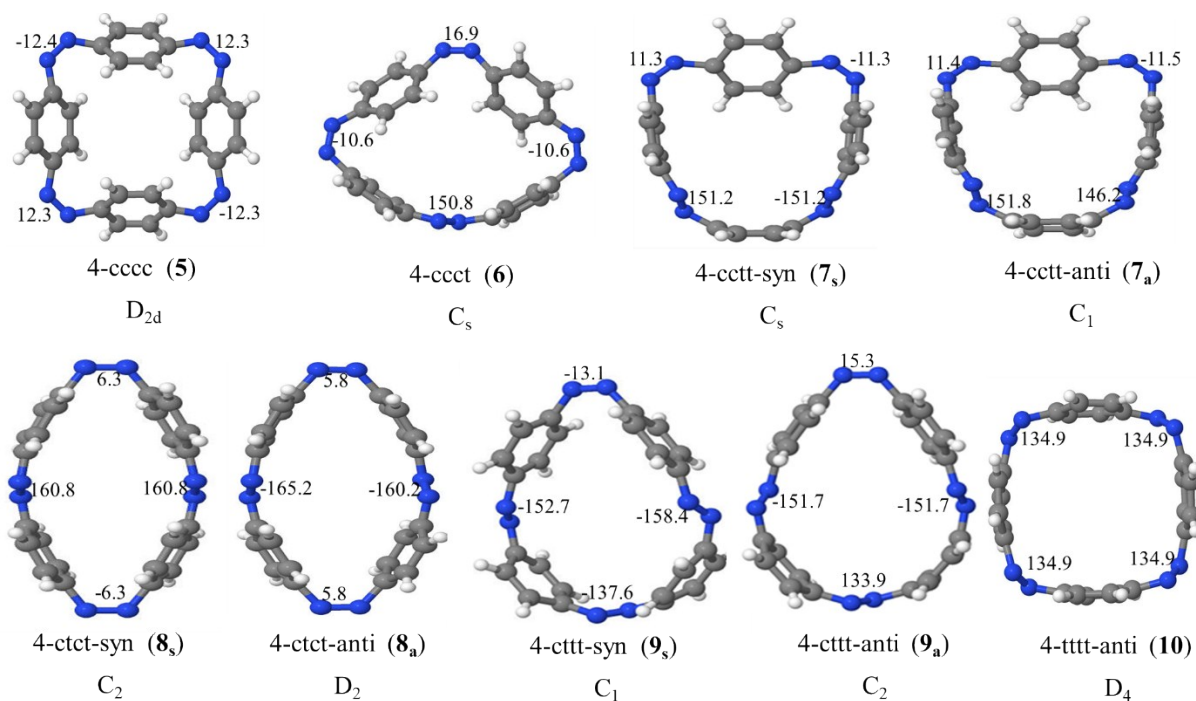


Figure S1 (b): Optimized structure of all-cis, cis-trans, and all-trans isomer of [4]CPPD obtained at B3LYP/6-31+G(d,p) level. The $\angle C-N=N-C-$ ($sp^2-sp^2-sp^2-sp^2$) angle is shown on the structure. The 4-ctct-anti is the most stable structure.

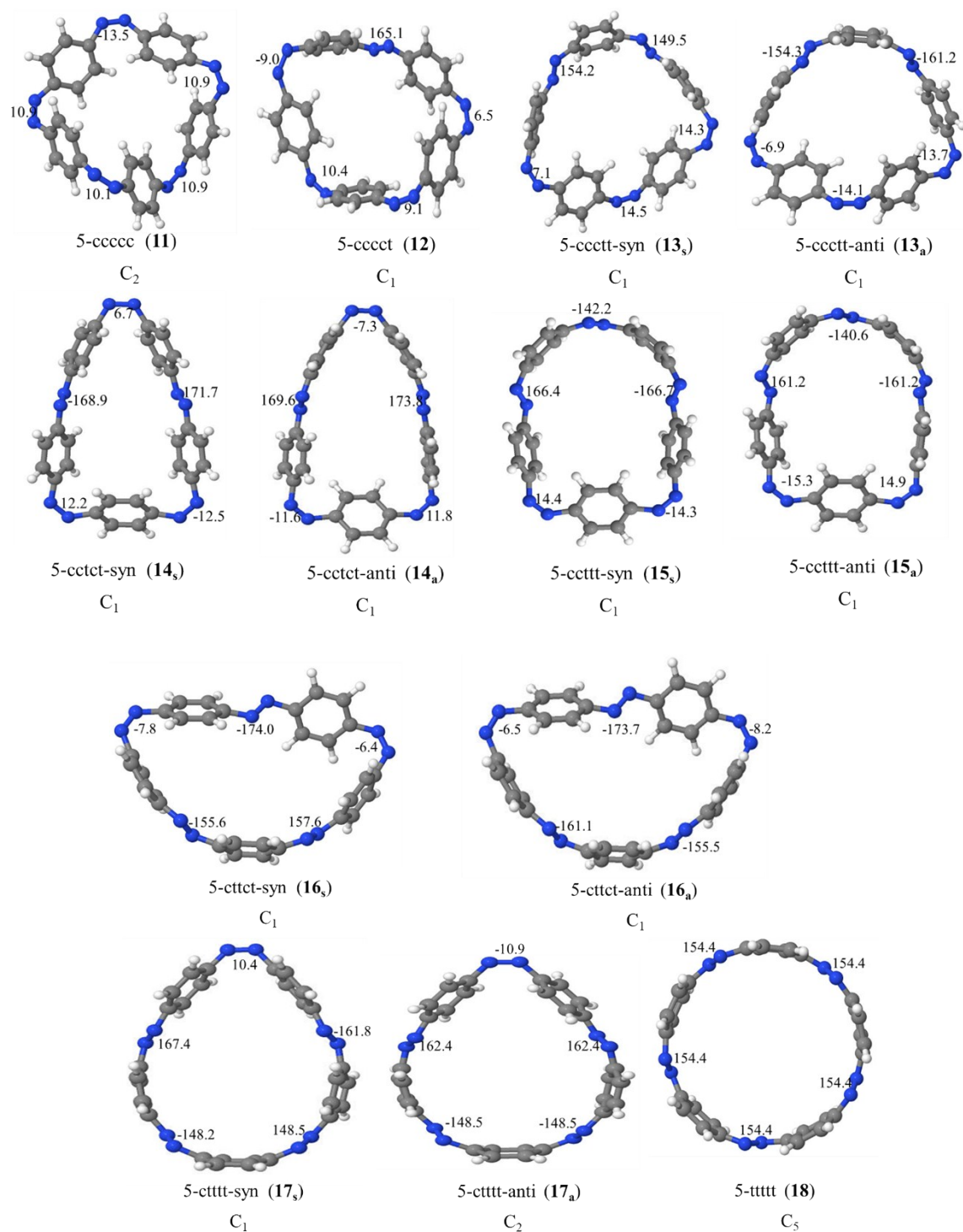
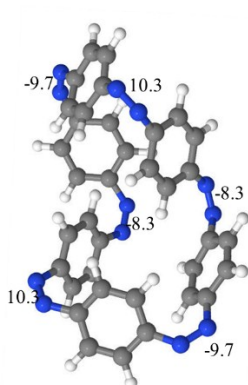
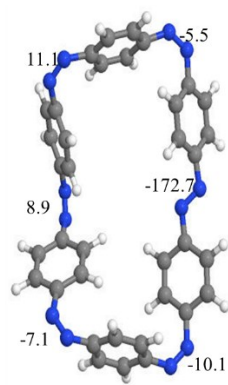


Figure S1(c): Optimized structure of all-cis, cis-trans and all-trans isomer of [5]CPPD obtained at B3LYP/6-31+G(d,p) level. The $\angle\text{C-N=N-C}$ (sp^2 - sp^2 - sp^2 - sp^2) angle is shown on the structure. The 5-cctct-anti is a most stable structure.



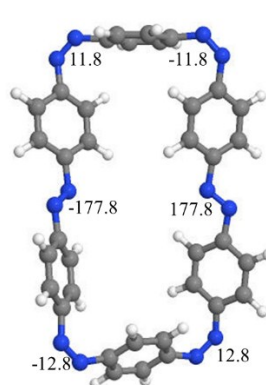
6-cccccc (19)

C_2



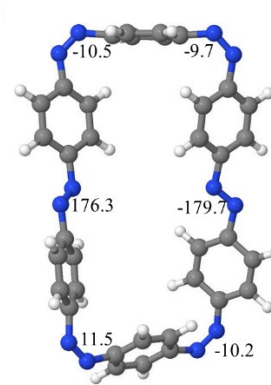
6-ccccct (20)

C_1



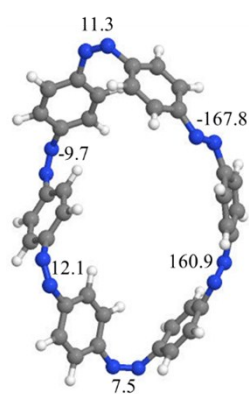
6-cctcct-syn (21_s)

C_s



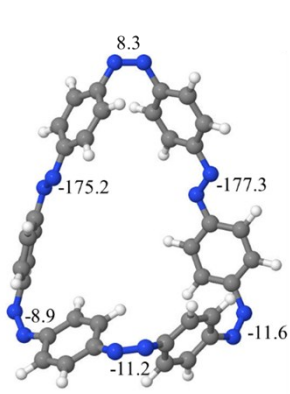
6-cctcct-anti (21_a)

C_1



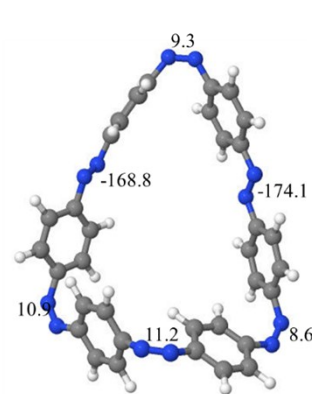
6-cccctt (22)

C_1



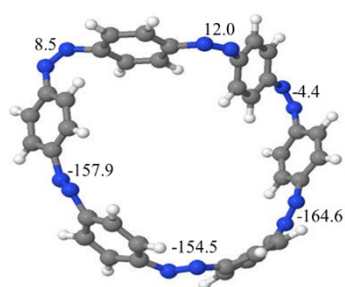
6-ctctcc-syn (23_s)

C_1



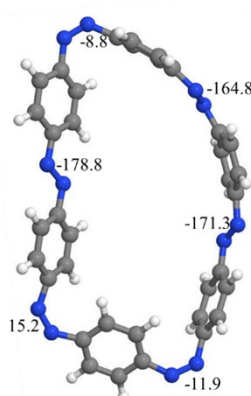
6-ctctcc-anti (23_a)

C_1



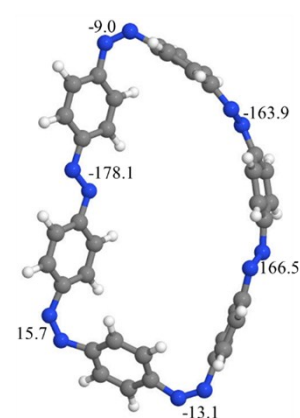
6-cccttt (24)

C_1



6-cttctc-syn (25_s)

C_1



6-cttctc-anti (25_a)

C_1

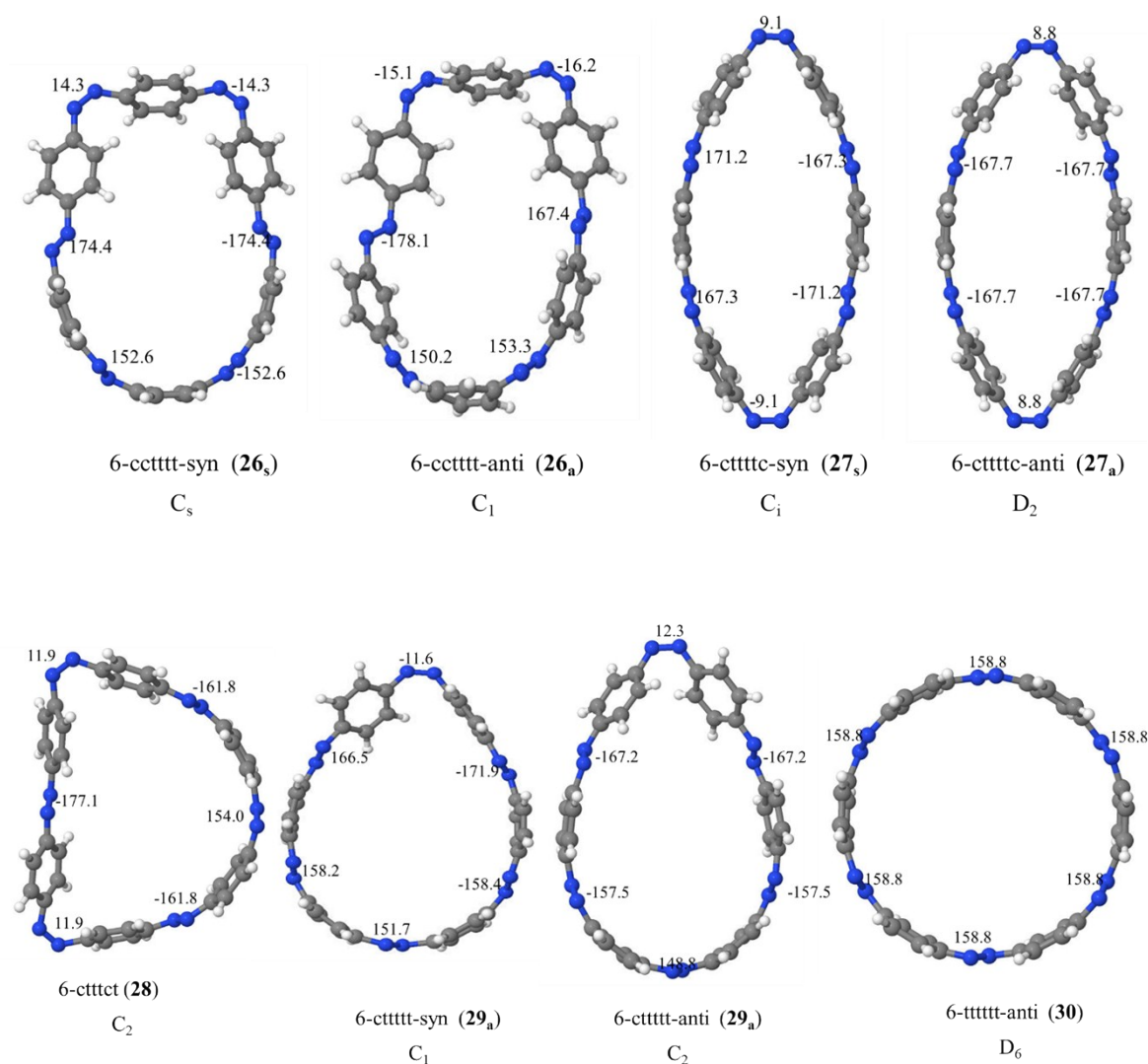


Figure S1 (d): Optimized structure of all-cis, cis-trans, and all-trans isomer of [6]CPPDs obtained at B3LYP/6-31+G(d,p) level. The $\angle C-N=N-C$ ($sp^2-sp^2-sp^2-sp^2$) angle is shown on the structure. The 6-ccttttc-anti is the most stable structure.

Full Reference of Gaussian 09

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