

Supporting Informations

Intramolecular boron-locking strategy induced the remarkable first hyperpolarizability: role of torsion angles between donor and acceptor units

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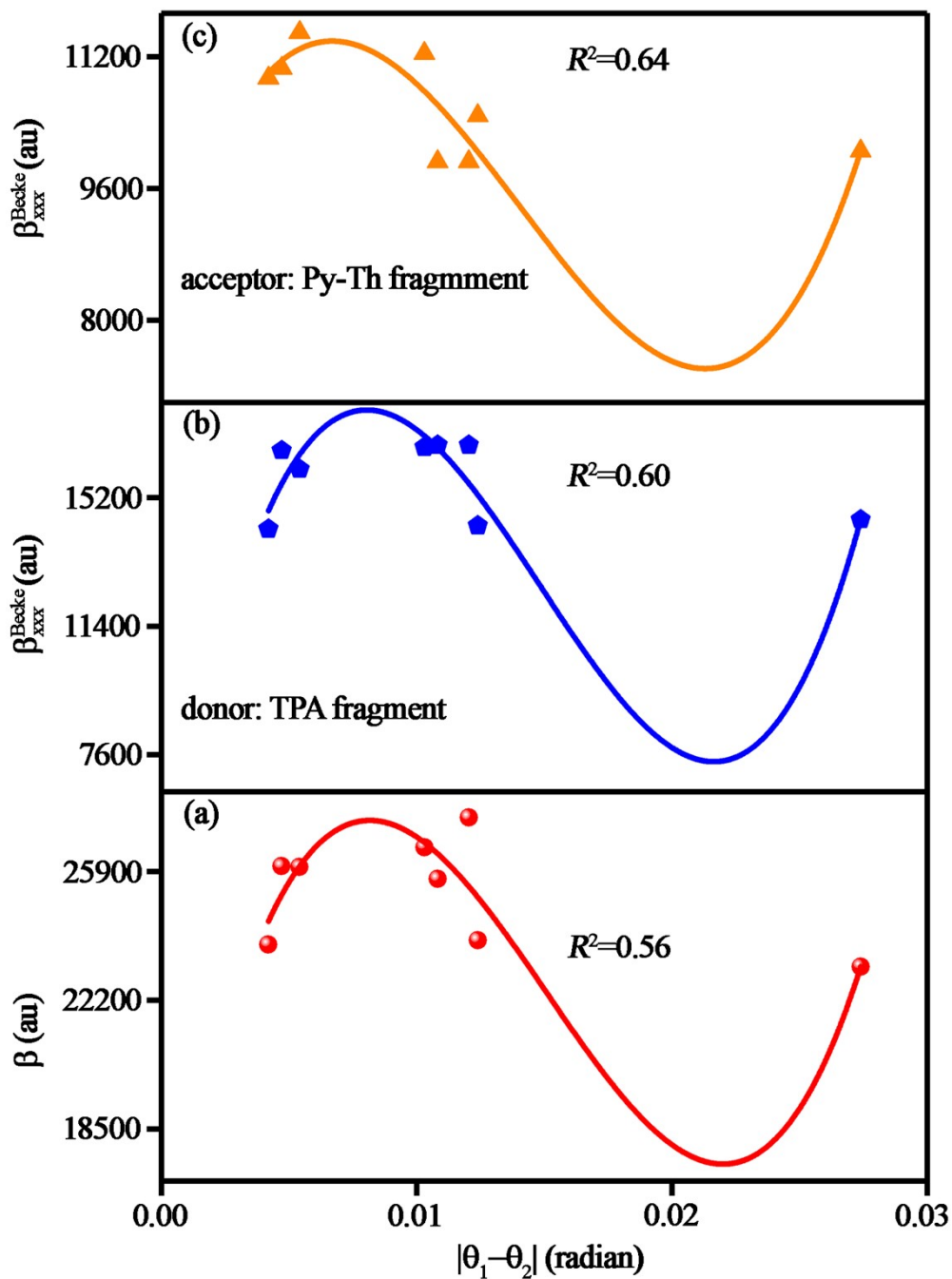


Figure S1: Correlations between $|\theta_1 - \theta_2|$ and $\beta/\beta_{xxx}^{\text{Becke}}$, where coefficient of determination, (a) $R^2=0.78$ for correlation between $|\theta_1 - \theta_2|$ and β in Py-Th-TPA and B-R-locking-Py-Th-TPA, (b) $R^2=0.77$ for correlation between $|\theta_1 - \theta_2|$ and $\beta_{xxx}^{\text{Becke}}$ in TPA fragment (donor part) of Py-Th-TPA and B-R-locking-Py-Th-TPA, and (c) $R^2=0.90$ for correlation between $|\theta_1 - \theta_2|$ and $\beta_{xxx}^{\text{Becke}}$ in Py-Th fragment (acceptor part) of Py-Th-TPA and B-R-locking-Py-Th-TPA, where R=TXO, DPzS, DPyS, DTC, TXO2-CF₃, DSCZ, and TXO2.

Py-Th-TPA

N	5.03709700	-0.80631500	0.22653400
C	0.80071900	-0.93331000	0.24404300
C	3.63428800	-0.84722800	0.23093600
C	2.88521300	0.17039800	0.84682700
H	3.39933300	1.00457400	1.32801400
C	5.37937100	-0.49624400	2.63341700
H	4.53662100	-1.16201300	2.83550200
C	5.74450200	-0.22885000	1.31137800
C	1.55256800	-1.94346400	-0.37434000
H	1.05118800	-2.77625600	-0.87330700
C	2.94105600	-1.90599600	-0.38057300
H	3.49965300	-2.70844900	-0.86597900
C	1.49748400	0.12156300	0.85225100
H	0.94042300	0.92042900	1.34899400
C	5.77127400	-1.33745500	-0.86406700
C	5.38056000	-1.09322200	-2.18323400
H	4.49364200	-0.48553600	-2.37897600
C	6.07896300	0.08119900	3.69332000
H	5.75517100	-0.15563100	4.70811400
C	7.26191900	-2.38892200	-3.04222900
C	6.91878600	-2.11012600	-0.63931600
H	7.23855500	-2.31190800	0.38582400
C	7.64693100	-2.61431000	-1.71043700
H	8.53676900	-3.21240600	-1.49432100
C	6.11026900	-1.62052400	-3.24894800
H	5.76471600	-1.40440100	-4.26119600
C	7.17540100	0.92456700	3.47788300
C	7.53740300	1.17055300	2.14332100
H	8.38529600	1.82444900	1.92038200
C	6.83765800	0.61656900	1.07779500
H	7.13795000	0.83571900	0.05030300
C	-0.68174200	-0.93430100	0.22916200
C	-1.37305200	0.22275000	-0.04933200
C	-1.44807000	-2.12546600	0.51649300
C	-2.79452800	0.26338500	-0.07216200
H	-0.84219200	1.14668900	-0.28776500
C	-2.82422800	-2.12256400	0.49658000
C	-3.53526900	-0.92910300	0.19717200
H	-3.39782500	-3.02266200	0.72413100
C	-4.74462200	1.40482900	-0.37426400
C	-5.47115200	2.62282500	-0.67483200
C	-5.49285700	0.19508200	-0.09729900
C	-6.86268700	2.62520100	-0.69475000

C	-6.94192400	0.24297400	-0.12799200
C	-7.59919200	1.43397500	-0.42074500
C	-0.79119100	-3.35452100	0.88926300
N	-0.29655500	-4.35163900	1.19610900
N	-3.42561800	1.41653900	-0.35700300
N	-4.87879200	-0.93856200	0.18046200
C	-9.16044400	-0.45625000	0.00947100
C	-7.84590900	-0.83015800	0.11644100
C	-5.87846300	4.85350900	-1.21226400
C	-4.92097100	3.90248000	-0.97242200
C	8.09257900	-2.97723400	-4.18699800
C	7.97039200	1.57155100	4.61646100
C	8.10651300	-4.51042900	-4.06949700
H	7.08271800	-4.91811000	-4.13058700
H	8.70284000	-4.95161800	-4.88774700
H	8.54740300	-4.84264800	-3.11452700
C	9.53277600	-2.44635800	-4.09704200
H	10.14559800	-2.86237400	-4.91624400
H	9.55149900	-1.34570800	-4.17730700
H	10.01177800	-2.72558800	-3.14360900
C	7.52470300	-2.60305500	-5.55929500
H	6.49931200	-2.98697900	-5.69512200
H	7.50916500	-1.51012800	-5.71001200
H	8.15386800	-3.04196200	-6.35238400
C	9.44261600	1.13798300	4.52205700
H	9.89834000	1.44726300	3.56642200
H	10.02908400	1.59561900	5.33835400
H	9.53534100	0.04125600	4.60403600
C	7.43450300	1.16630300	5.99275500
H	6.38571900	1.47983200	6.13089800
H	7.49390900	0.07564000	6.14860000
H	8.03520400	1.65091200	6.78129500
C	7.88170400	3.10180500	4.49264000
H	6.83344700	3.44093800	4.55849600
H	8.45210500	3.58534700	5.30542300
H	8.29411000	3.45814000	3.53364200
H	-7.50774900	-1.83846400	0.35629800
H	-3.84642600	4.08455900	-0.99854300
S	-7.48917100	4.18426200	-1.07584800
S	-9.31110900	1.23816000	-0.39527200
C	-5.68722400	6.27144200	-1.54705000
C	-6.76619500	7.14742900	-1.72410200
C	-4.40115800	6.80845800	-1.70359700
C	-6.51501400	8.48128600	-2.04038100

H	-7.80029400	6.80882000	-1.61836000
C	-4.26464200	8.15717100	-2.01942100
H	-3.50977700	6.19013700	-1.58489100
H	-7.35297000	9.17286400	-2.18067500
H	-3.26446200	8.58642200	-2.14400800
C	-10.35829300	-1.28720800	0.19307600
C	-11.64715200	-0.80507800	-0.07013500
C	-10.25454600	-2.61099800	0.64402100
C	-12.74090300	-1.64625300	0.12557800
H	-11.81306600	0.21386200	-0.42999900
C	-11.41417700	-3.36455600	0.80261000
H	-9.28546400	-3.05619500	0.87639800
H	-13.75234000	-1.27743900	-0.07728600
H	-11.34462400	-4.39958700	1.15471200
N	-5.29344000	8.98696200	-2.18712600
N	-12.63831300	-2.90204300	0.55228900
B-TXO-locking-Py-Th-TPA			
N	4.79017300	-0.85606700	-0.33109600
C	0.64642800	-1.68823600	-0.46470100
C	3.42693700	-1.14877600	-0.37259300
C	2.48081900	-0.09963800	-0.23014400
H	2.82309200	0.93086100	-0.11262300
C	4.93079200	0.73552400	1.52749100
H	4.46675400	-0.00857800	2.18051900
C	5.19776100	0.40649800	0.19882300
C	1.56000400	-2.72691200	-0.60165100
H	1.24597400	-3.76241800	-0.74683600
C	2.93588400	-2.45398200	-0.54122500
H	3.63879400	-3.28380100	-0.63347100
C	1.13007700	-0.37447700	-0.25394500
C	5.77111100	-1.66241200	-0.96115700
C	5.54658300	-2.26436800	-2.20249300
H	4.58663300	-2.12942500	-2.70633300
C	5.21114300	2.01532900	2.00835400
H	4.95943600	2.24283600	3.04478200
C	7.79547400	-3.21449800	-2.21282600
C	7.02281400	-1.83131900	-0.35373900
H	7.21699800	-1.36042200	0.61291500
C	8.00965900	-2.58749200	-0.97461800
H	8.97259600	-2.69634000	-0.46772300
C	6.54108500	-3.03375200	-2.80696200
H	6.31879300	-3.48568100	-3.77493100
C	5.78028400	2.99490800	1.18423200
C	6.08255300	2.62914800	-0.13802600

H	6.52485100	3.36204300	-0.81808600
C	5.79687000	1.35970900	-0.62994500
H	6.01174900	1.10742000	-1.67156200
C	-0.84230600	-1.65381000	-0.50439800
C	-1.32492700	-0.35805700	-0.30504500
C	-1.76349200	-2.72697200	-0.71364100
C	-2.71819100	-0.10103800	-0.26780700
C	-3.12556700	-2.48599700	-0.71529000
C	-3.63635800	-1.17996700	-0.49085900
H	-3.84031100	-3.29427600	-0.88019100
C	-4.47689700	1.32490200	0.02486800
C	-5.00723700	2.63540900	0.34513700
C	-5.40204500	0.23751800	-0.23858800
C	-6.38242000	2.84763400	0.36959500
C	-6.82671600	0.50972200	-0.22026300
C	-7.29232400	1.78772800	0.07286200
C	-1.30375000	-4.07490400	-0.93085100
N	-0.93963800	-5.15661400	-1.10580100
N	-3.17320600	1.14041300	-0.00906400
N	-4.96710600	-0.98167300	-0.48481400
C	-9.12550000	0.16690700	-0.37997600
C	-7.88507300	-0.40899800	-0.47475600
C	-5.07222800	4.87909500	0.97074900
C	-4.26808200	3.80607300	0.68796400
C	8.91172500	-4.04650200	-2.85193300
C	6.02218200	4.43379300	1.65217800
C	9.29208900	-5.19874100	-1.90728500
H	8.42550400	-5.85620000	-1.72046300
H	10.09789900	-5.80850500	-2.35293500
H	9.65165400	-4.82581400	-0.93342400
C	10.14172500	-3.15415100	-3.08740300
H	10.95592800	-3.73973200	-3.54989900
H	9.89526400	-2.31498600	-3.76060100
H	10.52563400	-2.73113100	-2.14388000
C	8.48383600	-4.64385600	-4.19573300
H	7.61609600	-5.31630600	-4.08555500
H	8.22471400	-3.85925000	-4.92687900
H	9.31381500	-5.23493100	-4.61907700
C	7.47075100	4.85282600	1.35751300
H	7.70321000	4.81410300	0.28050300
H	7.63995700	5.88988200	1.69662000
H	8.18535400	4.19747100	1.88518300
C	5.77005400	4.59663200	3.15434400
H	4.72642600	4.35840100	3.41854600

H	6.43508400	3.94665500	3.74958200
H	5.96474700	5.64221300	3.44982300
C	5.05516000	5.35702600	0.89068500
H	4.00590500	5.05475700	1.04999300
H	5.16225900	6.40272000	1.23086300
H	5.23813600	5.33309800	-0.19713000
H	-7.70844200	-1.45336100	-0.73353000
H	-3.17812700	3.82449400	0.74440200
S	-6.76506800	4.46994400	0.80415600
S	-9.01380500	1.86072600	0.03622700
C	-4.67663100	6.23237300	1.38709200
C	-5.59270100	7.12150500	1.96573600
C	-3.35973300	6.68665200	1.22964200
C	-5.15909200	8.38800300	2.35148800
H	-6.63495800	6.83669200	2.13255900
C	-3.03356100	7.97389000	1.65209200
H	-2.58487700	6.06648600	0.77262400
H	-5.86762700	9.08877400	2.80694600
H	-2.00746500	8.33017000	1.51896300
C	-10.43651600	-0.46477100	-0.58241400
C	-11.60863400	0.28631000	-0.74036500
C	-10.56259900	-1.86051600	-0.62944400
C	-12.81918300	-0.37712300	-0.93225900
H	-11.59160000	1.37945800	-0.72755800
C	-11.82180000	-2.41875100	-0.83174300
H	-9.69615800	-2.51142800	-0.49843200
H	-13.74138700	0.20094300	-1.05697500
H	-11.93315000	-3.50791300	-0.87016200
N	-3.90769600	8.81526400	2.20455000
N	-12.93465900	-1.70159100	-0.98018400
C	0.03113300	2.12241500	0.16082000
C	-0.61059500	3.08286100	-0.63958400
C	0.88014600	2.56701400	1.18445300
C	-0.35647400	4.44272300	-0.47167100
H	-1.30443100	2.76276800	-1.42094300
C	1.10226600	3.92735500	1.41453600
C	0.49859200	4.84736000	0.55003300
H	-0.81775200	5.18837700	-1.12486800
C	1.91850100	4.31764300	2.60979900
C	1.95800200	5.75563500	3.03691800
C	1.46721300	6.81302200	2.26042200
C	2.46073200	6.04848100	4.30902200
C	1.47215100	8.12691700	2.71908900
C	2.47778500	7.35903800	4.77907200

H	2.82609400	5.22361300	4.92403000
H	1.07825400	8.92804000	2.08851200
C	1.98102000	8.39678000	3.98857600
H	2.87307500	7.57252200	5.77452500
H	1.98451700	9.42322800	4.36177800
S	0.96076900	6.56130500	0.57597400
O	-0.22184800	7.37377600	0.30454400
O	2.12986500	6.72437100	-0.27861200
H	1.38189200	1.85483600	1.84549000
O	2.48444200	3.47253200	3.26579200
B	-0.09316100	0.59108800	-0.11058500

B-DPzS-locking-Py-Th-TPA

N	5.04880200	-0.78505500	-0.28181600
C	0.91834600	-1.55821500	-0.73975900
C	3.69184200	-1.06099500	-0.46526900
C	2.75637800	0.00519500	-0.40204600
H	3.11320200	1.02813800	-0.26210400
C	4.96580700	0.59678600	1.73333600
H	4.45112700	-0.21935600	2.24750900
C	5.38857100	0.41240400	0.41712500
C	1.82343300	-2.60785700	-0.83124100
H	1.50334000	-3.63880300	-0.99380500
C	3.19795900	-2.35532900	-0.68430400
H	3.89395100	-3.19504900	-0.73066800
C	1.40599100	-0.24730200	-0.51488100
C	6.08459600	-1.56222300	-0.85128500
C	5.95918300	-2.14647300	-2.11551900
H	5.03759100	-2.01475100	-2.68713800
C	5.15678800	1.82302000	2.37125800
H	4.79421600	1.93437900	3.39430200
C	8.21532700	-3.07089300	-1.97773900
C	7.29193700	-1.72820100	-0.15744200
H	7.41200400	-1.27464100	0.82916200
C	8.33039000	-2.46212600	-0.71774600
H	9.25530100	-2.56785800	-0.14377600
C	7.00474800	-2.89392900	-2.65779000
H	6.85773600	-3.33163900	-3.64648400
C	5.78560500	2.89266200	1.72149700
C	6.25580000	2.66636400	0.41658700
H	6.75979600	3.47076000	-0.12580200
C	6.06221200	1.45110600	-0.23224500
H	6.40310600	1.31021800	-1.26120800
C	-0.57018100	-1.51562100	-0.80701500
C	-1.05084300	-0.22049600	-0.59979300

C	-1.48938200	-2.58648000	-1.03046700
C	-2.44509400	0.03905300	-0.55358600
C	-2.85092900	-2.34533200	-1.02068900
C	-3.36039400	-1.04298200	-0.77354700
H	-3.56731400	-3.15162100	-1.18807600
C	-4.20729600	1.45367400	-0.22762100
C	-4.74529100	2.76396000	0.08803700
C	-5.12976300	0.35675200	-0.46355900
C	-6.12217300	2.95094800	0.17782700
C	-6.55619600	0.60572100	-0.38315400
C	-7.02823000	1.87445900	-0.06610400
C	-1.03008100	-3.93114000	-1.26745000
N	-0.66573500	-5.01032600	-1.45677200
N	-2.90282200	1.27564600	-0.27831900
N	-4.69174500	-0.85664900	-0.72970200
C	-8.85359500	0.22017100	-0.42150600
C	-7.60945700	-0.33237700	-0.58253400
C	-4.83099300	5.01966900	0.65905200
C	-4.01461900	3.96114700	0.35971100
C	9.38502000	-3.87972000	-2.54690900
C	5.93770600	4.27826100	2.35679600
C	9.71283200	-5.04087700	-1.59363700
H	8.84353800	-5.71083400	-1.47698500
H	10.55528300	-5.63502200	-1.98984800
H	9.99900900	-4.67784200	-0.59213500
C	10.61672400	-2.96904500	-2.68234400
H	11.46933800	-3.53774800	-3.09385800
H	10.40739700	-2.12331100	-3.35987800
H	10.92743100	-2.55502700	-1.70828200
C	9.06111900	-4.46275000	-3.92558500
H	8.19557300	-5.14586200	-3.88644700
H	8.84558300	-3.67092900	-4.66310400
H	9.92594000	-5.03896100	-4.29636500
C	7.41902600	4.68883400	2.35913400
H	7.83283600	4.74032300	1.33817300
H	7.53505100	5.68681300	2.81692700
H	8.02662400	3.97160400	2.93789800
C	5.42449300	4.30694300	3.79952000
H	4.34802200	4.07147100	3.85308300
H	5.97129400	3.59620700	4.44291300
H	5.56392700	5.31736400	4.21981100
C	5.12261300	5.29142300	1.53359400
H	4.05061000	5.03004500	1.52387900
H	5.21827200	6.30254600	1.96704900

H	5.47130100	5.33979500	0.48786800
H	-7.42559800	-1.37410900	-0.84642300
H	-2.92383400	4.01452500	0.36630400
S	-6.51853000	4.57397900	0.60184100
S	-8.75030200	1.91704900	-0.01291000
C	-4.43960100	6.38815000	1.03096000
C	-5.12033100	7.10073600	2.02835200
C	-3.33581300	7.00602700	0.43446200
C	-4.65018200	8.35980500	2.39517100
H	-5.98684800	6.67080100	2.53798900
C	-2.95127200	8.27165200	0.87841400
H	-2.76476500	6.51168800	-0.35430700
H	-5.16026800	8.92428100	3.18373900
H	-2.07439400	8.75124100	0.43052300
C	-10.16208800	-0.43599900	-0.54946100
C	-11.35968000	0.29034600	-0.58053000
C	-10.26133300	-1.83132600	-0.64841600
C	-12.56696400	-0.39483000	-0.70473100
H	-11.36662500	1.38185700	-0.51873600
C	-11.52007700	-2.41248200	-0.77356100
H	-9.37361500	-2.46574700	-0.62007500
H	-13.50843500	0.16477700	-0.72995700
H	-11.60973500	-3.50152400	-0.85171500
N	-3.58181300	8.93676000	1.84500100
N	-12.65701400	-1.71857300	-0.80109000
C	0.27649900	2.26710700	-0.16215300
C	1.03033600	2.79471800	0.90725200
C	-0.22538000	4.39384100	-0.83264400
C	0.48914600	4.87342600	0.26376300
H	-0.70725600	5.07558100	-1.53968600
C	0.11350600	7.77118100	3.05785900
C	-0.26396300	6.77336600	2.16233500
C	-1.60918500	7.13832900	4.39430300
C	-1.95234800	6.11748800	3.49649800
H	-2.18546500	7.28739200	5.31275400
H	-2.78918800	5.44093100	3.69442200
S	0.57611400	6.63966600	0.57547600
O	-0.24806500	7.27993700	-0.44640400
O	1.95324100	7.06003900	0.77598100
H	1.55999600	2.13320500	1.60075200
H	0.97594400	8.41619900	2.86436700
N	-0.33913500	3.08508500	-1.02835800
N	-0.58044900	7.94982100	4.17910600
N	1.11716400	4.10011300	1.12813200

N	-1.27324300	5.94651600	2.36881600
B	0.18426600	0.71992100	-0.41350500
B-TTR-locking-Py-Th-TPA			
N	4.82240500	-0.64762100	-0.47440200
C	0.68140500	-1.46179300	-0.62275100
C	3.45487300	-0.91656300	-0.52676700
C	2.50956900	0.13978500	-0.44684300
H	2.86307300	1.17145300	-0.37570100
C	4.80660300	0.97698100	1.37521600
H	3.99461500	0.42699900	1.85853100
C	5.32645600	0.52059200	0.16016300
C	1.59501000	-2.50281700	-0.72646300
H	1.28348500	-3.54280100	-0.83785700
C	2.96817700	-2.22599300	-0.66449000
H	3.67418800	-3.05589900	-0.72482000
C	1.15649100	-0.13613500	-0.46550700
C	5.75844800	-1.54843300	-1.05490300
C	5.60531200	-1.99316200	-2.36909900
H	4.74997500	-1.65073800	-2.95715900
C	5.31191600	2.13013400	1.97766200
H	4.85366600	2.46257600	2.91016200
C	7.64811600	-3.31731300	-2.21223200
C	6.86559600	-1.98696200	-0.31937600
H	6.99761100	-1.64168400	0.70896800
C	7.79159100	-2.84879400	-0.89587200
H	8.64561300	-3.17040900	-0.29332000
C	6.53247200	-2.87116500	-2.93109900
H	6.37292700	-3.19481300	-3.96077500
C	6.37739300	2.84329200	1.41525600
C	6.89712000	2.36244700	0.20297000
H	7.72476200	2.88868000	-0.28077400
C	6.38133600	1.23399900	-0.42360900
H	6.80077800	0.89445900	-1.37357100
C	-0.80523800	-1.45094000	-0.63608900
C	-1.31018400	-0.15854500	-0.46445800
C	-1.70093000	-2.55497000	-0.78766700
C	-2.71120300	0.06341300	-0.38711600
C	-3.06626400	-2.34952100	-0.74820700
C	-3.60179600	-1.05145100	-0.54035200
H	-3.76658200	-3.17861900	-0.86415900
C	-4.51161400	1.43780400	-0.06946300
C	-5.08464800	2.73824000	0.22454300
C	-5.40563600	0.30885200	-0.25462900
C	-6.46709700	2.88993500	0.30423000

C	-6.83809600	0.51908400	-0.17802200
C	-7.34483800	1.78477800	0.09241100
C	-1.22010800	-3.89839900	-0.98623700
N	-0.84919700	-4.97988200	-1.14738400
N	-3.20289000	1.29660000	-0.15213600
N	-4.93599000	-0.90012400	-0.48300300
C	-9.12378500	0.07100800	-0.20643500
C	-7.86487300	-0.45378700	-0.34533500
C	-5.23468900	5.00369000	0.75718900
C	-4.39071200	3.95858000	0.48369000
C	8.69128700	-4.27393200	-2.79833000
C	6.98929200	4.08613600	2.06825100
C	8.74248100	-5.55300000	-1.94627500
H	7.76229900	-6.06027600	-1.93998400
H	9.49110800	-6.25454600	-2.35495600
H	9.01953200	-5.33607400	-0.90089500
C	10.07067400	-3.59452000	-2.78195100
H	10.83533800	-4.27295800	-3.19982400
H	10.06128200	-2.67150200	-3.38702900
H	10.38169400	-3.32634100	-1.75832000
C	8.36293600	-4.66691900	-4.24168400
H	7.39185100	-5.18576400	-4.31262600
H	8.33705800	-3.78792100	-4.90798500
H	9.13771900	-5.35356900	-4.62329300
C	8.47085000	3.81382100	2.37767200
H	9.04472600	3.58992000	1.46227900
H	8.92931400	4.69861600	2.85417700
H	8.57965700	2.95698700	3.06534700
C	6.27831600	4.45038600	3.37506100
H	5.21140400	4.66297900	3.20060000
H	6.35903000	3.64205900	4.12235300
H	6.74093300	5.35471600	3.80692500
C	6.87654900	5.27935900	1.10493200
H	5.81914200	5.49100300	0.87688200
H	7.32274700	6.17986700	1.56377900
H	7.40824100	5.08863700	0.15709600
H	-7.65221800	-1.49901200	-0.57103300
H	-3.30175900	4.03480300	0.48710500
S	-6.90980400	4.50806200	0.68832100
S	-9.06755000	1.78368200	0.14071800
C	-4.90176100	6.39932400	1.07736300
C	-5.83342600	7.25654100	1.67942800
C	-3.63973200	6.93382300	0.78487600
C	-5.47054400	8.57438200	1.94824000

H	-6.83321800	6.90865800	1.95236600
C	-3.38666600	8.27029100	1.08781900
H	-2.85505900	6.33915300	0.31164600
H	-6.19090000	9.25013400	2.42239800
H	-2.41049800	8.69405400	0.83272300
C	-10.41408600	-0.62374300	-0.31436000
C	-11.63154600	0.06824600	-0.35408600
C	-10.47460900	-2.02287400	-0.38491200
C	-12.81970100	-0.65258200	-0.45919700
H	-11.66901700	1.16008500	-0.31294600
C	-11.71712900	-2.64140300	-0.49234400
H	-9.56937200	-2.63143400	-0.34924300
H	-13.77653100	-0.12008200	-0.49125400
H	-11.77650800	-3.73385700	-0.54838700
N	-4.27524600	9.08268200	1.65965900
N	-12.87302700	-1.97999700	-0.52869100
C	0.01587100	2.35535200	-0.10778500
C	-0.73817400	3.28293300	-0.84147800
C	0.95424700	2.84058400	0.82213600
C	-0.55171300	4.65857900	-0.68506800
H	-1.49019500	2.92732500	-1.54951500
C	1.13388500	4.20563900	0.98698300
C	0.39244200	5.11393700	0.22728100
H	-1.13818800	5.37941300	-1.26077600
C	1.54675900	6.15510100	2.91792700
C	0.81099500	7.06806000	2.15471300
C	1.66021800	6.31345600	4.29261600
C	0.18861600	8.15119500	2.76114600
C	1.05423300	7.41660100	4.90040900
H	2.20909100	5.57189300	4.87778100
H	-0.40341400	8.84522500	2.16034800
C	0.32533900	8.32840600	4.14084900
H	1.14414700	7.55197600	5.98031100
H	-0.15811600	9.18099000	4.62235800
S	0.65725800	6.87858500	0.37915900
O	-0.57151700	7.54453500	-0.03874200
O	1.91711000	7.22596800	-0.24794800
H	1.54234000	2.15373600	1.43802100
O	2.54613400	3.73012200	3.16465700
O	3.52124800	5.25256800	1.40866900
S	2.37224500	4.76305100	2.15085800
B	-0.08458300	0.81311200	-0.33508200
B-DPyS-locking-Py-Th-TPA			
N	5.17178900	-0.73255500	-0.30900800

C	1.02338700	-1.46788700	-0.60053800
C	3.80067200	-0.98507800	-0.42239700
C	2.87689100	0.08320600	-0.29131400
H	3.24612700	1.09969900	-0.13195300
C	5.14400900	0.50205400	1.80323100
H	4.46965000	-0.25118500	2.21935200
C	5.60863100	0.35639800	0.49450000
C	1.91827700	-2.51971700	-0.74862200
H	1.58828100	-3.54595900	-0.91912700
C	3.29684800	-2.27214700	-0.65436000
H	3.99207500	-3.10794600	-0.75566500
C	1.52092800	-0.16112000	-0.37090600
C	6.13600800	-1.49544100	-1.01326900
C	5.91929300	-1.90096500	-2.33323100
H	4.98579700	-1.63572600	-2.83547300
C	5.51992900	1.60526200	2.56990800
H	5.12757100	1.68394500	3.58503700
C	8.10577800	-2.98307300	-2.42077500
C	7.35000100	-1.83524300	-0.40060600
H	7.53787600	-1.52636900	0.63043800
C	8.31104800	-2.55720100	-1.09851400
H	9.24540900	-2.80252700	-0.58570300
C	6.88585700	-2.63973700	-3.01553000
H	6.67041700	-2.93414700	-4.04391100
C	6.38463900	2.58500700	2.06720900
C	6.86763600	2.40359400	0.76049500
H	7.54633100	3.14178900	0.32459700
C	6.48784800	1.31670100	-0.01915400
H	6.86247800	1.21165800	-1.04039000
C	-0.46595400	-1.42621800	-0.61876100
C	-0.94234100	-0.12630200	-0.43404500
C	-1.38605000	-2.51017200	-0.76500400
C	-2.33824400	0.13258200	-0.38331600
C	-2.74666200	-2.27750300	-0.70039200
C	-3.25347000	-0.96639600	-0.50080200
H	-3.46432700	-3.09432900	-0.79603700
C	-4.10647000	1.56374700	-0.17374500
C	-4.65237000	2.90316600	-0.05647500
C	-5.02479000	0.44197300	-0.24602200
C	-6.02777400	3.09386400	0.04803800
C	-6.44915400	0.68733600	-0.12536000
C	-6.92606700	1.98446800	0.02915000
C	-0.93302600	-3.86282000	-0.96591200
N	-0.58038300	-4.95041800	-1.12704500

N	-2.80121900	1.38761900	-0.22223800
N	-4.58356000	-0.78748500	-0.41441900
C	-8.74035600	0.27957400	-0.00135900
C	-7.49580100	-0.27824100	-0.14256200
C	-4.75175100	5.23091200	0.02635400
C	-3.93353900	4.13515700	-0.06966000
C	9.19454500	-3.78111800	-3.14485700
C	6.79777800	3.82337800	2.86852000
C	9.47841700	-5.07740200	-2.36792300
H	8.57076200	-5.70167200	-2.30043400
H	10.26328900	-5.66405900	-2.87732900
H	9.82585500	-4.87059700	-1.34167100
C	10.47909900	-2.93878700	-3.21745800
H	11.27561100	-3.50006900	-3.73727100
H	10.30230500	-1.99986400	-3.77000200
H	10.85244400	-2.67660800	-2.21317500
C	8.77959900	-4.15349500	-4.57129900
H	7.87220900	-4.78109300	-4.58136300
H	8.58961000	-3.25846900	-5.18785100
H	9.58891900	-4.72702800	-5.05447400
C	8.32920700	3.86357700	2.99934900
H	8.82326900	3.91385300	2.01458600
H	8.63865000	4.75307800	3.57578000
H	8.70309700	2.96655100	3.52260200
C	6.19214200	3.82460000	4.27519700
H	5.08920000	3.83438700	4.24446700
H	6.51647900	2.94691000	4.86007500
H	6.51741700	4.72869200	4.81722500
C	6.31424500	5.08354300	2.13086800
H	5.21547900	5.08134500	2.02456100
H	6.60217900	5.98957500	2.69254100
H	6.75316900	5.15844800	1.12162900
H	-7.30433400	-1.34520400	-0.25864800
H	-2.84640600	4.18264200	-0.15529900
S	-6.43227500	4.76600800	0.14414900
S	-8.64443300	2.01905900	0.15346000
C	-4.37809100	6.65237800	0.01420300
C	-5.22693400	7.65139000	0.50990200
C	-3.14267300	7.06281600	-0.50336400
C	-4.80394800	8.97839400	0.47174900
H	-6.20104000	7.40750800	0.94287500
C	-2.81951300	8.41848500	-0.49481400
H	-2.44270300	6.34044400	-0.92755000
H	-5.45291100	9.76720700	0.86725900

H	-1.84975000	8.74402600	-0.88428600
C	-10.04350500	-0.39915900	0.03078400
C	-11.24770900	0.30648500	0.15427500
C	-10.13303800	-1.79576300	-0.06171000
C	-12.44997000	-0.39789200	0.17891000
H	-11.26605900	1.39694800	0.23048600
C	-11.38777400	-2.39748400	-0.02735900
H	-9.24122200	-2.41720600	-0.15806700
H	-13.39578600	0.14641200	0.27533700
H	-11.46855500	-3.48763000	-0.09920700
N	-3.62722300	9.36367400	-0.01674600
N	-12.53043200	-1.72273500	0.09054000
C	0.38204300	2.31102400	0.22065400
C	1.00024700	2.64412700	1.43809200
C	-0.11704000	4.51128800	-0.20699000
C	0.97856900	3.96499700	1.87576000
C	0.37969300	4.90033400	1.03966000
H	-0.50360500	5.26344700	-0.90387200
C	-1.99586100	7.85773300	2.56210800
C	-1.41324500	6.59885800	2.36375400
C	-2.08247000	5.45582100	2.78631800
C	-3.81959800	6.91358700	3.55969100
H	-1.66650200	4.45620400	2.63459600
C	-3.32480500	5.62133200	3.39798400
H	-4.79227700	7.07510500	4.03725800
H	-3.90052600	4.75868800	3.73875100
S	0.19552800	6.58071600	1.57914900
O	0.10522400	7.43923900	0.40255400
O	1.20289400	6.83653000	2.59984200
H	1.47377100	1.86623600	2.04294600
H	1.41064300	4.27213400	2.83214600
H	-1.49004800	8.76577900	2.21381700
N	-0.14083800	3.24483800	-0.59497400
N	-3.17239600	8.00769000	3.15302200
B	0.30083900	0.80691900	-0.22243800
B-DTC-locking-Py-Th-TPA			
N	4.75226200	-0.66926100	-0.40744800
C	0.60174800	-1.47890500	-0.49381100
C	3.38514100	-0.94827100	-0.42616200
C	2.44414700	0.10628200	-0.29780200
H	2.78770500	1.13827500	-0.19874500
C	4.89084500	1.04315900	1.34893900
H	4.33891400	0.38046900	2.02169800
C	5.20211300	0.60197700	0.05693600

C	1.51077700	-2.52433600	-0.61112300
H	1.19285800	-3.56189100	-0.73031400
C	2.88720600	-2.25522300	-0.56275200
H	3.58598100	-3.08974600	-0.64157400
C	1.09161700	-0.16465600	-0.30983900
C	5.70954500	-1.53058400	-1.00669300
C	5.48641000	-2.12329300	-2.25178500
H	4.54853600	-1.93706700	-2.78069600
C	5.25401400	2.32148800	1.75834600
H	4.98322700	2.64458000	2.76780100
C	7.67518400	-3.20154700	-2.19096600
C	6.92956400	-1.76704800	-0.36059900
H	7.12012400	-1.30256800	0.61002200
C	7.88965700	-2.58144900	-0.94919900
H	8.82976000	-2.74352200	-0.41453900
C	6.45193000	-2.95211300	-2.82415800
H	6.23293600	-3.39641000	-3.79638200
C	5.95701000	3.19732600	0.91277200
C	6.30029600	2.72056600	-0.35735500
H	6.85354900	3.35296800	-1.05321500
C	5.92533400	1.44569300	-0.78523700
H	6.18149200	1.10713600	-1.79237000
C	-0.88748600	-1.43987500	-0.52211100
C	-1.36620700	-0.13857400	-0.35002700
C	-1.80964300	-2.51915800	-0.69010500
C	-2.76024600	0.12104600	-0.31832200
C	-3.17141900	-2.27919300	-0.67991300
C	-3.67920700	-0.96648400	-0.49283500
H	-3.88833800	-3.09187700	-0.81012900
C	-4.52010100	1.55984200	-0.09573800
C	-5.05212800	2.89018100	0.12647100
C	-5.44549000	0.45817800	-0.29160900
C	-6.42759400	3.10428100	0.12472700
C	-6.87066000	0.72716000	-0.27658800
C	-7.33728500	2.02217100	-0.07604300
C	-1.35236200	-3.87295300	-0.87294900
N	-0.99154200	-4.95994800	-1.01985200
N	-3.21615600	1.37335500	-0.12034000
N	-5.01021400	-0.77056900	-0.48191200
C	-9.17023800	0.36696500	-0.39112100
C	-7.92805200	-0.21003000	-0.45513800
C	-5.11935800	5.18832500	0.50472100
C	-4.31465200	4.08988100	0.35321800
C	8.75790500	-4.10435900	-2.79022800

C	6.29542800	4.61209900	1.39293500
C	9.02722100	-5.27681100	-1.83235500
H	8.11363900	-5.87683600	-1.67932200
H	9.80856800	-5.93795600	-2.24711900
H	9.37218400	-4.92532500	-0.84530000
C	10.05101600	-3.29419800	-2.98001900
H	10.84083300	-3.93225800	-3.41435100
H	9.88432000	-2.44116500	-3.66024400
H	10.42838000	-2.89718200	-2.02267600
C	8.34104900	-4.67487200	-4.14896000
H	7.42983200	-5.29191100	-4.07048900
H	8.15730700	-3.87605300	-4.88756000
H	9.14691800	-5.31695900	-4.54352100
C	7.06676300	5.40764700	0.33652700
H	6.47964600	5.52963600	-0.58942000
H	7.29012000	6.41587900	0.72456700
H	8.02591500	4.92564900	0.08066300
C	7.15184900	4.53215500	2.66725500
H	6.62048800	4.01297600	3.48320400
H	8.09618700	3.99334300	2.47672100
H	7.39961000	5.54793500	3.02249100
C	4.98775200	5.35739100	1.71177800
H	4.43417100	4.85520000	2.52281200
H	5.20400800	6.39014400	2.03883100
H	4.32812400	5.41252000	0.82803200
H	-7.74566000	-1.27089800	-0.62799100
H	-3.22412600	4.12151200	0.38484700
S	-6.81167300	4.76263000	0.38849800
S	-9.05880100	2.08869900	-0.10612100
C	-4.72054600	6.58573000	0.72671500
C	-5.59168000	7.65033200	0.45879900
C	-3.44311100	6.90883700	1.20536900
C	-5.15297900	8.95505700	0.67380900
H	-6.59919900	7.47740000	0.07116900
C	-3.10512100	8.25067000	1.37744600
H	-2.71187300	6.13907200	1.46522600
H	-5.82559100	9.79489700	0.46641800
H	-2.10711000	8.50166900	1.75003600
C	-10.48200100	-0.28044000	-0.53057200
C	-11.67931500	0.44625500	-0.49231200
C	-10.58692300	-1.66732700	-0.71075900
C	-12.89024000	-0.22912200	-0.63290600
H	-11.68531600	1.53096500	-0.35609400
C	-11.84903000	-2.23944000	-0.84178200

H	-9.70082600	-2.30329100	-0.74722900
H	-13.83073200	0.33194300	-0.60416200
H	-11.94178200	-3.32180100	-0.98344200
N	-3.93722900	9.26022200	1.11956000
N	-12.98526100	-1.54471200	-0.80533300
C	0.00826200	2.29234900	0.30630500
C	-0.59392100	3.36699300	-0.37292700
C	0.82472200	2.55577100	1.42156300
C	-0.36996900	4.68912900	0.01944000
H	-1.23979200	3.16670200	-1.23127200
C	1.00708600	3.86253300	1.86409800
C	0.42151600	4.90172500	1.13835600
H	-0.80841100	5.52602500	-0.53076600
C	1.78165900	4.33065800	3.03545200
C	1.79458900	5.72212100	3.15998900
C	2.47194300	3.56628700	3.97466000
C	2.47607800	6.38789100	4.16538700
C	3.16570600	4.21615700	4.99911800
H	2.47162100	2.47529100	3.91045200
H	2.46814900	7.47872900	4.22766000
C	3.17448700	5.61108300	5.09430800
H	3.70997600	3.62373000	5.73854600
H	3.72562000	6.09818500	5.90164400
S	0.83523800	6.48453100	1.85816300
O	-0.35941500	7.11225600	2.41461300
O	1.68616000	7.25950600	0.96810200
H	1.30996700	1.73111800	1.95243500
B	-0.12851600	0.80272600	-0.13581900
B-TXO2-CF ₃ -locking-Py-Th-TPA			
N	4.85116000	-0.77131300	-0.38884800
C	0.70710900	-1.57414700	-0.41161600
C	3.47777800	-1.03607400	-0.38864600
C	2.54255200	0.01965800	-0.22696000
H	2.90393300	1.04569000	-0.11583100
C	4.95056400	0.59278200	1.64674400
H	4.20410900	-0.05457300	2.11416200
C	5.37824800	0.32365500	0.34429800
C	1.61263600	-2.61128000	-0.58553100
H	1.29093600	-3.64429100	-0.73045100
C	2.98757300	-2.33781100	-0.56100200
H	3.69240400	-3.16238300	-0.68256200
C	1.18662200	-0.24893300	-0.22110700
C	5.75285100	-1.59669300	-1.11216300
C	5.48443900	-1.97650400	-2.42920500

H	4.56287600	-1.64002200	-2.91079900
C	5.46278700	1.68335300	2.34987600
H	5.08878800	1.86256900	3.35914600
C	7.58024400	-3.22060900	-2.55481700
C	6.94540000	-2.02956200	-0.51884800
H	7.17001200	-1.73910000	0.51033400
C	7.83875200	-2.81845500	-1.23436300
H	8.75970500	-3.13641500	-0.73763000
C	6.38103900	-2.78300500	-3.13022400
H	6.12820000	-3.05672800	-4.15575900
C	6.43243500	2.52541900	1.79319600
C	6.86896100	2.22417300	0.49275700
H	7.62652900	2.85087700	0.01407900
C	6.35183400	1.15364900	-0.22666400
H	6.70026400	0.95444100	-1.24289500
C	-0.78234000	-1.57553300	-0.39061100
C	-1.27163800	-0.29254100	-0.16803200
C	-1.70300000	-2.65842000	-0.56114600
C	-2.66321700	-0.06175700	-0.04638100
C	-3.06922700	-2.43502400	-0.50509700
C	-3.58871500	-1.13750400	-0.24803200
H	-3.77663700	-3.25362600	-0.65014500
C	-4.40387900	1.35096400	0.34543200
C	-4.89297800	2.66334600	0.69238600
C	-5.34400800	0.28421100	0.07330000
C	-6.25362000	2.93994400	0.69067600
C	-6.76080800	0.60178300	0.10577900
C	-7.18932200	1.89910300	0.39237900
C	-1.24149500	-4.00095200	-0.80730600
N	-0.87696600	-5.07864800	-1.00493600
N	-3.10535700	1.16478900	0.27390400
N	-4.92110100	-0.93630500	-0.19735900
C	-9.07052700	0.32939500	-0.05846800
C	-7.84748700	-0.28324100	-0.14779800
C	-4.83897700	4.90644500	1.28192700
C	-4.09411600	3.78636400	1.04111500
C	8.59365500	-4.09640200	-3.29840900
C	7.02021000	3.72998700	2.53432100
C	8.78996300	-5.41375200	-2.52997000
H	7.83840300	-5.96703100	-2.44900700
H	9.51891900	-6.05663500	-3.05433500
H	9.16933200	-5.23882200	-1.50912200
C	9.93732300	-3.35384200	-3.38845300
H	10.68018600	-3.97143500	-3.92366600

H	9.82382200	-2.40115400	-3.93402700
H	10.34570600	-3.12653100	-2.38932700
C	8.12996600	-4.43037800	-4.71935400
H	7.17733400	-4.98701400	-4.71738400
H	7.99991500	-3.52113100	-5.33063500
H	8.88590300	-5.06214200	-5.21616500
C	8.52899500	3.51377800	2.73606700
H	9.05419000	3.39746900	1.77287100
H	8.97297600	4.37806000	3.26126900
H	8.71952100	2.60879500	3.33851700
C	6.36894900	3.93075200	3.90598900
H	5.28219100	4.09716200	3.81850400
H	6.53679800	3.06456900	4.56841400
H	6.80628900	4.81680200	4.39713600
C	6.79663400	5.00159200	1.69884100
H	5.72269600	5.16808700	1.51117200
H	7.19313500	5.88333600	2.23251800
H	7.30579300	4.94411700	0.72229300
H	-7.70193500	-1.33371800	-0.40160600
H	-3.00420300	3.75577200	1.08692300
S	-6.55020900	4.59651400	1.09277900
S	-8.90739300	2.02112800	0.34869800
C	-4.30223400	6.22086600	1.66000400
C	-4.83101300	7.42465200	1.18761400
C	-3.17483500	6.28550800	2.49014900
C	-4.19882300	8.61628400	1.54368200
H	-5.69884200	7.44017600	0.52314500
C	-2.63257500	7.53084900	2.78988400
H	-2.73896700	5.37715300	2.91124500
H	-4.58652800	9.56941500	1.16737000
H	-1.75169300	7.59891600	3.44096500
C	-10.39939100	-0.26420300	-0.25906200
C	-11.55390200	0.51957100	-0.38472500
C	-10.56257700	-1.65487900	-0.33608900
C	-12.78355200	-0.10792500	-0.57551300
H	-11.50906500	1.61120900	-0.34580100
C	-11.83829900	-2.17591400	-0.53373800
H	-9.71192700	-2.33116800	-0.23291300
H	-13.69186600	0.49650500	-0.67458800
H	-11.97803900	-3.26075600	-0.59512600
N	-3.12369700	8.67897500	2.32485000
N	-12.93420800	-1.42752200	-0.65138900
C	-0.13689800	2.26553100	-0.06372200
C	-0.98098900	2.93676300	-0.96443000

C	0.57396400	3.01854100	0.87688600
C	-1.06758100	4.31701300	-0.94148700
H	-1.56734100	2.37358700	-1.69443100
C	0.44101500	4.41956500	0.98951900
C	-0.36545200	5.03677800	0.03009200
H	-1.69357000	4.85561100	-1.65755800
C	1.17977600	5.18996600	2.10997200
C	0.93914600	6.71756300	2.19620800
C	0.21698100	7.45655300	1.25519700
C	1.43337900	7.44358800	3.29651300
C	-0.01664000	8.82806700	1.37914300
C	1.20586100	8.80898400	3.43532100
H	2.01204500	6.94803400	4.07126200
H	-0.61507000	9.33901300	0.62116000
C	0.47713000	9.51283800	2.47818400
H	1.60713000	9.32348700	4.31103000
H	0.28538800	10.58156100	2.59159900
S	-0.42374200	6.78225900	-0.24283500
O	-1.81316900	7.19808500	-0.39602500
O	0.51187900	7.08558100	-1.31763600
H	1.23204300	2.48272700	1.55695000
C	2.70244200	4.95754700	1.89757400
C	0.75315500	4.59145200	3.49262000
B	-0.05815800	0.70255700	-0.10298100
F	1.63297100	4.88751500	4.45039600
F	0.64151200	3.27050000	3.50012400
F	-0.42881600	5.08651500	3.85005000
F	3.03179700	5.25866300	0.65107400
F	3.45649600	5.69869100	2.70376100
F	3.03555300	3.68535600	2.12702300

B-DSCZ-locking-Py-Th-TPA

N	4.62919100	-0.81407800	-0.00834800
C	0.52074600	-1.62927100	-0.54308600
C	3.27025700	-1.09239900	-0.19577500
C	2.30981800	-0.06413600	-0.01978900
H	2.64209900	0.94700700	0.22853200
C	4.47927900	0.31277400	2.15807200
H	3.80699000	-0.47524200	2.50748400
C	5.00564100	0.24073100	0.86667400
C	1.45259600	-2.64128400	-0.73784800
H	1.16129400	-3.65476800	-1.01922900
C	2.81650000	-2.36965900	-0.55188100
H	3.53965000	-3.17618800	-0.68810600
C	0.96444500	-0.33652500	-0.16889800

C	5.64122000	-1.50798000	-0.71752000
C	5.49585200	-1.82330300	-2.07139200
H	4.58139300	-1.54021200	-2.59829600
C	4.78550700	1.39032500	2.98924500
H	4.34212600	1.41193100	3.98614100
C	7.70473500	-2.86091200	-2.12613800
C	6.83139300	-1.86894800	-0.07130900
H	6.96298800	-1.62992800	0.98672200
C	7.83879500	-2.52443100	-0.76939200
H	8.75252700	-2.79004300	-0.23020400
C	6.50829300	-2.49658700	-2.75515200
H	6.34815900	-2.72271300	-3.81062200
C	5.64234700	2.41558800	2.57071600
C	6.19518000	2.30416500	1.28424900
H	6.87380400	3.07819500	0.91511000
C	5.88339200	1.24428700	0.44011700
H	6.30845900	1.19536700	-0.56547000
C	-0.96400000	-1.62256300	-0.66018600
C	-1.49067200	-0.36238500	-0.37110600
C	-1.83774600	-2.70143300	-1.00185700
C	-2.89554300	-0.15269500	-0.37146800
C	-3.20528000	-2.50350300	-1.03656200
C	-3.76598100	-1.23869700	-0.71967100
H	-3.88687900	-3.31484300	-1.29803200
C	-4.71905600	1.18523200	-0.04253500
C	-5.31052400	2.45408200	0.33489000
C	-5.59269600	0.08999100	-0.42310200
C	-6.69234900	2.61908900	0.30209000
C	-7.02638600	0.30717300	-0.44012700
C	-7.55041500	1.54732200	-0.09010800
C	-1.33144100	-4.01293700	-1.31656400
N	-0.93678500	-5.06783400	-1.57107100
N	-3.40906100	1.04574300	-0.03272700
N	-5.10265800	-1.08907600	-0.74663400
C	-9.30244500	-0.10710400	-0.71033000
C	-8.03875100	-0.63169400	-0.79106000
C	-5.48461000	4.66835000	1.04184300
C	-4.63105400	3.63252500	0.76458100
C	8.84071200	-3.59286600	-2.84753100
C	5.97106000	3.63443400	3.43724000
C	9.10300100	-4.93798800	-2.15005800
H	8.20185300	-5.57476900	-2.17299100
H	9.92063500	-5.47909700	-2.65834900
H	9.39503600	-4.80036900	-1.09530800

C	10.11531800	-2.73435800	-2.79370700
H	10.94504300	-3.24946500	-3.30935300
H	9.95436400	-1.76055200	-3.28768600
H	10.43328600	-2.54028700	-1.75551300
C	8.50431900	-3.86719200	-4.31620400
H	7.60880800	-4.50367000	-4.41720200
H	8.33128600	-2.93264100	-4.87663600
H	9.34599900	-4.39478700	-4.79642600
C	7.49070600	3.72149500	3.65253800
H	8.03406400	3.82216400	2.69816800
H	7.73818700	4.59977400	4.27455100
H	7.86743700	2.81961000	4.16511400
C	5.29105500	3.56575100	4.80777500
H	4.19147100	3.54302800	4.71745600
H	5.61073800	2.67726400	5.37845200
H	5.55875200	4.45807800	5.39886100
C	5.48228500	4.90369600	2.71840900
H	4.39142800	4.86698800	2.54932400
H	5.70678600	5.79636900	3.32897300
H	5.97131500	5.03253200	1.73759800
H	-7.81492900	-1.65114200	-1.10677300
H	-3.54452900	3.69181500	0.85088900
S	-7.15276000	4.20563100	0.78700800
S	-9.27123500	1.56178300	-0.19147500
C	-5.16083700	6.02686800	1.50211200
C	-6.11221200	7.05669700	1.47633500
C	-3.88610100	6.34868700	1.98578600
C	-5.75317100	8.32322100	1.92931400
H	-7.12483000	6.88837400	1.10005200
C	-3.63145300	7.65294300	2.40821700
H	-3.09103200	5.60199600	2.05239600
H	-6.48993400	9.13422200	1.91499900
H	-2.63450800	7.90641200	2.78050500
C	-10.57918700	-0.77475300	-0.99718300
C	-11.76387600	-0.05829600	-1.21068000
C	-10.65623000	-2.17269400	-1.07203600
C	-12.93907000	-0.75665700	-1.48205000
H	-11.78133400	1.03439100	-1.18139400
C	-11.88262200	-2.76735100	-1.35589000
H	-9.77718500	-2.79592200	-0.89715400
H	-13.87122400	-0.20639200	-1.65088900
H	-11.95606800	-3.85871400	-1.41696300
N	-4.54121500	8.62604100	2.38830600
N	-13.00792400	-2.08323400	-1.55735200

B	-0.29054700	0.59648900	-0.02771500
C	-0.26645300	2.10425400	0.36875000
C	0.51461100	2.52856300	1.46112800
C	-0.98541100	3.06823100	-0.35688500
C	0.54490600	3.86523400	1.84865900
H	1.08975700	1.79629900	2.03553500
C	-0.92129500	4.41905400	-0.01915500
H	-1.60934600	2.75926200	-1.19899200
C	-0.16615400	4.79346900	1.08967300
H	1.12158300	4.18227400	2.72231400
H	-1.46579300	5.17824600	-0.58609000
S	-0.20458100	6.50265400	1.60209800
C	1.49224900	7.04512900	1.54844000
C	2.11795100	7.17764900	0.30879200
C	2.12960200	7.37671900	2.74081900
C	3.43156300	7.63744900	0.27107900
H	1.58259400	6.92854900	-0.61138800
C	3.44114400	7.84974300	2.68679500
H	1.59549800	7.27284000	3.68788000
C	4.08887300	7.97463800	1.45767600
H	3.94185300	7.74394800	-0.68875800
H	3.95781300	8.12076200	3.61048900
H	5.11809600	8.34035900	1.42132600
O	-0.95620600	7.24298500	0.59276100
O	-0.63042000	6.53185300	3.00278600

B-DMPS-locking-Py-Th-TPA

N	5.06461900	-0.79965800	-0.50255300
C	0.93024700	-1.64406700	-0.81850000
C	3.70798400	-1.09923300	-0.64401600
C	2.75364400	-0.06111200	-0.48240000
H	3.08066900	0.96256000	-0.28846700
C	5.04802800	0.60036400	1.50400200
H	4.62327500	-0.23858300	2.06194600
C	5.39507300	0.42049600	0.16556000
C	1.85225300	-2.66957700	-0.99769100
H	1.54629100	-3.70041800	-1.18762700
C	3.22723800	-2.39328300	-0.90365500
H	3.93523000	-3.21604000	-1.01970300
C	1.40730500	-0.33912600	-0.55340000
C	6.09729900	-1.53214200	-1.13349800
C	5.93877300	-2.09106800	-2.40534400
H	4.99093500	-1.97666000	-2.93616500
C	5.18262500	1.85231300	2.10588300
H	4.87305000	1.96203700	3.14645500

C	8.22871300	-2.93910400	-2.38306400
C	7.33740700	-1.67238900	-0.49387700
H	7.48205900	-1.23682900	0.49760600
C	8.37559200	-2.35719800	-1.11350600
H	9.32642300	-2.44543400	-0.58036800
C	6.98572300	-2.78878400	-3.00848700
H	6.81314600	-3.20798800	-4.00107600
C	5.67995000	2.95300200	1.39622800
C	6.09029100	2.73129500	0.07043900
H	6.49413500	3.55915900	-0.51851500
C	5.95053300	1.48998200	-0.54242500
H	6.23210100	1.35275500	-1.58977900
C	-0.56036600	-1.61784500	-0.80200500
C	-1.04178300	-0.33408200	-0.53234500
C	-1.48414400	-2.69335200	-0.98780600
C	-2.43267900	-0.09125100	-0.42334700
C	-2.84589700	-2.47045300	-0.88726200
C	-3.35426200	-1.17573000	-0.59908800
H	-3.56090000	-3.28422800	-1.02129700
C	-4.18245300	1.32712400	-0.05851100
C	-4.70246100	2.65437800	0.19914100
C	-5.11202000	0.22596300	-0.22742400
C	-6.07464400	2.86548500	0.28920800
C	-6.53391800	0.48882400	-0.10789500
C	-6.99075100	1.77901400	0.14652500
C	-1.02337900	-4.02819300	-1.27336900
N	-0.65586900	-5.09847800	-1.50286000
N	-2.88150300	1.14973100	-0.15504200
N	-4.68328300	-0.99152000	-0.49385300
C	-8.83397100	0.12090400	-0.06519500
C	-7.59839200	-0.44984600	-0.22903100
C	-4.74562700	4.95761700	0.53994200
C	-3.95143900	3.85637500	0.35086900
C	9.40122200	-3.69116800	-3.01998300
C	5.73304600	4.36632400	1.98584000
C	9.80680500	-4.86423600	-2.11238400
H	8.96670500	-5.56775300	-1.98038700
H	10.65308100	-5.41711600	-2.55725100
H	10.11966000	-4.51727800	-1.11314000
C	10.59440500	-2.73439000	-3.17935600
H	11.44938000	-3.26227800	-3.63771700
H	10.32937100	-1.88050100	-3.82648700
H	10.92850600	-2.33297200	-2.20779700
C	9.04210600	-4.24917300	-4.40027800

H	8.20303600	-4.96353000	-4.34584000
H	8.76943200	-3.44639300	-5.10635600
H	9.91070500	-4.78406600	-4.82089700
C	7.15780600	4.93053400	1.87028700
H	7.49774800	4.98530500	0.82253500
H	7.19330400	5.95257400	2.28617800
H	7.87598000	4.30607800	2.42980100
C	5.32083600	4.39010500	3.46046700
H	4.27483800	4.07024500	3.59706200
H	5.97482200	3.74885500	4.07670200
H	5.39242100	5.42075800	3.84623900
C	4.75944900	5.25900800	1.19571600
H	3.73328600	4.85687600	1.24395900
H	4.73789300	6.27842200	1.61802600
H	5.04830800	5.33198200	0.13297500
H	-7.42961600	-1.51092800	-0.41549000
H	-2.85944300	3.87868100	0.32304100
S	-6.44206300	4.52860400	0.55079700
S	-8.71081900	1.83778100	0.23671100
C	-4.33233300	6.36026600	0.67981100
C	-5.20988100	7.35933000	1.11935300
C	-3.02533400	6.75415600	0.35977900
C	-4.75259700	8.67393500	1.20215100
H	-6.24160900	7.13003300	1.39937600
C	-2.67174300	8.09476400	0.48298200
H	-2.29031200	6.03041200	0.00130200
H	-5.43173100	9.46456300	1.54016100
H	-1.65248700	8.41124000	0.23450600
C	-10.14905700	-0.53237100	-0.11810700
C	-11.30640400	0.08356500	0.37560800
C	-10.29325000	-1.81359000	-0.66895900
C	-12.52157300	-0.59442800	0.29755500
H	-11.27319100	1.07749400	0.82979900
C	-11.55545100	-2.40100800	-0.69119000
H	-9.43894700	-2.34732700	-1.08986400
H	-13.43258400	-0.12200100	0.68102200
H	-11.68129800	-3.40164900	-1.11901700
N	-3.51392800	9.04527000	0.88980600
N	-12.65421100	-1.81232400	-0.22118800
C	0.35117400	2.04980800	0.28846600
C	-0.01246900	3.23783000	-0.38513700
C	0.98397300	2.12758700	1.53895400
C	0.26038400	4.46776500	0.21838000
C	1.22262800	3.35310200	2.15861000

C	0.85443300	4.50740500	1.48032200
H	0.03206800	5.40386300	-0.30046400
C	-0.61084800	7.94484400	3.07898800
C	-0.41483200	6.57579800	2.91079800
C	-1.80104300	8.41775400	3.64177400
C	-1.38062600	5.64272800	3.28387900
C	-2.77832800	7.48168000	4.00548400
H	-1.21717100	4.57105200	3.14452100
C	-2.57563700	6.11336100	3.82732400
H	-3.71950600	7.83501400	4.43692600
H	-3.35552600	5.40344200	4.11396800
S	1.17210100	6.08068800	2.24898100
O	1.52426900	7.04732700	1.21017000
O	2.08923200	5.85388500	3.36378500
H	1.30122400	1.21019800	2.04457600
H	1.70230800	3.41985600	3.13761400
H	0.16407300	8.64653200	2.75636000
B	0.19080400	0.60825300	-0.29366200
C	-0.64420100	3.17032900	-1.75023600
H	-1.57438000	2.57673000	-1.70978600
H	-0.88366400	4.17374700	-2.13681000
H	0.03357900	2.68389700	-2.47410500
C	-2.04302900	9.89525800	3.78648300
H	-2.44442300	10.29923000	2.83944500
H	-2.77501400	10.10387400	4.58282900
H	-1.10987000	10.43260400	4.01910700

B-TXO2-locking- Py-Th-TPA

N	4.72203500	-0.65602200	-0.28691400
C	0.58124600	-1.45221000	-0.36280600
C	3.34577800	-0.92732400	-0.32241700
C	2.41684900	0.13421300	-0.20529500
H	2.79256400	1.15883200	-0.13031700
C	4.73352200	0.46539000	1.89151200
H	3.94630500	-0.20810800	2.23959300
C	5.22422800	0.33844100	0.58851600
C	1.48307800	-2.49834700	-0.51085900
H	1.15959700	-3.53238600	-0.63985200
C	2.85929900	-2.23001800	-0.47893300
H	3.56634300	-3.05631000	-0.57840000
C	1.05880700	-0.12594200	-0.20535900
C	5.63074100	-1.42363600	-1.05879200
C	5.34631700	-1.74394300	-2.38888800
H	4.41241400	-1.39829500	-2.83896500
C	5.25025400	1.43396000	2.75356300

H	4.83941800	1.49051100	3.76312500
C	7.45864000	-2.94616300	-2.61116200
C	6.83905000	-1.86978100	-0.50679700
H	7.07759200	-1.63194900	0.53259200
C	7.73166800	-2.60734100	-1.27597400
H	8.66486500	-2.93625400	-0.81007900
C	6.24295700	-2.50016400	-3.14352900
H	5.97675800	-2.72603300	-4.17731800
C	6.28125400	2.29475300	2.35903800
C	6.75851800	2.15623800	1.04485300
H	7.55638600	2.81102500	0.68353600
C	6.24209500	1.20714800	0.17053100
H	6.63286000	1.12677200	-0.84663500
C	-0.90816500	-1.44568200	-0.35402400
C	-1.40956400	-0.15177500	-0.20895800
C	-1.80420700	-2.55518500	-0.45841700
C	-2.81010600	0.06757000	-0.11024000
C	-3.16954900	-2.35259600	-0.39472700
C	-3.70349900	-1.05064300	-0.21108100
H	-3.86895500	-3.18701000	-0.47153000
C	-4.60233500	1.45119600	0.20098000
C	-5.16238900	2.76421800	0.45334700
C	-5.50117900	0.31862900	0.07547200
C	-6.54059000	2.92804000	0.56428200
C	-6.93044700	0.53910800	0.18244900
C	-7.42546500	1.81685000	0.42083900
C	-1.32748900	-3.90413300	-0.62776900
N	-0.96118800	-4.99061600	-0.76431900
N	-3.29670200	1.30605900	0.09903500
N	-5.03710600	-0.89759400	-0.12489700
C	-9.21845100	0.10090100	0.22638500
C	-7.96513900	-0.43365400	0.07470700
C	-5.28056500	5.05117100	0.87626700
C	-4.45160200	3.98815600	0.63087700
C	8.47354200	-3.76552300	-3.41452800
C	6.90373100	3.33721400	3.29288800
C	8.70136200	-5.11849700	-2.72006400
H	7.75927500	-5.68962000	-2.65369400
H	9.43085100	-5.72177900	-3.28890200
H	9.09483600	-4.99197800	-1.69740200
C	9.80444200	-2.99833700	-3.48500900
H	10.54917700	-3.57653100	-4.06015400
H	9.66882700	-2.02164300	-3.98084200
H	10.22317700	-2.81448800	-2.48123500

C	7.99297700	-4.03102900	-4.84429400
H	7.05014600	-4.60392300	-4.85814000
H	7.83744000	-3.09255300	-5.40320400
H	8.75159000	-4.62143100	-5.38592100
C	8.39533200	3.01614000	3.48501100
H	8.94350000	3.04155000	2.52815800
H	8.86158600	3.75466700	4.16090800
H	8.52755600	2.01315500	3.92614200
C	6.23008000	3.34831700	4.66822800
H	5.15339900	3.57963100	4.59258500
H	6.34001000	2.38003100	5.18528300
H	6.69638300	4.12098000	5.30298800
C	6.76032500	4.73598300	2.67273500
H	5.69614900	4.98985100	2.52782500
H	7.21086900	5.49647100	3.33470200
H	7.26055200	4.80524900	1.69221200
H	-7.76104700	-1.48690600	-0.11926700
H	-3.36241400	4.05609200	0.59896700
S	-6.96075400	4.56764600	0.88257400
S	-9.14631800	1.82441400	0.51298600
C	-4.91587900	6.45433000	1.11564700
C	-5.78707400	7.34575900	1.75646700
C	-3.67360000	6.95495600	0.70512900
C	-5.38220800	8.66419100	1.95315300
H	-6.76795600	7.02298200	2.11560400
C	-3.37383700	8.29343300	0.94911500
H	-2.94269100	6.33443900	0.18153100
H	-6.05318800	9.36904600	2.45670700
H	-2.41177300	8.68758200	0.60843500
C	-10.51359800	-0.59107400	0.17326300
C	-11.73037000	0.10338100	0.18289200
C	-10.58103400	-1.99029000	0.10732100
C	-12.92361800	-0.61455100	0.12849500
H	-11.76427400	1.19529000	0.22495500
C	-11.82837400	-2.60587400	0.05332300
H	-9.67704400	-2.60166000	0.10441000
H	-13.87949700	-0.07941700	0.13559300
H	-11.89245500	-3.69828200	0.00145800
N	-4.20217400	9.13906900	1.56184600
N	-12.98339700	-1.94194400	0.06390500
C	-0.11684700	2.39399600	-0.15259400
C	-0.94216400	3.15247500	-0.99750400
C	0.85143400	3.05746700	0.62130000
C	-0.77234700	4.52912700	-1.08632900

H	-1.71795200	2.66388600	-1.59114600
C	1.04031500	4.44387300	0.57706900
C	0.21142300	5.14359100	-0.31287400
H	-1.40005900	5.13728300	-1.74304600
C	2.13202200	5.14846400	1.39981700
C	1.64115600	6.51540600	1.90860000
C	0.89207700	7.38487700	1.09947700
C	1.95320500	6.99158800	3.18880900
C	0.48254400	8.65213000	1.50928500
C	1.55838600	8.26003900	3.61603300
H	2.51143800	6.36708500	3.88510800
H	-0.10650200	9.27522000	0.83194600
C	0.82831300	9.10090700	2.77966300
H	1.82306600	8.58768800	4.62422300
H	0.51683400	10.09203100	3.11563600
S	0.40985100	6.89434000	-0.53589800
O	-0.89925500	7.47759600	-0.83338700
O	1.49314900	7.15077600	-1.48115500
H	1.47027900	2.45607100	1.28856200
C	3.36173500	5.38076500	0.48442800
H	3.77137900	4.40710200	0.16324700
H	3.10576500	5.96890400	-0.40850900
H	4.14243700	5.92088800	1.04569200
C	2.59957200	4.26604700	2.56292900
H	1.78256600	4.03305900	3.26668400
H	3.02491500	3.32402800	2.18497000
H	3.41100500	4.76466000	3.11394000
B	-0.18491100	0.83727800	-0.14546100