

Supporting Information for

From byproducts to NLO-active dyes: catalyst-free transfer hydrogenation in the modular synthesis of merocyanines

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Table. Cartesian coordinates for the optimized geometries at B3LYP-D3(BJ)/ma-TZVP level.

TCF1-based (Path I)

JD1'

O	2.77731800	1.49763900	-0.10614600
N	-0.86644000	-1.62654800	0.05485100
C	-2.84089500	0.54927200	0.08190100
C	-3.15711500	-0.91072000	0.42580000
C	-2.24935900	-1.86293800	-0.31660200
H	-2.38815100	-1.76602000	-1.40430700
C	0.04819300	-2.67440800	-0.35007200
H	-0.42391200	-3.63352200	-0.13397100
H	0.23237700	-2.64279900	-1.43520200
C	1.33432100	-2.53074200	0.42282700
H	2.01655400	-3.35051000	0.18857500
H	1.09705200	-2.59886000	1.48771500
C	2.03895900	-1.19538200	0.13544200
C	1.00444500	-0.05944500	0.05375200
C	1.42959100	1.27932200	-0.03097700
C	0.52313800	2.33365600	-0.05258400
H	0.85549500	3.35749400	-0.11443200
C	-0.83199000	2.05217800	0.00486300
H	-1.52613300	2.88183600	-0.00631200
C	-1.32435600	0.75960100	0.05546000
C	-0.39405700	-0.31429800	0.04945600
C	-3.43602500	0.90072200	-1.29460900
H	-3.21383200	1.93570700	-1.55803200
H	-4.52203900	0.77694500	-1.28237600
H	-3.02740300	0.26490700	-2.08071800
C	-3.50618300	1.43792500	1.14546800
H	-3.41213700	2.49868500	0.91333300
H	-3.06371400	1.26322900	2.12765000
H	-4.57256400	1.20732700	1.20490400
C	2.80691300	-1.31872300	-1.19496000
H	3.30190200	-0.38484200	-1.45109600
H	2.13407000	-1.58238500	-2.01225400
H	3.56546100	-2.10178700	-1.11421100
C	3.03932200	-0.98765300	1.29044000
H	2.50724600	-0.80678700	2.22668300
H	3.63525500	-1.89554200	1.41382900
H	3.71283300	-0.15611800	1.11069300
C	3.25635100	2.83029300	-0.19267700
H	2.97130500	3.41628400	0.68466500

H	2.89099900	3.32917500	-1.09385100
H	-2.48830400	-2.89528000	-0.05780500
H	-3.02117700	-1.07165600	1.49867800
H	-4.20219500	-1.12632300	0.19345200
H	4.34003300	2.75361600	-0.23796500

TCF-A2

Cl	-2.65512000	-1.94412800	0.17497700
O	3.89157900	-1.43444000	-0.00780000
N	7.31015700	-2.05366600	-0.07591200
N	6.87207900	2.29134700	-0.12679100
N	3.43428700	3.30330400	-0.08188700
C	6.60341500	-1.13983900	-0.07403200
C	6.34458900	1.26396700	-0.10237700
C	3.40901700	2.14989300	-0.05902000
C	5.74490300	-0.01473900	-0.07215000
C	4.37355300	-0.19819900	-0.03905200
C	3.29911700	0.74471100	-0.03037300
C	2.09499300	0.05793400	0.01156200
C	2.41600200	-1.42242100	0.02759000
C	1.95682200	-2.16053100	-1.22386200
H	0.87173900	-2.23228500	-1.25084700
H	2.37101800	-3.16792600	-1.21754100
H	2.29373000	-1.64108100	-2.11994400
C	2.01892800	-2.12009500	1.32244800
H	0.93663900	-2.19209200	1.40305000
H	2.39623600	-1.57122500	2.18406500
H	2.43523300	-3.12657500	1.32917900
C	0.82427400	0.65709300	0.03463300
H	0.81828100	1.73864800	0.00950800
C	-0.36628300	-0.02185900	0.07972000
H	-0.34185400	-1.09935900	0.09484600
C	-1.65071600	0.57131300	0.08628900
C	-1.77813600	2.07999200	0.07191800
H	-1.59499100	2.44323000	-0.94514200
H	-0.99339900	2.50788200	0.69662800
C	-3.13625700	2.56338700	0.56002100
H	-3.22500000	2.37472900	1.63335400
C	-4.25701500	1.84049500	-0.17246600
H	-4.23281100	2.10470500	-1.23527000
H	-5.23178100	2.14699100	0.20373000
C	-4.11763600	0.34308800	-0.03084400
C	-2.79846600	-0.19504700	0.07682400
C	-5.21891000	-0.45273500	-0.03053600
H	-5.15569900	-1.52871800	0.06839900
H	-3.22121400	3.64060300	0.41316400
O	-6.43426800	0.06344600	-0.16104600
C	-7.54330300	-0.87069800	-0.11340100
H	-7.40497500	-1.60547000	-0.90880300
H	-7.51692300	-1.38235500	0.85057500
C	-8.81962000	-0.08892600	-0.29375300
H	-8.93991300	0.64779600	0.50104900
H	-8.82793200	0.42517400	-1.25531400
H	-9.66910800	-0.77214500	-0.26124600

INT-I-A

Cl	-0.43507900	-2.70403900	0.41737700
O	5.89944100	-1.07267100	0.63277100
N	9.26164700	-0.78623900	1.45694700
N	8.52055000	2.21834800	-1.62212500
N	5.09597300	2.21243700	-2.71762400
C	8.50832600	-0.28522800	0.73822000
C	8.08225500	1.37361600	-0.96702300
C	5.16283200	1.38235200	-1.91840800
C	7.59318900	0.33454800	-0.14501100
C	6.27420800	-0.08780100	-0.17517500
C	5.16308700	0.35510900	-0.95393500
C	4.04249800	-0.39210900	-0.61164000

C	4.46610600	-1.37926700	0.45730500
C	4.39670400	-2.83231800	0.00471900
H	3.36224700	-3.14858100	-0.11020200
H	4.87236700	-3.46463700	0.75328400
H	4.90758400	-2.96026600	-0.94857500
C	3.81428400	-1.13656300	1.81280800
H	2.75913100	-1.39766200	1.78590400
H	3.90450200	-0.09021000	2.10031400
H	4.30571100	-1.75707800	2.56116200
C	2.76639200	-0.23623100	-1.17029900
H	2.67813400	0.52712600	-1.93176400
C	1.65730400	-0.96254400	-0.81095000
H	1.76926600	-1.72030400	-0.05285800
C	0.36309100	-0.81339400	-1.35136400
C	0.12119000	0.20509200	-2.44483000
H	0.51652100	-0.18777200	-3.38782200
H	0.69752400	1.10468800	-2.22338600
C	-1.34652600	0.57385900	-2.60106300
H	-1.66297800	1.16764400	-1.74220900
C	-2.21044800	-0.67490600	-2.69618800
H	-1.97149200	-1.22449900	-3.61339700
H	-3.26539700	-0.41413700	-2.75487000
C	-1.99040100	-1.57436500	-1.50421900
C	-0.69396800	-1.59196700	-0.91606800
C	-2.99477000	-2.36087100	-1.03467700
H	-2.87145700	-2.99798300	-0.16985100
H	-1.47922700	1.19300000	-3.48946500
O	-1.68626300	-0.75058300	3.25236100
N	-2.52292900	2.71456300	0.03403900
C	-5.19586100	1.67240200	-0.50974100
C	-4.44782200	2.59479300	-1.47504300
C	-3.47213200	3.48733400	-0.74570500
H	-4.00777100	4.20457900	-0.10711500
C	-1.41439500	3.49808200	0.53608400
H	-1.07930900	4.15389600	-0.26946900
H	-1.73581800	4.15092600	1.36114000
C	-0.29122000	2.59299200	0.96923400
H	0.54473600	3.18961500	1.33969800
H	0.06792600	2.03865200	0.09828700
C	-0.71745100	1.59722900	2.05594400
C	-2.05169700	0.94605800	1.65123000
C	-2.49503300	-0.22804600	2.28381900
C	-3.71418500	-0.81591200	1.96671900
C	-4.53501000	-0.19126100	1.04211600
H	-5.49763400	-0.63530300	0.83236600
C	-4.18420500	0.98438400	0.40680200
C	-2.91768700	1.56094400	0.70293200
C	-6.17996000	2.48883900	0.35118300
H	-6.73242700	1.82766300	1.02065700
H	-6.89896600	3.01445300	-0.28309400
H	-5.66431800	3.22483000	0.96795200
C	-6.00400300	0.67069400	-1.34565400
H	-6.66655200	0.06111200	-0.73118600
H	-5.34884000	0.00162000	-1.90215600
H	-6.63045800	1.21198300	-2.05804300
C	-0.90421400	2.33359400	3.39636100
H	-1.20712800	1.63334200	4.17427400
H	-1.66677700	3.10975500	3.32586300
H	0.03494600	2.80277700	3.70243400
C	0.46126600	0.61437000	2.19382800
H	0.47967100	-0.08359900	1.36114800
H	1.39445900	1.18189900	2.17597900
H	0.42577600	0.04294300	3.11444300
C	-2.03659500	-1.98961500	3.84559900
H	-2.12450600	-2.77877200	3.09500100
H	-2.97265300	-1.91718200	4.40539500
H	-2.89953900	4.07878100	-1.46297900
H	-3.90410800	1.98986600	-2.20403300
H	-5.15950900	3.20947500	-2.03033500
H	-4.04101400	-1.72400400	2.44728600
O	-4.17495600	-2.39177500	-1.63517900

C	-5.18990800	-3.22660100	-1.02378300
H	-4.77801500	-4.22963800	-0.89788200
H	-5.41916500	-2.81369100	-0.04037500
C	-6.39901000	-3.23027800	-1.92415100
H	-6.79379500	-2.22238200	-2.04909900
H	-6.15118700	-3.63593000	-2.90546500
H	-7.17710800	-3.85264000	-1.48059600
H	-1.22687900	-2.23129600	4.53009500

TS-I-A

Cl	-0.59378800	-2.70806300	0.01178700
O	5.69327500	-0.99465000	0.70281700
N	8.98199300	-0.80121500	1.75991500
N	8.63644600	2.01740500	-1.55355200
N	5.25909700	2.05466400	-2.92557000
C	8.31138700	-0.31621100	0.94957000
C	8.11000200	1.23600400	-0.88048900
C	5.25106900	1.28740000	-2.05853200
C	7.50623200	0.28173400	-0.04058300
C	6.15619300	-0.07955900	-0.15674700
C	5.14431700	0.34284900	-1.02882100
C	3.93353600	-0.34448500	-0.71199700
C	4.26257500	-1.26112500	0.45526500
C	4.16333600	-2.74249500	0.11606000
H	3.12664500	-3.03107400	-0.04582500
H	4.56356000	-3.33396800	0.93953000
H	4.72915200	-2.96306000	-0.78842300
C	3.53668400	-0.89261600	1.74212400
H	2.47445200	-1.10837100	1.65805100
H	3.65645600	0.16875500	1.95649900
H	3.94305300	-1.47204500	2.57108500
C	2.72916500	-0.18488000	-1.33859500
H	2.70848500	0.53037600	-2.15105800
C	1.52942700	-0.85802700	-1.00307300
H	1.58521200	-1.59523500	-0.21809500
C	0.29618600	-0.65709100	-1.55983000
C	0.06493600	0.34274400	-2.66920200
H	0.15268000	-0.16752500	-3.63529400
H	0.83871100	1.10788900	-2.64929700
C	-1.30604600	0.99733400	-2.56318600
H	-1.34098200	1.58246300	-1.64348900
C	-2.40944400	-0.04922800	-2.53861700
H	-2.50385400	-0.51655800	-3.52526400
H	-3.37449500	0.40982200	-2.33353100
C	-2.14435400	-1.12844500	-1.51737100
C	-0.86474100	-1.37529600	-1.11377000
C	-3.27085300	-1.88245600	-1.01406000
H	-3.04607000	-2.83550700	-0.55190700
H	-1.46097600	1.68742500	-3.39383700
O	-2.64513600	-1.86793900	2.47568500
N	-1.76659400	2.51473600	0.84784400
C	-4.45129700	2.74905400	-0.17225300
C	-3.32563800	3.60085200	-0.76194000
C	-2.18843100	3.76917000	0.21712400
H	-2.45603900	4.47347300	1.01038800
C	-0.44886200	2.62564500	1.46912100
H	0.21835300	3.08347300	0.73744500
H	-0.52595600	3.32396600	2.30817700
C	0.09401400	1.29463600	1.91544200
H	0.96449700	1.47063900	2.54859000
H	0.43124300	0.72318000	1.04862600
C	-0.95045300	0.46657800	2.67807700
C	-2.13298400	0.28335900	1.71815600
C	-2.90519700	-0.85806800	1.62684000
C	-3.95577500	-0.98069800	0.65020500
C	-4.48420600	0.25513000	0.14724400
H	-5.41989600	0.20702600	-0.38818300
C	-3.84159600	1.43276400	0.28350700
C	-2.54277500	1.42361600	0.94102300

C	-5.06976300	3.44526000	1.05701600
H	-5.90687900	2.85805500	1.43606100
H	-5.43704900	4.43727900	0.78562100
H	-4.35196300	3.55791300	1.86988700
C	-5.53707800	2.56772200	-1.23490000
H	-6.40165900	2.02759400	-0.84880500
H	-5.15818900	2.03366500	-2.10762100
H	-5.88530100	3.54820200	-1.56341500
C	-1.44905600	1.22223300	3.92510600
H	-2.14893300	0.59817300	4.48212100
H	-1.96315700	2.14903100	3.66949400
H	-0.60992000	1.46558900	4.58116200
C	-0.23201300	-0.80820900	3.14338600
H	0.03406000	-1.44865400	2.30597400
H	0.68795300	-0.50874300	3.64989500
H	-0.82771400	-1.38955900	3.83956300
C	-3.42399900	-3.06218900	2.46004400
H	-3.35357900	-3.57439000	1.50106300
H	-4.46869100	-2.85598400	2.69791400
H	-1.31493300	4.18125500	-0.28788600
H	-2.96310500	3.13255300	-1.67791300
H	-3.70068300	4.58941800	-1.03161000
H	-4.70353300	-1.73136000	0.86539500
O	-4.33835800	-1.90275400	-1.84687600
C	-5.34148700	-2.90072800	-1.58831200
H	-4.84804500	-3.86543900	-1.44375400
H	-5.87262500	-2.64382500	-0.66817200
C	-6.28738300	-2.92999400	-2.76421100
H	-6.76202000	-1.95780900	-2.90133300
H	-5.75923300	-3.19555400	-3.68036000
H	-7.06738000	-3.67137200	-2.58691200
H	-2.99586600	-3.69420900	3.23266300

INT-I-B

Cl	-0.62242900	-2.68550000	0.11125300
O	5.66386800	-0.95723000	0.76540800
N	8.92753100	-0.70913500	1.87775600
N	8.66651600	1.91083800	-1.60121300
N	5.29418900	1.89660900	-3.02583500
C	8.27591800	-0.26955200	1.02606900
C	8.12208900	1.17264700	-0.89347800
C	5.27584500	1.17366100	-2.12061800
C	7.49566000	0.27274700	-0.01304500
C	6.14245900	-0.09000300	-0.13819800
C	5.15190300	0.28438800	-1.04679900
C	3.92529100	-0.38626500	-0.71327200
C	4.23807600	-1.24004000	0.50667300
C	4.14701900	-2.73639700	0.23915200
H	3.11446900	-3.03154400	0.06239500
H	4.52437600	-3.28857600	1.10012000
H	4.73639000	-2.99981000	-0.63853500
C	3.49158200	-0.81386600	1.76374400
H	2.43303900	-1.04871500	1.68059700
H	3.59559300	0.25881000	1.92321100
H	3.89551500	-1.34298800	2.62704100
C	2.73812400	-0.26277700	-1.36495100
H	2.73167400	0.40223100	-2.21968800
C	1.51922300	-0.91150000	-1.00636500
H	1.56134800	-1.59510100	-0.17313400
C	0.30263600	-0.74399100	-1.58850800
C	0.07622300	0.17285100	-2.76667000
H	0.10049000	-0.41736400	-3.69017700
H	0.88247400	0.89995800	-2.83909600
C	-1.26416400	0.89218800	-2.66935100
H	-1.24964200	1.54274200	-1.79262100
C	-2.40371400	-0.10777400	-2.54244200
H	-2.53379100	-0.64384900	-3.48890100
H	-3.34816900	0.40088900	-2.36296900
C	-2.15465000	-1.12139500	-1.45209200

C	-0.88835900	-1.40778300	-1.08750500
C	-3.34710800	-1.77531400	-0.82220300
H	-3.07314600	-2.75837700	-0.44411800
H	-1.41743000	1.52868000	-3.54221100
O	-2.82255100	-1.81656200	2.42281600
N	-1.66933500	2.47531300	0.80212700
C	-4.33416800	2.87635000	-0.20578100
C	-3.16458100	3.65354300	-0.81626700
C	-1.99864600	3.74667700	0.13862400
H	-2.18936100	4.47988100	0.92611200
C	-0.34678200	2.51547800	1.43508400
H	0.35684800	2.87114900	0.68218800
H	-0.38652800	3.27442900	2.22051100
C	0.08326300	1.17858700	1.97831400
H	0.93501800	1.33548900	2.64069500
H	0.41845000	0.53909400	1.16025600
C	-1.04752700	0.46442800	2.73551600
C	-2.17827600	0.29884000	1.71369900
C	-2.95825100	-0.81523300	1.55484100
C	-3.92944100	-0.94095000	0.43417900
C	-4.43117300	0.37090900	-0.02785300
H	-5.34074500	0.35170800	-0.60738300
C	-3.79347900	1.51890900	0.20491000
C	-2.49668400	1.44536600	0.89577900
C	-4.87091000	3.58850700	1.05160900
H	-5.73288400	3.04950800	1.44566600
H	-5.18222800	4.60468800	0.80294100
H	-4.12717000	3.64667500	1.84655400
C	-5.45695300	2.77896800	-1.23847000
H	-6.33279600	2.26670900	-0.83953200
H	-5.12977500	2.25661100	-2.13867900
H	-5.76750300	3.78443100	-1.52551300
C	-1.55749800	1.32182800	3.90911200
H	-2.32859600	0.77987100	4.45762600
H	-1.98859900	2.26769700	3.58063900
H	-0.73859700	1.54223600	4.59727200
C	-0.44339800	-0.82539700	3.30643100
H	-0.15635300	-1.51891200	2.51957800
H	0.45400300	-0.55458300	3.86636500
H	-1.12229200	-1.33576200	3.98257400
C	-3.61783200	-3.00545800	2.36546200
H	-3.42686200	-3.56842400	1.45428000
H	-4.67862100	-2.77276700	2.45548500
H	-1.10016700	4.06986000	-0.38527100
H	-2.85271900	3.16391100	-1.73994700
H	-3.47751700	4.66547900	-1.07709100
H	-4.78406500	-1.52965700	0.76805200
O	-4.36769300	-1.90231400	-1.78402600
C	-5.30008500	-2.95646400	-1.54115100
H	-4.75471200	-3.90082600	-1.43552200
H	-5.84134500	-2.77621800	-0.60564600
C	-6.26524300	-3.01182900	-2.70276800
H	-6.80765800	-2.07025000	-2.79850800
H	-5.73512100	-3.20551000	-3.63605900
H	-6.98997000	-3.81166100	-2.54444700
H	-3.30366100	-3.59417000	3.22169300

TS-I-B

Cl	-0.35231100	-0.05357300	-1.81928600
O	-6.75574000	1.15307400	-0.80561700
N	-9.90945400	2.55732900	-0.90506900
N	-10.29811100	-1.02319000	1.55459800
N	-7.08172800	-2.75887000	1.88578200
C	-9.39771000	1.63265700	-0.42873500
C	-9.60098100	-0.34345600	0.92632700
C	-6.89253500	-1.83172100	1.21677900
C	-8.78848100	0.50608400	0.15545300
C	-7.41538600	0.26670400	-0.04468000
C	-6.56390400	-0.74172500	0.40303700

C	-5.23665100	-0.50104800	-0.10161100
C	-5.33396000	0.77339500	-0.92682000
C	-5.08299700	0.55711500	-2.41311500
H	-4.04097900	0.29980000	-2.59288300
H	-5.31613400	1.46917200	-2.96317800
H	-5.70816000	-0.25309600	-2.78726100
C	-4.53828700	1.93655800	-0.34986600
H	-3.46959500	1.74793400	-0.43184700
H	-4.78427000	2.07749200	0.70223400
H	-4.77321800	2.85079400	-0.89554800
C	-4.13770800	-1.26630600	0.12551200
H	-4.28964700	-2.14376300	0.74229800
C	-2.82148900	-1.01770000	-0.37364100
H	-2.69413500	-0.15411900	-1.00782000
C	-1.71129900	-1.76314000	-0.13899700
C	-1.72353100	-3.00508500	0.72192500
H	-1.86948400	-3.88606600	0.08537700
H	-2.56499700	-2.97481500	1.41156300
C	-0.42010600	-3.16121400	1.49861900
H	-0.30818500	-2.31479500	2.18119400
C	0.76705400	-3.20906900	0.54720100
H	0.78187900	-4.17186200	0.02466800
H	1.70998900	-3.16904900	1.09604100
C	0.73522800	-2.08864400	-0.46145700
C	-0.41644000	-1.43989600	-0.71312000
C	2.04905500	-1.68832900	-1.10017300
H	1.86076700	-1.39503400	-2.13417800
H	-0.44859400	-4.06582600	2.10810500
O	3.27200900	0.47726000	-2.53059200
N	2.79056300	3.40637700	1.18249200
C	1.96571200	1.27016400	2.95738000
C	1.51864100	2.71812100	3.16831800
C	2.51088900	3.69550000	2.58713000
H	3.44877300	3.69463000	3.15133800
C	3.37607700	4.50090600	0.41680700
H	3.12020100	5.43084800	0.91989200
H	4.46696000	4.41317900	0.42776600
C	2.82847600	4.47809000	-0.98697100
H	3.22658600	5.31678200	-1.55960200
H	1.74444100	4.60478600	-0.93328600
C	3.16325600	3.16683800	-1.71261000
C	2.92991200	1.98157300	-0.75986400
C	2.97397200	0.68205100	-1.22297600
C	2.69427800	-0.47329000	-0.39619100
C	2.23890500	-0.16286600	0.92958200
H	1.94809300	-0.99556600	1.55109200
C	2.26418300	1.07379500	1.47450500
C	2.65452900	2.18653700	0.63835900
C	3.24463700	0.97260900	3.76312100
H	3.52804400	-0.07372700	3.64177100
H	3.07954800	1.16514300	4.82552500
H	4.08751100	1.57945500	3.43142200
C	0.84215800	0.34569700	3.44263500
H	1.13522300	-0.70359900	3.42537600
H	-0.05430300	0.46226900	2.83197700
H	0.58947500	0.59281800	4.47516100
C	4.62914600	3.21222000	-2.17864000
H	4.89698500	2.31256300	-2.72638500
H	5.31469600	3.31126600	-1.33602000
H	4.77865100	4.06836000	-2.84021900
C	2.22743100	3.10762200	-2.93587700
H	1.19107300	2.98161000	-2.61761100
H	2.29931400	4.04985400	-3.48366900
H	2.48136400	2.29690200	-3.61038700
C	4.35942500	-0.40434600	-2.85661500
H	4.26723500	-1.36907200	-2.36423900
H	5.30587500	0.06089900	-2.57403600
H	2.11355400	4.70922700	2.63329600
H	0.54608000	2.86735500	2.69221500
H	1.39664000	2.92248300	4.23297400
H	3.91086000	-0.87660900	-0.06017200

O	2.97151900	-2.77713600	-1.10379600
C	2.71260300	-3.73976100	-2.12449700
H	1.69001500	-4.12004200	-2.03387400
H	2.79568900	-3.25401000	-3.10454600
C	3.71689600	-4.86108100	-1.98873700
H	4.73527100	-4.48106800	-2.08369300
H	3.61817000	-5.35234900	-1.01950200
H	3.55345300	-5.60548100	-2.76917900
C	6.07249200	-0.22460200	0.63771500
C	7.31028400	-0.46802500	1.20856200
C	7.64073500	-1.77565400	1.54515900
C	6.72617100	-2.79312800	1.30187300
C	5.50748500	-2.46974900	0.72721800
N	5.20467400	-1.21151200	0.40593000
H	8.59986900	-1.99827500	1.99267700
H	5.75735400	0.77135300	0.35540500
H	7.99517800	0.34877700	1.38447800
H	6.95004800	-3.82055200	1.55038000
H	4.75016800	-3.20782600	0.50325900
H	4.32304400	-0.53131200	-3.93471600

INT-I-C

Cl	-0.83483900	0.50672100	-1.81964000
O	-7.23233600	1.43623900	-0.50691200
N	-10.42538900	2.74817600	-0.38832400
N	-10.63632000	-1.03439200	1.76603200
N	-7.35210600	-2.68994800	1.86337900
C	-9.87122400	1.80365200	-0.00818900
C	-9.97663700	-0.28406000	1.17904100
C	-7.21480900	-1.70639600	1.26599300
C	-9.21212600	0.65126200	0.46024600
C	-7.84047900	0.47077300	0.19839200
C	-6.94627900	-0.54473300	0.53324400
C	-5.64516100	-0.22414200	0.00552800
C	-5.80643600	1.10982700	-0.70791200
C	-5.60514300	1.02238000	-2.21487100
H	-4.56423600	0.81046300	-2.45117700
H	-5.88187600	1.96906900	-2.67954600
H	-6.22269300	0.22766000	-2.63240400
C	-5.02070800	2.24482800	-0.06538600
H	-3.95132200	2.09524900	-0.20117700
H	-5.22990200	2.29194200	1.00293400
H	-5.30045800	3.19326800	-0.52469900
C	-4.51890000	-0.97359800	0.12868600
H	-4.62511800	-1.90375600	0.67364000
C	-3.23013100	-0.65013400	-0.39831600
H	-3.14575300	0.26853900	-0.95765500
C	-2.09950700	-1.39258700	-0.27864100
C	-2.06605400	-2.70598600	0.47028200
H	-2.30079800	-3.52391200	-0.22151100
H	-2.83876400	-2.71612100	1.23730400
C	-0.70369100	-2.96649600	1.10313500
H	-0.50308000	-2.19973100	1.85684300
C	0.38834300	-2.93295500	0.04396600
H	0.29506500	-3.81268600	-0.60309200
H	1.37640700	-3.01521500	0.49782600
C	0.31999800	-1.67904100	-0.79302900
C	-0.83906000	-1.00094100	-0.88721200
C	1.59120700	-1.19464300	-1.45886400
H	1.34945500	-0.77944000	-2.43675900
H	-0.70319600	-3.93084400	1.61368600
O	2.85042400	1.09256500	-2.63747300
N	4.27934200	2.75440000	1.67105000
C	3.01818700	0.48858600	3.03789900
C	3.52537600	1.75139900	3.74570000
C	4.69173400	2.36955100	3.00795000
H	5.54444400	1.67559100	2.97080600
C	5.09376400	3.75336100	1.01239700
H	5.35937300	4.51033200	1.75048300

H	6.03377900	3.31974700	0.63981000
C	4.29144400	4.36086800	-0.11127000
H	4.84118600	5.18024000	-0.57688000
H	3.37808700	4.78149200	0.31654200
C	3.92979300	3.32444100	-1.18846600
C	3.48180100	2.01349500	-0.51404300
C	2.89600900	0.98073200	-1.26156600
C	2.30354800	-0.13430100	-0.65526400
C	2.35294000	-0.21645300	0.72909700
H	1.87615300	-1.05619800	1.21041300
C	2.99630400	0.71216900	1.52264700
C	3.59599000	1.83635600	0.89768000
C	3.93846400	-0.69862800	3.37475400
H	3.61996200	-1.60009700	2.84957200
H	3.91146400	-0.90338700	4.44747100
H	4.97152000	-0.49704900	3.09327600
C	1.60611700	0.18276000	3.56418800
H	1.22560500	-0.76893500	3.19374100
H	0.90528300	0.96629800	3.27256100
H	1.62416400	0.12657300	4.65470900
C	5.15676900	3.11671200	-2.09382300
H	4.91759200	2.50080700	-2.95494500
H	5.97889900	2.64559900	-1.55347600
H	5.50483100	4.08360700	-2.46453000
C	2.78404000	3.94031400	-2.01441300
H	1.89048600	4.05627100	-1.39829000
H	3.08413600	4.93203000	-2.36153500
H	2.53203000	3.33263000	-2.87791400
C	3.74953800	0.24961100	-3.36315200
H	3.52919500	-0.80465500	-3.20781600
H	4.78411900	0.43839600	-3.06910300
H	5.03356900	3.26845700	3.52067000
H	2.72248200	2.49102900	3.79689700
H	3.81136000	1.50789500	4.77074200
H	3.97488100	-2.24151900	-0.77982600
O	2.50560300	-2.29831300	-1.66435500
C	2.15922200	-3.15685300	-2.75981600
H	1.11570300	-3.46444400	-2.66108800
H	2.25260700	-2.59277300	-3.69370800
C	3.07937400	-4.35446200	-2.74903500
H	4.12271700	-4.04848600	-2.84262800
H	2.95946200	-4.92652700	-1.82762000
H	2.84318200	-5.00898500	-3.58865600
C	5.48340900	-1.05047500	-0.05225500
C	6.62461500	-0.99245300	0.71767000
C	7.07929300	-2.15041500	1.33708300
C	6.38109900	-3.34239900	1.17406300
C	5.24905100	-3.34956200	0.38825300
N	4.83925100	-2.21675200	-0.20043500
H	7.96923800	-2.12435300	1.95015200
H	5.05298400	-0.19476400	-0.54738300
H	7.13731900	-0.05022600	0.83612500
H	6.70675100	-4.25538800	1.64841700
H	4.65155600	-4.22989000	0.21045400
H	3.62292700	0.49945400	-4.41399100

TS-I-C

Cl	-1.31324100	1.99717100	-0.68013300
O	-7.80646100	1.50776700	0.20483700
N	-11.16990000	2.23224200	0.55523100
N	-10.83617700	-2.08602100	1.06509800
N	-7.37046500	-3.20214000	0.73500700
C	-10.48590400	1.29772000	0.58339100
C	-10.29027500	-1.08489900	0.86304400
C	-7.36089600	-2.05312800	0.59125100
C	-9.66585400	0.15243400	0.62060000
C	-8.28206800	0.27544500	0.42198400
C	-7.24902200	-0.66903200	0.40430000
C	-6.00697900	-0.00375000	0.15989700

C	-6.34289500	1.47198400	0.01590500
C	-6.08702200	2.02113500	-1.38133600
H	-5.01950900	2.06142200	-1.58842200
H	-6.49464600	3.02906200	-1.45935200
H	-6.56089400	1.38675100	-2.12971800
C	-5.75545800	2.34214900	1.11895700
H	-4.67246400	2.39783700	1.02808600
H	-5.99936700	1.92927900	2.09725900
H	-6.16285100	3.35063200	1.04651700
C	-4.77893700	-0.59486300	0.07587100
H	-4.76037500	-1.67024800	0.20169900
C	-3.55072200	0.07230000	-0.16849200
H	-3.58960900	1.13979200	-0.31573800
C	-2.32004000	-0.51461600	-0.25454900
C	-2.15116700	-2.00856200	-0.05914700
H	-2.43075500	-2.52618300	-0.98389100
H	-2.84579600	-2.35235700	0.70731500
C	-0.72990200	-2.40492300	0.32050700
H	-0.50157400	-2.04781600	1.32860600
C	0.25288800	-1.79601800	-0.66765500
H	0.04859800	-2.20543700	-1.66343800
H	1.27623900	-2.07881400	-0.44058200
C	0.11139400	-0.29020600	-0.72087500
C	-1.13132300	0.24128700	-0.56045000
C	1.27396000	0.54977700	-0.98813300
H	1.03548400	1.51672500	-1.40482000
H	-0.63615000	-3.49162300	0.33069300
O	3.12792600	2.58084100	-1.21581000
N	5.88243800	0.63221700	2.25483900
C	3.83769200	-1.37733900	2.82796200
C	4.95499600	-1.00075900	3.80508500
C	6.18996700	-0.53165600	3.07084000
H	6.60739300	-1.33262100	2.44830400
C	6.95635600	1.58973900	2.07866800
H	7.47560500	1.68648300	3.03292800
H	7.69180900	1.21930800	1.35415600
C	6.39160300	2.92023800	1.65558400
H	7.20400900	3.63346800	1.50996600
H	5.75739100	3.30595600	2.45820900
C	5.56927200	2.82493400	0.36187200
C	4.53513900	1.69690600	0.52011400
C	3.40185200	1.60937700	-0.28546600
C	2.43746000	0.58576100	-0.12641600
C	2.63028300	-0.32096100	0.91785400
H	1.86876500	-1.05675500	1.10873300
C	3.73412200	-0.31308500	1.73087000
C	4.74201700	0.67278300	1.50717500
C	4.13951200	-2.74612800	2.19138400
H	3.37089800	-3.01523600	1.46590300
H	4.16977100	-3.52026800	2.96161200
H	5.09432900	-2.74555500	1.66799000
C	2.52618700	-1.48106000	3.62308400
H	1.70572100	-1.86785100	3.01883600
H	2.23136500	-0.50756600	4.01766300
H	2.66186600	-2.16521500	4.46320600
C	6.51987700	2.51543900	-0.81034100
H	5.99238200	2.50716600	-1.76006100
H	7.00045100	1.54403500	-0.69361900
H	7.30102900	3.27745000	-0.86644100
C	4.94470100	4.21885300	0.16585500
H	4.16284700	4.39970500	0.90515200
H	5.72303600	4.97196000	0.30756600
H	4.51550600	4.35911500	-0.81965300
C	3.56359400	2.42523800	-2.57246800
H	2.69111200	2.42137300	-3.22364100
H	4.11141800	1.49651100	-2.71198400
H	6.96537800	-0.24104300	3.77807300
H	4.61471900	-0.19509800	4.46075700
H	5.19771400	-1.85699900	4.43697100
H	2.54301400	-0.93395300	-2.36607400
O	1.94456800	-0.09025900	-2.55453100

C	1.03955300	-0.24177200	-3.66271100
H	0.31579800	-1.02905900	-3.44744900
H	0.50008800	0.70138900	-3.74487700
C	1.81684300	-0.54197700	-4.92776900
H	2.53373700	0.25120800	-5.14028400
H	2.35480000	-1.48716100	-4.84491100
H	1.12462700	-0.61887500	-5.76781200
C	4.73729300	-1.58755000	-1.50003700
C	5.75000400	-2.45415700	-1.12465600
C	5.54689000	-3.81927600	-1.27675900
C	4.34018200	-4.26711900	-1.79960700
C	3.38259500	-3.33092700	-2.15662100
N	3.57946800	-2.01783300	-2.00946300
H	6.31426500	-4.52443200	-0.98726600
H	4.84440000	-0.51791100	-1.38177300
H	6.66969600	-2.06322100	-0.71355000
H	4.14088000	-5.32105700	-1.93029800
H	2.42861400	-3.63187800	-2.57049200
H	4.20189800	3.27124200	-2.83015300

Type-I product (TCF1-based)

Cl	-0.82380700	-1.90789800	-0.06243300
O	-7.32678400	-1.38434300	0.32068700
N	-10.72015800	-2.01100200	0.69228600
N	-10.36997300	2.27302400	-0.07225900
N	-6.94487300	3.28587700	-0.51355200
C	-10.03258800	-1.10565700	0.48249000
C	-9.82375300	1.26280400	0.05860900
C	-6.90643400	2.14775800	-0.32053900
C	-9.20036500	0.00780700	0.22585000
C	-7.82419100	-0.16289300	0.14849000
C	-6.77506800	0.76521000	-0.09273700
C	-5.55196000	0.08869800	-0.07153900
C	-5.85523200	-1.37114600	0.20471000
C	-5.32246400	-1.86407800	1.54430600
H	-4.23671500	-1.92901200	1.52525100
H	-5.72581100	-2.85514600	1.74902300
H	-5.61601300	-1.18667900	2.34520000
C	-5.51503900	-2.29565200	-0.95732100
H	-4.43722700	-2.37128400	-1.08413700
H	-5.94811900	-1.91958900	-1.88331500
H	-5.91171100	-3.28995400	-0.75518100
C	-4.30223800	0.67304100	-0.27086900
H	-4.30761900	1.73984100	-0.45203200
C	-3.09461200	-0.00072600	-0.24246200
H	-3.11256100	-1.06014800	-0.04729900
C	-1.82953500	0.57681200	-0.41972300
C	-1.71133000	2.05821100	-0.69823800
H	-1.80010000	2.61277700	0.24263200
H	-2.54644300	2.37455700	-1.32317000
C	-0.40014400	2.40003800	-1.38238800
H	-0.39148400	1.96591000	-2.38604200
C	0.77770100	1.85595400	-0.58929400
H	0.85773100	2.39685300	0.36024800
H	1.69926300	2.04387200	-1.13770400
C	0.65942300	0.36933100	-0.32968300
C	-0.65575700	-0.16973700	-0.31005700
C	1.75537600	-0.45107500	-0.13048800
H	1.53346200	-1.50419700	-0.11951700
H	-0.30346600	3.48037500	-1.49695000
O	3.57568900	-2.52095000	-0.07877500
N	7.28058300	0.52084500	0.07792400
C	5.53534900	2.76739500	0.60584800
C	6.91127800	2.94659700	-0.04145300
C	7.85530800	1.83347100	0.34252300
H	8.13773500	1.90411800	1.39905600
C	8.23019900	-0.57974000	0.06091000
H	9.19387000	-0.18155100	-0.25300200
H	8.36034600	-0.98032000	1.07279800

C	7.75374800	-1.63983300	-0.89769100
H	8.47926800	-2.45271000	-0.94907400
H	7.68824100	-1.19685000	-1.89476000
C	6.38610300	-2.21008600	-0.49545400
C	5.43989800	-1.04437200	-0.15270400
C	4.07074500	-1.23721200	-0.05643900
C	3.13611000	-0.16050700	0.00962800
C	3.68555400	1.12509100	0.20297900
H	3.01589000	1.94812500	0.36808700
C	5.02842700	1.37030200	0.26221100
C	5.94430600	0.28723200	0.05039400
C	5.63482400	2.89779300	2.13810500
H	4.64333700	2.81624100	2.58562400
H	6.05778300	3.86744700	2.41133100
H	6.25755400	2.11715600	2.57515600
C	4.61378400	3.87258400	0.07488700
H	3.64526400	3.88100800	0.57453400
H	4.44656000	3.76447400	-0.99795700
H	5.07700400	4.84483000	0.25243200
C	6.57333500	-3.16080000	0.70008000
H	5.65217300	-3.68701300	0.93351700
H	6.89493400	-2.62809400	1.59550600
H	7.33193000	-3.90876000	0.45806100
C	5.88855200	-3.01227900	-1.71304700
H	5.68914500	-2.34625600	-2.55457900
H	6.66810200	-3.71421200	-2.01789900
H	4.98583800	-3.57315600	-1.49495200
C	3.13912100	-3.01867400	1.19476100
H	2.24516600	-2.49946900	1.54332700
H	3.92698000	-2.90856900	1.94101400
H	8.77791100	1.90711800	-0.23449400
H	6.79551500	2.96377400	-1.12839000
H	7.34534400	3.90243400	0.25646700
H	2.91476200	-4.07249900	1.04854500

EtOH

O	-1.24310600	-0.25535100	-0.10877900
C	-0.07436500	0.55822200	0.04723100
H	-0.11778500	1.28368900	-0.76581700
H	-0.12756700	1.11328800	0.99012800
C	1.21201600	-0.24409300	-0.02184900
H	1.26179800	-0.97206300	0.79174600
H	1.28393900	-0.77997400	-0.96985000
H	2.07619300	0.41800800	0.06757100
H	-1.25763700	-0.90491600	0.60415500

Pyridine

C	-1.14208500	-0.71936100	0.00000000
C	-1.19406700	0.66942100	-0.00000200
C	0.00000000	1.37841300	0.00000000
C	1.19406600	0.66942200	0.00000100
C	1.14208500	-0.71936000	-0.00000100
N	0.00000000	-1.41232700	0.00000200
H	-0.00000100	2.46055400	0.00000500
H	-2.05789400	-1.30010800	0.00000300
H	-2.14886200	1.17736900	-0.00000100
H	2.14886200	1.17737100	0.00000200
H	2.05789400	-1.30010700	-0.00000600

TCF1-based (Path II)

INT-II-A

Cl	-1.35622800	0.77928800	-1.73602900
O	5.06890400	-0.42790400	-1.43904400

N	8.27131300	-1.69373600	-1.90688400
N	8.62119800	1.34858000	1.20692400
N	5.47231700	2.88946300	1.95122900
C	7.74945500	-0.90116900	-1.24799100
C	7.92722200	0.78606300	0.47455700
C	5.24177300	2.11446100	1.12792200
C	7.11830700	0.07166300	-0.43685500
C	5.75648300	0.28747500	-0.55795100
C	4.88390800	1.19019400	0.12544500
C	3.59349300	1.02120300	-0.35377900
C	3.63839000	-0.06345200	-1.40999400
C	3.29782800	0.42699000	-2.81140200
H	2.23653900	0.65192600	-2.89145900
H	3.54067700	-0.35394500	-3.53086100
H	3.86466600	1.32500600	-3.05284100
C	2.88969600	-1.32849600	-1.01441500
H	1.81680200	-1.15452300	-0.99120500
H	3.20295200	-1.66650600	-0.02835600
H	3.10073600	-2.10946400	-1.74322100
C	2.46814400	1.73988900	0.08155600
H	2.65333700	2.48325100	0.84540900
C	1.19446700	1.55940500	-0.39089400
H	1.03254800	0.81568300	-1.15379200
C	0.05112000	2.28046800	0.02401900
C	0.17394600	3.32891100	1.10828800
H	0.57630000	4.25066900	0.67448100
H	0.90301400	2.99166700	1.84553300
C	-1.15214600	3.61264900	1.79989200
H	-1.44718000	2.73966400	2.38725000
C	-2.23608500	3.92745000	0.78006700
H	-2.01181000	4.87837700	0.28500000
H	-3.20339700	4.05153300	1.26565100
C	-2.34511000	2.84184800	-0.26539800
C	-1.18104200	2.06910200	-0.56037900
C	-3.51845100	2.63997300	-0.91923500
H	-3.62406500	1.89604300	-1.69743600
H	-1.03785500	4.44412200	2.49601900
O	-4.59105200	3.37118900	-0.64418300
C	-5.80131300	3.04076000	-1.37350000
H	-5.59587700	3.14497400	-2.44047200
H	-6.05425700	2.00021700	-1.16177400
C	-6.89004500	3.97942800	-0.92022100
H	-7.07708000	3.87004700	0.14841600
H	-6.62129800	5.01569900	-1.12704600
H	-7.81146100	3.74901900	-1.45627300
O	-4.26542800	0.39180700	0.20055200
O	0.70522200	-3.38149900	0.58271500
N	-3.37503600	-1.02070700	1.48790900
C	-4.65669900	-2.13906700	-0.90695600
C	-5.40886200	-1.44050400	0.23269500
C	-4.54954900	-0.39848800	0.90920900
C	-2.65002700	-0.20017600	2.43636100
H	-3.37878800	0.32412000	3.05525900
H	-2.05239100	0.56444500	1.92096100
C	-1.77309000	-1.09137000	3.27914200
H	-1.27163800	-0.51326000	4.05799900
H	-2.41504100	-1.82219900	3.77748500
C	-0.71325400	-1.81831000	2.43503300
C	-1.32133500	-2.27260500	1.09597900
C	-0.58284500	-3.09207300	0.22371500
C	-1.12822000	-3.57788800	-0.95985900
H	-0.55407600	-4.20235200	-1.62549400
C	-2.43811900	-3.25583500	-1.27572700
H	-2.85605800	-3.65577900	-2.19005900
C	-3.21763400	-2.43805200	-0.47641300
C	-2.63642800	-1.90284900	0.70311600
C	-4.65170400	-1.23959500	-2.15571200
H	-4.12658300	-1.72350600	-2.98018700
H	-5.67413600	-1.02749600	-2.47798700
H	-4.14815800	-0.29476200	-1.95977800
C	-5.41080600	-3.43673900	-1.24150600

H	-4.98988900	-3.94316400	-2.11001700
H	-5.38404200	-4.12806100	-0.39756000
H	-6.45610600	-3.21035400	-1.46548700
C	0.46346700	-0.85429800	2.19880000
H	1.22919800	-1.30872400	1.57652400
H	0.12652600	0.05747000	1.70795600
H	0.91471700	-0.57720200	3.15510100
C	-0.23717300	-3.01607600	3.28117500
H	-1.03922800	-3.74913400	3.38882300
H	0.03206500	-2.66397400	4.28024200
H	0.62606800	-3.51003800	2.84672000
C	1.41604700	-4.36766900	-0.14927900
H	1.59090800	-4.05782000	-1.18186500
H	-5.10051100	0.08595800	1.71630200
H	-5.70598900	-2.17901100	0.98194400
H	-6.32205000	-0.98328700	-0.15443100
H	2.37245800	-4.48133000	0.35521600
H	0.88475800	-5.32250200	-0.14591400

TS-II-A

Cl	1.34206000	-0.55460600	-1.74912100
O	-5.06737800	0.52049200	-1.30979100
N	-8.23723200	1.85094000	-1.70357000
N	-8.70695800	-1.54766800	0.99197800
N	-5.52273300	-3.18999000	1.63548600
C	-7.73924800	0.97577800	-1.13199100
C	-7.98606700	-0.90297500	0.35598800
C	-5.29413100	-2.31355100	0.91520000
C	-7.14437300	-0.09311000	-0.43041400
C	-5.76575700	-0.31266800	-0.53260500
C	-4.92400500	-1.27776500	0.04496300
C	-3.58821800	-1.05204600	-0.38681300
C	-3.63663800	0.15632900	-1.30743300
C	-3.28182900	-0.16898700	-2.75240400
H	-2.22628600	-0.41851900	-2.84018100
H	-3.48859100	0.69554200	-3.38301400
H	-3.86829000	-1.01637500	-3.10577500
C	-2.89837800	1.37446200	-0.77054900
H	-1.82276700	1.21464500	-0.77780200
H	-3.20605200	1.58823400	0.25176600
H	-3.12487000	2.23705000	-1.39647900
C	-2.49083500	-1.79764500	-0.03851100
H	-2.67644900	-2.64062300	0.61492600
C	-1.16965500	-1.54222500	-0.45506300
H	-1.01541500	-0.68919200	-1.09628100
C	-0.04482900	-2.25507600	-0.12045100
C	-0.09338600	-3.48598900	0.75405200
H	-0.15732600	-4.37483900	0.11609300
H	-0.99379700	-3.47582800	1.36505700
C	1.13466500	-3.59336200	1.65117500
H	1.12539600	-2.76756100	2.36590800
C	2.42172300	-3.55775500	0.83734600
H	2.58862500	-4.52561000	0.35247100
H	3.28268600	-3.40738500	1.49146700
C	2.42064700	-2.48477100	-0.22516600
C	1.24822800	-1.88759900	-0.60374000
C	3.69630500	-2.07369500	-0.76175000
H	3.69743100	-1.67393300	-1.77380300
H	1.09402600	-4.51372400	2.23505800
O	4.72753400	-2.91456600	-0.48813900
C	5.93787000	-2.67096100	-1.22942600
H	5.69725200	-2.65859300	-2.29578100
H	6.32872000	-1.68831500	-0.95515400
C	6.92509600	-3.76154900	-0.89486500
H	7.15359600	-3.76360200	0.17141300
H	6.53068200	-4.73968500	-1.17179000
H	7.85206300	-3.59505400	-1.44490300
H	3.98304100	-0.92872800	-0.13274100
O	-0.63482900	3.44932600	0.78526500

N	3.17656200	0.59584400	1.25690100
C	4.55379800	1.90217500	-0.98243400
C	5.24290100	1.00950700	0.05981100
C	4.32551400	0.06754800	0.77413800
C	2.47656300	-0.10374200	2.33755400
H	3.20529000	-0.71985300	2.85914600
H	1.71865100	-0.75929600	1.91461200
C	1.84391300	0.91492000	3.24727800
H	1.39362500	0.41326700	4.10464100
H	2.62121400	1.58199900	3.62813300
C	0.76785200	1.72573800	2.51045500
C	1.30582900	2.15385000	1.13702200
C	0.60008300	3.08363800	0.34879400
C	1.14665400	3.59472500	-0.82300400
H	0.60496400	4.31081000	-1.42013100
C	2.41663100	3.20405500	-1.21360000
H	2.83954100	3.64757500	-2.10421200
C	3.14610700	2.26312200	-0.50907500
C	2.54230600	1.69112400	0.63216100
C	4.50428500	1.19973900	-2.34919000
H	4.06625400	1.85637300	-3.10106100
H	5.51318300	0.93702100	-2.67379000
H	3.90356700	0.29565200	-2.31905300
C	5.40768900	3.17541500	-1.12478200
H	5.03172200	3.82371400	-1.91519000
H	5.41929400	3.74187000	-0.19279100
H	6.43535600	2.90496600	-1.37713100
C	-0.50610400	0.87295900	2.36899300
H	-1.29025800	1.42996700	1.86425000
H	-0.32214400	-0.03520800	1.79647700
H	-0.86842700	0.58646400	3.35881700
C	0.47376100	2.95139500	3.39888700
H	1.34259300	3.61076900	3.44223000
H	0.26036400	2.60845500	4.41372800
H	-0.37754400	3.52210700	3.04315200
C	-1.33812300	4.47328300	0.09316600
H	-1.55982300	4.18058000	-0.93485100
H	4.80160800	-0.62242100	1.46495400
H	5.67163400	1.64095500	0.84663200
H	6.07182000	0.46520900	-0.38889000
H	-2.26933000	4.60980300	0.63617500
H	-0.77302500	5.40797900	0.09223100

INT-II-B

Cl	1.04853700	-0.07225500	-1.78049700
O	-5.43590400	1.01594700	-0.82644800
N	-8.58668900	2.42416200	-0.75194400
N	-8.94798800	-1.37077200	1.36833200
N	-5.73073300	-3.14013000	1.47386200
C	-8.07104200	1.45788200	-0.37282300
C	-8.25921800	-0.63701500	0.79429800
C	-5.55008700	-2.15155600	0.89697000
C	-7.45637900	0.27998400	0.09337200
C	-6.08753200	0.06061000	-0.14675200
C	-5.23041900	-0.98618100	0.19083600
C	-3.90991300	-0.69737700	-0.30364400
C	-4.01716800	0.65129800	-1.00029900
C	-3.77661200	0.56906900	-2.50159500
H	-2.73814900	0.31303400	-2.70472300
H	-3.99713600	1.53042000	-2.96619900
H	-4.41386200	-0.19530100	-2.94501200
C	-3.21915000	1.76517600	-0.33807400
H	-2.15770900	1.63506500	-0.52943900
H	-3.38446300	1.77357000	0.73861200
H	-3.51979300	2.72702500	-0.75313100
C	-2.81993300	-1.50120100	-0.18649100
H	-2.98894600	-2.45016000	0.30752100
C	-1.49753500	-1.22122200	-0.64893000
H	-1.32130100	-0.24219000	-1.06750200

C	-0.44258500	-2.08058500	-0.63835400
C	-0.59018300	-3.52571400	-0.21422600
H	-0.92089600	-4.10623400	-1.08367700
H	-1.37610300	-3.61947400	0.53341800
C	0.70270600	-4.12417000	0.32379200
H	0.94686500	-3.65428000	1.27917800
C	1.85878500	-3.93013800	-0.64827800
H	1.74630500	-4.60281700	-1.50825500
H	2.80366100	-4.20446400	-0.18072300
C	1.95718300	-2.51605700	-1.15924300
C	0.87512900	-1.71357200	-1.12803700
C	3.25699500	-2.07874500	-1.77658500
H	3.19696100	-2.17634500	-2.87233300
H	0.56410000	-5.18695600	0.52786500
O	4.33088700	-2.86296700	-1.29053800
C	5.58301900	-2.44870100	-1.82357700
H	5.55427200	-2.51468500	-2.91861100
H	5.76090000	-1.39748800	-1.56285700
C	6.67098800	-3.33429200	-1.25941600
H	6.70987700	-3.25634400	-0.17208100
H	6.49709400	-4.37772100	-1.52634200
H	7.64049800	-3.03413600	-1.65989700
H	3.44435700	-1.02233400	-1.56207200
O	3.42257200	3.91238400	-1.18034900
N	1.30307400	0.73341500	1.70508500
C	3.76179300	-0.59600300	2.25697400
C	2.42999700	-1.34528200	2.23172800
C	1.26313300	-0.45788700	2.19533000
C	0.03097700	1.47247400	1.54905800
H	-0.64743400	1.12406400	2.32208700
H	-0.37050100	1.18061000	0.58080400
C	0.28763300	2.94966800	1.62873200
H	-0.66434500	3.47744700	1.57307500
H	0.73136000	3.18429700	2.59913800
C	1.20772300	3.43275800	0.49880800
C	2.41040400	2.48837500	0.40096500
C	3.53619600	2.82107400	-0.38636700
C	4.69027200	2.05007300	-0.34117700
H	5.54885900	2.31411300	-0.93796900
C	4.76545900	0.94681900	0.49869000
H	5.69507900	0.40128900	0.55553300
C	3.67802500	0.53548100	1.24142800
C	2.49237200	1.28512300	1.11700400
C	4.87974300	-1.59560900	1.95817800
H	5.86338900	-1.13647900	2.05121300
H	4.83368700	-2.41406400	2.67842200
H	4.77752500	-2.01580200	0.95813300
C	3.98357700	0.02215000	3.65151100
H	4.92506900	0.57111400	3.67090900
H	3.18457500	0.71481400	3.92083200
H	4.02473600	-0.76282700	4.40907000
C	0.42748400	3.49056900	-0.82677400
H	1.06350200	3.84841900	-1.63237700
H	0.04435500	2.51301300	-1.11538800
H	-0.41870500	4.17203500	-0.72333200
C	1.65796300	4.85359400	0.89560300
H	2.29125900	4.82275200	1.78369700
H	0.77250700	5.44662500	1.13290100
H	2.20075200	5.34905700	0.09805700
C	4.53275500	4.30594700	-1.98173800
H	4.79632200	3.52585100	-2.69880400
H	0.29541900	-0.80759200	2.52966400
H	2.33694100	-2.03991100	3.06703700
H	2.35631400	-1.95003400	1.31588000
H	4.20833800	5.19497200	-2.51484600
H	5.39990400	4.54584300	-1.36309100

TS-II-B

Cl	1.06442700	-0.08993100	-1.68502400
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O	-5.44382300	0.96699300	-0.85488400
N	-8.67377500	2.21272500	-0.96160900
N	-8.95028600	-1.63065900	1.08565400
N	-5.70401700	-3.22629300	1.38235500
C	-8.12982900	1.27290500	-0.56300900
C	-8.26796500	-0.85399300	0.56724400
C	-5.51887000	-2.22868900	0.82845400
C	-7.47575600	0.12131000	-0.07242900
C	-6.09839400	-0.01302000	-0.23221000
C	-5.20266400	-1.03759200	0.15300000
C	-3.89984200	-0.68953100	-0.25198300
C	-4.00121700	0.66651700	-0.92455000
C	-3.64301200	0.65022000	-2.40441500
H	-2.57645100	0.48344800	-2.53964200
H	-3.90255000	1.61014200	-2.84984500
H	-4.18612200	-0.14101700	-2.91951900
C	-3.30210200	1.77341300	-0.14870300
H	-2.22562800	1.63566500	-0.18311100
H	-3.61954900	1.77047600	0.89319300
H	-3.53841400	2.73925500	-0.59348800
C	-2.76679200	-1.46184200	-0.05924300
H	-2.92996200	-2.40522600	0.44489000
C	-1.47284000	-1.14457600	-0.46874500
H	-1.31823600	-0.20955900	-0.98420100
C	-0.35478700	-1.96455500	-0.31488500
C	-0.51408000	-3.33407600	0.31796600
H	-0.99855500	-3.98897900	-0.41435200
H	-1.19993100	-3.26480000	1.16274500
C	0.79138700	-3.96411700	0.78615300
H	1.10161200	-3.49901300	1.72320300
C	1.90140800	-3.81529800	-0.24377000
H	1.67647800	-4.41369400	-1.13393800
H	2.84312300	-4.19034300	0.15278200
C	2.08570200	-2.36240200	-0.66178700
C	0.90087700	-1.62316600	-0.83883500
C	3.23935500	-2.08880100	-1.61143200
H	2.90121200	-2.21342300	-2.65073300
H	0.62742600	-5.01955400	1.00839400
O	4.29961800	-2.98616300	-1.35134300
C	5.43342600	-2.73686300	-2.17305400
H	5.14848500	-2.83056000	-3.22860900
H	5.77856500	-1.70647700	-2.01611300
C	6.51911500	-3.72661300	-1.81577200
H	6.80849000	-3.62039700	-0.76920400
H	6.17841600	-4.75006500	-1.97945800
H	7.40032600	-3.55424800	-2.43556800
H	3.58825200	-1.05653800	-1.50625700
O	3.01855000	4.17937500	-1.11571000
N	1.50255000	0.66817000	1.77268200
C	4.07481400	-0.52698400	1.88392400
C	2.79073100	-1.33650400	1.95160800
C	1.62684800	-0.60384500	2.15745200
C	0.16124900	1.25090500	1.76055100
H	-0.40014800	0.81765200	2.58487300
H	-0.32721400	0.94557000	0.83082200
C	0.25359900	2.74781500	1.87726600
H	-0.74992600	3.17248300	1.91716300
H	0.74631400	2.99381300	2.82102000
C	1.02736400	3.37904700	0.70952400
C	2.29939000	2.56409400	0.44668700
C	3.29989100	3.04094100	-0.42797800
C	4.50295200	2.36423500	-0.58312500
H	5.26219200	2.73587200	-1.25268100
C	4.74788900	1.21006200	0.14858200
H	5.70738000	0.72516500	0.04624300
C	3.79322600	0.67215700	0.98745300
C	2.54527400	1.32965200	1.07387100
C	5.23571500	-1.39855400	1.40645100
H	6.17976400	-0.85483900	1.43890800
H	5.33294900	-2.25823100	2.07216900
H	5.07606600	-1.77613400	0.40061900

C	4.41542300	-0.00532900	3.30067200
H	5.33404800	0.58320100	3.26899300
H	3.61832800	0.62497800	3.69607700
H	4.56320400	-0.84253700	3.98594100
C	0.13522800	3.42580300	-0.54383000
H	0.66020700	3.89282400	-1.37350900
H	-0.16231700	2.42725200	-0.86046500
H	-0.76700900	4.00388900	-0.33493600
C	1.36496000	4.81664700	1.15425300
H	2.07056900	4.80444800	1.98687300
H	0.44926800	5.30422400	1.49590900
H	1.78922500	5.40654600	0.34885500
C	3.99939400	4.71765000	-1.99388900
H	4.23496200	4.01982200	-2.80051800
H	0.72306600	-1.05910800	2.53731000
H	2.85053200	-2.28503000	2.47425800
H	2.48612600	-1.79362400	0.60501600
H	3.55769700	5.61815900	-2.41192200
H	4.91402200	4.97596400	-1.45565700

JD1'(-2H)

O	-2.71995500	-1.51893800	-0.11227200
N	0.89171400	1.63661500	-0.10058900
C	2.88011000	-0.47432400	0.07851100
C	3.17411300	0.94056900	-0.33827000
C	2.22731600	1.87621900	-0.37696400
C	-0.05253800	2.70323500	-0.39320900
H	0.43189200	3.65196000	-0.16606900
H	-0.30614600	2.70997300	-1.46092900
C	-1.28380500	2.51360900	0.45457000
H	-1.98186100	3.33775100	0.29703200
H	-0.98287700	2.53706800	1.50529600
C	-1.99842900	1.18634700	0.15267400
C	-0.96401300	0.05822800	0.01268300
C	-1.37527300	-1.28628400	-0.06715900
C	-0.45328200	-2.32568900	-0.11245600
H	-0.77455300	-3.35377800	-0.16350800
C	0.90142900	-2.03212400	-0.07960700
H	1.60245500	-2.85505100	-0.08317400
C	1.37622600	-0.73290300	-0.04388900
C	0.42627600	0.31911300	-0.03557600
C	3.70641000	-1.43288900	-0.79707600
H	3.62982600	-2.46697100	-0.46051700
H	4.76053800	-1.15164300	-0.74988800
H	3.38570600	-1.38304800	-1.83849200
C	3.30540700	-0.66446100	1.55372900
H	3.12495200	-1.69214500	1.87759500
H	2.74076700	0.00562500	2.20331600
H	4.36916400	-0.44479900	1.67516300
C	-2.81336500	1.33734400	-1.14573900
H	-3.32405500	0.41006200	-1.39552300
H	-2.17200200	1.60792500	-1.98557600
H	-3.56308100	2.12325300	-1.02402800
C	-2.95622900	0.94384000	1.33662000
H	-2.39138900	0.74184100	2.24890000
H	-3.55140400	1.84503000	1.50304500
H	-3.63168800	0.11373100	1.15829300
C	-3.18647900	-2.85860900	-0.16781800
H	-2.87062500	-3.42818200	0.70960800
H	-2.83972200	-3.36504000	-1.07194300
H	2.45071100	2.90461700	-0.62663400
H	4.19936800	1.21361000	-0.55100000
H	-4.27158000	-2.79393000	-0.18480600

TCF-A2(+2H)

CI	2.92150100	-1.54907000	-1.47249800
O	-3.57787400	-1.41324000	-0.26212100
N	-6.95176200	-2.16042500	0.16336600

N	-6.51708100	2.07123000	1.15014300
N	-3.15119200	3.20600300	0.81042900
C	-6.25502200	-1.24556200	0.26576300
C	-5.99698700	1.09853600	0.80916200
C	-3.11538500	2.08873700	0.52836700
C	-5.40719200	-0.11781900	0.39431200
C	-4.06092800	-0.24021300	0.11916500
C	-2.99903100	0.72761800	0.17031700
C	-1.82071000	0.11731000	-0.19411500
C	-2.12388400	-1.33212800	-0.50400500
C	-1.47698300	-2.31273500	0.46656300
H	-0.40025700	-2.34647000	0.31667000
H	-1.88310600	-3.30775200	0.29055400
H	-1.67676000	-2.02113300	1.49662800
C	-1.91537100	-1.69985600	-1.96809100
H	-0.85641100	-1.69880500	-2.21617800
H	-2.42629000	-0.99115900	-2.61834400
H	-2.31232100	-2.69848400	-2.14471200
C	-0.56056500	0.76477400	-0.25699500
H	-0.56386200	1.81248800	0.01267500
C	0.60467400	0.16625400	-0.61412600
H	0.59726600	-0.88035000	-0.87301100
C	1.88686500	0.81157500	-0.64993300
C	1.97389200	2.28812600	-0.32621500
H	1.86494400	2.42380700	0.75470300
H	1.12518600	2.79585700	-0.78706800
C	3.27245300	2.92265100	-0.80596100
H	3.26392800	2.99090800	-1.89796300
C	4.45788600	2.09017500	-0.35080700
H	4.45516000	2.01775600	0.73891900
H	5.40165500	2.55328400	-0.64264300
C	4.41223500	0.67476800	-0.94026900
C	3.01243800	0.12246300	-0.95769400
C	5.39396300	-0.24537300	-0.21415600
H	5.50002800	-1.19783400	-0.74210100
H	3.34702300	3.94106800	-0.42226100
O	4.92989900	-0.46713900	1.10267400
C	5.77954400	-1.32492300	1.85381900
H	5.87332600	-2.28914000	1.33781600
H	6.78306300	-0.88425600	1.91495600
C	5.18962100	-1.51016900	3.23386700
H	5.10728900	-0.55296200	3.75107700
H	4.19659000	-1.95808800	3.17209600
H	5.82687000	-2.16756000	3.82741700
H	6.37773700	0.24035500	-0.19831700
H	4.74838800	0.71278600	-1.98426900

INT-II-C

Cl	1.31224400	-0.53243400	-1.71658200
O	-5.10822200	0.58267500	-1.34710600
N	-8.30936300	1.88566400	-1.70086700
N	-8.65172700	-1.38374500	1.17401200
N	-5.49818900	-2.97998800	1.78593300
C	-7.78600200	1.04420300	-1.10669300
C	-7.95962900	-0.76850000	0.48321100
C	-5.27254400	-2.14588000	1.02077700
C	-7.15355400	0.01159300	-0.37492700
C	-5.79198300	-0.19771300	-0.51889300
C	-4.91897600	-1.15065900	0.08787400
C	-3.62902700	-0.94976600	-0.38659900
C	-3.67962400	0.21026600	-1.35985300
C	-3.35635700	-0.18248700	-2.79584800
H	-2.30159300	-0.42897500	-2.89631000
H	-3.58134800	0.65459900	-3.45549700
H	-3.94647200	-1.04599200	-3.09975600
C	-2.91980300	1.44176400	-0.88629000
H	-1.84655900	1.26992000	-0.90845300
H	-3.20449100	1.70167200	0.13173000
H	-3.15134500	2.27697600	-1.54555000

C	-2.50417000	-1.70064500	-0.01676200
H	-2.68595600	-2.50449400	0.68408100
C	-1.22910500	-1.47621100	-0.47347700
H	-1.07216900	-0.66796100	-1.16873300
C	-0.08122200	-2.21529300	-0.11738600
C	-0.20119400	-3.37249500	0.85089600
H	-0.59408200	-4.24417700	0.31653000
H	-0.93886400	-3.12233500	1.61393500
C	1.11897900	-3.72545800	1.52191600
H	1.39161100	-2.93436500	2.22419700
C	2.22635900	-3.89206900	0.49189500
H	2.02623000	-4.77561900	-0.12379400
H	3.18539000	-4.06365900	0.97892800
C	2.33559900	-2.68069000	-0.40504200
C	1.15782100	-1.91910700	-0.65574300
C	3.52694400	-2.35291700	-0.97517200
H	3.63663800	-1.50165500	-1.63120200
H	1.00553000	-4.64127400	2.10298400
O	4.61364100	-3.07113700	-0.74468900
C	5.81925600	-2.71688400	-1.46758300
H	5.85927800	-3.35049500	-2.35484000
H	5.74477600	-1.67530900	-1.77951000
C	7.00652400	-2.94438000	-0.56532200
H	6.95753300	-2.29940000	0.31242100
H	7.05194400	-3.98284000	-0.23628100
H	7.92359600	-2.71706900	-1.11063900
O	-0.53752600	3.32526700	0.67424700
N	3.36225600	0.64735400	1.42783400
C	4.72800500	1.79425800	-0.89083900
C	5.22960300	0.63648400	-0.07376100
C	4.56842600	0.15280300	0.97707100
C	2.64492500	-0.08897200	2.45325200
H	3.37325300	-0.63981300	3.04640300
H	1.97233400	-0.82098400	1.99528500
C	1.87441400	0.88664000	3.30628600
H	1.37467900	0.36361500	4.12367900
H	2.58459600	1.58793100	3.75201800
C	0.82477800	1.65861900	2.48960000
C	1.42217100	2.08585500	1.13850900
C	0.72549800	2.97022500	0.29413700
C	1.29398700	3.45155000	-0.87959400
H	0.75814600	4.13574200	-1.51807800
C	2.57650300	3.05344000	-1.22368700
H	3.01479400	3.46182500	-2.12424000
C	3.30026000	2.15136600	-0.46468800
C	2.69202100	1.63577600	0.70482300
C	4.78890400	1.41122300	-2.38353600
H	4.55601600	2.25746700	-3.03067700
H	5.79461200	1.06891200	-2.63724000
H	4.08559800	0.60936800	-2.60858400
C	5.65426400	3.00983200	-0.65934800
H	5.33909500	3.86232800	-1.26468200
H	5.63718400	3.30733700	0.38981000
H	6.68346900	2.75932100	-0.92891400
C	-0.40559500	0.75742000	2.28261800
H	-1.16376200	1.25937300	1.68754500
H	-0.13593300	-0.16608300	1.77277900
H	-0.84213600	0.49645200	3.24994200
C	0.43139600	2.87844100	3.34698400
H	1.26991400	3.57258500	3.43086800
H	0.17437600	2.53862500	4.35316400
H	-0.41951200	3.41254500	2.93697700
C	-1.20206800	4.36129000	-0.03364700
H	-0.62298600	5.28755800	-0.01431600
H	-1.39729700	4.08010800	-1.07068900
H	4.95389800	-0.67314300	1.55906400
H	6.19163600	0.21365000	-0.33094400
H	-2.14844300	4.51213900	0.47954000

Cl	1.37833900	-0.52208500	-1.84261600
O	-5.08029700	0.20573400	-1.39733500
N	-8.33681800	1.23191600	-1.94051600
N	-8.53788200	-1.64533100	1.33273400
N	-5.23212900	-2.98803600	2.12829600
C	-7.77304200	0.50535900	-1.23605800
C	-7.87221500	-1.08500200	0.56852800
C	-5.07972800	-2.22437800	1.27127000
C	-7.09886000	-0.38164500	-0.37336400
C	-5.70661500	-0.52909000	-0.47019900
C	-4.79583400	-1.32189200	0.23787200
C	-3.47677700	-1.08262300	-0.25937200
C	-3.62649100	-0.04938200	-1.36551100
C	-3.25995500	-0.58446100	-2.74328100
H	-2.18871400	-0.76515500	-2.80932500
H	-3.53847100	0.14304900	-3.50575600
H	-3.78120200	-1.52127000	-2.93729600
C	-2.97698700	1.29160800	-1.05538200
H	-1.89333800	1.20504600	-1.03542300
H	-3.30918600	1.65896900	-0.08572300
H	-3.25331500	2.01565100	-1.82161800
C	-2.33187200	-1.69072900	0.16943800
H	-2.45047900	-2.43353200	0.94838900
C	-1.02731200	-1.42395700	-0.31639600
H	-0.93482500	-0.64889100	-1.06040700
C	0.13370700	-2.03484500	0.06411700
C	0.16542300	-3.17188700	1.05887300
H	0.09857700	-4.11898600	0.51074100
H	-0.70732100	-3.12795400	1.70779200
C	1.43318200	-3.17200000	1.90435800
H	1.42718500	-2.30163400	2.56205700
C	2.68217100	-3.14987000	1.03504000
H	2.85175800	-4.13804000	0.59478800
H	3.56651700	-2.95326900	1.64436300
C	2.61069500	-2.13959100	-0.08574300
C	1.40540800	-1.65904200	-0.49764900
C	3.86865300	-1.73451600	-0.68403700
H	3.81678400	-1.26611100	-1.65780100
H	1.45072500	-4.04989200	2.55167600
O	4.84698800	-2.65534600	-0.54065600
C	5.97749700	-2.55542000	-1.42642800
H	5.61108100	-2.41916500	-2.44665300
H	6.56906400	-1.67832900	-1.15350700
C	6.79170100	-3.81880700	-1.29074500
H	7.14086100	-3.94542900	-0.26548300
H	6.20290200	-4.69216800	-1.57212200
H	7.66196300	-3.76249400	-1.94569400
O	-0.55458500	3.59136000	-0.07264900
N	2.87907300	0.72010900	1.63242600
C	4.58975200	1.22927400	-0.60717500
C	4.65166600	-0.04877500	0.21717300
C	3.93550400	-0.03593300	1.41836100
C	2.05965200	0.46897400	2.82859400
H	2.70682900	0.03383600	3.58561100
H	1.29703900	-0.26344300	2.56570800
C	1.42673700	1.75120000	3.28845600
H	0.87107000	1.56729400	4.20824400
H	2.21042700	2.47712000	3.51901400
C	0.47816700	2.32535900	2.22678600
C	1.19826700	2.32982100	0.87250800
C	0.68888600	3.06693800	-0.21754700
C	1.43486800	3.23617400	-1.37693700
H	1.05347900	3.82546400	-2.19566100
C	2.68817500	2.65401900	-1.48666000
H	3.25683700	2.82414000	-2.38841000
C	3.19600000	1.83745300	-0.49516300
C	2.41526900	1.65721600	0.66254100
C	5.01901600	0.99351600	-2.06083200
H	5.19770900	1.93949300	-2.56984800
H	5.95473800	0.43526700	-2.08522900
H	4.27026900	0.44725700	-2.63227900

C	5.59605100	2.22370200	0.02837500
H	5.57624200	3.16846700	-0.51632300
H	5.34844700	2.42322700	1.07159900
H	6.60904000	1.81811700	-0.01416400
C	-0.81232700	1.48994800	2.16286500
H	-1.50719500	1.92032300	1.44743300
H	-0.61960400	0.46181000	1.85770300
H	-1.29231900	1.47502800	3.14366500
C	0.14411600	3.75660800	2.69389300
H	1.02865200	4.39421500	2.64472300
H	-0.18472700	3.71668700	3.73441700
H	-0.64336000	4.20989400	2.10210100
C	-1.09612500	4.38852700	-1.11940800
H	-0.48293900	5.27423100	-1.29884100
H	-1.19173400	3.81587400	-2.04406900
H	4.16685400	-0.74197000	2.20408900
H	5.64317000	-0.47357500	0.30789100
H	-2.08234600	4.69058800	-0.77834900

INT-II-D

Cl	0.91679400	-0.25441100	-1.24027300
O	-5.49336900	1.14495200	-0.84680600
N	-8.57513100	2.67223400	-1.18958100
N	-9.35884900	-1.12283300	0.81369300
N	-6.26024700	-2.99102000	1.38063200
C	-8.15030000	1.68664900	-0.75255000
C	-8.57180600	-0.40846600	0.35308600
C	-5.96404600	-2.01451000	0.83230800
C	-7.64737300	0.48510400	-0.21698900
C	-6.26856300	0.21662500	-0.26921700
C	-5.50631900	-0.86554100	0.17599600
C	-4.12483300	-0.63084100	-0.13502700
C	-4.07916300	0.72262500	-0.82735100
C	-3.64272500	0.64922100	-2.28443400
H	-2.59214600	0.37487000	-2.35739600
H	-3.78206000	1.62068400	-2.75911600
H	-4.23202100	-0.09538300	-2.81859800
C	-3.33241500	1.78546500	-0.03331500
H	-2.26969500	1.55791800	0.00163700
H	-3.70926500	1.83070200	0.98797400
H	-3.46295400	2.75960200	-0.50479800
C	-3.08488400	-1.46390000	0.14385100
H	-3.34075600	-2.39110800	0.64145700
C	-1.71472900	-1.22576000	-0.16740400
H	-1.48409900	-0.30926100	-0.68742500
C	-0.66539000	-2.04477300	0.11385700
C	-0.83177000	-3.36287500	0.83519600
H	-0.95747600	-4.16540100	0.09890000
H	-1.73848300	-3.34698700	1.43701200
C	0.36983000	-3.68079400	1.71859300
H	0.44627000	-2.92422400	2.50541000
C	1.64791300	-3.69164000	0.89275200
H	1.66466300	-4.57303000	0.24269800
H	2.52500800	-3.79453800	1.53614500
C	1.78826400	-2.45274400	0.04369200
C	0.69486500	-1.72666500	-0.27588500
C	3.19739200	-2.10566400	-0.39149800
H	3.15751700	-1.37422200	-1.20028300
H	0.23257700	-4.64382300	2.21206200
O	3.90449100	-3.25437300	-0.81894200
C	3.50124600	-3.71372100	-2.10981200
H	2.42664200	-3.92675600	-2.10949500
H	3.68122900	-2.92052300	-2.84537800
C	4.29622800	-4.95450800	-2.44393900
H	5.36552600	-4.73835500	-2.44989400
H	4.10440400	-5.74334700	-1.71520100
H	4.01354700	-5.32246400	-3.43132200
O	2.48239300	4.40162700	-0.97931800
N	2.72832400	0.40044400	1.64017100

C	5.09668900	-0.46791900	0.34860600
C	4.02166400	-1.48411900	0.77605800
C	3.05052200	-0.84593200	1.69920200
C	1.59107600	0.85784700	2.47814200
H	1.62354500	0.28739200	3.40216100
H	0.68236900	0.59106200	1.93959700
C	1.68504200	2.33590600	2.71796600
H	0.84648800	2.64025800	3.34439000
H	2.60068900	2.55530000	3.27219600
C	1.66522200	3.14167700	1.41168500
C	2.70665400	2.54941000	0.45885600
C	3.14214100	3.25687600	-0.68389500
C	4.18628200	2.77634200	-1.46328900
H	4.52550100	3.32897000	-2.32510500
C	4.81859400	1.58478300	-1.13430800
H	5.65163200	1.25902600	-1.73804600
C	4.38776300	0.81153600	-0.07560100
C	3.29323600	1.29316800	0.66821800
C	5.98804300	-1.05043300	-0.75004000
H	6.82552700	-0.38356300	-0.95273800
H	6.39472600	-2.00647300	-0.42394300
H	5.44738700	-1.21351600	-1.68071600
C	5.98526400	-0.14790300	1.57099600
H	6.73883900	0.58952500	1.29588600
H	5.41070200	0.25627900	2.40540700
H	6.49326800	-1.05137800	1.91280900
C	0.26566500	3.09686900	0.77354000
H	0.24393400	3.68739800	-0.13988700
H	-0.02735500	2.07937200	0.51810800
H	-0.47260400	3.50377700	1.46691100
C	2.01050500	4.59004700	1.81267000
H	3.04848300	4.66294100	2.14188900
H	1.37103700	4.87995400	2.64862400
H	1.85449600	5.29128700	1.00109200
C	2.89805800	5.17254800	-2.10295700
H	3.93209100	5.50496600	-1.99153700
H	2.79108900	4.60624600	-3.03033500
H	2.54460400	-1.43298400	2.45237900
H	4.49126200	-2.31386900	1.30664200
H	2.23851400	6.03528900	-2.12599200

TS-II-D

Cl	1.10524800	0.45566900	-2.09786800
O	7.32656000	-1.40272900	-0.96169100
N	10.44486600	-2.86214000	-1.24529300
N	10.63515400	-0.37127200	2.33023700
N	7.46870200	1.38995500	2.88980100
C	9.90462700	-2.12572900	-0.53160600
C	9.99969600	-0.74806100	1.43767700
C	7.32522900	0.74089200	1.94066700
C	9.26047700	-1.23040400	0.34336500
C	7.92379700	-0.85807600	0.10848200
C	7.05431200	-0.00572500	0.78829300
C	5.78195500	0.00788100	0.11650700
C	5.93374400	-0.92623500	-1.07478600
C	5.83974500	-0.21931800	-2.42024100
H	4.82628200	0.13513400	-2.59794000
H	6.11143000	-0.91001300	-3.21886100
H	6.51419200	0.63606000	-2.44560900
C	5.05781400	-2.16904200	-0.99029600
H	4.00745600	-1.90558600	-1.09864400
H	5.19307800	-2.66155600	-0.02780900
H	5.32613700	-2.86408200	-1.78626400
C	4.68310600	0.71600500	0.48808900
H	4.79156700	1.33112200	1.37302200
C	3.42110400	0.72136900	-0.18115700
H	3.33956500	0.12309100	-1.07530100
C	2.31173600	1.41361800	0.18545400
C	2.26173600	2.30087800	1.40741200

H	2.48597200	3.33381600	1.11531900
H	3.02923400	2.00335400	2.11933600
C	0.88897300	2.25728300	2.07113900
H	0.69004900	1.23796200	2.41477900
C	-0.19301900	2.68548700	1.08992400
H	-0.15359200	3.76935800	0.93843300
H	-1.18418900	2.48798700	1.50395400
C	-0.07198200	1.98865800	-0.24209100
C	1.08087900	1.38466300	-0.58644900
C	-1.30882400	1.98847100	-1.11128200
H	-1.00640300	1.88983000	-2.15650000
H	0.87274600	2.90183600	2.95134900
O	-1.99788600	3.23263200	-0.96759600
C	-1.39219900	4.30035700	-1.69035300
H	-0.34494400	4.41258900	-1.38810100
H	-1.40057800	4.06107300	-2.76105600
C	-2.16867200	5.56780600	-1.41438700
H	-3.21379000	5.45140100	-1.70525200
H	-2.12891900	5.82420900	-0.35445100
H	-1.74388300	6.39711900	-1.98168400
O	-6.75680800	-3.45099800	0.37735900
N	-2.45317400	-1.36543700	0.10180200
C	-3.29832900	0.45487100	-1.90056300
C	-2.30408000	0.86557400	-0.79295200
C	-1.80953600	-0.22355000	-0.06914500
C	-1.90861800	-2.32504300	1.07782200
H	-0.82546500	-2.30896100	0.98377200
H	-2.16877800	-1.98333900	2.08128600
C	-2.46587900	-3.69415500	0.80359200
H	-2.03335900	-4.40505600	1.50814200
H	-2.16418700	-4.00600500	-0.19949700
C	-3.99751900	-3.73636200	0.91533200
C	-4.58463400	-2.57035500	0.11307500
C	-5.96267000	-2.50981700	-0.19295600
C	-6.46698600	-1.51797900	-1.02351200
H	-7.51821700	-1.48082000	-1.26114600
C	-5.61449600	-0.56934200	-1.57153600
H	-6.03108700	0.16789300	-2.24023500
C	-4.26851000	-0.54063600	-1.26222100
C	-3.78591300	-1.52276800	-0.37303700
C	-4.02202300	1.66520900	-2.49520000
H	-4.68620600	1.35313800	-3.30074500
H	-3.30257000	2.36016400	-2.92134200
H	-4.60645500	2.20111900	-1.74869900
C	-2.55240900	-0.27273200	-3.04179800
H	-3.26829800	-0.60008600	-3.79723500
H	-2.01890800	-1.14961900	-2.67464300
H	-1.82961500	0.38745400	-3.52186200
C	-4.42536900	-3.64938600	2.39139700
H	-5.50872400	-3.69643600	2.47896700
H	-4.09134800	-2.72018200	2.85435000
H	-3.99680200	-4.48303700	2.95168800
C	-4.42235200	-5.09912500	0.33196400
H	-4.22993100	-5.13453100	-0.74182900
H	-3.82850400	-5.88331500	0.80604000
H	-5.47190700	-5.31178100	0.50232700
C	-8.14938100	-3.45150700	0.08319000
H	-8.32752000	-3.59144100	-0.98509600
H	-8.62368800	-2.52543300	0.41533700
H	-0.87589700	-0.14640300	0.47186100
H	-3.13338700	1.39270700	0.17814900
C	-4.91934900	1.07923400	1.65191400
C	-5.87205800	1.54542900	2.54075400
C	-5.93412300	2.91010200	2.79654000
C	-5.04223600	3.76247100	2.15743600
C	-4.11466900	3.22292000	1.28217100
N	-4.06670200	1.90967300	1.04698800
H	-6.66978900	3.30398300	3.48455000
H	-4.83446800	0.02925700	1.40739300
H	-6.54955700	0.85144100	3.01658200
H	-5.06200500	4.82876900	2.33018600

H	-3.39355100	3.81999100	0.74349000
H	-8.56584200	-4.29021200	0.63412700

INT-II-E

Cl	1.45171200	0.95192700	-1.85807500
O	7.78628800	-0.86383300	-1.37274900
N	11.01620700	-1.85868500	-2.10771400
N	10.95966900	-1.13196700	2.19202000
N	7.65309200	-0.03023700	3.31114800
C	10.40766100	-1.53982500	-1.17409600
C	10.36722000	-1.13579500	1.19621900
C	7.57568900	-0.20431200	2.16811000
C	9.68208900	-1.15344500	-0.03132100
C	8.32365300	-0.80225200	-0.14536800
C	7.38175000	-0.38570500	0.79413000
C	6.12359800	-0.15417600	0.13419800
C	6.36402900	-0.46783900	-1.33475900
C	6.24209700	0.74637100	-2.24559100
H	5.20861000	1.08303700	-2.29948800
H	6.57651600	0.48816300	-3.25066800
H	6.85298000	1.56546400	-1.86725900
C	5.57893000	-1.67204000	-1.83673000
H	4.51416000	-1.44884600	-1.86788600
H	5.73380000	-2.52544500	-1.17720700
H	5.90899400	-1.93494700	-2.84205900
C	4.97195100	0.26155900	0.72318200
H	5.02374200	0.43736900	1.79075700
C	3.72397900	0.49487900	0.06734700
H	3.69341300	0.33860300	-0.99969800
C	2.57250700	0.91352400	0.65380100
C	2.47114900	1.18042500	2.13874300
H	2.72799900	2.22793700	2.33724000
H	3.19847900	0.57448800	2.67632200
C	1.07060900	0.90231500	2.67172300
H	0.84332500	-0.16115400	2.55273300
C	0.04287500	1.72849800	1.91366000
H	0.14217000	2.78404300	2.18904600
H	-0.96737900	1.44733800	2.20948400
C	0.18320400	1.57779600	0.41888800
C	1.35933100	1.17841900	-0.10174200
C	-1.02744300	1.87884200	-0.43540600
H	-0.68580900	2.26922000	-1.39220000
H	1.02068300	1.12644100	3.73837000
O	-1.82954000	2.92162600	0.19164000
C	-1.26625600	4.24352700	0.16118200
H	-1.69638000	4.76146000	1.01878500
H	-0.18725600	4.17581100	0.31858900
C	-1.57860700	4.98338000	-1.12475900
H	-1.13389900	4.49316500	-1.99079800
H	-2.65564500	5.05296200	-1.28010600
H	-1.17220100	5.99508400	-1.06852300
O	-7.60829400	-2.11419300	-0.45597200
N	-2.91609200	-1.33591500	0.11480500
C	-2.83671900	0.62269500	-1.91131500
C	-1.94411000	0.71020400	-0.67451000
C	-1.98528700	-0.31817100	0.18119500
C	-2.87102500	-2.33995800	1.17272500
H	-1.83085100	-2.62870900	1.31683000
H	-3.22870100	-1.91235800	2.11644100
C	-3.70616700	-3.52764700	0.76858300
H	-3.63783800	-4.30471800	1.53142800
H	-3.29515900	-3.94176100	-0.15572400
C	-5.18416300	-3.16134600	0.55267300
C	-5.26704900	-1.87550600	-0.28021900
C	-6.48706000	-1.43512100	-0.83010300
C	-6.54049700	-0.34773300	-1.69482800
H	-7.47616300	-0.02357400	-2.12146500
C	-5.37077400	0.31966000	-2.02943000
H	-5.43316500	1.13605900	-2.73331600

C	-4.15001800	-0.02958900	-1.48079500
C	-4.12242600	-1.10066900	-0.55609600
C	-3.06229900	1.97590700	-2.59024400
H	-3.64081800	1.85275800	-3.50474600
H	-2.11162500	2.41908900	-2.88071600
H	-3.58134300	2.68429000	-1.94710900
C	-2.14185600	-0.30868700	-2.93616300
H	-2.76571600	-0.42072800	-3.82550900
H	-1.97022000	-1.29576000	-2.50714500
H	-1.17762700	0.10743100	-3.23249200
C	-5.87562800	-2.99089200	1.91675100
H	-6.91148400	-2.68286900	1.79218800
H	-5.37057300	-2.24411700	2.52835700
H	-5.85908800	-3.93798900	2.46112700
C	-5.81398000	-4.35398100	-0.19466900
H	-5.40194500	-4.43433000	-1.20235300
H	-5.57566300	-5.27565800	0.34110800
H	-6.89317700	-4.26824300	-0.26903600
C	-8.86619800	-1.70232400	-0.97250500
H	-8.89807000	-1.78938500	-2.06098600
H	-9.09607500	-0.67368500	-0.68408600
H	-1.29311800	-0.41254200	1.00478600
H	-3.24050000	2.45560000	0.98628800
C	-5.24741400	2.14589100	0.68379700
C	-6.38768700	1.50135600	1.11638000
C	-6.32294000	0.72324200	2.26377300
C	-5.12613700	0.62412700	2.96750300
C	-4.01891200	1.29029900	2.49422200
N	-4.10775600	2.02460500	1.37600700
H	-7.19956700	0.19440200	2.60991700
H	-5.20812700	2.75648800	-0.20318700
H	-7.30007200	1.59556400	0.55009200
H	-5.04868100	0.03325500	3.86710800
H	-3.05327800	1.25327400	2.97237200
H	-9.60023300	-2.37354300	-0.53436400

TS-II-E

Cl	1.68455900	1.92332300	-0.97734800
O	8.09908800	0.54866700	-1.31490500
N	11.45215100	0.56573300	-2.15799600
N	11.02172500	-2.51533100	0.89986200
N	7.55665100	-2.79059500	2.03295300
C	10.75262600	-0.00807800	-1.43432400
C	10.50402400	-1.70560600	0.25356200
C	7.57460600	-1.95864500	1.22740100
C	9.91307500	-0.71344000	-0.54980200
C	8.54199400	-0.41485700	-0.49711400
C	7.49598100	-0.94145400	0.26757100
C	6.27699300	-0.27403500	-0.07762100
C	6.64653800	0.74699700	-1.14216600
C	6.47140100	2.18960100	-0.68640700
H	5.41677000	2.42799000	-0.56365200
H	6.89630100	2.86376500	-1.43020200
H	6.97486300	2.34869600	0.26664600
C	6.02083500	0.46833800	-2.50215900
H	4.94579300	0.63437900	-2.47187200
H	6.20323600	-0.56410600	-2.79851300
H	6.45417900	1.13460700	-3.24823400
C	5.04606900	-0.51890100	0.45661100
H	5.00445700	-1.28686100	1.21898300
C	3.83945700	0.14579900	0.10793400
H	3.90388800	0.92236800	-0.63744900
C	2.60492200	-0.09164900	0.63779700
C	2.38458100	-1.15777000	1.68993800
H	2.60406000	-0.74068900	2.67964200
H	3.08858400	-1.97451600	1.53562300
C	0.96037900	-1.69889000	1.68299500
H	0.77697800	-2.23955800	0.75019300
C	-0.03269800	-0.55451400	1.80948800

H	0.07559600	-0.09388400	2.79820100
H	-1.05392200	-0.92221700	1.76848400
C	0.18923600	0.49975000	0.74765000
C	1.44358900	0.67790300	0.25725500
C	-0.92898700	1.34420300	0.30434200
H	-0.59499100	2.29968800	-0.07034200
H	0.82453600	-2.40702600	2.50149000
O	-1.61705500	2.00711500	1.79855700
C	-0.73999000	2.66735800	2.73413400
H	-1.16369600	2.50561600	3.72607100
H	0.23779600	2.18370300	2.69771200
C	-0.63216300	4.13872400	2.40277900
H	-0.20628600	4.28640400	1.40967100
H	-1.61062800	4.61787900	2.43779300
H	0.02235700	4.62905600	3.12528000
O	-8.18891500	-0.64749200	-1.20972000
N	-3.42137500	-1.06019300	-1.01204100
C	-3.02095300	1.73696200	-1.18910800
C	-2.08150700	0.82749200	-0.39643600
C	-2.30517500	-0.50694600	-0.48205000
C	-3.54248800	-2.51764400	-0.93447200
H	-2.57706600	-2.94684100	-1.19591300
H	-3.77137800	-2.80757100	0.09566100
C	-4.61580200	-2.98261000	-1.88187900
H	-4.67773900	-4.07141300	-1.85859100
H	-4.33554500	-2.69404500	-2.89827000
C	-5.99213400	-2.39015100	-1.54126200
C	-5.84254500	-0.88312400	-1.30090000
C	-6.96935500	-0.04215700	-1.20345800
C	-6.83139700	1.33530100	-1.08061200
H	-7.69726300	1.97441000	-1.01327100
C	-5.56502700	1.90246900	-1.06715400
H	-5.48854000	2.97764800	-1.00959400
C	-4.42091700	1.12743100	-1.11468000
C	-4.58118400	-0.27397700	-1.17020400
C	-3.00283000	3.19214300	-0.71082000
H	-3.61811800	3.81164100	-1.36170600
H	-1.99452500	3.60057800	-0.75962600
H	-3.35956700	3.29786400	0.31182100
C	-2.55854300	1.71714000	-2.66745100
H	-3.22247000	2.33148900	-3.27871400
H	-2.56568800	0.70192700	-3.06433200
H	-1.54285500	2.10991100	-2.75061000
C	-6.56284500	-3.08936400	-0.29455900
H	-7.52942700	-2.66958800	-0.02426400
H	-5.89815600	-2.98199400	0.56232100
H	-6.69197000	-4.15570000	-0.49382900
C	-6.89279800	-2.68544200	-2.75711400
H	-6.56047100	-2.11612200	-3.62723600
H	-6.81962100	-3.74746400	-3.00190700
H	-7.93366000	-2.44717900	-2.56586100
C	-9.35848300	0.15640000	-1.12918200
H	-9.42519500	0.84669500	-1.97315000
H	-9.38878800	0.72079300	-0.19421500
H	-1.58692700	-1.22761500	-0.12578500
H	-2.29958200	1.32652100	2.24176000
C	-4.63812000	0.83550700	2.19215800
C	-5.76890100	0.03907300	2.26740100
C	-5.66516100	-1.20295100	2.87725100
C	-4.43906600	-1.59820600	3.39871100
C	-3.35808700	-0.73990400	3.28099700
N	-3.45526100	0.45141700	2.68209400
H	-6.52526300	-1.85499200	2.94385200
H	-4.66855800	1.80293900	1.71234600
H	-6.69814300	0.38318200	1.83859400
H	-4.31729300	-2.55546900	3.88488400
H	-2.38516700	-1.00843300	3.66975000
H	-10.19547200	-0.53611600	-1.16056400

Type-II product (TCF1-based)

Cl	-1.24306900	-2.11162700	-0.02711700
O	-7.71383700	-1.23357300	0.42944000
O	9.22791400	-0.20105100	0.04239700
N	-11.12826400	-1.68122100	0.83904500
N	-10.58772200	2.53517200	-0.15036500
N	-7.10880500	3.36148500	-0.65365100
N	4.59543700	0.92534100	0.53808700
C	-10.40062000	-0.82042100	0.58094800
C	-10.08663000	1.50953300	0.03293300
C	-7.12742900	2.23450300	-0.39970700
C	-9.52003000	0.23859100	0.26488900
C	-8.15174200	0.00103600	0.19336500
C	-7.06280400	0.86213100	-0.09843000
C	-5.86965200	0.12842500	-0.04323600
C	-6.24399500	-1.29817900	0.31063800
C	-5.73048000	-1.74384800	1.67393300
H	-4.64877400	-1.85823500	1.65749700
H	-6.17743900	-2.70331600	1.93215200
H	-5.99064300	-1.01171600	2.43737500
C	-5.95404300	-2.29913700	-0.80050000
H	-4.88176100	-2.43651600	-0.92280600
H	-6.36958100	-1.95067700	-1.74519700
H	-6.40058600	-3.25994700	-0.54669100
C	-4.59697700	0.63808200	-0.27335600
H	-4.54972600	1.69337100	-0.50839500
C	-3.41902100	-0.09246600	-0.21529000
H	-3.48736700	-1.14040000	0.02630300
C	-2.13300800	0.41530500	-0.41735700
C	-1.94486400	1.88148100	-0.74029300
H	-2.04977900	2.46957600	0.17827300
H	-2.74449300	2.20661600	-1.40638900
C	-0.59848000	2.16039200	-1.38432500
H	-0.57270800	1.71783100	-2.38386300
C	0.52624000	1.56974900	-0.54710600
H	0.57476800	2.09563800	0.41308500
H	1.48235600	1.73356300	-1.04490500
C	0.34017000	0.08568900	-0.32253400
C	-0.99203800	-0.38647800	-0.29351700
C	1.41159400	-0.78900100	-0.18691400
H	1.14080100	-1.83399500	-0.21487700
C	3.74598400	-1.73877500	-0.25644300
C	2.79386600	-0.55936300	-0.05169500
C	3.29819600	0.64387000	0.38516800
H	2.64024300	1.43559000	0.70014500
C	4.98330500	2.17083200	1.19778900
H	4.11570900	2.82583800	1.21383700
H	5.25871900	1.95107100	2.23243100
C	6.13117200	2.78569000	0.43943300
H	6.39207100	3.74957700	0.87819800
H	5.80612500	2.97207100	-0.58720100
C	7.37199500	1.87909800	0.43789000
C	6.95479200	0.42304100	0.18357000
C	7.92371500	-0.57100300	-0.06037400
C	7.55127200	-1.87073100	-0.38401000
H	8.29519800	-2.62652700	-0.57943100
C	6.20935800	-2.20399200	-0.46238100
H	5.95009100	-3.21946900	-0.72598200
C	5.20764800	-1.28758700	-0.19017200
C	5.60496000	0.01376500	0.16651200
C	3.50041100	-2.78603700	0.85341000
H	4.15407400	-3.64799800	0.71834700
H	2.46959300	-3.14207300	0.83757000
H	3.69930000	-2.35408900	1.83476200
C	3.47377300	-2.37268300	-1.63662200
H	4.10305500	-3.24579800	-1.80366300
H	3.66646000	-1.65160700	-2.43170600
H	2.43539800	-2.69595200	-1.71354000
C	8.08964600	2.00125300	1.79570000
H	8.96853800	1.36210100	1.83036500
H	7.43336100	1.71894900	2.62008700
H	8.40700700	3.03454200	1.95259800

C	8.28610000	2.41339400	-0.68278500
H	7.83019700	2.24635600	-1.66042900
H	8.41375100	3.49012900	-0.55083700
H	9.26548500	1.94721000	-0.67336800
C	10.24341200	-1.16074300	-0.22340200
H	10.17518300	-1.53712800	-1.24648200
H	10.19247100	-1.99688400	0.47755000
H	-0.45267200	3.23482900	-1.50229800
H	11.18582100	-0.63581100	-0.09239100

TCF1-based (Path II-c)

INT-II-A(c)

Cl	-1.49802300	-3.67011500	0.28824200
O	4.84767700	-2.13122000	0.66434700
N	8.22994900	-2.01527200	1.44910400
N	7.49402400	1.38057400	-1.19336500
N	4.09188500	1.52703500	-2.28246700
C	7.47476000	-1.41295200	0.81546800
C	7.05118300	0.46248600	-0.64991300
C	4.13281700	0.61982300	-1.57077300
C	6.55676500	-0.66894800	0.03653100
C	5.23074200	-1.06121900	-0.02136500
C	4.11493400	-0.50285500	-0.71881500
C	2.98507500	-1.25971500	-0.44414900
C	3.40517300	-2.38434300	0.48090500
C	3.29575200	-3.76650500	-0.15158100
H	2.25340600	-4.05335500	-0.27174000
H	3.78310400	-4.49482400	0.49529300
H	3.77517600	-3.77908200	-1.12939600
C	2.78387400	-2.30450500	1.86950100
H	1.71650400	-2.50765000	1.82635400
H	2.93153700	-1.31515300	2.29928900
H	3.25282500	-3.04592000	2.51490400
C	1.69649900	-0.99843800	-0.93655400
H	1.60122600	-0.12107500	-1.56069100
C	0.58561100	-1.75267500	-0.66084200
H	0.70467300	-2.63365500	-0.05155100
C	-0.72837200	-1.47799900	-1.10601100
C	-0.98585800	-0.25076300	-1.95237200
H	-0.64794000	-0.44795500	-2.97564300
H	-0.37177900	0.56225000	-1.56954900
C	-2.44387300	0.18238900	-1.95148900
H	-2.69112200	0.61047200	-0.97911000
C	-3.36015000	-0.99820300	-2.23645800
H	-3.17911900	-1.37469800	-3.24926100
H	-4.40617600	-0.69924800	-2.19432800
C	-3.12059000	-2.11190000	-1.24558200
C	-1.78491500	-2.30097800	-0.77544300
C	-4.14549200	-2.89628400	-0.82197900
H	-4.00401900	-3.69406600	-0.10421800
H	-2.59605000	0.96814700	-2.69127800
O	-5.37946500	-2.71625000	-1.27625500
C	-6.40799100	-3.56629900	-0.70766000
H	-6.12240300	-4.60683800	-0.87374900
H	-6.44991500	-3.37748800	0.36674800
C	-7.71434500	-3.23317600	-1.38247500
H	-7.98163300	-2.18894200	-1.21784400
H	-7.65551600	-3.41699500	-2.45565800
H	-8.50492100	-3.86016200	-0.96846800
O	-4.08178500	1.71606000	2.19048400
N	0.49759300	1.94812900	0.75310900
C	-0.18094100	3.86817700	-1.36238400
C	1.16323100	3.13959800	-1.26101500
C	1.51155000	2.80877900	0.16966400
H	1.63489500	3.72726600	0.76332100
C	0.90951800	1.32252100	1.99254300
H	1.91238800	0.92047900	1.84230800

H	0.98146900	2.06240700	2.80459800
C	-0.05343800	0.22002000	2.34703400
H	0.27477600	-0.29486900	3.25209700
H	-0.04533500	-0.50976900	1.53717500
C	-1.48691100	0.72961100	2.55142800
C	-1.83292800	1.76030600	1.46425600
C	-3.15905600	2.20258900	1.30739200
C	-3.51514000	3.10525300	0.31189100
H	-4.53501300	3.43339700	0.19112900
C	-2.53071900	3.59305000	-0.53072000
H	-2.82126500	4.29458000	-1.30101900
C	-1.20013300	3.23194100	-0.41247700
C	-0.84048400	2.31663000	0.61250200
C	0.00746500	5.35121600	-0.99070300
H	-0.94022700	5.88810300	-1.04939400
H	0.71381700	5.82759200	-1.67537200
H	0.38759000	5.46154100	0.02556500
C	-0.65027400	3.78300000	-2.82380200
H	-1.55274700	4.36735300	-3.00206500
H	-0.85274100	2.74931500	-3.10716300
H	0.12921500	4.17046500	-3.48387900
C	-1.59866200	1.37413900	3.94610200
H	-2.59884500	1.76862000	4.11408200
H	-0.88691700	2.19294000	4.05982800
H	-1.38671700	0.62962100	4.71815800
C	-2.38687000	-0.52188400	2.49204700
H	-2.45547700	-0.89622600	1.47102000
H	-1.94304100	-1.30823000	3.10728400
H	-3.39116100	-0.32824500	2.85309000
C	-5.44274100	2.08712300	2.03920700
H	-5.83348800	1.78302100	1.06490000
H	-5.58130400	3.16406700	2.16316400
H	2.46152700	2.27607900	0.21367400
H	1.12292700	2.21114000	-1.83389800
H	1.95062600	3.74879000	-1.70768200
H	-5.98239200	1.56271600	2.82413600

TS-II-A(c)

Cl	-0.92403200	-3.09651800	1.29193000
O	5.40609800	-1.24808500	0.99524400
N	8.84074200	-1.07599700	1.38212500
N	7.97866600	0.82418400	-2.45405600
N	4.39194100	0.93221600	-3.11401400
C	8.04858300	-0.75231600	0.60253900
C	7.56059600	0.29615000	-1.51293100
C	4.52824100	0.37031500	-2.11168900
C	7.09218300	-0.35300800	-0.35414200
C	5.73569900	-0.61134100	-0.13335400
C	4.58992200	-0.31717300	-0.89121000
C	3.44023600	-0.79735600	-0.20456600
C	3.94898600	-1.45993600	1.06489000
C	3.73927300	-2.96927800	1.06875900
H	2.67971400	-3.21046900	1.12893300
H	4.24434500	-3.40687600	1.92959500
H	4.14208500	-3.40887100	0.15719200
C	3.48617900	-0.79229500	2.35195300
H	2.43449900	-1.00244700	2.53496600
H	3.63175900	0.28601000	2.30203500
H	4.05962000	-1.18734200	3.19000500
C	2.14868400	-0.68499200	-0.63235300
H	2.00420000	-0.21019900	-1.59348100
C	0.97608200	-1.08490500	0.09891700
H	1.14436000	-1.78169000	0.90848500
C	-0.27380600	-1.31887400	-0.62928000
C	-0.52541100	-0.50206900	-1.87626300
H	0.06706200	-0.91708600	-2.69889200
H	-0.15299900	0.51218500	-1.71694200
C	-1.99412600	-0.44527500	-2.26859400
H	-2.52705000	0.19610800	-1.56514900

C	-2.61172800	-1.83804700	-2.25991200
H	-2.13862000	-2.45205800	-3.03423000
H	-3.67322200	-1.79496000	-2.49922600
C	-2.42947200	-2.50516000	-0.91764400
C	-1.20464300	-2.21089000	-0.21059100
C	-3.37816900	-3.31434500	-0.40713900
H	-3.27366100	-3.79264000	0.55787200
H	-2.09624900	0.00825900	-3.25528100
O	-4.51554600	-3.56502700	-1.07360000
C	-5.51484800	-4.31144800	-0.34793200
H	-5.07759800	-5.26003600	-0.02614100
H	-5.79914000	-3.73947600	0.53884300
C	-6.69503500	-4.53019800	-1.26187500
H	-7.12051400	-3.57782800	-1.58025600
H	-6.40137600	-5.09649100	-2.14647000
H	-7.46633400	-5.09219000	-0.73362700
O	-5.05913600	2.49274200	-0.58628600
N	-0.95928300	1.31590200	1.62534000
C	0.45609900	3.36357000	0.33885700
C	1.20700600	2.07987400	0.70829600
C	0.38495600	1.13283400	1.53870600
H	0.81837400	0.80174700	2.47610000
C	-1.69733900	0.66090600	2.70340900
H	-1.02508800	-0.03861300	3.19506900
H	-1.98643800	1.42061900	3.43416200
C	-2.90106500	-0.05343000	2.14047700
H	-3.44244800	-0.54560100	2.94982500
H	-2.55450200	-0.83196700	1.46402400
C	-3.86321600	0.87811400	1.38884500
C	-3.06682400	1.84363800	0.49976600
C	-3.71190600	2.63376600	-0.47587400
C	-2.99732300	3.51336000	-1.27990000
H	-3.49381900	4.08567400	-2.04724500
C	-1.63770300	3.69804400	-1.06869400
H	-1.11727600	4.42924100	-1.66945400
C	-0.96170400	3.00520200	-0.08415700
C	-1.68164800	2.04591000	0.66029700
C	0.36762200	4.28794400	1.57091400
H	-0.17333100	5.20052500	1.31857300
H	1.36902500	4.56180800	1.90966400
H	-0.15284800	3.80505900	2.39887800
C	1.24804300	4.07267900	-0.76227100
H	0.83902000	5.05844600	-0.98325200
H	1.25830600	3.48670200	-1.68257300
H	2.28019100	4.21204000	-0.43660100
C	-4.68245900	1.70184800	2.40201600
H	-5.36222700	2.37922600	1.88842100
H	-4.03670700	2.29657100	3.04934200
H	-5.27307000	1.03171000	3.03086400
C	-4.81293200	-0.04850200	0.60313200
H	-4.29970700	-0.51742200	-0.23426000
H	-5.15051000	-0.84602600	1.26887200
H	-5.68344000	0.47605100	0.22600600
C	-5.75601900	3.24387100	-1.57222000
H	-5.40505300	3.00054300	-2.57750400
H	-5.65264300	4.31747300	-1.39943100
H	0.63182900	-0.05078600	0.85339300
H	1.53820000	1.57902000	-0.20546900
H	2.12037500	2.32270500	1.25267300
H	-6.80042300	2.95987800	-1.47483600

INT-II-B(c)

Cl	-1.87458100	-2.68505500	1.76768800
O	4.25193700	-2.09876500	1.23180200
N	7.55980300	-3.00507500	1.60723700
N	7.20891300	-1.53788500	-2.48388400
N	3.72083700	-0.56408300	-3.24537600
C	6.87906200	-2.57155900	0.77431900
C	6.67575700	-1.76237100	-1.47920800

C	3.75326800	-0.91162100	-2.13951900
C	6.06649600	-2.04376600	-0.24525800
C	4.69610000	-1.80494100	-0.00323400
C	3.67730200	-1.30730700	-0.80206100
C	2.44661600	-1.25256900	-0.02691800
C	2.81101800	-1.80258700	1.34693200
C	2.12915600	-3.12584700	1.66176900
H	1.05678700	-2.98822300	1.78477100
H	2.53490500	-3.54189700	2.58452300
H	2.29368300	-3.83448400	0.85050900
C	2.68504700	-0.78074400	2.46796300
H	1.64604000	-0.48858100	2.61114000
H	3.27007600	0.10745900	2.23117200
H	3.05772900	-1.20282200	3.40150700
C	1.25859400	-0.79671000	-0.44625300
H	1.20571500	-0.43782300	-1.46798600
C	-0.00702900	-0.67927300	0.35576400
H	0.08432200	-1.16943900	1.31696800
C	-1.22945200	-1.17043900	-0.37067500
C	-1.47299100	-0.55947200	-1.73030800
H	-0.88208100	-1.09604500	-2.48115200
H	-1.09307900	0.46371600	-1.72601800
C	-2.94284200	-0.57624900	-2.12321300
H	-3.49550700	0.11180700	-1.47854000
C	-3.51339700	-1.98063100	-1.96701600
H	-3.01137400	-2.65326500	-2.67215400
H	-4.57379800	-2.00277800	-2.21500200
C	-3.31832300	-2.49646100	-0.55988400
C	-2.12096500	-2.03899100	0.13214400
C	-4.20430300	-3.33896300	-0.00588200
H	-4.08839300	-3.73142600	0.99554100
H	-3.06318100	-0.22854800	-3.15062300
O	-5.29629400	-3.76187100	-0.68637100
C	-6.20341600	-4.59164400	0.05864300
H	-5.66437000	-5.47348600	0.41698900
H	-6.56427600	-4.03250200	0.92685000
C	-7.34383200	-4.98215100	-0.85034700
H	-7.87855100	-4.09935900	-1.20339600
H	-6.97781200	-5.53776300	-1.71474200
H	-8.04644400	-5.61531700	-0.30676700
O	-3.80885200	2.82426500	-0.67527000
N	0.43372100	2.96519800	1.57525700
C	1.85187300	3.35751900	-0.84501600
C	2.43048500	2.52090700	0.30741200
C	1.70421100	2.76037200	1.56113700
H	2.20814700	2.77509000	2.51807600
C	-0.27988000	3.19740400	2.84408300
H	0.42576100	3.04293400	3.65503800
H	-0.60208500	4.23821300	2.84938700
C	-1.44200500	2.23807400	2.89704600
H	-1.93418100	2.32190400	3.86566100
H	-1.05583800	1.21921400	2.81966300
C	-2.46639200	2.50531200	1.78236500
C	-1.74272600	2.80584900	0.46265200
C	-2.46159400	2.93323400	-0.74736100
C	-1.80037000	3.15449700	-1.94959400
H	-2.35565500	3.23028500	-2.87096000
C	-0.41842500	3.26018400	-1.98767400
H	0.06309500	3.41825100	-2.94079500
C	0.34022600	3.17211700	-0.83657800
C	-0.35149000	2.97122500	0.37156100
C	2.17637800	4.84779300	-0.62920000
H	1.76701100	5.43927700	-1.44796500
H	3.25694200	4.99912600	-0.59981400
H	1.75266900	5.22704400	0.30236600
C	2.49553700	2.87654400	-2.14765800
H	2.20752400	3.50345700	-2.99055900
H	2.22472400	1.84521000	-2.37060800
H	3.58124700	2.92895100	-2.05759900
C	-3.33981000	3.71144900	2.18076000
H	-4.07176200	3.93432900	1.40903100

H	-2.73775000	4.60609000	2.34505000
H	-3.87165000	3.48399500	3.10629100
C	-3.33672000	1.23760600	1.68464800
H	-2.75693600	0.39385100	1.31186000
H	-3.69634700	0.98412400	2.68386400
H	-4.19439500	1.37888700	1.03617100
C	-4.58565300	2.98808800	-1.85913700
H	-4.34327900	2.22361400	-2.59923600
H	-4.43805500	3.97993400	-2.29066300
H	-0.18510500	0.38309700	0.56839900
H	2.33132000	1.44905500	0.07743400
H	3.49148800	2.71577000	0.45517600
H	-5.61974100	2.87562200	-1.54671400

TS-II-B(c)

Cl	-0.92403200	-3.09651800	1.29193000
O	5.40609800	-1.24808500	0.99524400
N	8.84074200	-1.07599700	1.38212500
N	7.97866600	0.82418400	-2.45405600
N	4.39194100	0.93221600	-3.11401400
C	8.04858300	-0.75231600	0.60253900
C	7.56059600	0.29615000	-1.51293100
C	4.52824100	0.37031500	-2.11168900
C	7.09218300	-0.35300800	-0.35414200
C	5.73569900	-0.61134100	-0.13335400
C	4.58992200	-0.31717300	-0.89121000
C	3.44023600	-0.79735600	-0.20456600
C	3.94898600	-1.45993600	1.06489000
C	3.73927300	-2.96927800	1.06875900
H	2.67971400	-3.21046900	1.12893300
H	4.24434500	-3.40687600	1.92959500
H	4.14208500	-3.40887100	0.15719200
C	3.48617900	-0.79229500	2.35195300
H	2.43449900	-1.00244700	2.53496600
H	3.63175900	0.28601000	2.30203500
H	4.05962000	-1.18734200	3.19000500
C	2.14868400	-0.68499200	-0.63235300
H	2.00420000	-0.21019900	-1.59348100
C	0.97608200	-1.08490500	0.09891700
H	1.14436000	-1.78169000	0.90848500
C	-0.27380600	-1.31887400	-0.62928000
C	-0.52541100	-0.50206900	-1.87626300
H	0.06706200	-0.91708600	-2.69889200
H	-0.15299900	0.51218500	-1.71694200
C	-1.99412600	-0.44527500	-2.26859400
H	-2.52705000	0.19610800	-1.56514900
C	-2.61172800	-1.83804700	-2.25991200
H	-2.13862000	-2.45205800	-3.03423000
H	-3.67322200	-1.79496000	-2.49922600
C	-2.42947200	-2.50516000	-0.91764400
C	-1.20464300	-2.21089000	-0.21059100
C	-3.37816900	-3.31434500	-0.40713900
H	-3.27366100	-3.79264000	0.55787200
H	-2.09624900	0.00825900	-3.25528100
O	-4.51554600	-3.56502700	-1.07360000
C	-5.51484800	-4.31144800	-0.34793200
H	-5.07759800	-5.26003600	-0.02614100
H	-5.79914000	-3.73947600	0.53884300
C	-6.69503500	-4.53019800	-1.26187500
H	-7.12051400	-3.57782800	-1.58025600
H	-6.40137600	-5.09649100	-2.14647000
H	-7.46633400	-5.09219000	-0.73362700
O	-5.05913600	2.49274200	-0.58628600
N	-0.95928300	1.31590200	1.62534000
C	0.45609900	3.36357000	0.33885700
C	1.20700600	2.07987400	0.70829600
C	0.38495600	1.13283400	1.53870600
H	0.81837400	0.80174700	2.47610000
C	-1.69733900	0.66090600	2.70340900

H	-1.02508800	-0.03861300	3.19506900
H	-1.98643800	1.42061900	3.43416200
C	-2.90106500	-0.05343000	2.14047700
H	-3.44244800	-0.54560100	2.94982500
H	-2.55450200	-0.83196700	1.46402400
C	-3.86321600	0.87811400	1.38884500
C	-3.06682400	1.84363800	0.49976600
C	-3.71190600	2.63376600	-0.47587400
C	-2.99732300	3.51336000	-1.27990000
H	-3.49381900	4.08567400	-2.04724500
C	-1.63770300	3.69804400	-1.06869400
H	-1.11727600	4.42924100	-1.66945400
C	-0.96170400	3.00520200	-0.08415700
C	-1.68164800	2.04591000	0.66029700
C	0.36762200	4.28794400	1.57091400
H	-0.17333100	5.20052500	1.31857300
H	1.36902500	4.56180800	1.90966400
H	-0.15284800	3.80505900	2.39887800
C	1.24804300	4.07267900	-0.76227100
H	0.83902000	5.05844600	-0.98325200
H	1.25830600	3.48670200	-1.68257300
H	2.28019100	4.21204000	-0.43660100
C	-4.68245900	1.70184800	2.40201600
H	-5.36222700	2.37922600	1.88842100
H	-4.03670700	2.29657100	3.04934200
H	-5.27307000	1.03171000	3.03086400
C	-4.81293200	-0.04850200	0.60313200
H	-4.29970700	-0.51742200	-0.23426000
H	-5.15051000	-0.84602600	1.26887200
H	-5.68344000	0.47605100	0.22600600
C	-5.75601900	3.24387100	-1.57222000
H	-5.40505300	3.00054300	-2.57750400
H	-5.65264300	4.31747300	-1.39943100
H	0.63182900	-0.05078600	0.85339300
H	1.53820000	1.57902000	-0.20546900
H	2.12037500	2.32270500	1.25267300
H	-6.80042300	2.95987800	-1.47483600

TCF-A2(+2H, c)

CI	1.56549200	-2.40475500	-2.10660100
O	-4.37522700	-1.76743700	-1.16981900
N	-7.63091000	-2.95014900	-1.08602200
N	-7.03266000	-0.84311100	2.68775900
N	-3.63348800	0.30308300	3.04699000
C	-6.91728100	-2.35218000	-0.39981400
C	-6.57156400	-1.18584300	1.68418600
C	-3.69548400	-0.13260400	1.97848000
C	-6.05434400	-1.62038600	0.44610100
C	-4.75397100	-1.34317000	0.03429900
C	-3.68954100	-0.66069400	0.67533900
C	-2.57709600	-0.63752300	-0.17954500
C	-2.95894300	-1.43148400	-1.41236700
C	-2.22361400	-2.76223200	-1.51602100
H	-1.17194200	-2.60668300	-1.74071700
H	-2.66621800	-3.35379100	-2.31715200
H	-2.30260500	-3.31465800	-0.58035100
C	-2.92104600	-0.62053600	-2.69875400
H	-1.89554700	-0.36612700	-2.95864500
H	-3.49432300	0.29928200	-2.59148300
H	-3.34454900	-1.20952500	-3.51142600
C	-1.39580400	0.08783600	0.00997900
H	-1.28415700	0.46607800	1.02113400
C	-0.07426400	-0.25564700	-0.65742300
H	-0.22664200	-0.66732900	-1.64843000
C	0.83390600	-1.13704000	0.15807400
C	0.95328700	-0.78464400	1.62239400
H	0.09774900	-1.20013600	2.16676300
H	0.87493600	0.30052200	1.72386200
C	2.25369700	-1.26962300	2.24724800

H	3.08369000	-0.67054100	1.86338700
C	2.49148300	-2.73706900	1.90996400
H	1.69287900	-3.34258600	2.35431400
H	3.42885200	-3.09126800	2.33634700
C	2.50829700	-2.95033000	0.41496000
C	1.60329300	-2.10983300	-0.35629200
C	3.30550600	-3.87158200	-0.14810800
H	3.33172200	-4.04355100	-1.21595500
H	2.22527500	-1.12664600	3.32867700
O	4.11519400	-4.65938600	0.59837900
C	4.99733100	-5.51545100	-0.14748700
H	4.40029600	-6.14630100	-0.81247800
H	5.65709700	-4.89572600	-0.76172300
C	5.78839700	-6.35003400	0.83066400
H	6.38163100	-5.71608200	1.49097100
H	5.12557100	-6.96584000	1.43999200
H	6.46642000	-7.00891500	0.28636900
O	3.96331600	2.52422600	1.58626100
N	0.56600500	3.01419200	-1.77072600
C	-1.43083800	3.57740600	0.12423800
C	-1.70084100	2.70565300	-1.10293600
C	-0.70664600	2.75636100	-2.07472600
H	-0.90681800	2.55658900	-3.11903000
C	1.59067900	3.08591100	-2.80913300
H	1.11009100	2.90909300	-3.76837400
H	2.00109700	4.09725800	-2.81922500
C	2.65189200	2.05418200	-2.51289200
H	3.40476400	2.05843800	-3.30202300
H	2.18397400	1.06704100	-2.52168500
C	3.34444400	2.29037000	-1.15834300
C	2.31451500	2.70325500	-0.09515600
C	2.66148200	2.75325200	1.27380700
C	1.70635200	3.01539600	2.24811500
H	1.97630600	3.02649400	3.29210700
C	0.38749900	3.25542200	1.88705600
H	-0.33883000	3.43638200	2.66564800
C	-0.00120300	3.27571500	0.56235400
C	0.98410700	3.02431900	-0.41439300
C	-1.53269500	5.06728700	-0.27446700
H	-1.32892000	5.69916200	0.59183600
H	-2.53683900	5.29294700	-0.63926000
H	-0.81830400	5.32156000	-1.05787000
C	-2.46531600	3.30138300	1.21610800
H	-2.37531100	4.01429600	2.03573100
H	-2.37545200	2.30042100	1.62931400
H	-3.46832400	3.40717500	0.79977600
C	4.40109700	3.39999600	-1.31530800
H	4.89868700	3.59962200	-0.36894100
H	3.95137700	4.33059000	-1.66482600
H	5.15416200	3.09115900	-2.04347300
C	4.03389500	0.95635600	-0.80701500
H	3.29390900	0.18453400	-0.59306500
H	4.61986100	0.62811500	-1.66817300
H	4.69742900	1.04567600	0.04597900
C	4.34079800	2.43275900	2.95510800
H	3.78734600	1.64031600	3.46366500
H	4.18431600	3.38045200	3.47480600
H	0.46807200	0.67850100	-0.80239100
H	-1.65580200	1.33850300	-0.61827700
H	-2.71845400	2.70685500	-1.48039200
H	5.40044600	2.19238600	2.95256800

TCF5-based (Path I)

TCF-A6

Cl	-2.92744600	-1.17032700	0.43788700
O	3.51092300	-0.25313700	0.18094100
N	6.95176200	-0.65250200	0.35596400

N	6.28218900	3.35713800	-1.25136400
N	2.79784200	4.17215100	-1.42338800
C	6.19866800	0.16005200	0.02956500
C	5.81263400	2.37833800	-0.85731700
C	2.83480800	3.08088900	-1.05038500
C	5.28230800	1.16196300	-0.37128500
C	3.92375800	0.92354600	-0.28056700
C	2.80046200	1.74818100	-0.59309700
C	1.63178600	1.04401700	-0.34332500
C	2.02931000	-0.34753500	0.13247900
C	0.33134300	1.55037700	-0.46924000
H	0.25557800	2.57876300	-0.79596000
C	-0.80763400	0.82584100	-0.21697500
H	-0.69410800	-0.20013600	0.09210300
C	-2.13087300	1.29610400	-0.35240300
C	-2.38075900	2.72676900	-0.77950400
H	-2.23443800	2.80592600	-1.86218200
H	-1.63010900	3.37021900	-0.31971900
C	-3.77180400	3.21834100	-0.40554800
H	-3.84079900	3.32162500	0.68074200
C	-4.83274100	2.23964400	-0.88711300
H	-4.83808000	2.21079400	-1.98210300
H	-5.82731500	2.55808100	-0.57856600
C	-4.56971900	0.84990000	-0.35645900
C	-3.21423600	0.46626700	-0.13092300
C	-5.60265400	-0.00509000	-0.12804400
H	-5.45103300	-1.00675400	0.25322500
H	-3.94505200	4.20525200	-0.83571200
O	-6.85285400	0.35557200	-0.37650400
C	-7.88672800	-0.60801100	-0.04386700
H	-7.64512100	-1.55179600	-0.53603700
H	-7.87393300	-0.75783600	1.03726400
C	-9.20787100	-0.05568100	-0.51482300
H	-9.42959400	0.89296200	-0.02517300
H	-9.20268000	0.09722400	-1.59439900
H	-10.00179600	-0.76247300	-0.27065800
C	1.55585900	-0.60157600	1.55772700
C	0.59496100	-1.56308500	1.85347000
C	2.05337300	0.20072000	2.58546900
C	0.13144700	-1.72958300	3.15301900
H	0.19151400	-2.19165300	1.07401000
C	1.60934000	0.04289600	3.88875700
H	2.79672000	0.95728000	2.37608900
C	0.65124100	-0.92272100	4.14497400
H	-0.61730200	-2.47188900	3.39020200
H	1.99270400	0.65498400	4.69284200
F	0.20924800	-1.07937800	5.41362200
C	1.73829500	-1.46988200	-0.84883800
C	2.23659000	-2.74218600	-0.55531200
C	1.05914300	-1.26852800	-2.04568100
C	2.04338700	-3.80026100	-1.42764700
H	2.78285100	-2.90874200	0.36247300
C	0.85130000	-2.32122600	-2.93074400
H	0.68028200	-0.29258400	-2.30635100
C	1.34551000	-3.56629900	-2.60054800
H	2.42386200	-4.78803800	-1.20916900
H	0.31997900	-2.17504600	-3.86046100
F	1.14679100	-4.59625500	-3.45422300

FP-INT-I-A

CI	0.67008000	2.16523300	0.86528600
O	-5.25230700	-0.39619600	0.14496000
N	-8.52681800	-1.41148000	0.65009800
N	-7.21824400	-3.36775700	-3.02993500
N	-3.76961100	-2.64408800	-3.78147400
C	-7.68388400	-1.58779700	-0.11985500
C	-6.94380600	-2.66592300	-2.15448200
C	-4.01495400	-2.02969100	-2.83574100
C	-6.65636600	-1.81092200	-1.06722700

C	-5.42878000	-1.19348300	-0.90516300
C	-4.23513800	-1.25109400	-1.68253800
C	-3.27314000	-0.42743700	-1.10915900
C	-3.90733900	0.23262700	0.10914500
C	-1.96295700	-0.26539900	-1.56917100
H	-1.70297500	-0.82060100	-2.46047400
C	-1.02225600	0.53225700	-0.96071600
H	-1.31219400	1.05612800	-0.06496000
C	0.29740700	0.73688600	-1.40335200
C	0.77276900	0.08613300	-2.68463000
H	0.33259700	0.61671600	-3.53570700
H	0.38350000	-0.93263100	-2.72564200
C	2.28921900	0.05449200	-2.81172900
H	2.70150500	-0.66720100	-2.10499400
C	2.88159400	1.42771000	-2.52945100
H	2.55227100	2.14027500	-3.29361100
H	3.96847600	1.39934100	-2.57633400
C	2.45864100	1.92199700	-1.16760800
C	1.17305500	1.54262200	-0.69472200
C	3.27278900	2.73095500	-0.43697300
H	3.00644800	3.07228200	0.55417400
H	2.56869300	-0.27859500	-3.81213800
O	1.99886100	-0.65287800	2.88589800
N	4.09610800	-2.59363300	-0.97070800
C	6.33292300	-0.72814900	-0.79935500
C	5.95311700	-1.46075500	-2.08889700
C	5.27513600	-2.77737400	-1.79617500
H	5.97947900	-3.47569500	-1.32118900
C	3.29464000	-3.79025000	-0.82336000
H	3.27683200	-4.30031700	-1.78753600
H	3.75287400	-4.48534700	-0.10392600
C	1.89733200	-3.41578200	-0.40399800
H	1.27507800	-4.30904900	-0.31916800
H	1.46050300	-2.79028300	-1.18688200
C	1.86416300	-2.65586200	0.92919800
C	2.98253000	-1.59854800	0.95653900
C	3.00009800	-0.60984200	1.95733700
C	4.00120600	0.35228800	2.01807700
C	5.03265000	0.30231100	1.09432600
H	5.82225300	1.03613300	1.17151400
C	5.10554300	-0.66415900	0.10933200
C	4.06450700	-1.63038500	0.03258000
C	7.46222500	-1.48107600	-0.06877900
H	7.75531000	-0.93727800	0.83068200
H	8.33995700	-1.57638300	-0.71384200
H	7.15164000	-2.47962500	0.23792800
C	6.85309200	0.66285900	-1.18378100
H	7.25394800	1.20497300	-0.32727400
H	6.06663800	1.26928800	-1.63053200
H	7.66337300	0.56076700	-1.90901300
C	2.07051600	-3.64911500	2.08920600
H	2.05706800	-3.13014300	3.04623500
H	3.02295800	-4.17329600	2.00054700
H	1.26968200	-4.39356000	2.08999700
C	0.44915000	-2.06018500	1.02500800
H	0.32446000	-1.25288400	0.30753200
H	-0.28082200	-2.83616300	0.78347700
H	0.22185100	-1.67529300	2.01028300
C	1.98674500	0.30327100	3.93238500
H	1.87566900	1.31854800	3.54454600
H	2.89456800	0.24460600	4.53822800
H	4.95271000	-3.24825400	-2.72724000
H	5.27737500	-0.83232500	-2.67470400
H	6.84394500	-1.63529700	-2.69597600
H	3.99729800	1.11791800	2.77699100
O	4.42682500	3.15480400	-0.92427600
C	5.24807600	3.96383800	-0.04415400
H	4.62472200	4.75712500	0.37200700
H	5.59717400	3.32635000	0.76936200
C	6.39408200	4.51972200	-0.85030400
H	6.99989100	3.71718700	-1.27016100

H	6.02844700	5.14807500	-1.66289200
H	7.02801700	5.12709500	-0.20324000
C	-3.20713900	-0.16298400	1.40347900
C	-2.50131000	0.76065700	2.16774000
C	-3.23994200	-1.49707900	1.81105200
C	-1.83852500	0.36974100	3.32446000
H	-2.45753400	1.79724200	1.86982200
C	-2.59413500	-1.90253800	2.96794500
H	-3.77564600	-2.23277500	1.22773000
C	-1.90283900	-0.95560900	3.70225500
H	-1.28413500	1.08145700	3.91885000
H	-2.61301000	-2.93331500	3.29196400
C	-4.17420600	1.72176200	-0.03752900
C	-4.92150400	2.35282700	0.96088400
C	-3.76320800	2.45904000	-1.14264000
C	-5.23609600	3.69842100	0.87124600
H	-5.26270200	1.78753000	1.81669400
C	-4.06560700	3.81298900	-1.24630100
H	-3.20056400	1.99326300	-1.93642500
C	-4.79328300	4.40460800	-0.23453800
H	-5.81236900	4.19536700	1.63882800
H	-3.74576400	4.39483000	-2.09909200
F	-1.25777100	-1.34653200	4.82589900
F	-5.09057000	5.72104800	-0.32597200
H	1.12640900	0.05563000	4.54865000

FP-TS-I-A

Cl	0.88140600	1.88301300	0.76297300
O	-5.26154500	-0.37053100	0.14927500
N	-8.58238000	-1.12066700	0.71365100
N	-7.65361900	-2.76373000	-3.22257300
N	-4.14527900	-2.19283700	-4.10425300
C	-7.79701700	-1.28440900	-0.12136700
C	-7.27334600	-2.18810600	-2.29293500
C	-4.31128200	-1.69887200	-3.07059800
C	-6.85019600	-1.49118900	-1.14532200
C	-5.54347400	-1.01056900	-0.99482400
C	-4.41490200	-1.07454200	-1.82028400
C	-3.31894700	-0.42564800	-1.17511200
C	-3.87211700	0.14841400	0.12473500
C	-2.03765600	-0.34962300	-1.63698300
H	-1.85628100	-0.80701000	-2.60092900
C	-0.96278300	0.30372100	-0.98480800
H	-1.16017600	0.72072400	-0.00941100
C	0.29171500	0.47743900	-1.50132500
C	0.64908000	-0.03096600	-2.88088900
H	0.32404600	0.70344200	-3.62687700
H	0.09949100	-0.94788000	-3.08902500
C	2.13967800	-0.28743300	-3.03048100
H	2.41935100	-1.10347300	-2.36405300
C	2.94132900	0.94952000	-2.66452200
H	2.77860800	1.73839000	-3.40743700
H	4.00937600	0.74062700	-2.67942900
C	2.55906100	1.47289900	-1.30289700
C	1.31395000	1.20984000	-0.80625500
C	3.52612400	2.28300500	-0.60117400
H	3.15591000	2.89175400	0.21472000
H	2.37024000	-0.60261500	-4.04899000
O	3.55971000	1.15341000	2.68782100
N	3.06091000	-2.67231700	-0.09801600
C	5.56541500	-2.12078800	-1.42839600
C	4.51479100	-3.01164500	-2.09515900
C	3.57237400	-3.62629400	-1.08597500
H	4.05916800	-4.44267000	-0.54342700
C	1.85889400	-3.16333700	0.57419500
H	1.13752900	-3.42788800	-0.20105800
H	2.11976600	-4.09041200	1.09361900
C	1.26794600	-2.15895400	1.53062500
H	0.54943600	-2.67281400	2.16987800
H	0.72054900	-1.39012100	0.98197500

C	2.35162100	-1.48268000	2.38468300
C	3.28353200	-0.77989100	1.39230000
C	3.84107900	0.47172200	1.56214700
C	4.67945900	1.05853400	0.55436600
C	5.27924200	0.15211200	-0.37908700
H	6.09576700	0.52884600	-0.97634300
C	4.84596600	-1.11698700	-0.54036700
C	3.69410300	-1.53748100	0.24063600
C	6.49262700	-2.96642100	-0.53116100
H	7.26598300	-2.33520000	-0.09208500
H	6.97615700	-3.74937700	-1.11926500
H	5.94998700	-3.44043700	0.28724100
C	6.40631800	-1.45707400	-2.52086600
H	7.22482600	-0.86798500	-2.10711100
H	5.79908100	-0.80881500	-3.15414100
H	6.84771400	-2.22896500	-3.15333000
C	3.17390100	-2.53112900	3.16217900
H	3.89653200	-2.02928600	3.80683500
H	3.72727600	-3.20170900	2.50489300
H	2.51573200	-3.13489700	3.79131200
C	1.62976900	-0.60204000	3.41099200
H	1.07906700	0.20478400	2.93488500
H	0.91791800	-1.23140900	3.94586600
H	2.31267500	-0.17234300	4.13690400
C	4.22429700	2.37810300	2.99126300
H	3.98118400	3.15879300	2.27071200
H	5.30549800	2.23992900	3.04000900
H	2.70895200	-4.05676300	-1.59288900
H	3.95241600	-2.42311200	-2.81946600
H	5.00279500	-3.81656600	-2.64726000
H	5.32646700	1.85769400	0.88584600
O	4.42016400	2.89537400	-1.40835800
C	5.16949200	3.98635800	-0.84341500
H	4.47763700	4.65753200	-0.32820300
H	5.87878200	3.59123100	-0.11170500
C	5.89242200	4.68941400	-1.96643500
H	6.57037700	4.00485100	-2.47713600
H	5.18456000	5.09041000	-2.69225000
H	6.47845500	5.51529500	-1.56159900
C	-3.18346800	-0.43454800	1.35135000
C	-2.51029300	0.35241200	2.27923500
C	-3.22129800	-1.81775300	1.53683600
C	-1.90113800	-0.22037600	3.39050700
H	-2.45165400	1.42232900	2.14733400
C	-2.62085400	-2.40628400	2.63803300
H	-3.73037800	-2.44575400	0.81861800
C	-1.97684700	-1.58806500	3.54949200
H	-1.37748800	0.38410600	4.11657700
H	-2.65027700	-3.47555500	2.79365400
C	-4.01539000	1.66335800	0.14361900
C	-4.78306700	2.23861300	1.16033600
C	-3.44893200	2.48923900	-0.82037500
C	-4.96832800	3.61003300	1.22694500
H	-5.24414300	1.60799900	1.90737900
C	-3.61962700	3.86950100	-0.76698900
H	-2.86849700	2.06689900	-1.62542500
C	-4.37373200	4.40070200	0.25845000
H	-5.56071000	4.06230500	2.00991500
H	-3.18000400	4.51792600	-1.51180300
F	-1.39215800	-2.15608100	4.63225500
F	-4.54531400	5.74324700	0.31907000
H	3.85263500	2.67127200	3.96891500

FP-INT-I-B

Cl	0.86441500	1.80387700	0.77558700
O	-5.25619100	-0.43358200	0.19503700
N	-8.54646600	-1.22405200	0.85053500
N	-7.79745700	-2.60158400	-3.22255900
N	-4.29693200	-2.00868300	-4.19330800

C	-7.79768000	-1.33523800	-0.02666300
C	-7.37341200	-2.09382800	-2.27172000
C	-4.42986400	-1.57068300	-3.12917200
C	-6.89730800	-1.47754000	-1.10048600
C	-5.58018300	-1.00501900	-0.97757000
C	-4.48948100	-1.01638400	-1.84529100
C	-3.36165300	-0.40108700	-1.20064400
C	-3.87752700	0.10779700	0.14226400
C	-2.10060300	-0.30342200	-1.69263000
H	-1.94592400	-0.70946900	-2.68428600
C	-0.99637100	0.31354500	-1.03100700
H	-1.16902400	0.66622000	-0.02622700
C	0.23764800	0.51961600	-1.56032800
C	0.58165500	0.10745800	-2.97361300
H	0.31743400	0.92290500	-3.65717600
H	-0.01878000	-0.75144200	-3.26839400
C	2.05948000	-0.21880900	-3.12978000
H	2.29163700	-1.09499300	-2.52128500
C	2.91489000	0.95251200	-2.67667200
H	2.79242600	1.79324900	-3.36798000
H	3.97230600	0.69877200	-2.70984800
C	2.54590100	1.41264200	-1.28831300
C	1.29604000	1.19565100	-0.82837700
C	3.59755900	2.14354400	-0.50637600
H	3.12219500	2.81323700	0.20940100
H	2.28460600	-0.47448700	-4.16620300
O	3.62911500	1.23426900	2.58687400
N	3.07927600	-2.62333000	-0.09368500
C	5.58410400	-2.14226000	-1.42622400
C	4.50546200	-2.97860600	-2.12136500
C	3.52311400	-3.56554000	-1.13383800
H	3.95148600	-4.42854400	-0.61797200
C	1.90003500	-3.11769700	0.62725500
H	1.14442100	-3.35490900	-0.12200000
H	2.18705900	-4.05910700	1.10217600
C	1.36460200	-2.13497800	1.63839000
H	0.69969400	-2.67231600	2.31414500
H	0.77013700	-1.36650200	1.14162400
C	2.49001400	-1.45561500	2.43524300
C	3.34702900	-0.73998800	1.38780700
C	3.84274900	0.53087800	1.47492700
C	4.56129500	1.17106200	0.34010600
C	5.22492800	0.18914200	-0.54415400
H	6.01153600	0.57115800	-1.17623700
C	4.86693600	-1.09508800	-0.59514700
C	3.71492800	-1.50636600	0.22021400
C	6.42771200	-3.01808600	-0.47857000
H	7.21496800	-2.42026800	-0.01866500
H	6.89248200	-3.83303800	-1.03636100
H	5.83237600	-3.45374200	0.32422300
C	6.49975600	-1.53026400	-2.48575100
H	7.31065600	-0.95571800	-2.03725100
H	5.94789300	-0.87875800	-3.16480600
H	6.95056200	-2.32929100	-3.07574800
C	3.36179800	-2.49906800	3.16117900
H	4.12503900	-1.99539400	3.75520900
H	3.87077300	-3.17562300	2.47482600
H	2.74513500	-3.09898500	3.83368800
C	1.82368800	-0.57484100	3.49816100
H	1.24417500	0.22878800	3.05132600
H	1.14583200	-1.20461600	4.07540100
H	2.54682500	-0.14047900	4.18187900
C	4.26414000	2.49348600	2.83443500
H	3.94436900	3.25267100	2.12355500
H	5.34914600	2.39133000	2.81963000
H	2.62771700	-3.91437600	-1.64656400
H	3.98095200	-2.35476300	-2.84521300
H	4.96357800	-3.79848100	-2.67632000
H	5.32709000	1.84027300	0.73267700
O	4.39280700	2.88523500	-1.40331800
C	4.99138100	4.05715200	-0.84973200

H	4.20638200	4.70203600	-0.43923200
H	5.66756700	3.78754800	-0.03052100
C	5.75528700	4.76294200	-1.94637400
H	6.53968700	4.11878400	-2.34595100
H	5.08748300	5.04597400	-2.76091000
H	6.22047000	5.66692700	-1.55091600
C	-3.13839300	-0.50860600	1.32218700
C	-2.45274400	0.25443700	2.26076700
C	-3.13926500	-1.89876300	1.45076200
C	-1.79065500	-0.34921200	3.32480800
H	-2.42303700	1.33000500	2.17224100
C	-2.48777400	-2.51824300	2.50515800
H	-3.65870500	-2.50723600	0.72313700
C	-1.82928900	-1.72363100	3.42726300
H	-1.25566100	0.23700000	4.05753400
H	-2.48753300	-3.59350000	2.61626700
C	-4.03877000	1.61938100	0.22767600
C	-4.80443700	2.14287300	1.27325100
C	-3.48049600	2.49213100	-0.69888700
C	-4.99830000	3.50879200	1.40324200
H	-5.25732600	1.47546300	1.99283900
C	-3.65964100	3.86751500	-0.58200900
H	-2.90010100	2.10882500	-1.52335900
C	-4.41317400	4.34651200	0.46926700
H	-5.58999700	3.92115000	2.20850700
H	-3.22691600	4.55228600	-1.29783700
F	-1.19036000	-2.32307000	4.46237400
F	-4.59346900	5.68431500	0.59137800
H	3.94086400	2.77927100	3.83059600

FP-TS-I-B

Cl	-0.28076300	-1.82901700	1.31128000
O	5.64876400	0.31347100	0.27747000
N	8.71244600	1.78131300	0.84877000
N	9.03177500	-0.11359000	-3.07129200
N	5.88902000	-1.79771300	-3.98331800
C	8.20364400	1.16015700	0.01302000
C	8.37072100	0.11133300	-2.14684100
C	5.71925500	-1.30847600	-2.94680700
C	7.59757000	0.40609600	-1.01004700
C	6.26469400	-0.02015400	-0.87176300
C	5.41882100	-0.75585100	-1.69686500
C	4.14628800	-0.92552100	-1.04359000
C	4.22307700	-0.07990400	0.22858400
C	3.09871200	-1.67400800	-1.46912200
H	3.21570400	-2.18334300	-2.41819100
C	1.86068200	-1.79136600	-0.76381200
H	1.84591300	-1.36728500	0.22727500
C	0.69618200	-2.32686300	-1.20182500
C	0.50472600	-2.92051200	-2.57398500
H	0.51831900	-4.01425900	-2.50102900
H	1.32799600	-2.63694700	-3.22731900
C	-0.82687300	-2.47877100	-3.17908200
H	-0.81741500	-1.39357900	-3.30762600
C	-1.98738900	-2.86969800	-2.27261300
H	-2.13198500	-3.95537200	-2.31386800
H	-2.92349600	-2.44490800	-2.63354700
C	-1.76227200	-2.46534200	-0.83574800
C	-0.50936200	-2.27254200	-0.38647400
C	-2.97877500	-2.18200500	0.02700300
H	-2.75345300	-2.47729200	1.05149700
H	-0.95928600	-2.92116900	-4.16773700
O	-3.06890500	-0.54049700	2.42587700
N	-2.03281000	3.33394700	-0.12904200
C	-2.88432200	2.10456200	-2.59682100
C	-1.85558100	3.23518800	-2.59078400
C	-1.99393300	4.10825200	-1.36828900
H	-2.89429400	4.72777200	-1.42868900
C	-1.84593500	4.12748600	1.08084800

H	-1.23637600	4.98888900	0.81697800
H	-2.81559500	4.50477700	1.42124700
C	-1.16462800	3.30142700	2.13837700
H	-1.01734500	3.89993900	3.03839300
H	-0.17605500	3.01760400	1.77168500
C	-1.95567300	2.03648400	2.49566500
C	-2.42117800	1.35231400	1.19952300
C	-2.92668600	0.06609400	1.22155700
C	-3.29482100	-0.66848000	0.03300100
C	-3.10634200	0.04236300	-1.19945700
H	-3.36773100	-0.48308300	-2.10471400
C	-2.76581100	1.34780000	-1.27937000
C	-2.38186300	2.03681900	-0.06552700
C	-4.31520100	2.66903200	-2.69919700
H	-5.03497600	1.85134300	-2.75488500
H	-4.41919300	3.28480500	-3.59534700
H	-4.57820400	3.27723600	-1.83331600
C	-2.61037400	1.21646300	-3.81469800
H	-3.35772300	0.43261900	-3.93565400
H	-1.62740200	0.74884000	-3.74645000
H	-2.63402000	1.82764100	-4.71840200
C	-3.16958200	2.41169600	3.36335700
H	-3.72866700	1.52518600	3.65496300
H	-3.85014200	3.07934200	2.83341200
H	-2.83461300	2.91741500	4.27185000
C	-0.98138900	1.16257000	3.30986900
H	-0.16335600	0.81388000	2.67902900
H	-0.55412000	1.76888600	4.11150000
H	-1.46474700	0.29825300	3.75143100
C	-4.30984700	-1.18634800	2.73892800
H	-4.63434900	-1.87400100	1.96071900
H	-5.08411600	-0.43490600	2.90464300
H	-1.14659300	4.79014600	-1.29239800
H	-0.85486800	2.79915600	-2.62568500
H	-1.96730100	3.85463400	-3.48178500
H	-4.63424100	-0.58572400	0.03306100
O	-4.13072200	-2.89117800	-0.41372700
C	-4.10549100	-4.27663300	-0.06981500
H	-3.21216300	-4.75118500	-0.48839700
H	-4.04791100	-4.37291000	1.02124600
C	-5.35868800	-4.92960900	-0.60582000
H	-6.25007200	-4.47994600	-0.16589300
H	-5.41407700	-4.82524700	-1.69050900
H	-5.35745900	-5.99315500	-0.36318200
C	-6.46375400	0.82014000	0.40528100
C	-7.77908500	1.20692600	0.21451300
C	-8.62731200	0.35439600	-0.48278800
C	-8.13424700	-0.85097200	-0.96746800
C	-6.80514100	-1.16733700	-0.73766600
N	-6.00502200	-0.34306800	-0.06045300
H	-9.66050300	0.62805700	-0.64804500
H	-5.75375700	1.44155700	0.93564600
H	-8.12662300	2.15335800	0.60253700
H	-8.76525600	-1.53629800	-1.51471100
H	-6.35054300	-2.08383000	-1.08576900
C	3.44080900	1.22746200	0.15907300
C	3.77073600	2.24514100	1.05849400
C	2.41241600	1.44410300	-0.75078200
C	3.08440600	3.44985700	1.06127700
H	4.57416500	2.09544800	1.76557600
C	1.71044300	2.64533500	-0.75990800
H	2.14727700	0.67907000	-1.46307800
C	2.06027300	3.62258200	0.14728300
H	3.33445100	4.24056900	1.75463100
H	0.91156800	2.81960700	-1.46438200
C	3.95851300	-0.88153100	1.49583300
C	4.72021300	-2.02848500	1.72645600
C	2.96941900	-0.53532200	2.41003000
C	4.50634100	-2.81325400	2.84830300
H	5.48803100	-2.31556800	1.02082100
C	2.73386000	-1.31397800	3.53827300

H	2.35597700	0.33704800	2.24445100
C	3.51020400	-2.43686700	3.73377100
H	5.09235900	-3.70197900	3.03649500
H	1.95782800	-1.05630900	4.24519100
F	1.37849800	4.79566100	0.14290800
F	3.28953700	-3.20452800	4.82907200
H	-4.13259400	-1.73575700	3.65901900

FP-INT-I-C

Cl	-0.08508300	-1.08082800	-1.99559200
O	-5.70807600	0.88452200	0.46980400
N	-8.47020900	2.83656900	1.12644100
N	-9.08440500	-0.85590000	3.37035200
N	-6.25476200	-3.16314600	2.91649500
C	-8.07426600	1.78741500	1.41921100
C	-8.40348600	-0.25174200	2.65369200
C	-6.03001500	-2.22706700	2.27163600
C	-7.60461700	0.51111300	1.78389000
C	-6.37649300	0.04510300	1.28139500
C	-5.67180200	-1.14139700	1.46471100
C	-4.44238900	-1.08534900	0.71688900
C	-4.49106500	0.22960200	-0.06152600
C	-3.42404900	-1.97942100	0.74060700
H	-3.53981200	-2.83423900	1.39571500
C	-2.21607600	-1.83751800	-0.01165200
H	-2.20544400	-1.04809600	-0.74492200
C	-1.06930100	-2.54578500	0.11659700
C	-0.87547000	-3.66043900	1.11270200
H	-0.90009600	-4.62378100	0.59011900
H	-1.68907400	-3.67016900	1.83511500
C	0.46594700	-3.51676000	1.82958300
H	0.47097500	-2.57564000	2.38605800
C	1.61486700	-3.52377700	0.82846000
H	1.76667500	-4.54319000	0.45594600
H	2.55325100	-3.25420200	1.31461100
C	1.37285300	-2.60120600	-0.34137400
C	0.12472100	-2.20118000	-0.64063800
C	2.57266900	-2.03569300	-1.07510500
H	2.36470600	-2.00944000	-2.14453900
H	0.59839300	-4.32172200	2.55420600
O	3.30924300	0.09495200	-2.85059700
N	3.61844200	3.25913800	0.79089700
C	2.86222800	1.19839200	2.73401100
C	2.90288800	2.70127500	3.03985800
C	3.93979200	3.41086300	2.19788200
H	4.94926400	3.02916500	2.41213000
C	4.19651900	4.23479200	-0.10809300
H	4.13199600	5.21229600	0.37014500
H	5.26313200	4.03089900	-0.28613500
C	3.41599900	4.21925000	-1.39901900
H	3.76910400	5.00282600	-2.07119000
H	2.37149400	4.43690600	-1.16294800
C	3.51237100	2.86244400	-2.11693500
C	3.36723800	1.72378300	-1.09023500
C	3.20484800	0.39403000	-1.50636900
C	2.87834700	-0.63085100	-0.61093000
C	2.76171100	-0.30043300	0.73188100
H	2.47843000	-1.07471500	1.42803600
C	2.99762900	0.96621600	1.22606400
C	3.33372100	1.99666000	0.31019500
C	4.00983300	0.48815300	3.47399800
H	4.02547700	-0.57726600	3.23991300
H	3.88507600	0.59631200	4.55391600
H	4.97942500	0.90349700	3.20036100
C	1.52318900	0.64377400	3.24915500
H	1.47712400	-0.44313200	3.18493000
H	0.68753300	1.05290800	2.68109000
H	1.39142400	0.91596500	4.29864200
C	4.85915000	2.79743900	-2.85872600

H	4.92468900	1.91657700	-3.48989300
H	5.69895100	2.78256100	-2.16285400
H	4.96622000	3.67480300	-3.50088500
C	2.36247700	2.83353100	-3.14207700
H	1.39777300	2.83723900	-2.63178300
H	2.41445600	3.72863800	-3.76659600
H	2.40947500	1.95928500	-3.78371900
C	4.48585200	-0.61652100	-3.24226200
H	4.53810700	-1.59975900	-2.77756500
H	5.38570000	-0.05631100	-2.97864600
H	3.94700300	4.47737000	2.42229000
H	1.92851400	3.14410600	2.82621900
H	3.10887500	2.85345100	4.10120600
H	5.02690100	-2.10984300	0.01935800
O	3.74765900	-2.85103300	-0.87319500
C	3.78393700	-4.04494800	-1.66653700
H	2.88666700	-4.63697400	-1.47135000
H	3.77425900	-3.76463700	-2.72506800
C	5.03203300	-4.82173500	-1.31991400
H	5.92843200	-4.23376300	-1.52421100
H	5.03072200	-5.11128800	-0.26793800
H	5.07929700	-5.73024300	-1.92118100
C	6.05068100	-0.37098300	0.40736400
C	7.02408400	0.23648500	1.17016600
C	7.68930600	-0.51091700	2.13465900
C	7.36604000	-1.85163100	2.31596800
C	6.39019400	-2.41471200	1.52257700
N	5.76982700	-1.66804500	0.59774100
H	8.45126600	-0.05030300	2.74767800
H	5.47379800	0.14277300	-0.34505000
H	7.24348600	1.28176700	1.01551300
H	7.86110700	-2.45468000	3.06143400
H	6.07927900	-3.44489400	1.59847500
C	-3.32164100	1.14455700	0.28428800
C	-2.35993300	1.51297500	-0.65063600
C	-3.17904200	1.57690500	1.60362500
C	-1.27189300	2.29955700	-0.28767000
H	-2.43850400	1.17791600	-1.67374900
C	-2.10800200	2.37154300	1.98313800
H	-3.91082400	1.29127700	2.34675200
C	-1.17394900	2.71906700	1.02224700
H	-0.51423300	2.57737400	-1.00628000
H	-1.99282000	2.71558300	3.00142700
C	-4.73866200	0.07539700	-1.55519400
C	-5.06518400	1.21532500	-2.29466400
C	-4.68475700	-1.15346300	-2.20201000
C	-5.31931900	1.13618100	-3.65460200
H	-5.12351400	2.17602300	-1.80229800
C	-4.93145200	-1.25262400	-3.56827400
H	-4.44886900	-2.04715100	-1.64467100
C	-5.24135300	-0.10366900	-4.26571300
H	-5.57298000	2.01283300	-4.23407800
H	-4.88830700	-2.20439300	-4.07902300
F	-0.12613900	3.49923900	1.38394200
F	-5.48329500	-0.18933600	-5.59682400
H	4.43302700	-0.72545800	-4.32304900

FP-TS-I-C

Cl	0.32249300	-1.97802300	1.72804400
O	5.54442000	1.07520300	-0.15398400
N	8.00377900	3.48616200	-0.28206500
N	8.51412600	1.09114700	-3.89687800
N	6.04887900	-1.62229700	-4.04574500
C	7.64419500	2.59507200	-0.92935600
C	7.91767600	1.26799900	-2.91995500
C	5.83560900	-1.03122600	-3.07273900
C	7.21655600	1.51466500	-1.72572100
C	6.12640600	0.73025100	-1.31554600
C	5.50039300	-0.38099400	-1.87909300

C	4.40543700	-0.78667400	-1.04358800
C	4.40161800	0.18344400	0.14062700
C	3.53255000	-1.80316200	-1.26773400
H	3.65932600	-2.36841300	-2.18260700
C	2.39175900	-2.03986100	-0.44317800
H	2.41146800	-1.56909100	0.52549300
C	1.22772100	-2.64708600	-0.78272200
C	0.96841700	-3.28807500	-2.12098700
H	0.86034100	-4.37047700	-1.99153700
H	1.81450800	-3.13108900	-2.78653400
C	-0.31152800	-2.73124000	-2.74654200
H	-0.18596100	-1.65965800	-2.92481100
C	-1.49970400	-2.96113900	-1.82198800
H	-1.75246600	-4.02656100	-1.80224000
H	-2.39357700	-2.46719500	-2.19635300
C	-1.21862900	-2.52987000	-0.40001700
C	0.05342500	-2.48961400	0.05584500
C	-2.28305800	-2.00619200	0.47145900
H	-2.24992800	-2.35913100	1.49167800
H	-0.49708900	-3.20237500	-3.71284700
O	-3.13790700	-0.54157400	2.69250000
N	-3.58506800	3.41865400	0.02448200
C	-3.03880900	1.98126300	-2.41824600
C	-2.70572500	3.46886300	-2.27085500
C	-3.59012800	4.13616400	-1.24410700
H	-4.61805000	4.22657400	-1.61177700
C	-4.06903200	4.15863400	1.17873500
H	-3.99782400	5.21987400	0.94837900
H	-5.12714900	3.93378500	1.35376900
C	-3.22129000	3.80892000	2.37623400
H	-3.52480500	4.39812300	3.24255400
H	-2.18635200	4.06922300	2.14655600
C	-3.31647300	2.31547800	2.72532200
C	-3.23801200	1.48114000	1.43297500
C	-3.07563500	0.10226100	1.48040100
C	-2.72220600	-0.65712600	0.33364900
C	-2.65869700	0.02290700	-0.89605200
H	-2.38946000	-0.53617000	-1.77501100
C	-2.96482300	1.34415700	-1.03528100
C	-3.26625300	2.10839000	0.14063500
C	-4.46518000	1.79608300	-2.97049700
H	-4.67954400	0.73573900	-3.10803400
H	-4.56746700	2.29798700	-3.93549600
H	-5.22035900	2.19455700	-2.29464000
C	-2.04795800	1.35845900	-3.40874900
H	-2.29102800	0.32138700	-3.63941900
H	-1.02515700	1.39338400	-3.03120400
H	-2.07973000	1.91396100	-4.34744500
C	-4.63081300	2.07085600	3.48672700
H	-4.67760000	1.06150600	3.88379200
H	-5.50182600	2.22720600	2.84913000
H	-4.69865300	2.76171500	4.32996000
C	-2.11954900	2.01275900	3.64780100
H	-1.18091200	2.13968400	3.10595400
H	-2.12419000	2.71714600	4.48280900
H	-2.15610000	1.00424900	4.04756300
C	-4.30320700	-1.34032400	2.92475700
H	-4.43798200	-2.08799000	2.14617800
H	-5.19703100	-0.71666800	2.97691900
H	-3.23570800	5.14891600	-1.04747100
H	-1.66035900	3.57581500	-1.97093100
H	-2.82412900	3.97819300	-3.22848900
H	-4.58223500	-2.56041600	-0.25500000
O	-3.74227700	-3.13166200	-0.07660400
C	-3.98413900	-4.36817300	0.60880500
H	-3.00258000	-4.80395900	0.79680800
H	-4.46056300	-4.17593100	1.57348800
C	-4.83180200	-5.29131400	-0.24313200
H	-5.81902700	-4.86329700	-0.42301800
H	-4.35020400	-5.47900400	-1.20324600
H	-4.96567700	-6.24491100	0.27077700

C	-6.14619300	-0.47585300	-0.24643100
C	-7.09474000	0.35230100	-0.82393900
C	-7.67919800	-0.03822800	-2.02131800
C	-7.29211300	-1.24181500	-2.59593200
C	-6.33910500	-2.01133800	-1.94614900
N	-5.77893800	-1.63833800	-0.79198800
H	-8.41834900	0.58787900	-2.50259000
H	-5.65495700	-0.19599200	0.67427800
H	-7.35838200	1.28528900	-0.34662900
H	-7.71610800	-1.58126100	-3.53020900
H	-6.00611600	-2.95528400	-2.35976800
C	3.18723900	1.09576800	0.24947100
C	3.16356000	2.05365700	1.26680100
C	2.11098800	1.02898300	-0.63014900
C	2.07873600	2.90223800	1.42848900
H	3.99880900	2.13418000	1.94853700
C	1.00703100	1.86031100	-0.47434200
H	2.11394400	0.31503600	-1.43779600
C	1.01175000	2.77700000	0.55603200
H	2.05299000	3.64137200	2.21683800
H	0.15486300	1.79036500	-1.13366000
C	4.74639400	-0.54915700	1.43529900
C	6.02419500	-1.09326100	1.57834100
C	3.81608500	-0.74624000	2.45112600
C	6.37224300	-1.81247900	2.71142200
H	6.76198000	-0.95624800	0.80051400
C	4.14352500	-1.47153900	3.59164800
H	2.82094000	-0.33699600	2.36728800
C	5.41822300	-1.98850800	3.69827300
H	7.36160700	-2.23130800	2.83121200
H	3.42301600	-1.62891900	4.38190900
F	-0.06251200	3.58674500	0.71648400
F	5.74998500	-2.69256100	4.80797500
H	-4.14852300	-1.83428500	3.88038400

Type-I product (TCF5-based)

CI	-0.01719400	-1.18963600	0.54376900
O	6.39246800	-0.25964800	-0.01809400
N	9.83541800	-0.66175700	-0.00629300
N	9.11246300	3.47422200	-1.21612900
N	5.60178900	4.20308700	-1.47432100
C	9.07058400	0.17420000	-0.23273100
C	8.65588800	2.46016100	-0.90297100
C	5.66209500	3.11503100	-1.09309600
C	8.14185700	1.20379300	-0.51332100
C	6.78399800	0.95517700	-0.39730400
C	5.65214200	1.78641500	-0.62731900
C	4.48965800	1.06883900	-0.35140100
C	4.91564100	-0.31420100	0.12653800
C	3.18524700	1.53076700	-0.52668800
H	3.08857500	2.53693300	-0.91242000
C	2.05339800	0.79135000	-0.25115500
H	2.18692100	-0.20915400	0.12483900
C	0.72904500	1.22179000	-0.43581900
C	0.47547500	2.62710400	-0.94136900
H	0.74334900	2.67176100	-2.00243900
H	1.15004000	3.31303300	-0.42637500
C	-0.96558000	3.08159600	-0.76234300
H	-1.16306700	3.29729000	0.29116900
C	-1.90471900	1.98430200	-1.23942200
H	-1.67571600	1.75406200	-2.28678200
H	-2.93741800	2.30797200	-1.22173100
C	-1.70998000	0.71313000	-0.44166300
C	-0.35009300	0.38278500	-0.17392000
C	-2.73292100	-0.13160900	-0.08199400
H	-2.43775400	-1.10988200	0.27067500
H	-1.13465800	4.00336400	-1.32014000
O	-4.41112200	-2.30102700	-0.36889800
N	-8.31863800	0.43515800	0.16846000

C	-6.71212400	2.85794300	0.39938000
C	-8.13738100	2.74149600	0.94656800
C	-8.95507000	1.74284700	0.16242200
H	-9.11120100	2.08322400	-0.86843900
C	-9.18242800	-0.69686900	-0.11544400
H	-10.17837300	-0.45592700	0.25365000
H	-9.26737600	-0.84994400	-1.19841700
C	-8.64053900	-1.92260700	0.57464200
H	-9.30286600	-2.77333500	0.40772000
H	-8.62302100	-1.72869600	1.65013400
C	-7.22734900	-2.28301200	0.09236000
C	-6.37165000	-1.00635200	0.02049500
C	-4.99602500	-1.07545100	-0.15394500
C	-4.14843500	0.06150600	-0.09942400
C	-4.77319800	1.30321500	0.10613400
H	-4.15071900	2.17237000	0.23752000
C	-6.12976200	1.45519900	0.22163400
C	-6.96454200	0.29517200	0.13985800
C	-6.72075700	3.57581200	-0.96377500
H	-5.70338700	3.68305000	-1.34238400
H	-7.15739300	4.57247000	-0.86481600
H	-7.29244000	3.02351800	-1.70986400
C	-5.89250900	3.69465100	1.39287700
H	-4.89492800	3.92347400	1.01869900
H	-5.79088600	3.17816000	2.34859000
H	-6.39827300	4.64590200	1.56986900
C	-7.32839100	-2.96402000	-1.28411400
H	-6.35871200	-3.31872100	-1.62181600
H	-7.72243900	-2.28480500	-2.04075200
H	-7.99656600	-3.82594600	-1.21911500
C	-6.67080200	-3.28582000	1.12149500
H	-6.52728700	-2.80053400	2.08873600
H	-7.39230800	-4.09511600	1.25587400
H	-5.72531600	-3.71487600	0.80658100
C	-3.85307100	-2.51294000	-1.67238800
H	-2.96181900	-1.90564500	-1.83326300
H	-4.58878000	-2.28263200	-2.44513000
H	-9.94203000	1.62777100	0.61039200
H	-8.09973800	2.42309900	1.99175400
H	-8.62647600	3.71661200	0.91894600
C	4.67430700	-0.58687700	1.60157400
C	5.21038800	-1.75608100	2.14824900
C	4.00088900	0.30144900	2.43285400
C	5.06117200	-2.04577400	3.49428100
H	5.75158500	-2.44702500	1.51722200
C	3.83686300	0.02383400	3.78610100
H	3.59251600	1.21942700	2.03989700
C	4.36844100	-1.14644800	4.28722200
H	5.47112500	-2.94787600	3.92604400
H	3.31034400	0.70601400	4.43841100
C	4.42082000	-1.40484700	-0.81474600
C	4.87135500	-1.40914600	-2.13554200
C	3.48502700	-2.35355700	-0.41560600
C	4.40563200	-2.34782200	-3.04264000
H	5.59442500	-0.67715100	-2.46750100
C	2.99999700	-3.29712300	-1.31356600
H	3.11693800	-2.36525200	0.59921800
C	3.47343600	-3.27505200	-2.60980000
H	4.75264700	-2.36319500	-4.06614700
H	2.26966500	-4.03441000	-1.01195900
F	4.21292400	-1.42555400	5.60180000
F	3.01029300	-4.19136900	-3.49107200
H	-3.58801300	-3.56657200	-1.72023200

TCF5-based (Path II)

FP-INT-II-A

Cl	-0.01775400	-2.31888300	1.45886800
O	5.14518200	1.39463400	0.15223000

N	7.85545500	3.54513800	0.39041800
N	7.48409800	2.54189800	-3.84565000
N	4.65240600	0.43026700	-4.48386700
C	7.28827600	2.96873700	-0.43415800
C	7.06814100	2.40585200	-2.77692000
C	4.67768200	0.56582200	-3.33831600
C	6.59826600	2.26626700	-1.45147500
C	5.51259000	1.47673100	-1.12271000
C	4.64297200	0.68575800	-1.93430200
C	3.71055100	0.05457700	-1.12498800
C	4.01727400	0.44163600	0.31555000
C	2.66855200	-0.76996100	-1.57093700
H	2.61790600	-0.92958500	-2.63951900
C	1.75437500	-1.37146300	-0.74252400
H	1.83432800	-1.18303900	0.31530200
C	0.71934300	-2.24182300	-1.14577600
C	0.56489100	-2.60059700	-2.60818100
H	1.31295900	-3.35792300	-2.86581300
H	0.79343400	-1.72449500	-3.21534100
C	-0.82867700	-3.10554000	-2.95358100
H	-1.53815800	-2.27695900	-2.90288200
C	-1.26064000	-4.20284800	-1.99121500
H	-0.62337900	-5.08320100	-2.12615500
H	-2.28094800	-4.52229800	-2.19790700
C	-1.16539500	-3.74031200	-0.55634900
C	-0.14799600	-2.79736700	-0.22454000
C	-2.03395700	-4.20943600	0.37877200
H	-1.99317900	-3.89566500	1.41371000
O	-2.98549500	-5.07198000	0.05480500
C	-3.85619900	-5.51455000	1.12922900
H	-3.25951100	-6.10994200	1.82244100
H	-4.23156300	-4.63275100	1.65065000
C	-4.97476800	-6.32024200	0.51992600
H	-5.55757800	-5.71455100	-0.17462100
H	-4.58383500	-7.18780300	-0.01222700
H	-5.63830000	-6.67159700	1.31088100
H	-2.87705200	-1.04479900	0.52285300
O	-6.27427000	4.22882500	0.68242600
N	-3.12318800	0.79848000	-0.47996100
C	-5.27538100	-1.15545400	-0.89885700
C	-3.83614900	-1.33549200	-1.39152700
C	-2.85183300	-0.62498700	-0.49381600
C	-2.06832600	1.60268500	0.10372400
H	-1.11277400	1.21325100	-0.24961000
H	-2.06443300	1.51555300	1.20060700
C	-2.25256300	3.03513800	-0.32785300
H	-1.43484600	3.65672100	0.03872100
H	-2.21880800	3.06309000	-1.42004500
C	-3.58524400	3.62390400	0.16372900
C	-4.70660200	2.57775700	0.04089900
C	-6.04450500	2.94207900	0.28125400
C	-7.08733600	2.03405800	0.13140000
H	-8.11038000	2.32035500	0.31557000
C	-6.79550200	0.73874100	-0.26345200
H	-7.61669800	0.04494800	-0.38446400
C	-5.50189300	0.30156400	-0.48920200
C	-4.43834300	1.22552200	-0.30423400
C	-5.53104900	-2.08375300	0.30282700
H	-6.54442000	-1.95327600	0.68431700
H	-5.41199400	-3.12734900	0.00287100
H	-4.83976500	-1.87970100	1.12116800
C	-6.21745300	-1.56651700	-2.04192000
H	-7.26289400	-1.56868400	-1.73381000
H	-6.11343900	-0.88978400	-2.89162400
H	-5.97093200	-2.57692000	-2.37685200
C	-3.41934800	4.06063600	1.63210800
H	-4.34917800	4.46053100	2.02952000
H	-3.11183900	3.22166300	2.25710100
H	-2.64915800	4.83207700	1.70488900
C	-3.85072300	4.86202400	-0.71599300
H	-4.05844300	4.56045000	-1.74474500

H	-2.95718100	5.49142600	-0.72530900
H	-4.68499200	5.45491000	-0.35539100
C	-7.60775800	4.64756000	0.92612600
H	-8.06677300	4.07245400	1.73426400
H	-1.83502200	-0.75878800	-0.86092500
H	-3.74114600	-0.92674100	-2.40110000
H	-3.60047000	-2.39883300	-1.44639900
H	-7.54157000	5.69218200	1.22048900
C	2.87267300	1.22381600	0.94744000
C	2.13126300	0.71378000	2.00867700
C	2.53207100	2.46879000	0.41713700
C	1.07284600	1.43402100	2.54834800
H	2.37096200	-0.25100900	2.42945800
C	1.48655700	3.20606300	0.95035900
H	3.08961400	2.87995200	-0.41281800
C	0.77992400	2.67230700	2.01397100
H	0.49209800	1.04531800	3.37258100
H	1.22406600	4.17739500	0.55613300
C	4.57421300	-0.68048700	1.17553600
C	4.69693300	-1.98995000	0.72329800
C	5.04261600	-0.35532900	2.45162900
C	5.25234600	-2.97323100	1.53538100
H	4.36149100	-2.26562700	-0.26420400
C	5.60307000	-1.32061700	3.27121700
H	4.97122800	0.66230700	2.80889900
C	5.69070800	-2.61764600	2.79426400
H	5.34667200	-3.99431700	1.19407500
H	5.96688500	-1.07894900	4.25987500
F	-0.23280900	3.39011600	2.54691400
F	6.23077000	-3.56746100	3.59121300
H	-8.22436400	4.56276500	0.02783400
H	-0.84416500	-3.47731000	-3.97848600

FP-TS-II-A

Cl	-0.42744700	-1.26164400	1.22774400
O	5.58696900	1.03193100	0.20077600
N	8.54297900	2.78708200	0.50813900
N	9.24328800	-0.16975200	-2.62753300
N	6.23444900	-2.12336400	-3.30475200
C	8.12651700	1.91674800	-0.13132200
C	8.50096200	0.28096500	-1.86268000
C	5.97175000	-1.41228900	-2.43061000
C	7.62958500	0.85581200	-0.91710800
C	6.31645900	0.41210900	-0.73682600
C	5.56415100	-0.58845300	-1.37127700
C	4.26522100	-0.63900100	-0.79563800
C	4.24758700	0.40971200	0.31357100
C	3.22570800	-1.43566600	-1.19310600
H	3.41802100	-2.08873000	-2.03457000
C	1.95819500	-1.47374500	-0.57428500
H	1.82414600	-0.86300000	0.30329000
C	0.88623300	-2.23346100	-0.96601900
C	0.94973800	-3.12494700	-2.18681600
H	1.36700000	-4.09745400	-1.90142100
H	1.63385600	-2.69516700	-2.91715100
C	-0.42005400	-3.32957800	-2.82107500
H	-0.78398500	-2.37520800	-3.21215700
C	-1.40859600	-3.86496300	-1.79686100
H	-1.15385500	-4.89654000	-1.53006600
H	-2.41466000	-3.90945100	-2.21504600
C	-1.42488800	-3.02472200	-0.54186000
C	-0.33601900	-2.25611500	-0.22403000
C	-2.62802400	-3.03747600	0.25038100
H	-2.55695600	-2.69970100	1.28099200
O	-3.44972800	-4.10258700	0.04749700
C	-3.94429400	-4.75719600	1.23660800
H	-3.09847600	-5.24117300	1.73064500
H	-4.35644500	-4.00854300	1.91505500
C	-4.98681100	-5.76382900	0.81874700

H	-5.82770700	-5.27560100	0.32492200
H	-4.56147200	-6.49968100	0.13576400
H	-5.36073500	-6.28725400	1.69953000
H	-3.34618800	-1.96830500	-0.23505200
O	-5.55529400	4.35891800	0.66784200
N	-3.80859800	0.14986400	-0.82733200
C	-6.28369000	-1.20148800	-0.24174500
C	-5.32019400	-1.69449400	-1.32758800
C	-3.93556300	-1.15945800	-1.16478500
C	-2.46862100	0.72808700	-0.84439500
H	-1.83181500	0.07522500	-1.43854500
H	-2.07055600	0.72956100	0.17270100
C	-2.52908900	2.11740700	-1.42070000
H	-1.52388900	2.53392900	-1.48609100
H	-2.92067600	2.05322800	-2.43899100
C	-3.41193300	3.05367000	-0.58356000
C	-4.69932900	2.32559100	-0.17235000
C	-5.76923300	3.04280100	0.40212900
C	-6.98229800	2.42681700	0.68488100
H	-7.80276800	2.98623200	1.10526500
C	-7.14265500	1.07588300	0.42422400
H	-8.09527900	0.61902100	0.64892100
C	-6.11455600	0.30229700	-0.08126500
C	-4.88163500	0.93562200	-0.35258300
C	-5.98191300	-1.87046100	1.11018900
H	-6.67376000	-1.50285200	1.86820800
H	-6.10318400	-2.95103800	1.03549500
H	-4.97218200	-1.64970600	1.45641600
C	-7.70348700	-1.58890900	-0.67520100
H	-8.43819300	-1.38214400	0.10179800
H	-7.99795100	-1.05510900	-1.57977200
H	-7.74076900	-2.66014800	-0.88130900
C	-2.63899300	3.50562500	0.66998100
H	-3.25823100	4.14035800	1.29921600
H	-2.31625400	2.65132000	1.26711900
H	-1.75535100	4.07175900	0.37276200
C	-3.69573600	4.27330600	-1.48406800
H	-4.34686300	3.99325400	-2.31426200
H	-2.75073900	4.62662100	-1.90210100
H	-4.15860700	5.09042600	-0.94203700
C	-6.61074600	5.13633400	1.21897000
H	-6.91389000	4.75718200	2.19747600
H	-3.21412400	-1.46064100	-1.92228700
H	-5.67947000	-1.36518300	-2.30963500
H	-5.28737500	-2.78360400	-1.35051200
H	-6.21000600	6.14048900	1.32843000
C	3.22989100	1.50320800	0.01217200
C	2.07376400	1.66815500	0.76719500
C	3.43141500	2.31840800	-1.10258700
C	1.12801400	2.62823600	0.42534400
H	1.89205100	1.04704000	1.63141900
C	2.50326500	3.28534500	-1.45612800
H	4.32088600	2.20255800	-1.70578800
C	1.36538800	3.41917200	-0.68030200
H	0.22853100	2.75898200	1.00802500
H	2.65366200	3.92444700	-2.31485400
C	4.18517000	-0.14125700	1.72834000
C	4.07554900	-1.50048900	1.99965600
C	4.30660600	0.75486800	2.79366000
C	4.06040400	-1.96659700	3.31047000
H	3.99783000	-2.21143000	1.19142300
C	4.29885800	0.30892900	4.10539200
H	4.40993000	1.81296000	2.59735500
C	4.16913900	-1.05006600	4.33590700
H	3.97029800	-3.02107200	3.53028000
H	4.39125300	0.99483100	4.93573400
F	0.45295200	4.36130500	-1.02212000
F	4.15306400	-1.49376300	5.61536000
H	-7.47582600	5.16021200	0.55258400
H	-0.34446200	-4.01641200	-3.66485400

FP-INT-II-B

Cl	1.46207800	0.35963100	1.48988000
O	-4.99571200	-0.61760500	-0.09514500
N	-8.19303000	-1.87430600	-0.37209400
N	-7.70036800	0.84959700	-3.75043800
N	-4.32608300	2.32301500	-3.77766700
C	-7.51127300	-1.13501000	-0.94769300
C	-7.22972200	0.36787500	-2.80794700
C	-4.39221200	1.64188600	-2.84284900
C	-6.69211900	-0.23520100	-1.65678700
C	-5.38825300	0.03084500	-1.20560400
C	-4.36986600	0.84551700	-1.69256000
C	-3.21806200	0.73486900	-0.83552800
C	-3.64377500	-0.17209600	0.31493300
C	-2.03436300	1.37436200	-0.99766600
H	-1.98853000	2.07143100	-1.82610500
C	-0.87423400	1.25108300	-0.16635100
H	-0.80255900	0.36508700	0.44737900
C	0.12243800	2.16978600	-0.07293500
C	-0.00277200	3.52831000	-0.73599700
H	-0.65844200	4.14299200	-0.10859500
H	-0.51379000	3.42877300	-1.69322400
C	1.32013200	4.25737200	-0.93647300
H	1.88605900	3.79403700	-1.74681900
C	2.16342600	4.23953800	0.32871000
H	1.71384900	4.88934200	1.09034200
H	3.15800600	4.63807000	0.13206700
C	2.30063000	2.85565200	0.91002500
C	1.31987100	1.95250900	0.72196800
C	3.53380500	2.60875800	1.72128600
H	3.49898000	3.22034900	2.63675900
H	1.12695400	5.28525800	-1.24695300
O	4.67335400	2.97692500	0.95384900
C	5.89017400	2.75294100	1.65216300
H	5.87699400	3.30626400	2.60039400
H	5.98194500	1.68668000	1.89516800
C	7.04219200	3.20849300	0.78508700
H	7.06363200	2.65706300	-0.15552900
H	6.95809900	4.27229600	0.55810000
H	7.98827300	3.04068500	1.30208200
H	3.61132800	1.56354000	2.02333900
O	5.22272500	-2.68644700	1.43422100
N	1.87893900	-1.14901600	-1.63478600
C	3.64246300	0.80183400	-2.75943700
C	2.12746300	1.00302900	-2.72534400
C	1.37500500	-0.19440000	-2.33707500
C	0.97520800	-2.21910400	-1.15506000
H	0.16641200	-2.30812600	-1.87353900
H	0.55952700	-1.87525900	-0.20909200
C	1.74972300	-3.49616700	-0.99806400
H	1.06860900	-4.29529500	-0.71095000
H	2.18253200	-3.77155600	-1.96286200
C	2.85895700	-3.36742400	0.05504400
C	3.64362100	-2.07945800	-0.20813300
C	4.87049800	-1.82828700	0.44645200
C	5.66069800	-0.74483100	0.08682700
H	6.60291400	-0.56542700	0.57957400
C	5.26105300	0.10458200	-0.93427000
H	5.91710200	0.90948900	-1.22430100
C	4.04332300	-0.04990300	-1.56351100
C	3.22670300	-1.11214600	-1.13495900
C	4.31344300	2.17806200	-2.75695000
H	5.38341400	2.09979600	-2.94680100
H	3.88677100	2.79394000	-3.55008600
H	4.17098800	2.68518300	-1.80259800
C	4.02792300	0.04095300	-4.04310100
H	5.10345800	-0.13473900	-4.06629200
H	3.52667600	-0.92665400	-4.10419200
H	3.75266000	0.62427600	-4.92402200
C	2.25062500	-3.36546100	1.46857100

H	3.03020100	-3.28191600	2.22144900
H	1.55858300	-2.53641900	1.60915500
H	1.70449700	-4.29507000	1.63452300
C	3.75572300	-4.60950500	-0.12173900
H	4.27432500	-4.57664300	-1.08138000
H	3.12379200	-5.49976600	-0.11010600
H	4.49258200	-4.69980500	0.66879700
C	6.46255400	-2.49431300	2.10861900
H	6.48791100	-1.52935300	2.61900800
H	0.32596400	-0.28297700	-2.58560400
H	1.74737400	1.37820300	-3.67649700
H	1.85875400	1.75689200	-1.97667100
H	6.52482500	-3.29423500	2.84084600
H	7.30328900	-2.56618100	1.41553000
C	-2.81614800	-1.44577700	0.43673700
C	-2.04868000	-1.73180200	1.56145000
C	-2.86407900	-2.37602800	-0.60289200
C	-1.36991800	-2.94077200	1.67401100
H	-1.98309700	-1.02069300	2.37113800
C	-2.19692400	-3.58779100	-0.50790200
H	-3.44698500	-2.16562600	-1.48878700
C	-1.47382000	-3.85084600	0.64228100
H	-0.78443100	-3.17553900	2.55092100
H	-2.24252700	-4.32139300	-1.30051100
C	-3.84891300	0.55127200	1.64103100
C	-4.53069800	-0.12495800	2.65701000
C	-3.41783000	1.85204800	1.87245300
C	-4.76593000	0.47530600	3.88335900
H	-4.88495700	-1.13204400	2.48755500
C	-3.63946800	2.46982200	3.10011700
H	-2.90452100	2.39902800	1.09799200
C	-4.30703300	1.76650100	4.08078200
H	-5.29383600	-0.04095800	4.67289600
H	-3.30473300	3.48050200	3.28741500
F	-0.83791100	-5.04273000	0.75317200
F	-4.52794500	2.35975100	5.27906100

FP-TS-II-B

Cl	-0.95146400	-0.19631900	1.18537400
O	5.35112900	0.73350700	-0.16936000
N	8.49252600	2.13178300	-0.53057500
N	8.77269500	-1.88277500	-2.22800100
N	5.59327500	-3.62193600	-2.07459800
C	7.96666000	1.13112000	-0.77499100
C	8.10852000	-1.09010600	-1.71063600
C	5.41834500	-2.59532600	-1.57304000
C	7.33445900	-0.09499500	-1.07875100
C	5.99327300	-0.28004200	-0.75625400
C	5.11957300	-1.37273000	-0.94861700
C	3.84400700	-1.04270000	-0.45016100
C	3.96735900	0.33473100	0.19079800
C	2.70996100	-1.82526200	-0.53457000
H	2.83949200	-2.79913200	-0.98817100
C	1.44982700	-1.45386800	-0.06544400
H	1.34592700	-0.46011900	0.34167300
C	0.31843400	-2.26021900	-0.04724900
C	0.39431900	-3.69636400	-0.52740200
H	0.87292700	-4.29098600	0.25829400
H	1.05064700	-3.75532100	-1.39566200
C	-0.95926400	-4.30138400	-0.87824100
H	-1.29563400	-3.89804900	-1.83483200
C	-2.00538000	-4.01250800	0.18851700
H	-1.75466200	-4.53721300	1.11742600
H	-2.98071700	-4.38241400	-0.12154800
C	-2.11069900	-2.52199200	0.48097200
C	-0.89155900	-1.81932600	0.50884300
C	-3.17559400	-2.11520600	1.48883700
H	-2.75270800	-2.16742500	2.50322200
H	-0.85385500	-5.37856400	-1.01562100

O	-4.28705300	-2.98009500	1.39882800
C	-5.29729400	-2.65885900	2.34743800
H	-4.89715200	-2.78602100	3.36174900
H	-5.58266400	-1.60674400	2.23390200
C	-6.48614300	-3.56467400	2.11926700
H	-6.89689600	-3.42041500	1.11913600
H	-6.20182900	-4.61239900	2.22820800
H	-7.26819600	-3.34364300	2.84726700
H	-3.49474800	-1.08250200	1.32133500
O	-5.57915400	2.90651300	1.40663500
N	-2.71637900	0.73630000	-1.76361400
C	-4.51609200	-1.42921900	-2.11060500
C	-3.00760100	-1.60451600	-2.13216000
C	-2.26667200	-0.43259300	-2.22006600
C	-1.77050500	1.85404000	-1.69996900
H	-1.14182000	1.80592700	-2.58630100
H	-1.12986900	1.70957900	-0.82742800
C	-2.52012100	3.15542600	-1.62662200
H	-1.80849200	3.98017700	-1.61180200
H	-3.12652200	3.26683100	-2.52908700
C	-3.42501400	3.24022700	-0.38888300
C	-4.24857400	1.95132200	-0.29025200
C	-5.36912100	1.86175200	0.56283800
C	-6.20163300	0.74925600	0.54287400
H	-7.06587900	0.69571000	1.18562700
C	-5.92868900	-0.30401100	-0.31807700
H	-6.60398900	-1.14601600	-0.33855200
C	-4.80568600	-0.30795000	-1.12028300
C	-3.94662600	0.81284400	-1.05952900
C	-5.20298700	-2.75146300	-1.76414700
H	-6.28564900	-2.67335500	-1.86883800
H	-4.86476600	-3.52177300	-2.45974800
H	-4.97230400	-3.06784600	-0.75009400
C	-4.99445100	-0.98568200	-3.51349500
H	-6.07689800	-0.84589200	-3.50986500
H	-4.52895500	-0.04718100	-3.81629800
H	-4.74592800	-1.74730200	-4.25558300
C	-2.57374600	3.44373900	0.87704600
H	-3.20733000	3.50410900	1.75949300
H	-1.87024300	2.62466000	1.02472600
H	-2.00488000	4.37266200	0.79654800
C	-4.32028100	4.47617700	-0.61125100
H	-5.01804100	4.30253500	-1.43244600
H	-3.68665000	5.32345600	-0.88192100
H	-4.88772800	4.73997200	0.27431200
C	-6.71102500	2.88242000	2.26768100
H	-6.66528800	2.03743400	2.95841700
H	-1.24326900	-0.42931400	-2.57086800
H	-2.62861600	-2.44091400	-2.70829200
H	-2.57863800	-2.01967800	-0.78348300
H	-6.67350300	3.81173500	2.82954200
H	-7.64173300	2.83820600	1.69771700
C	3.05224900	1.37130000	-0.44678400
C	2.13467300	2.11325300	0.28924000
C	3.14514800	1.58028200	-1.82415500
C	1.33521700	3.06988400	-0.32742900
H	2.03109400	1.95600400	1.35204900
C	2.35554400	2.52696500	-2.45612000
H	3.84642600	1.00503600	-2.41325100
C	1.46884300	3.26077300	-1.68704100
H	0.62714100	3.65696800	0.23928000
H	2.42511300	2.70151800	-3.52052300
C	3.94241200	0.32399200	1.71351400
C	4.41042600	1.45901900	2.38211700
C	3.50374200	-0.76397000	2.45968700
C	4.42433800	1.51716200	3.76604200
H	4.77039200	2.30627700	1.81599200
C	3.50626900	-0.72135300	3.85065200
H	3.15590500	-1.65966300	1.97033000
C	3.96378500	0.42052000	4.47450400
H	4.78442400	2.39128900	4.29008000

H	3.16520100	-1.56281300	4.43708400
F	0.69988400	4.19444400	-2.29596500
F	3.96970600	0.47085900	5.82732800

TCF-A6(+2H)

Cl	3.05344000	-0.69001700	1.53655700
O	-3.22796800	0.43598700	0.19229700
N	-6.55958000	1.41152300	0.32367700
N	-5.92877000	-0.19977000	-3.68934500
N	-2.60949000	-1.43132200	-4.14474200
C	-5.83449800	0.93636200	-0.43832100
C	-5.46888700	0.03882600	-2.65793900
C	-2.61744800	-0.99143100	-3.07924200
C	-4.95054800	0.35158200	-1.37938300
C	-3.64066100	0.11223500	-1.02641300
C	-2.55653000	-0.47110000	-1.76805100
C	-1.42408000	-0.47197400	-0.98741800
C	-1.77511500	0.16509100	0.34919900
C	-0.16645300	-0.99924100	-1.36623800
H	-0.10969100	-1.41851800	-2.36188900
C	0.93437600	-0.96667400	-0.57067500
H	0.84096100	-0.54357900	0.41581900
C	2.24844600	-1.39077200	-0.94894600
C	2.46569300	-1.99089200	-2.32083100
H	2.40711400	-1.19715500	-3.07263900
H	1.64391500	-2.67723700	-2.53270200
C	3.79580300	-2.72368100	-2.43585900
H	3.75908900	-3.64381600	-1.84497500
C	4.92148000	-1.83376500	-1.93748100
H	4.94288500	-0.91388600	-2.52599900
H	5.89170800	-2.31783100	-2.05767000
C	4.74349500	-1.46966800	-0.45715400
C	3.30124000	-1.22460300	-0.11079400
C	5.61878200	-0.27054600	-0.08411900
H	5.65678100	-0.13911200	1.00133800
H	3.96666800	-3.01541800	-3.47292200
O	5.08263200	0.88581800	-0.69581600
C	5.77640000	2.07826400	-0.35282600
H	5.78939400	2.19140400	0.73877300
H	6.81847900	2.00822200	-0.69052900
C	5.07593500	3.24989600	-1.00420600
H	5.07060500	3.14249300	-2.09000700
H	4.04374900	3.32188600	-0.65739400
H	5.58901200	4.17958500	-0.75345300
H	6.64065500	-0.45763400	-0.43673600
H	5.08556700	-2.30724900	0.16280800
C	-1.62953000	-0.83615900	1.48877300
C	-0.66197700	-0.68658900	2.47755000
C	-2.44443400	-1.96891100	1.50024800
C	-0.50436000	-1.64716300	3.46894500
H	-0.01580500	0.17817100	2.48566200
C	-2.30736900	-2.93257900	2.48672800
H	-3.19889400	-2.10862400	0.73878700
C	-1.33371200	-2.75071300	3.45351400
H	0.24632600	-1.53977500	4.23886100
H	-2.93804300	-3.80998400	2.50855400
C	-1.14354800	1.52297700	0.60292900
C	-1.54418900	2.22769500	1.74132700
C	-0.24112200	2.11338100	-0.27619600
C	-1.03603400	3.48687100	2.01307900
H	-2.26026800	1.79025000	2.42267000
C	0.28448200	3.37398300	-0.01473600
H	0.07114900	1.60351400	-1.17388800
C	-0.12167200	4.03241700	1.12775600
H	-1.33769200	4.03887400	2.89192600
H	0.99307100	3.83586600	-0.68743000
F	-1.19069100	-3.68887800	4.41625100
F	0.38608600	5.25706400	1.39188900

FP-INT-II-C

Cl	-1.66811000	-0.98891600	0.92208100
O	4.75731800	0.19121400	0.78576900
N	7.92455800	1.30739200	1.64847400
N	8.46451600	-2.72007600	0.04229300
N	5.33518100	-4.25412200	-0.81840600
C	7.44339800	0.36002000	1.19550500
C	7.72652100	-1.87167700	0.30613500
C	5.06574700	-3.18590100	-0.47472900
C	6.86207100	-0.80529000	0.64063400
C	5.49434900	-0.86154500	0.44379100
C	4.65920500	-1.89825300	-0.07170600
C	3.33985300	-1.46530800	-0.07441500
C	3.33918300	-0.01054100	0.38027200
C	2.23203600	-2.23288200	-0.45688400
H	2.45758600	-3.20513700	-0.87646200
C	0.91977000	-1.86920300	-0.26816700
H	0.71999500	-0.94543100	0.24913100
C	-0.20175600	-2.63616000	-0.64405500
C	-0.04347700	-3.82684400	-1.56324500
H	0.18082700	-4.72201700	-0.97299300
H	0.81125000	-3.66230700	-2.21901000
C	-1.29901200	-4.05680700	-2.39584700
H	-1.44722500	-3.20258100	-3.06212200
C	-2.51574900	-4.22132900	-1.49743300
H	-2.45340700	-5.17476100	-0.96237300
H	-3.43065200	-4.26100100	-2.08898300
C	-2.63072400	-3.09987700	-0.48896200
C	-1.46796700	-2.34130500	-0.17046300
C	-3.82063800	-2.86203800	0.12854600
H	-3.94262900	-2.08985100	0.87520500
H	-1.17625700	-4.93942200	-3.02431400
O	-4.89141100	-3.57816000	-0.16797200
C	-6.08600100	-3.37533300	0.63014700
H	-6.12750900	-4.19680700	1.34639200
H	-5.98710200	-2.43544500	1.17202900
C	-7.28856000	-3.36925900	-0.28076000
H	-7.24251500	-2.53662500	-0.98296600
H	-7.35587000	-4.30063500	-0.84348600
H	-8.19399500	-3.26480300	0.31881800
O	-0.37868500	3.50217000	-0.19305000
N	-4.11641200	0.67665700	-1.19113200
C	-5.33613800	1.19733100	1.42363900
C	-5.89677700	0.28711200	0.36733400
C	-5.29398700	0.07308200	-0.80099400
C	-3.44867400	0.19777200	-2.38851400
H	-4.19970800	-0.25702500	-3.03296800
H	-2.72150000	-0.58163800	-2.13744800
C	-2.77992200	1.36014100	-3.07721500
H	-2.30465000	1.02798900	-4.00206000
H	-3.54753200	2.09024500	-3.34714000
C	-1.72200700	2.02891800	-2.18561000
C	-2.27409100	2.20729600	-0.76296000
C	-1.59606700	3.00338000	0.17712000
C	-2.12817800	3.25158100	1.43748900
H	-1.61372200	3.88170000	2.14563400
C	-3.33658300	2.67027600	1.78635200
H	-3.73951100	2.87639200	2.76890200
C	-4.02390400	1.82168500	0.93591100
C	-3.46961000	1.57555500	-0.34316600
C	-5.09684400	0.37806700	2.71064700
H	-4.77370000	1.01457600	3.53587900
H	-6.01905300	-0.12320400	3.01377100
H	-4.33021900	-0.37994200	2.54820600
C	-6.37119200	2.30143600	1.72886200
H	-6.02918200	2.95778500	2.53085600
H	-6.55443200	2.90855100	0.84154500
H	-7.31788400	1.85280200	2.03969600
C	-0.45922400	1.15346500	-2.16069000
H	0.30995400	1.60086300	-1.53853900

H	-0.66988300	0.15686200	-1.77564000
H	-0.05730800	1.04895200	-3.17023800
C	-1.39333100	3.37724600	-2.85764000
H	-2.24314300	4.05894600	-2.78609300
H	-1.18912100	3.20421300	-3.91691000
H	-0.52648800	3.85761700	-2.41660800
C	0.24730600	4.47217000	0.63517100
H	-0.41167200	5.32442200	0.81393400
H	0.55664400	4.04536900	1.59189800
H	-5.71154800	-0.59653400	-1.54051400
H	-6.84131100	-0.20060100	0.56990600
C	3.12714300	0.97260800	-0.76022300
C	3.21828100	2.33969600	-0.48695900
C	2.96745700	0.55693900	-2.07859800
C	3.12803800	3.27501600	-1.50434300
H	3.36733900	2.67941100	0.52809900
C	2.87898500	1.48208300	-3.11152300
H	2.89909900	-0.49268600	-2.31955500
C	2.95413400	2.82354500	-2.80099000
H	3.19700900	4.33476900	-1.30436200
H	2.74312600	1.16705100	-4.13621900
C	2.49191300	0.21945600	1.62078800
C	2.85107800	-0.43134300	2.80220600
C	1.33401700	0.99166900	1.59668400
C	2.07639600	-0.31007000	3.94479300
H	3.74367300	-1.04040600	2.83769200
C	0.54030300	1.11582700	2.73081200
H	1.02271000	1.49021800	0.69137600
C	0.93043000	0.46379500	3.88216700
H	2.34793100	-0.80687600	4.86549400
F	2.85616400	3.73280300	-3.79754800
F	0.16238800	0.57862900	4.99023900
H	-0.37105800	1.69588100	2.71160700
H	1.12766700	4.80182100	0.09127300

FP-TS-II-C

Cl	-1.71631500	-1.07287100	1.20273600
O	4.76977900	-0.64685700	0.75436000
N	8.08040300	-0.53295300	1.72513000
N	7.99822400	-2.94128800	-1.91767600
N	4.58953200	-3.30738900	-3.18805200
C	7.45494800	-0.99663300	0.86775600
C	7.39921000	-2.32485100	-1.14201700
C	4.52097300	-2.62995900	-2.25160400
C	6.70496600	-1.56620800	-0.18097900
C	5.31897300	-1.36848000	-0.23639300
C	4.33977800	-1.80366000	-1.13498900
C	3.05674300	-1.34759500	-0.69229100
C	3.34459700	-0.37068600	0.44627900
C	1.85176300	-1.72589300	-1.20746700
H	1.89904700	-2.39608300	-2.05736800
C	0.57246000	-1.41736000	-0.67693100
H	0.54566100	-0.84114900	0.23312500
C	-0.62515900	-1.85166100	-1.16946100
C	-0.74454000	-2.60868600	-2.47052400
H	-0.71047000	-3.68598700	-2.27023900
H	0.10256100	-2.38037700	-3.11494700
C	-2.04575800	-2.27172000	-3.18940900
H	-2.03250200	-1.21601200	-3.46927300
C	-3.24993200	-2.55942300	-2.30439500
H	-3.43571700	-3.63715300	-2.26135000
H	-4.15570900	-2.13068600	-2.74090100
C	-3.08645600	-2.04702000	-0.89410500
C	-1.85452200	-1.68276000	-0.43697600
C	-4.26972800	-2.04151700	-0.05719800
H	-4.11212800	-1.96072700	1.01002200
H	-2.12447200	-2.84091900	-4.11641900
O	-5.19749700	-2.94376700	-0.43867200
C	-6.16526500	-3.34324500	0.55150100

H	-5.63453200	-3.60392700	1.47013900
H	-6.82741900	-2.50081300	0.76413300
C	-6.94031400	-4.51564000	0.00253700
H	-7.45675900	-4.24115000	-0.91781400
H	-6.27801300	-5.35691500	-0.20286500
H	-7.68533700	-4.83235600	0.73336500
O	-0.15786900	3.32087200	0.62826900
N	-3.89916100	1.15007000	-1.44906900
C	-5.16578000	0.67655700	1.07274600
C	-5.33081900	-0.23767900	-0.13058300
C	-4.87219500	0.26586200	-1.34615600
C	-3.40857000	1.47156100	-2.80209400
H	-4.26939700	1.48099600	-3.46663200
H	-2.74343100	0.67197500	-3.12348100
C	-2.69759900	2.79432700	-2.80444200
H	-2.31941900	2.98279700	-3.80971500
H	-3.40612100	3.59195100	-2.56737500
C	-1.53262600	2.83540800	-1.80603400
C	-2.06700200	2.42427100	-0.43138600
C	-1.39308000	2.77017400	0.75710300
C	-1.96648200	2.53415500	2.00006900
H	-1.46410200	2.84068100	2.90414200
C	-3.18451000	1.88127600	2.08604400
H	-3.60714200	1.70579100	3.06393800
C	-3.83430400	1.40970100	0.96070200
C	-3.25544800	1.68472500	-0.29289600
C	-5.31021100	-0.09454300	2.39159800
H	-5.43232400	0.58891900	3.23061700
H	-6.20077600	-0.72274800	2.35747400
H	-4.44616500	-0.72341300	2.60002500
C	-6.30537400	1.72581400	1.00591900
H	-6.21917700	2.41811700	1.84442100
H	-6.25838700	2.29971100	0.07976300
H	-7.27926300	1.23490500	1.05860100
C	-0.41264400	1.87373500	-2.23107600
H	0.39611900	1.90843800	-1.50757600
H	-0.75470000	0.84163400	-2.28515000
H	-0.01470300	2.16045700	-3.20716600
C	-1.00643500	4.28455600	-1.84315900
H	-1.70804300	4.96757400	-1.36083300
H	-0.90458000	4.58886000	-2.88678100
H	-0.04052400	4.38664800	-1.36256400
C	0.43255800	3.96486400	1.75235700
H	-0.24023700	4.71580200	2.17107300
H	0.70707100	3.24856600	2.52937200
H	-5.24706900	-0.12194300	-2.28360100
H	-6.29037900	-0.73348400	-0.19272300
C	3.33249600	1.08664900	0.00014000
C	3.80222000	2.05633400	0.89085300
C	2.95923900	1.47354900	-1.28020900
C	3.88208800	3.38770700	0.51829600
H	4.11433400	1.76755800	1.88467400
C	3.03155600	2.80701800	-1.67269600
H	2.59967200	0.73784300	-1.98371600
C	3.48799600	3.73601500	-0.76289200
H	4.24173600	4.14458500	1.20117800
H	2.73185800	3.11742100	-2.66344500
C	2.56315400	-0.64623200	1.71761100
C	2.77761400	-1.84856800	2.39150700
C	1.59931800	0.23520600	2.19776300
C	2.05361600	-2.16488000	3.53094100
H	3.51774600	-2.54663600	2.02558800
C	0.86098400	-0.06623200	3.33610700
H	1.39745700	1.15514400	1.67032200
C	1.10694900	-1.26096200	3.98055100
H	2.21422500	-3.09238600	4.06243400
F	3.55426500	5.03832600	-1.13166800
F	0.39033100	-1.56564300	5.08954600
H	0.09989800	0.60480600	3.70759900
H	1.33263300	4.44304100	1.37843800

FP-INT-II-D

Cl	-1.68399900	-1.20159100	1.24083200
O	4.79972600	-0.66602200	0.68214700
N	8.12677800	-0.52955000	1.58423400
N	8.02089800	-2.70276600	-2.20200700
N	4.58458600	-3.02334900	-3.44764200
C	7.49292900	-0.95244800	0.71120100
C	7.42536300	-2.15034100	-1.37617100
C	4.52572600	-2.42411800	-2.45786400
C	6.73484700	-1.47157400	-0.35612300
C	5.33995600	-1.30410500	-0.37263700
C	4.35394300	-1.69364900	-1.27667700
C	3.06412600	-1.30040500	-0.76980700
C	3.36470500	-0.39537900	0.42334500
C	1.85820100	-1.66414800	-1.27585600
H	1.89239800	-2.27809800	-2.16812400
C	0.57737600	-1.39608900	-0.70228300
H	0.56799800	-0.89673500	0.25257900
C	-0.62178700	-1.77795900	-1.21069900
C	-0.77190300	-2.42594600	-2.56529900
H	-0.79982500	-3.51579900	-2.44878300
H	0.08902600	-2.19598900	-3.19016500
C	-2.05242200	-1.96774500	-3.25556800
H	-1.99096300	-0.89298300	-3.44356100
C	-3.26648900	-2.27794000	-2.39301600
H	-3.46630500	-3.35360800	-2.40589500
H	-4.16470300	-1.82512900	-2.81889200
C	-3.09729600	-1.85347200	-0.95310900
C	-1.86258500	-1.62814100	-0.46202200
C	-4.35103000	-1.80187600	-0.11862800
H	-4.08957700	-1.91549100	0.93081800
H	-2.15378500	-2.45293300	-4.22726800
O	-5.15892600	-2.88869200	-0.52656700
C	-6.09054700	-3.35023100	0.45003600
H	-5.55915100	-3.55871100	1.38506500
H	-6.83817700	-2.57605300	0.65718900
C	-6.76146700	-4.59479300	-0.08454800
H	-7.29216600	-4.37894300	-1.01287400
H	-6.02646200	-5.37725300	-0.27689000
H	-7.48213500	-4.96873500	0.64410200
O	-0.18706400	3.20545700	0.84672700
N	-3.93657000	1.23876600	-1.42418300
C	-5.17921200	0.51345800	1.00315000
C	-5.20462900	-0.44110100	-0.21536200
C	-4.82500500	0.30437800	-1.42194900
C	-3.55155800	1.81277700	-2.74370700
H	-4.47091100	1.97388800	-3.30047300
H	-2.96759900	1.05200800	-3.25633000
C	-2.76614000	3.08038600	-2.57970400
H	-2.42375000	3.38897700	-3.56777100
H	-3.41162600	3.87356400	-2.19644400
C	-1.55830900	2.91678900	-1.64488100
C	-2.08759300	2.40864400	-0.30276700
C	-1.42373900	2.65729800	0.91633200
C	-2.01876300	2.33156900	2.12908300
H	-1.52633000	2.56861800	3.05911400
C	-3.23530000	1.67044700	2.15836200
H	-3.66334700	1.41754400	3.11612800
C	-3.86707300	1.28036000	0.99373300
C	-3.27579900	1.66424800	-0.22159800
C	-5.41162200	-0.24923200	2.31088700
H	-5.60285300	0.44731100	3.12601500
H	-6.29203100	-0.88475100	2.21859000
H	-4.56283400	-0.86805300	2.59525800
C	-6.33726000	1.52455900	0.83579400
H	-6.33359500	2.22626700	1.66919700
H	-6.25357500	2.10049200	-0.08667000
H	-7.29591200	1.00261100	0.82632600
C	-0.54444500	1.90754200	-2.20564100
H	0.29016200	1.80871800	-1.51768400

H	-0.97265200	0.91487700	-2.33306700
H	-0.16047400	2.24832400	-3.16936200
C	-0.90440300	4.31025800	-1.56879400
H	-1.51756500	5.00252200	-0.98960000
H	-0.81886200	4.70395800	-2.58327700
H	0.08586600	4.27829000	-1.13105100
C	0.38563900	3.77468900	2.02111900
H	-0.29192400	4.50253100	2.47128700
H	0.64015700	3.00939300	2.75654200
H	-5.25931900	0.06189500	-2.38243600
H	-6.22973700	-0.78119000	-0.35640700
C	3.31423300	1.08787000	0.07381800
C	3.81295500	2.00717100	1.00122500
C	2.86697300	1.55021200	-1.15677400
C	3.84945500	3.36177500	0.71411800
H	4.18179600	1.66070900	1.95645900
C	2.89362200	2.90772700	-1.46317200
H	2.48889000	0.85209300	-1.88825800
C	3.38156100	3.78477300	-0.51874600
H	4.23145400	4.07997600	1.42609400
H	2.53887400	3.27568800	-2.41530000
C	2.61788400	-0.76579500	1.69150100
C	2.85035800	-2.01501100	2.26712600
C	1.66919400	0.07535800	2.26416500
C	2.15848800	-2.41716300	3.39939400
H	3.57870400	-2.68252000	1.82774900
C	0.96282000	-0.31125900	3.39718200
H	1.45545300	1.03220400	1.81299700
C	1.22550400	-1.55089500	3.94231800
H	2.33257000	-3.38200400	3.85476700
F	3.40502500	5.10988600	-0.80350700
F	0.54011700	-1.93934800	5.04530500
H	0.21475800	0.32967400	3.84147600
H	1.29513300	4.26857400	1.69430000

FP-TS-II-D

CI	0.39388700	-1.37567200	1.70416100
O	6.10904100	1.14029300	-0.13205300
N	8.99165000	3.03152600	-0.17377800
N	9.48757900	0.06750100	-3.33764400
N	6.51366000	-2.08131600	-3.61474300
C	8.54976800	2.13039400	-0.75296400
C	8.81384000	0.49217200	-2.49641900
C	6.32098700	-1.35144500	-2.73601300
C	8.02529400	1.03515300	-1.46624700
C	6.75737500	0.52590800	-1.13763300
C	5.99508300	-0.51558000	-1.66175800
C	4.75411700	-0.60883700	-0.94119200
C	4.82198600	0.46419500	0.14545500
C	3.71352900	-1.43730100	-1.20622900
H	3.82357600	-2.09687100	-2.05810300
C	2.50607600	-1.49114200	-0.44438800
H	2.49076700	-0.91652400	0.46724900
C	1.37879900	-2.18338600	-0.73777400
C	1.20575700	-3.01579000	-1.98333500
H	1.31367000	-4.07712300	-1.73077400
H	1.98249800	-2.78077800	-2.70799800
C	-0.17487700	-2.78512800	-2.59434900
H	-0.26705500	-1.73215300	-2.87528800
C	-1.27085000	-3.14759100	-1.60013000
H	-1.37875400	-4.23555000	-1.54217400
H	-2.23795500	-2.78049400	-1.95020300
C	-1.01618100	-2.60111300	-0.21743200
C	0.20384400	-2.14463300	0.11787800
C	-2.20839900	-2.53562300	0.71089200
H	-1.85786200	-2.62523700	1.74251700
H	-0.29081600	-3.37238200	-3.50652900
O	-3.09169700	-3.62565900	0.44708700
C	-2.65553900	-4.85690000	1.01568200

H	-1.64334100	-5.09385600	0.66907900
H	-2.61238500	-4.75433600	2.10719000
C	-3.62796000	-5.94194300	0.61290600
H	-4.63675200	-5.70122300	0.95169600
H	-3.64485700	-6.06426300	-0.47130500
H	-3.33284500	-6.89267900	1.05896800
O	-6.73012200	3.85229700	0.19408100
N	-2.81331300	1.10003200	0.03768000
C	-3.92291500	-0.84023000	1.77766300
C	-3.01737900	-1.23607600	0.59083600
C	-2.36247700	-0.14230300	0.01635500
C	-2.12243000	2.09812400	-0.79748200
H	-1.05567600	1.89771800	-0.73176700
H	-2.43201800	1.95620500	-1.83454200
C	-2.45622200	3.48015700	-0.31001900
H	-1.91616400	4.21095000	-0.91061300
H	-2.10600000	3.58716000	0.71966200
C	-3.96187900	3.77729600	-0.37412900
C	-4.72497100	2.61242200	0.26425200
C	-6.09378500	2.72308200	0.59648900
C	-6.74606200	1.70841500	1.28428400
H	-7.78910400	1.80005300	1.54258300
C	-6.05254500	0.56670400	1.66266600
H	-6.57809700	-0.18829500	2.22655300
C	-4.72899600	0.37563900	1.31678400
C	-4.10116600	1.39222400	0.56831200
C	-4.82490500	-1.99413200	2.22115900
H	-5.42731500	-1.69686100	3.07922000
H	-4.22222300	-2.84482800	2.52911200
H	-5.49045600	-2.32391100	1.42471100
C	-3.05971400	-0.40893400	2.98476400
H	-3.70718200	-0.08853400	3.80234600
H	-2.39920100	0.41933500	2.72805500
H	-2.44440900	-1.23507200	3.34220700
C	-4.40224300	3.97741400	-1.83532400
H	-5.46419100	4.20835100	-1.88657500
H	-4.22362300	3.08475400	-2.43578500
H	-3.84639400	4.80523400	-2.28056900
C	-4.16248300	5.08863300	0.41203800
H	-3.96483700	4.93404100	1.47429900
H	-3.45151400	5.83040300	0.04237500
H	-5.16486300	5.48720600	0.30133000
C	-8.10187000	4.02997900	0.52903500
H	-8.24705500	4.03318100	1.61136200
H	-8.72272700	3.25240400	0.07875100
H	-1.46080800	-0.28276000	-0.56365900
H	-3.92658600	-1.48585700	-0.41886800
C	-5.60502700	-0.67945100	-1.81670100
C	-6.62008900	-0.85056200	-2.74142700
C	-6.93584000	-2.13999400	-3.15313300
C	-6.22773300	-3.21407400	-2.62819100
C	-5.22340300	-2.96504500	-1.70790300
N	-4.93069000	-1.72066700	-1.32356300
H	-7.72567700	-2.30523400	-3.87324300
H	-5.32570400	0.29945000	-1.45127400
H	-7.15001500	0.00923000	-3.12482600
H	-6.44736300	-4.22986900	-2.92348200
H	-4.63248300	-3.74600600	-1.25183600
C	3.72991300	1.51106000	-0.04794600
C	2.65786800	1.63938300	0.82911400
C	3.77229800	2.32146200	-1.18345500
C	1.64028200	2.55676200	0.58748900
H	2.59834700	1.02120200	1.71211300
C	2.77186800	3.24688700	-1.43868800
H	4.59411600	2.23327800	-1.88003300
C	1.72194800	3.34425000	-0.54268100
H	0.80566300	2.66018700	1.26662600
H	2.80052100	3.88234400	-2.31273300
C	4.94596700	-0.05826400	1.56768100
C	5.15633000	0.86144900	2.59831500
C	4.91642600	-1.41450800	1.87124100

C	5.31645300	0.44115300	3.90904200
H	5.19730200	1.91854300	2.37524300
C	5.06962400	-1.85593800	3.18192700
H	4.76966100	-2.14046100	1.08598300
C	5.26370200	-0.91671900	4.17362200
H	5.47919900	1.14566500	4.71263600
H	5.04240500	-2.90840900	3.42705000
F	0.73929100	4.24615900	-0.78655200
F	5.41230200	-1.33613100	5.45371200
H	-8.38097100	4.99782500	0.12183300

FP-INT-II-E

Cl	0.70206600	1.47711600	-1.08200800
O	6.62185900	-1.11297100	-0.34146600
N	9.65858900	-2.58889200	-1.02803100
N	9.76660300	-1.60808600	3.22294600
N	6.59078800	-0.09521600	4.30930300
C	9.11638600	-2.13270100	-0.11105100
C	9.16512200	-1.58994900	2.23303300
C	6.50086200	-0.28375100	3.16968200
C	8.46809700	-1.58333600	1.01189500
C	7.17162100	-1.05488600	0.88453600
C	6.29647200	-0.47242500	1.79803900
C	5.07689100	-0.10948700	1.12569500
C	5.30051900	-0.44512500	-0.34823200
C	3.95013300	0.39069400	1.69123400
H	3.97480800	0.53785200	2.76395000
C	2.76220000	0.73921500	0.97757300
H	2.80090300	0.63972900	-0.09477000
C	1.59563700	1.18890900	1.50259400
C	1.37836200	1.37919400	2.98451700
H	1.56881500	2.42666100	3.24701000
H	2.08969000	0.77937500	3.54893300
C	-0.04770200	1.01755600	3.38729800
H	-0.22114200	-0.04280800	3.18227600
C	-1.04786700	1.85888400	2.60750700
H	-1.02952500	2.88924600	2.97847500
H	-2.06421600	1.50874800	2.78695200
C	-0.77353700	1.85430900	1.12350800
C	0.45103000	1.52679000	0.67109800
C	-1.91494700	2.19506600	0.19031400
H	-1.50873000	2.71675200	-0.67444800
H	-0.18871500	1.16696900	4.45881500
O	-2.84469800	3.10421200	0.84419500
C	-2.38023600	4.45402000	1.01308000
H	-2.93923900	4.84682900	1.86256100
H	-1.32302400	4.43659900	1.28820800
C	-2.60138900	5.31099900	-0.21800900
H	-2.02542600	4.95057500	-1.07033200
H	-3.65601900	5.32947100	-0.49404800
H	-2.28191500	6.33368900	-0.00845000
O	-8.15405500	-2.16083200	-0.98892300
N	-3.61769300	-1.16508500	0.18059000
C	-3.47233800	1.01316700	-1.60335100
C	-2.71720500	1.01023500	-0.27539600
C	-2.77216000	-0.10923200	0.45595100
C	-3.60532900	-2.28433500	1.11659800
H	-2.56659800	-2.52178800	1.34136900
H	-4.08976600	-1.99740600	2.05702100
C	-4.30251800	-3.46473300	0.49037500
H	-4.25403100	-4.32250700	1.16286500
H	-3.76927000	-3.73726600	-0.42400500
C	-5.77429600	-3.16814900	0.15652800
C	-5.86795800	-1.79939900	-0.53048100
C	-7.05454300	-1.37319500	-1.15900500
C	-7.10035800	-0.19532500	-1.89620400
H	-8.00951400	0.11981600	-2.38273200
C	-5.95491800	0.57773700	-2.02453600
H	-6.00549100	1.46673600	-2.63537300

C	-4.77362800	0.24089000	-1.38897000
C	-4.76210500	-0.92758700	-0.59012800
C	-3.71862300	2.42066100	-2.15179700
H	-4.20231600	2.37277700	-3.12639600
H	-2.77370200	2.94047500	-2.29877100
H	-4.33519600	3.02545000	-1.48928100
C	-2.61849700	0.24488600	-2.64335600
H	-3.14593300	0.19572800	-3.59839300
H	-2.41925200	-0.77180600	-2.30515100
H	-1.66237700	0.74786500	-2.79403800
C	-6.61028400	-3.20651000	1.44783700
H	-7.64730000	-2.94508200	1.24862600
H	-6.22235300	-2.51324400	2.19330600
H	-6.58253900	-4.21084000	1.87692300
C	-6.23451300	-4.29933400	-0.78480300
H	-5.71851700	-4.23174200	-1.74439700
H	-5.98257200	-5.26193000	-0.33397400
H	-7.30422000	-4.27329800	-0.96561900
C	-9.38000800	-1.76957000	-1.59102700
H	-9.29384700	-1.72611500	-2.67916000
H	-9.71486100	-0.80003500	-1.21445900
H	-2.16038800	-0.25464200	1.33408300
H	-4.31543500	2.46109100	1.38597100
C	-6.26424600	2.08540600	0.85397100
C	-7.39172400	1.32648800	1.08982700
C	-7.37404800	0.40487400	2.12727400
C	-6.23734000	0.27579900	2.91999100
C	-5.14004400	1.05823800	2.64279800
N	-5.18216000	1.93350200	1.62777700
H	-8.23993900	-0.21286100	2.31865400
H	-6.19144200	2.81147800	0.06110000
H	-8.25678100	1.44769600	0.45787800
H	-6.19759100	-0.42704900	3.73775100
H	-4.21721900	1.00619800	3.19780900
C	4.29717100	-1.47611300	-0.84987100
C	3.34362000	-1.17899100	-1.81756100
C	4.29539300	-2.74460700	-0.26770900
C	2.39715400	-2.12251200	-2.20304300
H	3.31855300	-0.20184200	-2.27597400
C	3.36603200	-3.70187100	-0.64433000
H	5.02574800	-2.99135500	0.49042500
C	2.43021600	-3.36645300	-1.60763900
H	1.64822500	-1.89421300	-2.94820800
H	3.36016400	-4.68799100	-0.20138500
C	5.46710000	0.76000700	-1.26166700
C	5.89780500	0.54300500	-2.57329000
C	5.24915900	2.06368900	-0.83202200
C	6.09311600	1.60185600	-3.44555400
H	6.08487200	-0.46479200	-2.91708200
C	5.43450300	3.13998900	-1.69478800
H	4.93050100	2.25210300	0.18169400
C	5.85037300	2.88471300	-2.98496900
H	6.42639500	1.44308300	-4.46159800
H	5.26358100	4.15656200	-1.36926800
F	1.51332100	-4.29480400	-1.97641800
F	6.03310900	3.92599800	-3.83334100
H	-10.10223900	-2.53370100	-1.31569900

FP-TS-II-E

Cl	-0.87226200	1.02200700	1.24602600
O	-7.06360000	-0.74842800	0.30499600
N	-10.38594200	-1.50607800	0.84613100
N	-9.85135000	-1.57972500	-3.48523400
N	-6.36106400	-0.91768700	-4.40061700
C	-9.67152600	-1.38208200	-0.05716400
C	-9.36590000	-1.42155200	-2.44586300
C	-6.42576500	-0.83167100	-3.24767600
C	-8.81364300	-1.23406400	-1.16524800
C	-7.46465900	-0.90511000	-0.96695700

C	-6.40306100	-0.70768800	-1.85276800
C	-5.22093200	-0.38050300	-1.11342300
C	-5.64478900	-0.32628600	0.35316100
C	-3.97152300	-0.19055200	-1.61797700
H	-3.86763300	-0.29330300	-2.69074600
C	-2.82480400	0.15212400	-0.84968800
H	-2.97696700	0.29703200	0.20714100
C	-1.56066900	0.33961300	-1.31921800
C	-1.20992800	0.15992300	-2.77914300
H	-1.35028400	1.11119000	-3.30559300
H	-1.89276000	-0.55373400	-3.23705600
C	0.22902000	-0.30561300	-2.96796400
H	0.35114800	-1.30224500	-2.53460200
C	1.18333900	0.66495800	-2.29060000
H	1.16304300	1.62067300	-2.82629700
H	2.20824500	0.31142200	-2.36240500
C	0.81572000	0.90476200	-0.84308400
C	-0.47509600	0.74770100	-0.45535000
C	1.84484100	1.34359300	0.11282600
H	1.43272300	1.93243300	0.91806300
H	0.46385800	-0.38118700	-4.03040600
O	2.63409700	2.73226300	-0.67937400
C	1.82037700	3.82179000	-1.15858000
H	2.32235500	4.22649200	-2.03845600
H	0.85353700	3.42349200	-1.47184800
C	1.65385000	4.86570100	-0.07727100
H	1.15605700	4.44603000	0.79770200
H	2.62059300	5.26485200	0.22989100
H	1.04070100	5.68690200	-0.45219300
O	9.05201700	-1.13407800	0.87370300
N	4.33829600	-1.38721000	0.06995300
C	3.77733100	0.80663400	1.76585900
C	2.95177900	0.51305900	0.51314900
C	3.23812800	-0.63378200	-0.15355600
C	4.53854800	-2.54884800	-0.79983800
H	3.58095900	-3.05531700	-0.90440900
H	4.84887500	-2.20761800	-1.79202000
C	5.56935300	-3.46072400	-0.19022700
H	5.68904400	-4.34635300	-0.81560500
H	5.20771200	-3.79704800	0.78493100
C	6.93270200	-2.77199000	-0.02213100
C	6.72084800	-1.39501800	0.61817000
C	7.80523700	-0.64149900	1.11097200
C	7.60236600	0.55820600	1.78250200
H	8.43553200	1.12587100	2.16508300
C	6.31162500	1.02550300	1.98450900
H	6.18167500	1.94071800	2.54189600
C	5.21040700	0.35679600	1.48277600
C	5.44125100	-0.82581600	0.74747600
C	3.71033300	2.27231700	2.20531100
H	4.24564900	2.41066800	3.14353200
H	2.67956300	2.57077600	2.39186900
H	4.12736100	2.94795800	1.46135100
C	3.21155900	-0.06089900	2.91770800
H	3.79509800	0.09317800	3.82741000
H	3.24543800	-1.11999200	2.66202400
H	2.17261600	0.20978000	3.11763200
C	7.61928600	-2.64055100	-1.39326900
H	8.57721200	-2.13351500	-1.29919300
H	7.00639500	-2.07412000	-2.09395400
H	7.79266400	-3.63227500	-1.81738300
C	7.76601700	-3.69832500	0.88568100
H	7.34868000	-3.72349900	1.89406300
H	7.73220200	-4.71271400	0.48197200
H	8.80340200	-3.38755000	0.94911700
C	10.18066700	-0.40741800	1.34133900
H	10.17032700	-0.31342800	2.42957100
H	10.22635600	0.58678500	0.89060200
H	2.58831800	-1.02211900	-0.92151400
H	3.39212200	2.41435000	-1.34700300
C	5.75901900	2.05711800	-1.32942300

C	6.96146800	1.47834100	-1.70108900
C	7.00870400	0.74659500	-2.87886300
C	5.85625500	0.62939100	-3.64656800
C	4.69594300	1.24235000	-3.20288400
N	4.64720900	1.93789800	-2.06203600
H	7.92776900	0.27141700	-3.19326100
H	5.67217000	2.62258200	-0.41272100
H	7.82914300	1.58686300	-1.06788900
H	5.85139900	0.07079500	-4.57150700
H	3.77722200	1.17542300	-3.76968400
C	-4.90855700	-1.36962100	1.18440400
C	-3.98968000	-1.02212400	2.16890000
C	-5.11644600	-2.72026000	0.90083200
C	-3.28292200	-1.99771700	2.86372500
H	-3.80680500	0.01608300	2.40199400
C	-4.42805200	-3.70789800	1.58829300
H	-5.82288400	-3.00976400	0.13538500
C	-3.51959200	-3.32233400	2.55877300
H	-2.56347900	-1.73367600	3.62592100
H	-4.58651700	-4.75644200	1.37842200
C	-5.66557800	1.06487600	0.96714600
C	-6.21815600	1.21702900	2.24168000
C	-5.20607700	2.19075500	0.29374200
C	-6.29580500	2.46320400	2.84232100
H	-6.59376500	0.35245700	2.77105400
C	-5.27048000	3.45001600	0.88266100
H	-4.79037900	2.09674700	-0.69767500
C	-5.81185200	3.55814900	2.14682200
H	-6.72120900	2.58985600	3.82798200
H	-4.91134900	4.32981200	0.36740300
F	-2.83875200	-4.28180300	3.23176400
F	-5.87767200	4.77967800	2.72951700
H	11.05008600	-0.98354800	1.03596100

Type-II product (TCF5-based)

Cl	-0.27070500	1.38975500	0.32652400
O	-6.61038500	0.18701500	-0.34850600
N	-10.01319800	0.51470000	-0.87918300
N	-9.34361100	-3.71384700	-0.02113900
N	-5.85637600	-4.39526600	0.70127700
C	-9.26302700	-0.32686200	-0.62288700
C	-8.87829400	-2.66297000	-0.14568700
C	-5.91292800	-3.27031700	0.44382100
C	-8.35455800	-1.36300800	-0.30879900
C	-7.00159800	-1.07663400	-0.17321600
C	-5.89162300	-1.89706900	0.14301800
C	-4.72410500	-1.11828900	0.14725200
C	-5.13460700	0.29754100	-0.24274300
C	-3.45275800	-1.55684900	0.47961700
H	-3.36794300	-2.60085900	0.75081700
C	-2.31541100	-0.75716500	0.46894600
H	-2.43771800	0.27396600	0.18231000
C	-1.02019400	-1.17436700	0.76569900
C	-0.75721700	-2.61313600	1.15148200
H	-0.74524500	-3.23232600	0.24757300
H	-1.58234600	-2.97705600	1.76380700
C	0.55061100	-2.77250400	1.90612000
H	0.46857700	-2.29177900	2.88471000
C	1.69501300	-2.13714000	1.13081300
H	1.85971700	-2.70054600	0.20496400
H	2.61483800	-2.20708400	1.71205500
C	1.42689600	-0.68318500	0.81457600
C	0.07583100	-0.30134700	0.68014800
C	2.44731800	0.25849200	0.69883300
H	2.10437100	1.27945400	0.66242200
H	0.75932100	-3.82862200	2.08082000
O	9.99616800	0.64088900	-1.11893500
N	5.75981700	-1.23443800	0.09401700
C	4.76214700	1.28299200	1.02163900

C	3.84505600	0.11667400	0.64598900
C	4.44691600	-1.07062400	0.29112200
C	6.21683000	-2.54051600	-0.39326100
H	5.54062300	-3.29550000	0.00023800
H	6.14586400	-2.55564700	-1.48387400
C	7.63030100	-2.77173700	0.06932600
H	7.95555600	-3.76878600	-0.22977800
H	7.65074000	-2.73621900	1.16148600
C	8.60037100	-1.72815700	-0.50403300
C	7.97810600	-0.33191600	-0.37592400
C	8.73664700	0.82634400	-0.64223900
C	8.20481200	2.09293100	-0.43635000
H	8.78912900	2.97652400	-0.63831700
C	6.91796100	2.23231200	0.06274700
H	6.55724900	3.23033300	0.25678700
C	6.11077600	1.13833200	0.31761700
C	6.64336800	-0.13636600	0.03005300
C	4.11635500	2.64614700	0.74665100
H	4.77238900	3.45377100	1.06285400
H	3.19751900	2.76335700	1.31848700
H	3.88919900	2.77734700	-0.31205700
C	5.02229200	1.16878400	2.54689100
H	5.68283300	1.97252700	2.87646400
H	5.49183300	0.21565500	2.79243300
H	4.07959100	1.23902600	3.09329200
C	8.89888000	-2.06061900	-1.97785200
H	9.58476000	-1.33478300	-2.40795900
H	7.98930000	-2.06311000	-2.57972900
H	9.35486700	-3.05070500	-2.04678300
C	9.89385300	-1.84627400	0.32675100
H	9.71898300	-1.52497100	1.35517600
H	10.20438700	-2.89319700	0.34944500
H	10.70416400	-1.25585600	-0.08741600
C	10.81643100	1.77645900	-1.36566000
H	10.97591800	2.35526900	-0.45322800
H	10.38302800	2.41942200	-2.13490400
H	3.86277200	-1.94739700	0.07178000
C	-4.84877300	1.28945600	0.87750600
C	-3.90996000	2.30677800	0.74214400
C	-5.50543700	1.13058200	2.09871300
C	-3.62383600	3.15838400	1.80303700
H	-3.38427500	2.44448200	-0.19066000
C	-5.23943000	1.97495000	3.16502900
H	-6.23465000	0.34259900	2.22570500
C	-4.29769400	2.97485700	2.99321900
H	-2.89231800	3.94807300	1.70660200
H	-5.74671000	1.86329800	4.11293700
C	-4.67283500	0.74408500	-1.62020000
C	-5.17244700	1.94920400	-2.12150600
C	-3.82670500	-0.01955300	-2.41661500
C	-4.81999800	2.39625100	-3.38421000
H	-5.84523000	2.54468400	-1.52042400
C	-3.45771400	0.41636400	-3.68525000
H	-3.44187600	-0.96215400	-2.05975000
C	-3.96024600	1.61775700	-4.14050300
H	-5.20045800	3.32742900	-3.77979900
H	-2.79664400	-0.16869200	-4.30886400
F	-4.02900400	3.80062900	4.03158800
F	-3.60561200	2.05091900	-5.37272000
H	11.76646400	1.38261400	-1.71656600

TCF5-based (Path II-c)

FP-INT-II-A(c)

Cl	0.61148300	2.90164300	0.46795900
O	-5.01472700	-0.39155200	0.38190600
N	-8.16834100	-1.64211100	1.09761300
N	-6.86163800	-3.68187900	-2.53921800

N	-3.53877800	-2.70172400	-3.51161400
C	-7.34966000	-1.78878800	0.29616200
C	-6.61199900	-2.91061000	-1.71656400
C	-3.78904300	-2.06501100	-2.58235800
C	-6.35114700	-1.97562300	-0.68971300
C	-5.17452400	-1.25288500	-0.61878100
C	-4.01711000	-1.25327400	-1.45326700
C	-3.10187200	-0.32851900	-0.96885500
C	-3.71360300	0.31506000	0.26867300
C	-1.83863500	-0.07863300	-1.51570100
H	-1.58472500	-0.65953700	-2.39183000
C	-0.93782800	0.82668000	-1.01099100
H	-1.23001300	1.39696600	-0.14473500
C	0.34767300	1.08710000	-1.52630800
C	0.85856300	0.33593100	-2.73672800
H	0.51407500	0.84266100	-3.64473900
H	0.42028300	-0.66027700	-2.75927900
C	2.37676300	0.22817500	-2.74302500
H	2.70031300	-0.38626100	-1.89994700
C	3.00249300	1.61042500	-2.64007300
H	2.80280800	2.17810000	-3.55509500
H	4.08619000	1.54085700	-2.55065500
C	2.46240300	2.37732600	-1.45454800
C	1.17023600	2.04123200	-0.95614700
C	3.21294200	3.35927700	-0.88524700
H	2.87247700	3.92715600	-0.02911900
H	2.71189100	-0.26829000	-3.65419700
O	4.41274300	3.65198200	-1.35891900
C	5.17657600	4.65466700	-0.63894700
H	4.70554300	5.62413500	-0.81033200
H	5.13135300	4.41987900	0.42559900
C	6.59217200	4.61810200	-1.15546100
H	7.04329500	3.64167900	-0.97731100
H	6.62158100	4.83132100	-2.22433100
H	7.18510600	5.37297400	-0.63772700
O	6.71066900	-1.57755600	0.11633100
N	2.03538800	-1.11270500	1.09215000
C	1.38439300	-3.50153300	-0.47405600
C	0.35932200	-2.43229100	-0.09578400
C	0.72272200	-1.72018800	1.18180800
H	0.66483100	-2.40573500	2.04006500
C	2.35351500	-0.25016000	2.21084800
H	1.45664400	0.31911000	2.45664000
H	2.61334500	-0.84150400	3.10226900
C	3.47138800	0.68151700	1.82347100
H	3.69795600	1.36730200	2.64272700
H	3.12791200	1.28350300	0.98334200
C	4.75436600	-0.06089100	1.42231000
C	4.40793000	-1.29509000	0.57177100
C	5.42868900	-2.00938000	-0.08213800
C	5.15367900	-3.11398700	-0.88026200
H	5.94024400	-3.65013100	-1.38645300
C	3.84064500	-3.53883100	-1.00337700
H	3.64197700	-4.40836600	-1.61471600
C	2.79064900	-2.91281400	-0.35624100
C	3.07480600	-1.77492100	0.44798800
C	1.25712700	-4.71483000	0.46595500
H	1.98012300	-5.48546400	0.19418000
H	0.25451900	-5.14578800	0.39971400
H	1.44332800	-4.43853200	1.50411200
C	1.07103000	-3.95502300	-1.90816200
H	1.67758000	-4.80621900	-2.21661100
H	1.23697300	-3.14376600	-2.61887900
H	0.02390900	-4.25841900	-1.97564100
C	5.49947400	-0.49598500	2.69881600
H	6.40327100	-1.05062200	2.45494200
H	4.86893900	-1.13033800	3.32352900
H	5.78099800	0.38404900	3.28340700
C	5.60761200	0.97025100	0.65564900
H	5.16972000	1.18228400	-0.31984800
H	5.62835600	1.90443700	1.22260800

H	6.62917200	0.63761100	0.50710700
C	7.77387600	-2.24847600	-0.54089700
H	7.66507500	-2.20274200	-1.62739500
H	7.84175900	-3.29378300	-0.22915800
H	0.00787100	-0.92087300	1.37425500
H	0.30488600	-1.69783100	-0.89666800
H	-0.63329300	-2.87709800	-0.00017900
C	-2.92415400	-0.02805000	1.52840000
C	-2.19326800	0.93236100	2.22098700
C	-2.90635900	-1.34868400	1.97938900
C	-1.46223100	0.59159900	3.35279100
H	-2.18672500	1.95981000	1.88984500
C	-2.19254700	-1.70391600	3.11312600
H	-3.45802500	-2.11400700	1.45239500
C	-1.48330100	-0.72093300	3.77939800
H	-0.88966100	1.33156100	3.89349100
H	-2.17621600	-2.72335000	3.47124600
C	-4.07398100	1.78318500	0.12451300
C	-4.74987700	2.40034400	1.18062000
C	-3.82623200	2.50871700	-1.03613200
C	-5.15145000	3.72278300	1.09231000
H	-4.96697900	1.84320800	2.08106800
C	-4.21692600	3.83944900	-1.13956400
H	-3.32371000	2.05150800	-1.87418700
C	-4.86858700	4.41929300	-0.07046800
H	-5.67331700	4.20912300	1.90428800
H	-4.02245400	4.41267400	-2.03490600
F	-0.77434400	-1.06171000	4.87900700
F	-5.25028600	5.71348600	-0.16112100
H	8.68110200	-1.72580900	-0.24737900

FP-TS-II-A(c)

Cl	0.84038100	2.80651200	0.84630800
O	-4.87838700	-0.06296700	0.09941500
N	-8.26131100	-0.72123400	0.29399600
N	-6.94722400	-2.36604800	-3.53561600
N	-3.33934100	-1.97418300	-3.98228900
C	-7.39522700	-0.90399600	-0.45151900
C	-6.65857700	-1.80932400	-2.56329200
C	-3.60990700	-1.45792500	-2.98289700
C	-6.34648600	-1.13386800	-1.36700600
C	-5.05377500	-0.69872200	-1.06772000
C	-3.83853400	-0.80943100	-1.76090500
C	-2.80721200	-0.18812400	-1.00379000
C	-3.47774900	0.39110200	0.23921300
C	-1.48629100	-0.12199400	-1.33042000
H	-1.19570800	-0.56007100	-2.27586100
C	-0.46660300	0.46354400	-0.50415400
H	-0.83040800	1.08473600	0.30111800
C	0.77090800	0.94798700	-1.10770600
C	1.30422800	0.21663800	-2.31803600
H	0.74428600	0.53619700	-3.20378300
H	1.10709100	-0.85118700	-2.20381800
C	2.79414600	0.43712100	-2.53296800
H	3.34842700	-0.09930400	-1.76103500
C	3.13613500	1.92069100	-2.47161000
H	2.65938200	2.44016500	-3.31016100
H	4.20885000	2.07674200	-2.57657800
C	2.66766500	2.53863800	-1.17536500
C	1.45575100	2.00482100	-0.60221000
C	3.37038300	3.52345100	-0.58036800
H	3.05939200	3.97356100	0.35327000
H	3.09670400	0.01879700	-3.49370000
O	4.50586700	3.99201800	-1.11724400
C	5.24259100	4.93318600	-0.30740900
H	4.59554800	5.78601100	-0.08753400
H	5.51055100	4.44591500	0.63331800
C	6.46973000	5.35527200	-1.07665800
H	7.10575300	4.49631800	-1.29357400

H	6.19310000	5.83357500	-2.01692500
H	7.04440600	6.06803900	-0.48383300
O	6.21877600	-1.81956400	-0.42533800
N	1.71209000	-1.55407200	1.21500700
C	0.92644800	-3.81947300	-0.22703100
C	-0.10974600	-2.71727200	0.01423800
C	0.38037400	-1.64259100	0.94803100
H	-0.22825000	-1.44531300	1.82200600
C	2.15077400	-0.78377000	2.37616300
H	1.28869900	-0.25235800	2.77247000
H	2.49769400	-1.48108600	3.14310400
C	3.23839700	0.17915200	1.96735900
H	3.55702500	0.75863200	2.83514100
H	2.82258400	0.87992800	1.24632200
C	4.46324200	-0.51420400	1.35169000
C	4.00997000	-1.61331800	0.38076500
C	4.92743400	-2.23868600	-0.49063200
C	4.52282900	-3.23676000	-1.36880500
H	5.22411200	-3.68327200	-2.05555500
C	3.21487900	-3.70152700	-1.33690700
H	2.94072100	-4.51588200	-1.99122500
C	2.28640100	-3.17685300	-0.46010400
C	2.68826800	-2.10066200	0.36052000
C	1.02755500	-4.72009100	1.02162600
H	1.76848500	-5.50397100	0.86143300
H	0.06365500	-5.19128700	1.22527300
H	1.32251000	-4.15205300	1.90465100
C	0.45196400	-4.66177300	-1.41338500
H	1.07886800	-5.54098700	-1.56122700
H	0.44838000	-4.07902800	-2.33584800
H	-0.56488800	-5.01187700	-1.22828000
C	5.30652500	-1.15790600	2.47010500
H	6.17558700	-1.66508700	2.05537000
H	4.72751800	-1.88740800	3.03790500
H	5.65426800	-0.38584500	3.16028700
C	5.28286200	0.60420000	0.67708300
H	4.78712200	0.96532400	-0.22213800
H	5.36095100	1.44577300	1.36909200
H	6.28379300	0.28104100	0.41434700
C	7.18108100	-2.40147500	-1.29560200
H	6.92689900	-2.22482200	-2.34308700
H	7.27722200	-3.47523400	-1.11950600
H	-0.00523900	-0.52724500	0.26811000
H	-0.39669100	-2.27664300	-0.94313000
H	-1.02444900	-3.14401800	0.42570700
C	-2.94717700	-0.23850900	1.52244400
C	-2.21302300	0.48655400	2.45675800
C	-3.17872200	-1.59581100	1.75123900
C	-1.72044800	-0.12183100	3.60598300
H	-2.01525000	1.53651900	2.30076900
C	-2.69872000	-2.21959400	2.89280200
H	-3.74290400	-2.17718600	1.03566500
C	-1.97714600	-1.46495100	3.80185100
H	-1.15056400	0.43560600	4.33578200
H	-2.87611900	-3.26944800	3.07823600
C	-3.54832700	1.91078700	0.27337000
C	-4.31134200	2.50929000	1.27995400
C	-2.93105800	2.71882400	-0.67464200
C	-4.44077600	3.88640100	1.35339800
H	-4.81125500	1.89349100	2.01456200
C	-3.04402800	4.10407600	-0.61293400
H	-2.35264200	2.27934400	-1.47248000
C	-3.79458900	4.65856200	0.40280600
H	-5.02821400	4.35761700	2.12879700
H	-2.56087300	4.73875000	-1.34229300
F	-1.50349600	-2.06543700	4.91660100
F	-3.90928200	6.00565100	0.47264800
H	8.12240500	-1.91039400	-1.06391500

Cl	2.41815800	1.02866900	1.57409800
O	-2.96538000	2.80871700	0.16585200
N	-5.54276300	5.09234800	0.22618700
N	-5.85753600	3.07294000	-3.63019700
N	-3.12837600	0.62609200	-4.06237300
C	-5.11766400	4.30003700	-0.50577300
C	-5.28311100	3.18349900	-2.62965600
C	-3.01428700	1.08455200	-3.00375900
C	-4.61420400	3.34124900	-1.40408000
C	-3.48806500	2.56898900	-1.05343700
C	-2.78573900	1.57529600	-1.71581000
C	-1.68520000	1.12093400	-0.88035300
C	-1.79507300	1.93969900	0.41132700
C	-0.77379100	0.19203100	-1.19453600
H	-0.87126200	-0.27172700	-2.16967900
C	0.39868900	-0.25828000	-0.37054500
H	0.28770200	0.03564800	0.66371400
C	1.72526100	0.21661600	-0.90471000
C	1.97198700	-0.04321400	-2.37045100
H	1.42247700	0.69629700	-2.96455000
H	1.53565800	-1.01235100	-2.62670500
C	3.44836400	-0.00981800	-2.73716700
H	3.94814500	-0.88341600	-2.30879400
C	4.09739700	1.25742800	-2.19315900
H	3.64074900	2.13011000	-2.67534900
H	5.15978600	1.28865900	-2.43131500
C	3.91322900	1.36400600	-0.69781800
C	2.67121200	0.82034700	-0.16837600
C	4.82806700	1.97484600	0.07075000
H	4.71173600	2.08111500	1.14087000
H	3.56996800	-0.06530200	-3.82025000
O	5.94862000	2.51971200	-0.46138700
C	6.86692600	3.08526000	0.48876600
H	6.34533500	3.84739100	1.07507100
H	7.20316400	2.29781400	1.16976300
C	8.02770600	3.68199000	-0.27001800
H	8.54407000	2.91830400	-0.85315400
H	7.68616200	4.46664700	-0.94642400
H	8.73966700	4.11855800	0.43183900
O	2.98226700	-4.15793400	-1.27814200
N	-1.04617600	-3.60192700	1.28059400
C	-2.65096600	-3.42331400	-1.03274900
C	-2.93180600	-2.56099500	0.20797300
C	-2.22083100	-3.08634500	1.38224200
H	-2.66199000	-3.07842900	2.36845200
C	-0.34560300	-4.12406400	2.46681600
H	-0.94859300	-3.88768800	3.33870200
H	-0.28714700	-5.20683200	2.36094700
C	1.01577300	-3.47652800	2.51211800
H	1.52554800	-3.77437600	3.42810600
H	0.88295700	-2.39301900	2.55350100
C	1.88382600	-3.85716900	1.30136100
C	1.04007900	-3.83287200	0.02008800
C	1.64530600	-3.95174200	-1.25181200
C	0.88874500	-3.85005400	-2.41337200
H	1.36315800	-3.91441100	-3.37972100
C	-0.48357600	-3.65892900	-2.35035600
H	-1.03907000	-3.57866900	-3.27239200
C	-1.13933600	-3.57276000	-1.13841700
C	-0.35403200	-3.67567800	0.02421900
C	-3.28617800	-4.81735000	-0.86742800
H	-3.08774200	-5.42145300	-1.75257500
H	-4.36713900	-4.72859200	-0.74496400
H	-2.88699600	-5.35076200	-0.00306600
C	-3.26550800	-2.72580500	-2.24698900
H	-3.18199300	-3.33846300	-3.14390700
H	-2.79273700	-1.76434300	-2.43885200
H	-4.32737200	-2.55280500	-2.06743500
C	2.45830000	-5.27189200	1.51136400
H	3.07118200	-5.57103600	0.66471100
H	1.66717400	-6.01279600	1.63476000

H	3.07965500	-5.28343100	2.40871800
C	3.02966900	-2.82753200	1.25727400
H	2.65732200	-1.84103300	0.98467800
H	3.47115800	-2.75550600	2.25322300
H	3.80727600	-3.10904800	0.55613900
C	3.65095500	-4.23801400	-2.53407900
H	3.53094100	-3.31474600	-3.10381300
H	3.28696100	-5.08350300	-3.12099500
H	0.41790900	-1.35078100	-0.38347600
H	-2.57291300	-1.53583100	0.03640900
H	-3.99645900	-2.49258700	0.42403800
C	-2.16640600	1.04681600	1.59172900
C	-1.21956700	0.61238000	2.51693200
C	-3.48193300	0.59995400	1.72102900
C	-1.56529300	-0.25787400	3.54343900
H	-0.19919600	0.95709900	2.45390100
C	-3.84992200	-0.26076500	2.74630100
H	-4.23601300	0.92432200	1.01960100
C	-2.87820100	-0.67565600	3.63754200
H	-0.83258000	-0.59754700	4.26188200
H	-4.86856600	-0.60691200	2.85163400
C	-0.63430100	2.88753400	0.65847400
C	-0.54439600	3.57243300	1.87179300
C	0.29578600	3.16499100	-0.33885200
C	0.47330400	4.48570000	2.10272200
H	-1.27273200	3.39208900	2.64984600
C	1.32522200	4.07306300	-0.12606300
H	0.23344200	2.65827900	-1.28903400
C	1.39638500	4.70792600	1.09654100
H	0.55599100	5.01338600	3.04256100
H	2.06539000	4.27214900	-0.88791200
F	-3.22376500	-1.53034300	4.63257400
F	2.40678200	5.58376500	1.32210400
H	4.70067300	-4.38429800	-2.29673100

FP-TS-II-B(c)

Cl	1.45307200	2.02297200	1.62941200
O	-4.04707400	0.79166500	0.18065600
N	-7.41292300	1.57064200	0.04941600
N	-6.42854300	-0.11836700	-3.85495600
N	-2.95247900	-1.08115500	-4.05668600
C	-6.61030400	1.11719200	-0.64844800
C	-6.05249300	0.17977100	-2.80321200
C	-3.08964900	-0.64404500	-2.99613500
C	-5.63771100	0.55974600	-1.50927000
C	-4.33079300	0.40277700	-1.06405300
C	-3.17505900	-0.12047900	-1.69374700
C	-2.08672800	-0.03973300	-0.81342600
C	-2.59939000	0.62470500	0.45918100
C	-0.81886600	-0.59685100	-1.01113900
H	-0.62430100	-0.84721400	-2.04955100
C	0.42480700	-0.19113000	-0.23537100
H	0.18377800	0.00959600	0.80025900
C	1.20769600	0.94527600	-0.82948100
C	1.50288000	0.83802800	-2.30572600
H	0.61909800	1.14317600	-2.87874400
H	1.66738200	-0.21600400	-2.54818300
C	2.70493100	1.67038600	-2.72868700
H	3.61617500	1.21637900	-2.32877800
C	2.57418300	3.09374700	-2.19984200
H	1.69928900	3.56907600	-2.65966200
H	3.43800500	3.69667100	-2.47683000
C	2.41414100	3.10530900	-0.69812100
C	1.70205300	1.97490000	-0.12408900
C	2.85746100	4.13663200	0.03745300
H	2.73825600	4.17913500	1.11174200
H	2.79556000	1.67556600	-3.81607500
O	3.46168900	5.20365100	-0.53603000
C	3.95241700	6.19846200	0.37874700

H	3.12161600	6.55217100	0.99609600
H	4.69810400	5.73988100	1.03470300
C	4.55293900	7.32636700	-0.42515500
H	5.37971900	6.96762800	-1.03964000
H	3.80437500	7.77949800	-1.07643900
H	4.93358900	8.09531300	0.24854700
O	5.17555800	-2.30605400	-0.94047000
N	0.98711700	-3.36621300	1.14716000
C	-0.22248200	-4.05946400	-1.30729200
C	-0.98070200	-3.33716200	-0.19624900
C	-0.33927400	-3.31763000	1.03527900
H	-0.88252600	-3.21244800	1.96258800
C	1.62781300	-3.33117200	2.45961200
H	0.84640800	-3.26024800	3.21201600
H	2.15857900	-4.27257100	2.61215100
C	2.56227600	-2.14736900	2.50574400
H	3.01250700	-2.06675500	3.49590200
H	1.97644200	-1.23969800	2.34342100
C	3.68110600	-2.24398700	1.45252600
C	3.11418600	-2.75655900	0.11932900
C	3.88031900	-2.69450600	-1.06619200
C	3.32202500	-3.00838700	-2.29909300
H	3.90565400	-2.92996600	-3.20255800
C	1.99945200	-3.42107400	-2.38065000
H	1.58402500	-3.63938700	-3.35331500
C	1.22065100	-3.56789700	-1.24981800
C	1.80696100	-3.25806600	-0.00491700
C	-0.24677500	-5.57975700	-1.02701900
H	0.30191500	-6.11163100	-1.80636400
H	-1.27533300	-5.94622900	-1.01541300
H	0.21144000	-5.81381500	-0.06560700
C	-0.88694700	-3.81025500	-2.66307200
H	-0.45408100	-4.44261700	-3.43804500
H	-0.80038400	-2.77467500	-2.98365700
H	-1.94825800	-4.05358900	-2.59728000
C	4.77626600	-3.19961300	1.96105800
H	5.57447700	-3.30037100	1.22914800
H	4.37471700	-4.19363200	2.16357000
H	5.20384300	-2.81000400	2.88744000
C	4.25250700	-0.81745900	1.31657700
H	3.53099600	-0.15603800	0.83551900
H	4.45331700	-0.42319800	2.31491000
H	5.17503000	-0.79594800	0.74685300
C	5.95014100	-2.08842600	-2.11400700
H	5.49015900	-1.33212200	-2.75395000
H	6.08497900	-3.01331700	-2.67888500
H	1.09336100	-1.05209900	-0.23843700
H	-0.99490900	-1.91417600	-0.54874500
H	-2.05377500	-3.49434200	-0.15979100
C	-2.49289300	-0.31170400	1.65839000
C	-1.51480600	-0.15361200	2.63757600
C	-3.38275100	-1.38155800	1.76330900
C	-1.43602000	-1.02522700	3.71718700
H	-0.80988900	0.66100600	2.57827400
C	-3.32353300	-2.25839700	2.83715000
H	-4.14427600	-1.53177900	1.01210700
C	-2.35219100	-2.05532600	3.80101800
H	-0.68267100	-0.90154100	4.48221900
H	-4.01721800	-3.08204800	2.92901000
C	-2.07675200	2.03440700	0.66762800
C	-2.34179000	2.70697300	1.86157600
C	-1.43926500	2.71737100	-0.36439500
C	-1.93938600	4.02135700	2.04093000
H	-2.86770500	2.20642600	2.66178500
C	-1.02578700	4.03283200	-0.20258800
H	-1.24898400	2.22710000	-1.30660400
C	-1.27639100	4.65336800	1.00396300
H	-2.13139100	4.54866700	2.96469400
H	-0.50691000	4.56003300	-0.98986900
F	-2.29076600	-2.90167400	4.85446100
F	-0.86182700	5.93027600	1.18004000

H 6.91650400 -1.73281600 -1.76706500

TCF-A6(+2H, c)

Cl 2.47126200 -2.26149400 -0.98993100
O -2.39588900 0.75679700 1.18786500
N -3.73806300 2.69320100 3.74814500
N -2.93368000 5.43730200 0.44221900
N -1.67334300 3.77958400 -2.42075100
C -3.34739200 2.84348900 2.67351800
C -2.89583000 4.35115800 0.82834000
C -1.77919300 2.94038500 -1.63987800
C -2.86899300 3.03453300 1.35058900
C -2.40372400 1.96031100 0.63752100
C -1.88058500 1.87241300 -0.71387900
C -1.53360600 0.58934000 -0.97348600
C -1.82221800 -0.24623100 0.26483200
C -1.08679200 0.06355600 -2.28987500
H -1.05595500 0.89122400 -2.99595000
C 0.23137500 -0.73321300 -2.34288300
H 0.15357100 -1.61928600 -1.72023100
C 1.47476700 0.03115700 -1.98351900
C 1.54585600 1.48017600 -2.39995600
H 0.93490100 2.08886000 -1.72342600
H 1.08837700 1.58662900 -3.38730100
C 2.96691100 2.02695800 -2.42275100
H 3.50798900 1.59249000 -3.26768900
C 3.69258000 1.67897100 -1.12864600
H 3.18969100 2.17234600 -0.28798300
H 4.71614700 2.05072600 -1.14102800
C 3.70050000 0.18705500 -0.90063400
C 2.52188100 -0.53115300 -1.35600500
C 4.71465400 -0.41382900 -0.25823300
H 4.73266800 -1.47886200 -0.06925800
O 5.76653200 0.29160100 0.21506200
C 6.81532400 -0.49155600 0.81250000
H 6.39219700 -1.08476800 1.62812900
H 7.21741700 -1.17626500 0.06041100
C 7.88068400 0.45041300 1.31859900
H 8.29797100 1.03986400 0.50117500
H 7.47304400 1.13053200 2.06765600
H 8.68837900 -0.12194600 1.77689500
H 0.31557200 -1.09320000 -3.37387600
H -1.87868000 -0.60510300 -2.64040900
C -2.89876200 -1.27761900 -0.04457400
C -2.57378100 -2.43062900 -0.76019000
C -4.22331900 -1.06071500 0.32613100
C -3.54877500 -3.35641500 -1.09887700
H -1.55261700 -2.62901600 -1.04866000
C -5.21117000 -1.98119000 -0.00240300
H -4.49670900 -0.17819900 0.88282300
C -4.85332700 -3.11082700 -0.71093600
H -3.30306200 -4.25378000 -1.64860700
H -6.24034700 -1.82416800 0.28791000
C -0.58384300 -0.77047500 0.97918100
C -0.57363800 -2.00985800 1.61291600
C 0.51629800 0.07639800 1.12397100
C 0.52685100 -2.41496300 2.35736700
H -1.42537000 -2.66853500 1.54161400
C 1.61785700 -0.30758100 1.87017700
H 0.52096100 1.05277500 0.66187000
C 1.60212600 -1.55534800 2.46495000
H 0.54882200 -3.37785400 2.84761300
H 2.47946400 0.33498300 1.97441400
F -5.80906000 -4.01041400 -1.03448900
F 2.68132500 -1.94711500 3.17890700
H 2.94789700 3.10765200 -2.57092700