

Structure and Formation Mechanism of Polymer Byproducts in Vinyl Carbonate Synthesis

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1 Figure S1

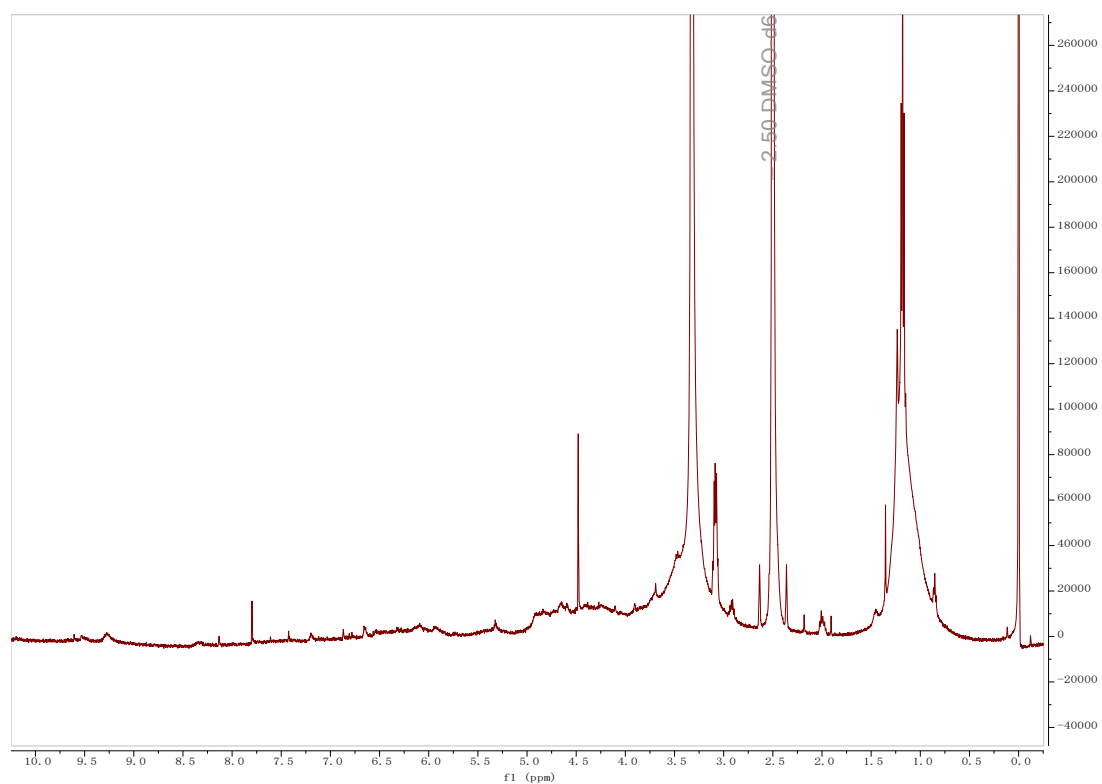


Figure S1. ¹H NMR spectrum of polyVC^{Sys} (measured at 25 °C).

The low solubility of polyVC^{Sys} in various common deuterated solvents, including deuterated dimethyl sulfoxide (DMSO-d₆), resulted in a ¹H NMR spectrum that reflects only the chemical shifts of the dissolved component.

2 Figure S2

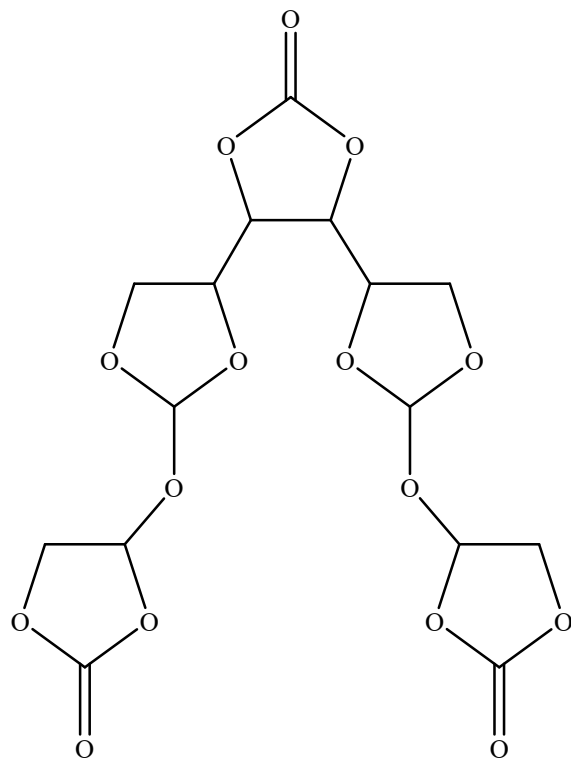


Figure S2. The structure reported in Ota's study.

3 Figure S3

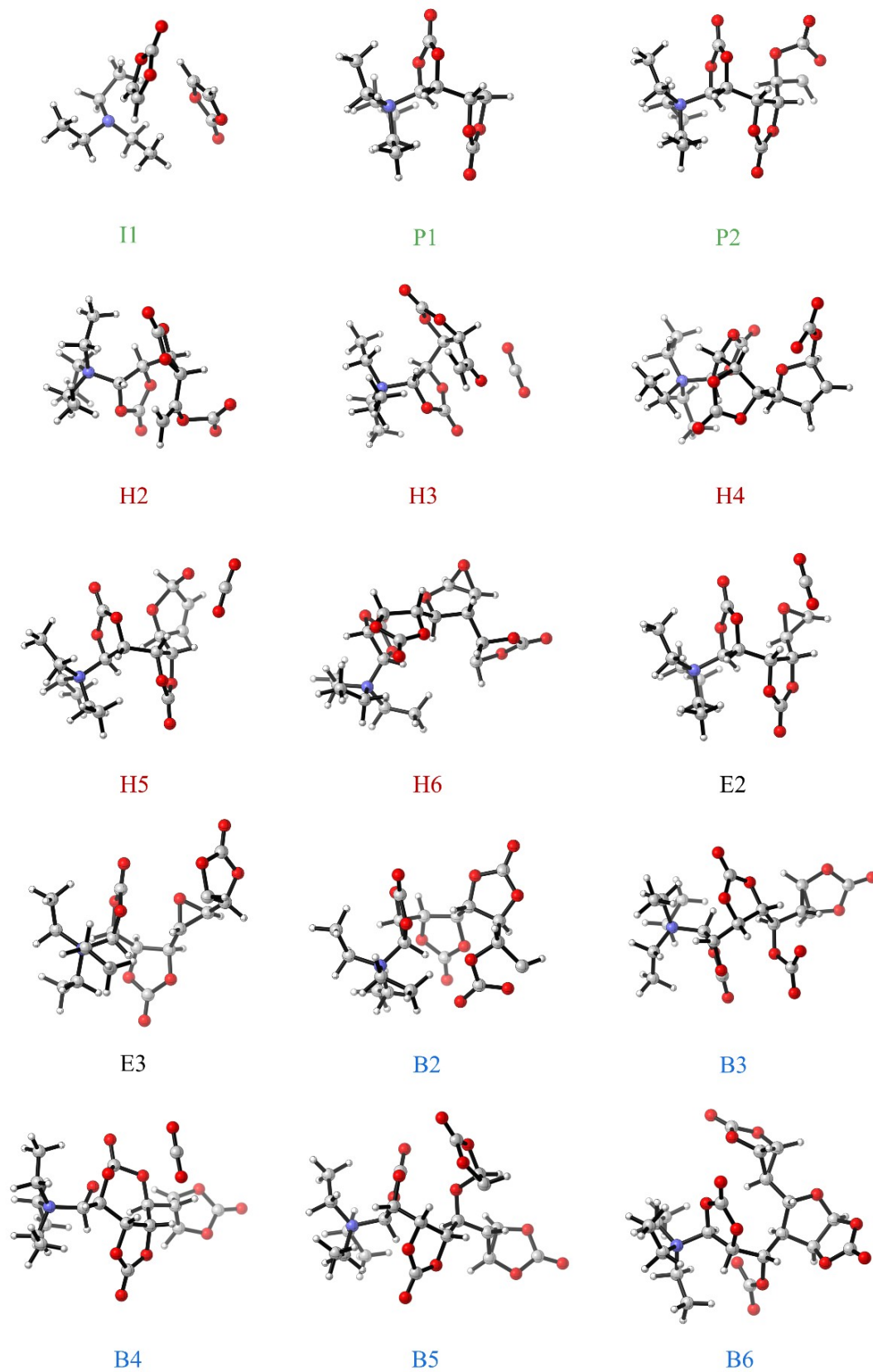


Figure S3. Structures of intermediates and minima.

4 Cartesian coordinates of the transition states

TS_II

N	-1.30633600	-1.19897900	0.07180800
C	-2.28967600	-1.50062900	-1.04432500
H	-3.01259100	-0.69302700	-1.04276800
H	-2.79708100	-2.41693100	-0.74389300
C	-0.27207800	-2.30621400	0.09796700
H	0.24457700	-2.25859300	-0.85661400
H	-0.83394900	-3.23908000	0.13043600
C	-2.05272900	-1.20154200	1.38278700
H	-1.31196000	-1.07669800	2.16503700
H	-2.46785000	-2.20555900	1.47306600
C	0.74171100	-2.25319900	1.22329800
H	0.30373400	-2.44348600	2.20119500
H	1.47435900	-3.03686900	1.03231600
H	1.28172900	-1.30848700	1.25574700
C	-3.13895500	-0.15791300	1.55150200
H	-3.90095300	-0.19349100	0.77601400
H	-3.63111000	-0.36408700	2.50226500
H	-2.73550300	0.84998700	1.61635200
C	-1.69448100	-1.64685200	-2.43176800
H	-1.04395600	-2.51404400	-2.52832100
H	-2.52715700	-1.78567800	-3.12158200
H	-1.15587000	-0.75510900	-2.74841600
C	0.09928500	0.90042400	0.85225600
C	-0.55847800	0.13397600	-0.23224700
O	-1.45228400	1.04418300	-0.82612600
H	0.13796600	0.47767500	1.84810200
H	0.16755800	-0.16094400	-1.01052600
C	2.16373200	0.93364600	-1.35510300
C	1.94584900	1.50414100	-0.14065000

H	1.94875700	1.20554100	-2.36896500
H	1.69894800	2.53629100	0.05326200
O	2.86365100	0.90958400	0.74694500
O	3.01618000	-0.18546600	-1.14614600
C	3.43796100	-0.13083500	0.11377400
O	4.20785400	-0.89703900	0.62816900
C	-1.49815900	2.19897000	-0.10274800
O	-2.21091700	3.11481900	-0.39654200
O	-0.67438200	2.13037100	0.91572100

TS_P1

N	-2.44543800	-0.42740900	0.43773100
C	-2.56978500	-0.96413900	1.86213600
H	-2.09516300	-1.93884100	1.86410600
H	-3.63864600	-1.09966500	2.01738100
C	-3.07611600	0.96619600	0.41554000
H	-2.38138500	1.62824700	0.92823600
H	-3.96383600	0.87387500	1.03851700
C	-3.23662300	-1.33600100	-0.48889700
H	-3.01671200	-1.02219300	-1.50490300
H	-4.27873000	-1.08764600	-0.29310800
C	-3.45962800	1.55051300	-0.92964400
H	-4.18043400	0.94068100	-1.46996000
H	-3.93907000	2.50546500	-0.71341800
H	-2.60630600	1.76901000	-1.56503300
C	-3.04569200	-2.83405200	-0.34446800
H	-3.39126400	-3.21064600	0.61568000
H	-3.66466800	-3.29314000	-1.11548700
H	-2.02611900	-3.17213700	-0.50731300
C	-1.97049400	-0.09390900	2.94788100
H	-2.44327700	0.88257900	3.02856300
H	-2.13357000	-0.61567300	3.89064900
H	-0.89398800	0.03589700	2.84113300

C	-0.56880200	-0.05945900	-1.35782400
C	-0.96531800	-0.31010000	0.10916800
O	-0.32240000	-1.50734200	0.43168700
H	-1.41152700	0.10823400	-2.02237400
H	-0.59388600	0.47368400	0.76152300
C	1.48004300	1.25394600	-0.44449300
C	0.45086300	1.07582300	-1.53109900
H	2.37886600	1.70543900	-0.86845300
H	0.89923400	0.95482800	-2.51542200
O	-0.31920900	2.30551200	-1.51749800
O	0.83714400	2.30895000	0.36299000
C	-0.09726500	2.92740200	-0.33806700
O	-0.71948600	3.88983800	0.01740700
C	0.20766100	-2.08969700	-0.68361300
O	0.69849800	-3.16535400	-0.69109200
O	0.03233900	-1.29481200	-1.73873700
C	3.47453800	0.74369200	1.56286500
C	2.33580900	0.14092500	1.10388600
H	1.43745700	0.00293500	1.68219500
O	2.76203000	-0.96658100	0.35275800
O	4.50762600	0.32245000	0.66395400
C	4.05612300	-0.74932100	0.02672400
O	4.69117200	-1.45230000	-0.71267100
H	3.62750800	1.69711700	2.03241000

TS_E1

N	-2.44733000	-0.33119200	0.13277300
C	-3.00744700	-0.75556100	1.48967400
H	-2.59660900	-1.73726100	1.69724400
H	-4.07944100	-0.85635700	1.32640200
C	-3.00451300	1.06149900	-0.17670400
H	-2.45550000	1.76225300	0.44869300
H	-4.02811600	1.03161300	0.19156200

C	-2.95267300	-1.30789500	-0.92054500
H	-2.40380500	-1.10259300	-1.83554700
H	-3.98602500	-1.01321700	-1.09189600
C	-3.00355000	1.53105200	-1.61851500
H	-3.57852700	0.88513900	-2.27804500
H	-3.49242800	2.50553400	-1.61134000
H	-2.01035000	1.68670600	-2.02831200
C	-2.91261100	-2.78885600	-0.59256400
H	-3.59084000	-3.05344500	0.21545300
H	-3.25740900	-3.30449800	-1.48888100
H	-1.92388500	-3.17394900	-0.36044500
C	-2.72080900	0.18170100	2.64471500
H	-3.13872400	1.17714600	2.50905400
H	-3.19703100	-0.25551400	3.52207500
H	-1.65844100	0.26200800	2.87138600
C	-0.12780700	-0.11969900	-1.05377300
C	-0.93103600	-0.25304500	0.25465900
O	-0.44131300	-1.42975000	0.81488800
H	-0.76032500	0.06306100	-1.91709000
H	-0.75159500	0.56903300	0.94135400
C	1.76557500	1.40672300	0.13545500
C	0.93414700	0.99323800	-1.08825900
H	2.65922200	1.89932600	-0.23860100
H	1.58596400	0.79491100	-1.93539200
O	0.20401800	2.20439900	-1.33644100
O	0.92285800	2.41745300	0.74041000
C	0.13800100	2.94119600	-0.20465300
O	-0.55727400	3.89826700	-0.07622100
C	0.29199500	-2.13885400	-0.10382100
O	0.64996500	-3.24905000	0.06375600
O	0.43833600	-1.40877100	-1.21643300
C	3.34035000	0.67149200	2.08193500
C	2.14833400	0.39305800	1.21192600
H	1.27371600	0.19344000	1.83535100

O	2.54560900	-0.86616700	0.68828000
O	4.10094400	0.16183700	-0.64790100
C	3.60790000	-0.92627200	-0.34702600
O	3.78057900	-2.07121400	-0.71966200
H	3.97654100	1.39031500	1.53712300

TS_E2

N	-2.32414600	-1.22734800	0.61007400
C	-1.86817800	-2.16273700	1.73432800
H	-1.30850800	-2.96434700	1.26725000
H	-2.79090800	-2.57479400	2.13838700
C	-3.20824500	-0.15004100	1.24779400
H	-2.53442900	0.61485700	1.62714400
H	-3.66404600	-0.62908800	2.11133900
C	-3.16310500	-2.03800800	-0.36320900
H	-3.58104700	-1.34170300	-1.08283200
H	-3.98963600	-2.40256900	0.24443600
C	-4.30128100	0.45990400	0.39156300
H	-5.09973600	-0.24749700	0.17933500
H	-4.72331200	1.27582000	0.97774900
H	-3.94257500	0.89736300	-0.53614100
C	-2.50513900	-3.19329400	-1.09313500
H	-1.99799000	-3.89548300	-0.43630600
H	-3.31128200	-3.73253500	-1.59124500
H	-1.81420400	-2.87053800	-1.86784700
C	-1.03411000	-1.51415000	2.81977700
H	-1.52720100	-0.66700500	3.29425900
H	-0.87590200	-2.27221800	3.58653700
H	-0.05045000	-1.21067000	2.46367700
C	-1.21739100	0.17881400	-1.31775800
C	-1.07595500	-0.58976900	0.02048100
O	-0.18826000	-1.62364700	-0.27093900
H	-2.21760200	0.07401300	-1.73653700

H	-0.65925800	0.03433600	0.80552000
C	0.14146300	2.41293500	-0.54843700
C	-0.93009400	1.69204800	-1.37710300
H	0.32679700	3.37226700	-1.03977300
H	-0.81370200	1.92899800	-2.43204600
O	-2.11687700	2.34845400	-0.90258900
O	-0.61343900	2.73848100	0.66283900
C	-1.89546000	2.85671300	0.33230900
O	-2.75595500	3.31338500	1.01955400
C	0.30710300	-1.49844400	-1.52379400
O	1.12378900	-2.21349800	-1.99219600
O	-0.32982800	-0.51564300	-2.17809200
C	2.30268500	1.12181400	-1.19126300
C	1.45655000	1.80208000	-0.21508300
H	1.95790000	2.32399600	0.60716200
O	1.52822700	0.40005200	-0.13209600
H	1.79706200	0.96342400	-2.15605300
C	4.30852100	0.96648700	-0.33161900
C	4.31061300	1.21556000	1.00266500
O	4.07550500	-0.02064400	1.66470800
O	4.38672900	-0.42883100	-0.46562700
C	4.15104800	-0.97235800	0.74228000
O	4.05222900	-2.15438600	0.94740900
H	4.78017200	1.54139500	-1.10613300
H	4.33776900	2.09831900	1.60905000

TS_H1

N	-2.45426700	-0.35067200	0.21915400
C	-2.88916300	-0.81838600	1.60778500
H	-2.46227300	-1.80552200	1.74514800
H	-3.97093300	-0.91615700	1.53945400
C	-3.03262600	1.05069700	0.00445100
H	-2.44452500	1.72761500	0.62072500

H	-4.02962700	1.00032800	0.43783600
C	-3.05346100	-1.29370300	-0.81592400
H	-2.58036800	-1.06480000	-1.76669700
H	-4.09583500	-0.98931500	-0.89186400
C	-3.12660400	1.57786100	-1.41440000
H	-3.72081200	0.94289900	-2.06774000
H	-3.63987400	2.53672900	-1.33986400
H	-2.16273100	1.77803800	-1.87279800
C	-2.99365400	-2.78338000	-0.53413700
H	-3.60879400	-3.07053800	0.31551200
H	-3.40627600	-3.27364300	-1.41587700
H	-1.99085600	-3.17469200	-0.38814200
C	-2.49885900	0.08244200	2.76173200
H	-2.92891500	1.07990600	2.69682800
H	-2.89345100	-0.38480900	3.66373300
H	-1.42021100	0.16016700	2.89624000
C	-0.24247900	-0.10183500	-1.15514900
C	-0.93563900	-0.27638100	0.20812200
O	-0.39765200	-1.46806400	0.68830900
H	-0.93498100	0.13668000	-1.95669800
H	-0.69986000	0.52785400	0.89958700
C	1.72883600	1.37066000	-0.01750600
C	0.84645500	0.98404300	-1.21901800
H	2.65213600	1.79682400	-0.41116400
H	1.45765400	0.77074100	-2.09198100
O	0.14360000	2.21644500	-1.43959700
O	0.96997600	2.42531900	0.59828200
C	0.15478400	2.96517700	-0.31519800
O	-0.49935900	3.94555800	-0.16174400
C	0.24822400	-2.14954900	-0.31642700
O	0.63263900	-3.25840900	-0.21195400
O	0.27388200	-1.39414200	-1.41977600
C	2.76032200	0.64054900	2.24709300
C	2.15419000	0.32068200	1.00648700

H	1.29616400	0.07431400	1.74008500
O	2.49683600	-0.84508800	0.35309100
O	4.51050700	0.17130100	0.03504600
C	3.88803300	-0.87646700	-0.14340500
O	4.15324700	-1.94551600	-0.66779700
H	2.44467600	1.66840100	2.49569900

TS_H2

N	-2.39791400	-0.37999200	0.21355400
C	-2.83189900	-0.99244400	1.54392800
H	-2.48417000	-2.01900200	1.53794400
H	-3.92015300	-0.99442300	1.50847300
C	-2.89240700	1.06851900	0.19318200
H	-2.21193900	1.63473400	0.82596300
H	-3.85634100	1.04080100	0.69680700
C	-3.07268100	-1.14125700	-0.91414000
H	-2.68558600	-0.73686700	-1.84469600
H	-4.12067700	-0.85262500	-0.84867500
C	-3.05250400	1.74309600	-1.15517000
H	-3.81073600	1.27045200	-1.77511800
H	-3.38789600	2.75869900	-0.94452300
H	-2.12646400	1.83281800	-1.71587600
C	-2.96781800	-2.65385900	-0.91285300
H	-3.42553200	-3.10836700	-0.03714200
H	-3.52552300	-2.99458900	-1.78546000
H	-1.95340200	-3.02830400	-1.01712600
C	-2.32149700	-0.28412800	2.78236700
H	-2.65152900	0.75068200	2.85428000
H	-2.73306200	-0.81793200	3.63867300
H	-1.23517600	-0.32518200	2.87059800
C	-0.18545800	-0.09997900	-1.16475000
C	-0.87623600	-0.38235000	0.18556900
O	-0.41152400	-1.64587400	0.54002000

H	-0.88825000	0.15864700	-1.95216600
H	-0.57972700	0.32364100	0.95531800
C	1.67425300	1.39401100	0.08389400
C	0.88236700	1.00921300	-1.18209000
H	2.64966700	1.77252800	-0.22626100
H	1.55091700	0.78212900	-2.00825900
O	0.19798900	2.23448400	-1.47573600
O	0.91937000	2.51238500	0.59299200
C	0.17108700	3.02614600	-0.38112700
O	-0.46620600	4.03000000	-0.30822700
C	0.32503300	-2.19804000	-0.46555600
O	0.74828200	-3.30107100	-0.44181900
O	0.37713600	-1.35590400	-1.50565900
C	1.60051200	0.46707600	2.39649200
C	1.89490800	0.29838900	1.10113700
O	2.36717400	-0.78988800	0.53762100
O	4.59189700	0.27540700	0.21456600
C	4.12291000	-0.76447800	-0.11566400
O	4.22355200	-1.80789300	-0.66130400
H	1.18413000	1.39436900	2.76404400
H	1.79208100	-0.33490600	3.09739800

TS_H3

N	-3.12535600	-0.00920800	0.16048600
C	-3.70146600	-0.56001700	1.46239800
H	-3.50197600	-1.62546000	1.45715900
H	-4.77617200	-0.40772700	1.37672800
C	-3.39310400	1.49594100	0.13826100
H	-2.68638200	1.94546900	0.83242500
H	-4.38666900	1.60610000	0.56842800
C	-3.86318500	-0.65731100	-1.00014000
H	-3.34234700	-0.36791400	-1.90822600
H	-4.83545700	-0.16713000	-1.01449800

C	-3.34303100	2.21131400	-1.19790600
H	-4.07478200	1.83472400	-1.90926500
H	-3.59707000	3.25070700	-0.98895000
H	-2.35746100	2.21951000	-1.65389000
C	-4.06482200	-2.16075300	-0.96131800
H	-4.72141000	-2.47331500	-0.15212600
H	-4.55628500	-2.42337200	-1.89832000
H	-3.14236100	-2.73172500	-0.90828000
C	-3.16122900	0.05797900	2.73574300
H	-3.34909100	1.12725200	2.81250100
H	-3.68292200	-0.42541200	3.56156500
H	-2.09815800	-0.13442900	2.87866500
C	-0.86115000	-0.06723800	-1.14939700
C	-1.61874200	-0.25395400	0.17827900
O	-1.37236400	-1.57740200	0.51599300
H	-1.47224800	0.39148200	-1.92122700
H	-1.24680600	0.40036000	0.96163400
C	1.30746700	0.86511100	0.16428200
C	0.41721500	0.78792600	-1.08551700
H	2.30844000	1.14410300	-0.16720400
H	1.00378200	0.53871500	-1.96577900
O	-0.02692100	2.15230000	-1.20582200
O	0.77196100	2.02721700	0.84873600
C	0.10886600	2.78556000	-0.02060700
O	-0.34166600	3.86698700	0.20369900
C	-0.74156500	-2.23194300	-0.51604000
O	-0.57118500	-3.40210500	-0.53843600
O	-0.61329500	-1.39628800	-1.55980400
C	2.26923600	-0.32775100	2.25834800
C	1.39593200	-0.37843700	1.07051400
H	0.52557900	-0.30557400	1.82322200
O	1.39942400	-1.46949400	0.31788700
H	2.40811100	0.73596800	2.54030000
C	4.20139300	-0.58845700	1.31870400

C	3.85914900	-1.56816900	0.45384800
H	4.51981900	-0.61570700	2.34326200
H	3.50636500	-2.56878600	0.59693000
O	4.14571700	-1.16236900	-0.81430600
O	4.72873400	0.46049700	0.54110900
C	4.65631600	0.09646300	-0.74401700
O	4.95826100	0.76053500	-1.68668900

TS_H4

N	-3.02647100	-0.35457400	-0.00919300
C	-3.62788200	-0.95249900	1.26113600
H	-3.23257100	-1.95875800	1.34197400
H	-4.69673700	-1.01482800	1.06275800
C	-3.56416900	1.07154900	-0.14562300
H	-3.04547900	1.67158200	0.59947500
H	-4.60603200	0.99954800	0.16014000
C	-3.50203900	-1.17525400	-1.19922700
H	-2.92313500	-0.85324100	-2.06028300
H	-4.52887200	-0.85263400	-1.36168900
C	-3.48367600	1.73670200	-1.50599300
H	-4.02130800	1.19135700	-2.27846700
H	-3.97110900	2.70513500	-1.39210400
H	-2.46898500	1.93731700	-1.83670300
C	-3.47221800	-2.68644900	-1.07085000
H	-4.17055900	-3.05237000	-0.32149000
H	-3.79480700	-3.07891500	-2.03534000
H	-2.48844100	-3.09989900	-0.86697200
C	-3.35497100	-0.18831700	2.54043700
H	-3.75309900	0.82436100	2.53276000
H	-3.85906800	-0.73107600	3.33988600
H	-2.29634700	-0.16093400	2.79702000
C	-0.66058300	-0.02348600	-1.07941300
C	-1.51376900	-0.30976500	0.17040500

O	-1.05748000	-1.55252600	0.59656800
H	-1.25444400	0.28799200	-1.93350100
H	-1.35514900	0.42283300	0.95585600
C	1.14926100	1.35566200	0.39469500
C	0.42709500	1.05563400	-0.92660200
H	2.09690300	1.82542600	0.13633700
H	1.15087700	0.89571000	-1.72106900
O	-0.24419500	2.30793600	-1.15377000
O	0.30276400	2.37061800	0.98421100
C	-0.38481800	2.97362000	0.01346400
O	-1.06172600	3.94516100	0.14410800
C	-0.26473600	-2.13428600	-0.36097400
O	0.11130500	-3.25214000	-0.30691200
O	-0.12220100	-1.29548100	-1.39269600
C	2.57567800	0.51224800	2.28613400
C	1.40742600	0.21974300	1.38177200
H	0.49852500	0.05287600	1.97970800
O	1.74685400	-0.92383400	0.66569600
H	2.58796100	1.35543100	2.96442200
C	3.52616000	-0.38170900	2.08964200
C	3.19549700	-1.40131300	1.01005300
H	4.48564800	-0.41103900	2.58916000
H	2.98343300	-2.39228600	1.46024600
O	3.98215100	-1.45322900	-0.02058900
O	3.85852900	1.02807700	-1.16901100
C	4.68088000	0.21666900	-1.34327900
O	5.61515800	-0.35134100	-1.74040800

TS_H5

N	-2.66285000	-1.01812000	0.34563000
C	-2.29907400	-2.19712300	1.24955000
H	-1.71775900	-2.87956300	0.64014900
H	-3.25114100	-2.66807600	1.48915600

C	-3.44621600	-0.01349300	1.19160800
H	-2.72072400	0.47727200	1.83768600
H	-4.08456100	-0.62695700	1.82452000
C	-3.56085600	-1.52451000	-0.77108300
H	-3.67989700	-0.70955700	-1.47957200
H	-4.52734100	-1.67921400	-0.29424500
C	-4.29437100	1.01550000	0.46971500
H	-5.07202900	0.56731500	-0.14459000
H	-4.78852000	1.59462500	1.24997700
H	-3.71986200	1.72056500	-0.12367000
C	-3.14949300	-2.79704500	-1.48719200
H	-3.15465300	-3.66469200	-0.83125800
H	-3.90130800	-2.96587000	-2.25823100
H	-2.18540900	-2.73943700	-1.98444900
C	-1.52965100	-1.84404700	2.50549600
H	-2.08974500	-1.20805300	3.18819400
H	-1.33107500	-2.78416200	3.01972900
H	-0.56071200	-1.39063500	2.29474900
C	-1.43319600	0.64322900	-1.26798400
C	-1.36186400	-0.37599400	-0.11410600
O	-0.50433000	-1.35894300	-0.60070600
H	-2.45335500	0.89494600	-1.54347600
H	-0.93876700	0.05186500	0.78914000
C	0.51582400	2.17872900	-0.15449700
C	-0.72384600	1.99285000	-1.05315200
H	1.06830000	3.03667600	-0.53609300
H	-0.53645600	2.40074900	-2.04301600
O	-1.67679100	2.83626700	-0.38915600
O	-0.07874000	2.55766100	1.10725500
C	-1.30128600	3.04060100	0.89319000
O	-1.99676600	3.55804700	1.70990000
C	-0.26238600	-1.18276600	-1.93264600
O	0.32778900	-1.95289200	-2.60536700
O	-0.87155000	-0.06874800	-2.35772000

C	2.81827500	1.39274200	0.62282600
C	1.47625400	1.01885100	0.07801200
H	1.00302500	0.29215900	0.76163800
O	1.71756000	0.38175900	-1.18223900
H	2.85243300	2.19730200	1.35021900
C	3.68981100	1.38943900	-0.50535800
C	2.99115800	0.80082800	-1.62725600
H	4.76217300	1.50660400	-0.48231200
H	3.36974200	0.08966400	-2.35575900
O	3.11678500	2.14797500	-1.89064300
C	3.26873300	-0.26708900	1.86405000
C	2.15922900	-0.90156000	2.36121200
H	3.98562800	0.28690800	2.44722500
H	1.70809100	-0.90622600	3.33496000
O	1.94640300	-2.06115800	1.55504500
O	3.83093400	-1.14374400	0.91229300
C	2.96861600	-2.16020600	0.71434600
O	3.11994600	-3.02384800	-0.10746800

TS_B1

N	2.83509300	0.82632900	-0.54699800
C	2.50291300	2.01837100	-1.44778400
H	2.11496600	1.60314900	-2.37135600
H	3.46651900	2.48136300	-1.65401500
C	3.33629400	1.38722600	0.78649100
H	2.46089700	1.76194300	1.31278700
H	3.94090000	2.24699600	0.50563200
C	3.95709100	0.03129400	-1.19969200
H	4.05553500	-0.89850100	-0.64616300
H	4.85355900	0.61781600	-1.00609000
C	4.14594500	0.47679000	1.68920600
H	5.04429200	0.09131100	1.21237900
H	4.46455500	1.09877500	2.52597800

H	3.57192500	-0.34144100	2.11334700
C	3.85733400	-0.24165100	-2.68910000
H	3.91699700	0.66737800	-3.28297700
H	4.72283000	-0.85396600	-2.94225200
H	2.97208200	-0.79643000	-2.98692000
C	1.52648000	3.02447900	-0.87797400
H	1.88765700	3.51034700	0.02633000
H	1.40742900	3.79848300	-1.63615000
H	0.53046900	2.62001800	-0.69877200
C	1.68466500	-1.34253000	0.34358000
C	1.55267000	0.04614800	-0.31341100
O	0.94291200	-0.23276800	-1.53741300
H	2.69224400	-1.54400100	0.69505100
H	0.91682400	0.72175300	0.25238200
C	-0.68620500	-1.13329500	1.64315200
C	0.76664300	-1.64291200	1.54006500
H	-1.24283900	-1.84592000	2.25572000
H	0.80067700	-2.71947600	1.68821400
O	1.37351200	-1.00883800	2.67150700
O	-0.53147700	0.07704200	2.40688000
C	0.62303500	0.04201900	3.07583400
O	0.97470500	0.82939400	3.89403400
C	0.94651500	-1.57670100	-1.79137500
O	0.61074500	-2.05314500	-2.81718800
O	1.42930000	-2.23321800	-0.73128000
C	-2.98705100	-0.54469400	0.61391000
C	-1.51196600	-0.80153900	0.39912600
H	-1.05587400	0.02599900	-0.14602600
O	-1.49394700	-1.96227700	-0.43725500
O	-3.52967600	-1.90875300	0.39353300
C	-2.68808600	-2.60992000	-0.32156000
O	-2.88780600	-3.67874500	-0.83226200
H	-3.23142600	-0.28668500	1.64630600
C	-3.89479600	0.86906200	-0.94845400

C	-4.75344100	1.81036200	-0.49445400
H	-4.10868600	0.01865700	-1.57049200
H	-5.75602200	1.76559900	-0.11674800
O	-3.95113000	2.89113300	-0.03259100
O	-2.66992300	1.51961800	-1.15722500
C	-2.72549900	2.69220500	-0.49632800
O	-1.79051700	3.44108500	-0.37256200

TS_B2

N	2.84387700	0.85341500	-0.08301400
C	2.54657900	2.31713700	-0.42350500
H	2.17052300	2.31799400	-1.44157600
H	3.51897000	2.80649400	-0.41548100
C	3.20966800	0.80617600	1.40228600
H	2.27858200	0.92232300	1.95357900
H	3.79031200	1.71252800	1.55865200
C	4.04364900	0.39735400	-0.90370500
H	4.09975000	-0.68457700	-0.81004500
H	4.90397000	0.80981500	-0.38040500
C	4.00334200	-0.37827800	1.92039100
H	4.94992100	-0.51725300	1.40327700
H	4.23405300	-0.14284800	2.95962400
H	3.45030600	-1.31147000	1.93269400
C	4.11180600	0.81482900	-2.36213400
H	4.18865100	1.89319400	-2.48170500
H	5.02964800	0.37810600	-2.75620900
H	3.28886000	0.45367600	-2.97127700
C	1.58397000	3.02677200	0.50695000
H	1.99854100	3.19556600	1.49836600
H	1.38843400	4.00269100	0.06269700
H	0.62174700	2.52321300	0.59700200
C	1.66927100	-1.48060400	-0.16928800
C	1.57902100	0.05713500	-0.34196400

O	1.22109600	0.21199500	-1.68775200
H	2.65656000	-1.80026100	0.15274000
H	0.79565400	0.51837500	0.26271200
C	-0.75732700	-1.63990400	0.95697300
C	0.67668800	-2.15793000	0.79091000
H	-1.36043100	-2.45088200	1.36904000
H	0.68935100	-3.22124800	0.56533100
O	1.19100600	-1.96266400	2.11096000
O	-0.59206500	-0.66646900	2.00183100
C	0.47517200	-0.99863800	2.73510500
O	0.78522800	-0.50527000	3.77022400
C	1.22609000	-0.97923400	-2.34623100
O	1.02511900	-1.09299600	-3.50472200
O	1.47781100	-1.97386300	-1.48928700
C	-2.48657100	0.00447000	0.11297700
C	-1.51441000	-1.09290100	-0.26052900
H	-0.84967200	-0.71653800	-1.02646500
O	-2.21032300	-2.17822200	-0.84663100
O	-3.86930600	-1.18703200	0.24484300
C	-3.54421700	-2.20685300	-0.45196200
O	-4.21798100	-3.14874100	-0.79918500
H	-2.56807300	0.33702300	1.13522400
C	-1.50713300	1.68484700	-0.47643900
C	-2.76848800	1.01824100	-0.91780900
H	-0.87174500	2.07428000	-1.26994600
H	-2.85845900	0.65258700	-1.93601900
O	-3.83974000	1.90860800	-0.61333400
O	-2.03095200	2.78560500	0.31598100
C	-3.34457200	2.90569600	0.15251300
O	-4.02337200	3.76947500	0.63107900

TS_B3

N	3.19169900	-0.48736400	0.86075100
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C	3.12572400	-0.70328600	2.36990000
H	2.91304600	0.26450800	2.80891600
H	4.13447600	-0.99968500	2.65317300
C	3.51111700	-1.83793600	0.21904000
H	2.59965300	-2.43006800	0.27122300
H	4.23608000	-2.29547000	0.88962600
C	4.32800100	0.47780300	0.56315200
H	4.26231800	0.72838800	-0.49129600
H	5.23241100	-0.11326200	0.69999500
C	4.05838200	-1.84309400	-1.19493000
H	5.00206600	-1.31011800	-1.28735500
H	4.25016000	-2.88866200	-1.43671200
H	3.35476900	-1.47640300	-1.93655100
C	4.42443500	1.73870700	1.40109500
H	4.64760700	1.53092700	2.44528300
H	5.26241000	2.30663200	0.99645100
H	3.54698200	2.37674700	1.34831600
C	2.10427600	-1.71699400	2.84412800
H	2.27108300	-2.71789500	2.45078100
H	2.20044400	-1.77184900	3.92828600
H	1.08064600	-1.40870500	2.63219700
C	1.70601700	0.57463600	-1.01844800
C	1.81352500	-0.02177200	0.39746500
O	1.37167500	1.00431800	1.22009300
H	2.60759200	0.43027800	-1.60727400
H	1.17944100	-0.89356100	0.52764200
C	-0.77310100	-0.45874200	-1.31096200
C	0.56161300	0.02792900	-1.89000200
H	-1.51644700	-0.38212800	-2.10394500
H	0.39493000	0.75042900	-2.68425000
O	1.07054500	-1.18576600	-2.47389800
O	-0.51842700	-1.87334700	-1.10454700
C	0.48411300	-2.25509000	-1.89368700
O	0.85141200	-3.37808600	-2.05461100

C	1.22889100	2.17369700	0.50624800
O	1.06233400	3.22822000	1.01368800
O	1.59446700	1.96066800	-0.77024600
C	-2.77062300	-0.09961200	0.12692900
C	-1.28949200	0.22809300	-0.03675700
H	-0.77997700	-0.27045300	0.81768700
O	-1.03523000	1.55610000	-0.07315600
O	-2.17472700	1.99905400	-2.43724200
C	-1.92499600	2.79536600	-1.61291000
O	-1.82728100	3.82063400	-1.06886700
H	-3.41706400	0.26470600	-0.66572400
C	-3.16927800	-1.37779100	0.80633800
C	-3.32160200	-0.07554700	1.51508100
H	-2.48604800	-2.17363000	1.05836500
H	-2.76708800	0.26225700	2.37691900
O	-4.72152700	0.11580000	1.62898900
O	-4.49312700	-1.82312500	0.56809200
C	-5.36370300	-0.91341800	1.04706900
O	-6.54901200	-1.00561000	0.95801500

TS_B4

N	-3.28558300	-1.08932100	-0.60032900
C	-3.28796300	-1.90818400	-1.88895600
H	-3.04779200	-1.21807900	-2.68996400
H	-4.31977600	-2.23434700	-2.01068800
C	-3.59784500	-2.04626700	0.55178200
H	-2.69659000	-2.63242100	0.72170700
H	-4.35285900	-2.71872600	0.14950000
C	-4.39325300	-0.04942500	-0.69056700
H	-4.25550100	0.63524500	0.14144500
H	-5.30863600	-0.60736100	-0.50156200
C	-4.09722900	-1.45658000	1.85656100
H	-5.01853200	-0.88988300	1.74190100

H	-4.31654500	-2.30750300	2.50179100
H	-3.35775100	-0.85510500	2.37623900
C	-4.54035500	0.71532400	-1.99275000
H	-4.85301500	0.07684700	-2.81615800
H	-5.33310500	1.44483000	-1.82670500
H	-3.65308600	1.26606100	-2.29198500
C	-2.34004000	-3.08967700	-1.92104100
H	-2.55245400	-3.83562600	-1.15791800
H	-2.47393600	-3.56787300	-2.89119000
H	-1.29309000	-2.79459800	-1.85691900
C	-1.70719800	0.58126900	0.65226800
C	-1.88489200	-0.51500100	-0.41526300
O	-1.47662900	0.10578200	-1.58955000
H	-2.58511300	0.70311400	1.27984700
H	-1.25856100	-1.38173300	-0.22822300
C	0.77292900	-0.31409200	1.25569600
C	-0.53645600	0.38373700	1.63177400
H	1.51667600	0.01509300	1.97923100
H	-0.32943400	1.34641200	2.09273800
O	-1.03882200	-0.51941700	2.63589900
O	0.46622000	-1.70617000	1.54072800
C	-0.50428300	-1.74630200	2.45509600
O	-0.88535700	-2.72502600	3.01845900
C	-1.34928000	1.46163000	-1.40346500
O	-1.19874400	2.22685200	-2.28898800
O	-1.58773700	1.76103400	-0.12062400
C	2.79185700	-0.56713500	-0.17441700
C	1.32351700	-0.16571800	-0.16917600
H	0.79566000	-0.90569400	-0.79252900
O	1.07940200	1.08267800	-0.68870300
H	3.44044700	-0.02478700	0.50570600
C	3.14079300	-2.00557400	-0.42877500
C	3.38547700	-0.98313200	-1.48365300
H	2.42140500	-2.80893400	-0.46115700

H	2.87618700	-0.89453000	-2.43060100
O	4.79391400	-0.88714900	-1.58062600
O	4.42729100	-2.41126000	-0.00461500
C	5.36257400	-1.72165600	-0.68861900
O	6.53626500	-1.82892800	-0.51837500
C	2.13182000	2.46807100	1.35641400
C	2.07672000	2.39195800	-0.02806900
H	3.04742600	2.58168700	1.91465000
H	2.93813700	2.20108600	-0.65091000
O	1.26042700	3.42666300	-0.48847600
O	1.11928100	3.44539700	1.70324200
C	0.65907300	3.98572900	0.58706700
O	-0.17887000	4.84432300	0.51070500

TS_B5

N	-3.23500600	-1.11830800	-0.60671300
C	-3.22084800	-1.88626200	-1.92673600
H	-3.01281900	-1.15765300	-2.70236800
H	-4.24171800	-2.24335100	-2.05359100
C	-3.52161000	-2.12906600	0.50818500
H	-2.60395100	-2.69155700	0.66550900
H	-4.25257600	-2.80844700	0.07418800
C	-4.36778000	-0.10227900	-0.65180700
H	-4.22904400	0.56617100	0.19383400
H	-5.26595500	-0.68458800	-0.45638600
C	-4.04642200	-1.60756400	1.83184600
H	-4.97848800	-1.05537900	1.73549400
H	-4.25326600	-2.49207200	2.43486200
H	-3.32000500	-1.02038800	2.38453200
C	-4.56450200	0.68561200	-1.93404900
H	-4.88234500	0.05555100	-2.76199000
H	-5.37073900	1.39130800	-1.73362600
H	-3.69899200	1.26374600	-2.24516800

C	-2.23225300	-3.03151700	-2.01263400
H	-2.39653400	-3.80193700	-1.26204300
H	-2.37541800	-3.49168900	-2.99014700
H	-1.19496800	-2.70030800	-1.96839500
C	-1.67509600	0.50368300	0.73393700
C	-1.84952600	-0.51786300	-0.40853500
O	-1.49183800	0.20162100	-1.54802100
H	-2.55959700	0.57674100	1.35937300
H	-1.18777500	-1.37048300	-0.30301400
C	0.86901500	-0.17348300	1.23559100
C	-0.51641500	0.23378800	1.71617100
H	-0.43881400	1.09848800	2.36518700
O	-0.96625200	-0.87368600	2.50642300
O	0.51165100	-1.82662400	1.17599900
C	-0.39464200	-2.04041400	2.08174100
O	-0.76728500	-3.09862400	2.51590000
C	-1.42445000	1.54121200	-1.27377500
O	-1.33361800	2.37381100	-2.10548700
O	-1.55792900	1.73826100	0.04135400
C	2.90057800	-0.36730900	-0.15962500
C	1.43479800	0.00848400	-0.17136200
H	0.90846500	-0.68178500	-0.83319400
O	1.20094100	1.26877600	-0.75199300
H	3.51786300	0.14845800	0.56930200
C	3.27379200	-1.78828600	-0.47129800
C	3.54516000	-0.71638400	-1.46765300
H	2.56059800	-2.59267400	-0.55683700
H	3.06905600	-0.58716800	-2.42678300
O	4.95244000	-0.59672600	-1.50458100
O	4.54611400	-2.19637100	-0.01480700
C	5.49892500	-1.46581100	-0.62992100
O	6.66580700	-1.56707500	-0.42001700
C	1.67406900	2.13764700	1.45119400
C	1.83245700	2.33488300	-0.00980200

H	2.55475400	2.45104500	2.01301600
H	2.85190900	2.43830600	-0.38325600
O	1.11243600	3.50834200	-0.34032700
O	0.61491800	3.10793400	1.76989300
C	0.35792600	3.86969100	0.72373400
O	-0.43432000	4.77149600	0.68766900
H	1.58182400	-0.20382600	2.04123300

5 Cartesian coordinates of the intermediates and minima

II

N	0.60000900	2.30778700	0.07005500
C	0.70259800	2.67675300	1.48400600
H	-0.08833700	3.39380300	1.70508100
H	1.65595500	3.19632900	1.67561300
C	1.83562300	1.67638200	-0.40168200
H	2.22913800	1.05424800	0.40179000
H	2.60292700	2.44066300	-0.60583700
C	0.26106500	3.47139300	-0.75397900
H	0.50321100	3.23370800	-1.79037800
H	0.89381600	4.33101200	-0.47769700
C	1.63008300	0.80031600	-1.62852000
H	1.24836400	1.36358200	-2.48155500
H	2.57695600	0.34963200	-1.93107600
H	0.91740900	0.00114600	-1.41378100
C	-1.20844500	3.85954300	-0.68360100
H	-1.52162700	4.11377200	0.33015000
H	-1.39322300	4.73202300	-1.31283500
H	-1.84124100	3.04425300	-1.03759400
C	0.55396800	1.49417100	2.42940600
H	1.33316500	0.74589100	2.27838900
H	0.62269200	1.83342400	3.46440800
H	-0.41644800	1.01276800	2.29519600

C	-2.42675000	-0.26222600	-1.41171300
C	-1.78674600	0.14541700	-0.32937800
O	-2.26433400	-0.58379200	0.74687600
H	-2.38211300	0.01387000	-2.44856500
H	-1.00626100	0.87990500	-0.14457300
C	0.78137000	-1.96226600	0.90542200
C	0.61721100	-2.67035600	-0.19817600
H	0.12470700	-1.66454400	1.70144400
H	-0.22184800	-3.17362500	-0.64123500
O	1.82438200	-2.72731400	-0.86471900
O	2.09823500	-1.55425500	0.96811600
C	2.72265500	-2.03153400	-0.13293800
O	3.86821800	-1.86475400	-0.40875000
C	-3.20371500	-1.43586500	0.27988200
O	-3.81938500	-2.21828300	0.93456900
O	-3.32096600	-1.25494500	-1.05230500

PI

N	0.99615900	-1.20572100	-0.02486400
C	1.77723900	-1.69076000	1.19297300
H	2.56727900	-0.96727200	1.35787200
H	2.22706500	-2.63196400	0.88018800
C	-0.14202300	-2.19977700	-0.26227900
H	-0.89128900	-1.99440200	0.49909100
H	0.29207900	-3.17419400	-0.04728200
C	1.92045400	-1.23060500	-1.22735800
H	1.35307400	-0.85023100	-2.07074800
H	2.10254400	-2.28895500	-1.40972900
C	-0.78242600	-2.22292200	-1.63588900
H	-0.09158300	-2.52847800	-2.41881800
H	-1.57218600	-2.97237600	-1.58405900
H	-1.26189600	-1.28605800	-1.90679400
C	3.24303700	-0.49684500	-1.11873200

H	3.88028300	-0.87660700	-0.32337500
H	3.76221000	-0.66679500	-2.06224900
H	3.13570100	0.57826700	-1.00379000
C	0.96939300	-1.86855400	2.46247700
H	0.18964800	-2.62239300	2.37385000
H	1.66659100	-2.20664200	3.22897900
H	0.53118200	-0.93615500	2.81621000
C	-0.16134100	0.99837600	-0.85183400
C	0.40074100	0.15296200	0.30585100
O	1.39497200	0.96022700	0.87362800
H	-0.12423500	0.51708400	-1.82504100
H	-0.36076800	-0.02149000	1.05968500
C	-1.85568600	1.79945000	0.88617700
C	-1.57158100	1.54618500	-0.55712000
H	-2.66402300	2.53376600	0.95857600
H	-1.70565100	2.42405500	-1.18769300
O	-2.50805000	0.51389600	-0.99055600
O	-2.54867500	0.49260800	1.21618900
C	-2.97490600	-0.09672100	0.12031700
O	-3.65692100	-1.09056700	0.07281500
C	1.53577500	2.11175200	0.17327700
O	2.30860900	2.96540200	0.46100600
O	0.73991600	2.10788800	-0.89408100

P2

N	-2.50927400	-0.28361600	0.28901000
C	-2.90886400	-0.74465000	1.69138500
H	-2.50068600	-1.74193100	1.81250500
H	-3.99457300	-0.81680300	1.65917100
C	-3.03320400	1.14409100	0.11128500
H	-2.38476600	1.78580900	0.70423100
H	-4.00907300	1.13356200	0.59244200
C	-3.18846800	-1.19103400	-0.72794400

H	-2.73264900	-0.98551700	-1.69274000
H	-4.21505300	-0.83272800	-0.77319800
C	-3.17217100	1.69085000	-1.29657200
H	-3.81699200	1.08502200	-1.92941900
H	-3.64810100	2.66567900	-1.18804200
H	-2.22193600	1.86349500	-1.79292600
C	-3.19839800	-2.68268100	-0.44960500
H	-3.79553600	-2.93862100	0.42268800
H	-3.66927500	-3.14773600	-1.31576000
H	-2.21281400	-3.12660400	-0.34014000
C	-2.46177300	0.14442200	2.83392900
H	-2.88388300	1.14635800	2.79027500
H	-2.82761800	-0.32378500	3.74749900
H	-1.37844300	0.21143900	2.92805500
C	-0.35386000	-0.09610100	-1.17529700
C	-0.99093200	-0.27781700	0.21518000
O	-0.49534000	-1.51075800	0.63744000
H	-1.07986300	0.16553600	-1.93892100
H	-0.68426200	0.49076600	0.91880300
C	1.76225200	1.25377000	-0.15361500
C	0.76127700	0.95580400	-1.28868700
H	2.67232500	1.63972000	-0.61839700
H	1.28938600	0.74689700	-2.21582100
O	0.09355400	2.21781700	-1.42046100
O	1.12320900	2.35400000	0.52838000
C	0.25911200	2.94847300	-0.29402700
O	-0.32210900	3.96363200	-0.07495800
C	0.09601200	-2.18122700	-0.40037700
O	0.46127400	-3.30094700	-0.33513100
O	0.12547600	-1.39592900	-1.48162000
C	3.42168300	0.50714900	1.69597200
C	2.16438700	0.20800600	0.89964300
H	1.31748600	-0.01631900	1.54601800
O	2.51297800	-0.97427200	0.16846700

O	4.41937200	0.00702900	0.64948300
C	3.86534100	-0.94687300	-0.03767500
O	4.40791500	-1.73583600	-0.76980000
H	3.59624700	1.59008600	1.70465100

H2

N	-2.35745600	-0.37471100	0.17065800
C	-2.82007800	-0.91546500	1.52299600
H	-2.45347000	-1.93365600	1.58764800
H	-3.90625600	-0.94169800	1.45505200
C	-2.86887400	1.06319500	0.04988700
H	-2.21663600	1.67548600	0.66948200
H	-3.84693500	1.04899100	0.52636500
C	-2.98896000	-1.21514400	-0.92777000
H	-2.53454500	-0.90575700	-1.86488000
H	-4.02891800	-0.89354300	-0.95292600
C	-2.99952600	1.65943000	-1.33848700
H	-3.71524000	1.12745100	-1.96084200
H	-3.38034600	2.67035400	-1.19265100
H	-2.05729600	1.75757000	-1.86930800
C	-2.93874300	-2.72440600	-0.78368200
H	-3.51636100	-3.08237300	0.06559700
H	-3.40048200	-3.12884700	-1.68454500
H	-1.93471600	-3.13472500	-0.72342400
C	-2.36572500	-0.12578600	2.73379300
H	-2.70797800	0.90739000	2.72998200
H	-2.80550700	-0.61227200	3.60417100
H	-1.28429100	-0.14992900	2.86986500
C	-0.10851400	-0.10149400	-1.15196300
C	-0.83715300	-0.36293400	0.18362300
O	-0.36889600	-1.61412800	0.57596000
H	-0.78781800	0.13542400	-1.96597100
H	-0.57222200	0.36350200	0.94500100

C	1.70345400	1.42408600	0.12707900
C	0.94647400	1.01991300	-1.15208400
H	2.64977300	1.87150200	-0.17242000
H	1.63749400	0.81073900	-1.96485400
O	0.24530400	2.23469300	-1.44657800
O	0.86205000	2.46338500	0.66197500
C	0.13474400	2.98525600	-0.32855100
O	-0.54824300	3.95594700	-0.24547400
C	0.36037800	-2.20081100	-0.41832900
O	0.75107700	-3.31385800	-0.37706800
O	0.47744700	-1.35796000	-1.45146600
C	1.68854300	0.47518700	2.43398200
C	1.98400600	0.35475200	1.14715800
H	1.92444200	-0.33050000	3.11545900
O	2.48812800	-0.79112000	0.62864300
O	4.29829400	0.35471100	-0.19833600
C	3.77914600	-0.75615400	-0.12547600
O	4.07060300	-1.86646400	-0.53057900
H	1.21835800	1.36847100	2.81892300

H3

N	-2.33969000	-0.57805300	-0.03900500
C	-2.94847800	-1.14878600	1.24021300
H	-2.49407100	-2.12199700	1.38655800
H	-4.00368800	-1.28920700	1.01010200
C	-2.95377700	0.80478400	-0.26295500
H	-2.45042500	1.47915700	0.42714400
H	-3.98512000	0.70764900	0.07056700
C	-2.71886900	-1.47941300	-1.20060800
H	-2.17696200	-1.12000000	-2.07080400
H	-3.77475100	-1.27558200	-1.37160600
C	-2.93772800	1.37281700	-1.66932300
H	-3.50720900	0.77128200	-2.37425500

H	-3.42360500	2.34639700	-1.60252900
H	-1.94082300	1.55026200	-2.06172800
C	-2.51924200	-2.97404900	-1.03380200
H	-3.13839000	-3.39413600	-0.24428600
H	-2.83642500	-3.42827400	-1.97274200
H	-1.48709400	-3.26679100	-0.86418300
C	-2.76250100	-0.30065400	2.48219500
H	-3.22750900	0.68057800	2.40425900
H	-3.25214000	-0.83148200	3.29857500
H	-1.71290700	-0.18156800	2.75639800
C	0.04393100	-0.10099100	-1.01590400
C	-0.84552100	-0.42562500	0.20109200
O	-0.33756300	-1.63293100	0.67588700
H	-0.52772700	0.05685800	-1.92633400
H	-0.75131500	0.31841900	0.98827900
C	1.48688000	1.60117000	0.48107000
C	0.97032400	1.11992600	-0.88884000
H	2.46588100	2.05808500	0.33034100
H	1.79284800	0.96052000	-1.57955200
O	0.21256900	2.25265000	-1.33877800
O	0.56441400	2.67081600	0.79933100
C	-0.06781500	3.06689400	-0.29871400
O	-0.81025300	3.99820400	-0.37489800
C	0.63466100	-2.11163800	-0.14793200
O	1.16142400	-3.16137900	-0.00573800
O	0.78768700	-1.29502600	-1.19876000
C	1.01914900	0.72393100	2.76704400
C	1.61373700	0.53052900	1.56155100
O	2.28748800	-0.47236300	1.14260800
O	4.13225300	0.37171200	-1.08789200
C	4.34450100	-0.65897300	-0.60141900
O	4.63229900	-1.69450600	-0.18024500
H	0.49038200	1.63832000	2.99607400
H	1.12081800	-0.02906800	3.53863000

H4

N	-2.89396800	-0.49576500	0.06981100
C	-3.47022400	-1.00840700	1.38856500
H	-3.01181500	-1.97391700	1.56884000
H	-4.53005100	-1.15994600	1.18928800
C	-3.51363500	0.87886300	-0.20019200
H	-2.99950600	1.58337200	0.45035100
H	-4.53755000	0.79320300	0.15816200
C	-3.31606200	-1.44638500	-1.03996700
H	-2.79321900	-1.13652000	-1.94013000
H	-4.37259200	-1.23266900	-1.19162600
C	-3.52589300	1.38713600	-1.62896800
H	-4.11541400	0.76021700	-2.29379500
H	-4.00539500	2.36533000	-1.59030700
H	-2.53791800	1.54286100	-2.05155500
C	-3.14185600	-2.93527100	-0.80923400
H	-3.74995000	-3.30678200	0.01233000
H	-3.49396400	-3.42121000	-1.71930200
H	-2.11355200	-3.24985700	-0.65688800
C	-3.26790500	-0.10574800	2.58851000
H	-3.72155300	0.87628200	2.47036200
H	-3.75904400	-0.59322300	3.43045600
H	-2.21883900	0.00924600	2.85890100
C	-0.54269300	-0.12521800	-1.02244700
C	-1.38813800	-0.34160300	0.24839900
O	-0.86259400	-1.50716200	0.79747700
H	-1.15116300	0.02520900	-1.90935500
H	-1.28003000	0.47012400	0.96167000
C	1.12043400	1.60018100	0.25630800
C	0.43489000	1.06296700	-1.00558200
H	1.98945100	2.15521300	-0.08657000
H	1.18727000	0.88836700	-1.76999900

O	-0.36575600	2.20561900	-1.36603400
O	0.14843200	2.55250700	0.75203900
C	-0.59139400	2.97124000	-0.27846400
O	-1.37208000	3.87055800	-0.24742200
C	-0.00784000	-2.11678000	-0.08241500
O	0.46278100	-3.18487200	0.09855100
O	0.11550300	-1.37036100	-1.18243100
C	2.80264400	1.10910100	2.05888800
C	1.53431600	0.65748900	1.39066600
H	0.70586400	0.58108100	2.10451400
O	1.82661900	-0.63096700	0.89763400
H	2.88366700	2.05164600	2.58056900
C	3.75206200	0.22147400	1.83727000
C	3.20920600	-0.95429300	1.06941500
H	4.78395400	0.27118100	2.15206700
H	3.25178600	-1.87272500	1.66015500
O	3.84718300	-1.30270800	-0.11425300
O	3.43110200	0.72196500	-1.07621900
C	3.99957900	-0.37292700	-1.19258600
O	4.68410800	-0.83545800	-2.10256800

H5

N	-3.05203100	-0.23813300	-0.06892100
C	-3.71809600	-0.87279500	1.15032200
H	-3.39275800	-1.90675600	1.17338200
H	-4.78414200	-0.84964300	0.93075500
C	-3.49919600	1.22410100	-0.12808400
H	-2.96641000	1.74242300	0.66661700
H	-4.55189900	1.19852700	0.14693600
C	-3.54756700	-0.95370000	-1.31715300
H	-2.92791500	-0.61659500	-2.14329600
H	-4.54748100	-0.55676800	-1.48133800
C	-3.34126000	1.96681200	-1.44104100

H	-3.87814000	1.49845800	-2.26290700
H	-3.78591300	2.94928300	-1.28129300
H	-2.30731300	2.13654800	-1.72593400
C	-3.61447400	-2.46894400	-1.28471700
H	-4.35451400	-2.83684400	-0.57767200
H	-3.93225100	-2.77855900	-2.28044000
H	-2.66358400	-2.95433400	-1.08377600
C	-3.42405800	-0.21074800	2.48118100
H	-3.74696100	0.82729500	2.53033700
H	-3.98736500	-0.76367300	3.23266500
H	-2.37330700	-0.27864500	2.76204000
C	-0.64437900	0.01381600	-1.06525900
C	-1.54455200	-0.29577300	0.14475400
O	-1.17358400	-1.58743700	0.50310600
H	-1.19662700	0.40963500	-1.91228700
H	-1.36335200	0.37866000	0.97632200
C	1.20363700	1.18742900	0.53270700
C	0.49813100	1.01635900	-0.82224200
H	2.19288100	1.59431100	0.32576800
H	1.22947000	0.86265300	-1.61079200
O	-0.09250100	2.31768900	-0.98727200
O	0.42215700	2.23306200	1.15811700
C	-0.20762100	2.92933900	0.21164700
O	-0.82030000	3.93666000	0.38390200
C	-0.38683800	-2.15507000	-0.46825100
O	-0.07795900	-3.29467900	-0.47489500
O	-0.17130800	-1.26604700	-1.44363900
C	2.46678500	0.14534500	2.44278900
C	1.34547400	-0.02521400	1.45028100
H	0.39666500	-0.18419200	1.98481300
O	1.67012500	-1.12732700	0.67328100
H	2.45447100	0.91233900	3.20649500
C	3.41744000	-0.73992900	2.20583700
C	3.17356500	-1.60783700	0.97823300

H	4.34661100	-0.83086100	2.75388100
H	2.95977900	-2.66194800	1.25290000
O	3.97786800	-1.44200200	-0.00869100
O	3.88790300	1.18919000	-1.32536400
C	4.78134000	0.47136500	-1.50696200
O	5.72688200	-0.13057100	-1.78916800

H6

N	2.84104400	-0.77968300	-0.97108100
C	2.33992200	-1.84986300	-1.94609100
H	2.07765500	-2.71278700	-1.34478100
H	3.21242000	-2.09757900	-2.54827100
C	3.23385800	0.44699700	-1.79893100
H	2.30485300	0.92890600	-2.09750000
H	3.68992900	0.03870000	-2.69828400
C	4.07757000	-1.30844400	-0.26490000
H	4.35998200	-0.56969700	0.47990700
H	4.84988600	-1.30197500	-1.03264600
C	4.17591600	1.45391300	-1.16905800
H	5.15721600	1.03749700	-0.95350300
H	4.31159200	2.24009500	-1.91193900
H	3.77832800	1.93409700	-0.27943600
C	4.00350900	-2.68939600	0.35695600
H	3.83456500	-3.47334400	-0.37745800
H	4.97985700	-2.86955200	0.80690300
H	3.26586100	-2.78454000	1.14878100
C	1.16139300	-1.44905700	-2.80960400
H	1.36243500	-0.58318200	-3.43833700
H	0.96980500	-2.29237200	-3.47340900
H	0.24331000	-1.29256900	-2.23618000
C	1.97299900	0.41813700	1.20030200
C	1.67935100	-0.41118000	-0.06780800
O	1.08768000	-1.57065200	0.43309700

H	3.00631300	0.74892100	1.25905900
H	0.97854900	0.08327800	-0.73282300
C	-0.34522600	1.80031900	0.96060200
C	1.12181200	1.68101600	1.42720900
H	-0.85776100	2.48991600	1.63388100
H	1.20590900	1.92088000	2.48409300
O	1.74399400	2.72690100	0.67390800
O	-0.20788900	2.44442300	-0.31813900
C	0.97563800	3.06261800	-0.38529400
O	1.32799500	3.78524900	-1.26016500
C	1.19053400	-1.63110200	1.79093900
O	0.86452600	-2.56213400	2.43960700
O	1.76697000	-0.51341000	2.25025200
C	-2.63627300	0.79680600	0.35122100
C	-1.17652400	0.55316800	0.77618900
H	-0.77078300	-0.10871100	0.00822000
O	-1.15983900	-0.16220700	2.01599200
H	-2.93431200	1.83722300	0.50356000
C	-3.39612700	-0.06809600	1.33693000
C	-2.44999300	-0.57603100	2.30466300
H	-4.32457900	-0.55990600	1.08008700
H	-2.49127500	-1.49914500	2.86565600
O	-3.32408600	0.46353700	2.68117600
C	-2.80374300	0.43644700	-1.14058400
C	-2.38388500	-0.94210600	-1.56201400
H	-2.29225300	1.20749500	-1.71876300
H	-2.23143100	-0.90349300	-2.65072500
O	-3.72758200	-1.62818500	-1.45201400
O	-4.22985200	0.52305200	-1.45044000
C	-4.69488100	-0.73926800	-1.53091700
O	-5.87297700	-0.99027900	-1.63294700

E2

N	-2.45959900	-0.55152800	0.00689000
C	-3.07775400	-1.08948800	1.29690100
H	-2.59449700	-2.03941100	1.49474000
H	-4.12104800	-1.27554700	1.04727900
C	-3.12003100	0.79666700	-0.29279000
H	-2.67621000	1.51658400	0.39186000
H	-4.15954900	0.66434200	0.00028900
C	-2.78636800	-1.51790500	-1.12039100
H	-2.23357300	-1.18629300	-1.99461700
H	-3.84230000	-1.34864500	-1.32481500
C	-3.06168700	1.31512200	-1.71588300
H	-3.56388600	0.66142900	-2.42525000
H	-3.60027300	2.26303300	-1.70913600
H	-2.05527600	1.53306700	-2.06000800
C	-2.55655000	-2.99705200	-0.87607100
H	-3.19613000	-3.39659900	-0.09246900
H	-2.82523600	-3.50100100	-1.80459900
H	-1.52576000	-3.25927700	-0.65518900
C	-2.95871200	-0.18781400	2.50825100
H	-3.43264400	0.78248100	2.37431800
H	-3.47596300	-0.69398500	3.32305700
H	-1.92721700	-0.04696100	2.82968000
C	-0.07088200	-0.08007400	-0.95949600
C	-0.97469000	-0.33339000	0.26186100
O	-0.43141900	-1.47596200	0.84400300
H	-0.63350900	0.01426600	-1.88443600
H	-0.93993600	0.48535600	0.97435600
C	1.54198200	1.60343600	0.40722600
C	0.83906300	1.15347700	-0.89550300
H	2.50721400	2.02661600	0.12859100
H	1.57271100	1.03405100	-1.68849900
O	0.00904200	2.27766900	-1.20747100
O	0.69439300	2.69104900	0.85092400
C	-0.09981200	3.09345700	-0.13474300

O	-0.83882900	4.02797000	-0.09551200
C	0.50827300	-2.04328100	0.02888500
O	1.00204400	-3.09729100	0.22567300
O	0.68997200	-1.27449800	-1.05185400
C	3.01864500	0.42557900	2.24946800
C	1.73437500	0.62278600	1.53530800
H	0.81118900	0.42689600	2.08666200
O	2.45788600	-0.50306100	1.13213400
O	3.93425700	0.21720800	-1.37962000
C	4.21245000	-0.79681300	-0.89174500
O	4.54232500	-1.81704900	-0.46507900
H	3.76190400	1.04376700	1.70668900

E3

N	-2.62275300	-1.17458600	0.47756500
C	-2.36783300	-1.92218800	1.78835800
H	-1.58371600	-2.64228000	1.58271100
H	-3.29394300	-2.46159100	1.97987600
C	-3.71787900	-0.13857100	0.74507700
H	-3.24773600	0.67480300	1.29384500
H	-4.40201100	-0.63817100	1.42782400
C	-3.12682100	-2.17371700	-0.55495100
H	-3.11754600	-1.66862300	-1.51694900
H	-4.16944300	-2.33889000	-0.29089800
C	-4.49714400	0.40429500	-0.43736700
H	-5.01678900	-0.36898200	-0.99842900
H	-5.25601400	1.06272300	-0.01365900
H	-3.90188900	1.01376900	-1.10985300
C	-2.42291800	-3.51528700	-0.64944800
H	-2.56754500	-4.12269000	0.24099000
H	-2.88914100	-4.04109500	-1.48271000
H	-1.35924500	-3.45200900	-0.86009200
C	-1.98508000	-1.06446500	2.97705800

H	-2.74061000	-0.32694500	3.24024700
H	-1.88314600	-1.74419900	3.82286500
H	-1.02025300	-0.57401000	2.85399800
C	-1.26981800	0.15750300	-1.31981700
C	-1.33676200	-0.46298400	0.09114800
O	-0.28542300	-1.37590500	0.09889100
H	-2.21866100	0.09551800	-1.84568300
H	-1.18035800	0.27165500	0.87663800
C	0.30427300	2.22326700	-0.56487500
C	-0.84295200	1.63012900	-1.41597300
H	0.79711000	2.99446000	-1.15811900
H	-0.66675300	1.82891700	-2.47021200
O	-1.96301200	2.40595400	-0.98748800
O	-0.40194400	2.87010400	0.50632900
C	-1.68280900	3.04582300	0.17042700
O	-2.48539400	3.65316500	0.80178800
C	0.23800800	-1.53725100	-1.15308000
O	1.04716600	-2.34634500	-1.43334000
O	-0.35128900	-0.67966400	-2.00021100
C	2.74791700	1.52240700	-0.08868800
C	1.31568700	1.28221800	0.01859300
H	1.02002200	0.67159100	0.86905500
O	2.08805800	0.58973700	-0.94946000
H	3.08754500	2.41638600	-0.60669000
C	3.68688900	0.95756800	0.95662100
C	3.24503200	-0.27488700	1.69137900
H	3.94434500	1.77381400	1.63516500
H	3.84097700	-0.31616300	2.61388100
O	3.91422300	-1.31542700	0.82543200
O	4.90186700	0.57007700	0.23209200
C	4.88292000	-0.77423800	0.12439300
O	5.68072500	-1.37714900	-0.55651900

B2

N	2.81384500	0.11554700	-0.53858700
C	2.94290700	0.28802800	-2.05698300
H	2.85680700	-0.70051600	-2.49130100
H	3.96357700	0.63897800	-2.19703300
C	2.95650300	1.51017300	0.08507500
H	2.00516100	2.01629100	-0.07943700
H	3.70739800	2.01103900	-0.52265700
C	3.97476300	-0.74665900	-0.07993300
H	3.94757300	-0.78402700	1.00380300
H	4.85706200	-0.16948200	-0.35053100
C	3.36773300	1.56497900	1.54239500
H	4.40465600	1.27272600	1.69633100
H	3.26973500	2.60611600	1.84911000
H	2.72875900	0.98386900	2.20273300
C	4.07470500	-2.14841500	-0.64776700
H	4.09602600	-2.17706100	-1.73430000
H	5.02144700	-2.55581500	-0.29327100
H	3.29863300	-2.81842100	-0.28429800
C	1.95023900	1.22771000	-2.70262400
H	2.01101100	2.24389200	-2.32031600
H	2.19579800	1.25183800	-3.76454000
H	0.92361300	0.88067200	-2.60863100
C	1.23997800	-1.20126600	1.10781800
C	1.42033600	-0.42222000	-0.22125100
O	1.05934300	-1.36485700	-1.19481300
H	2.15447100	-1.22246000	1.69493500
H	0.75613400	0.43510200	-0.31802700
C	-1.25269900	-0.29816300	1.65930100
C	0.14069100	-0.78406000	2.09873300
H	-1.95652400	-0.53616800	2.45936400
H	0.04584700	-1.61338500	2.79622600
O	0.62106800	0.35169300	2.81355100
O	-1.08170200	1.12406100	1.64094300

C	-0.07011700	1.45980800	2.45371000
O	0.19914000	2.55603300	2.81150100
C	0.85655200	-2.59455600	-0.65501900
O	0.60825300	-3.56332000	-1.28310200
O	0.97139900	-2.53110100	0.67767800
C	-2.90298700	0.22816800	-0.22308800
C	-1.88226900	-0.76984100	0.35452400
H	-1.14794400	-1.01128400	-0.40932700
O	-2.64738200	-1.94103000	0.61573400
O	-4.05885200	-0.59198000	-0.43228300
C	-3.88890600	-1.80552200	0.09767800
O	-4.71054200	-2.66513500	0.12019800
H	-3.17026300	1.00831700	0.48877300
C	-2.45025200	0.84836700	-1.56018200
C	-3.05670800	2.16917900	-1.99427200
H	-2.50726200	0.06972300	-2.32294100
H	-4.03262900	2.29187700	-1.50876200
O	-2.14412200	3.07814300	-1.14412200
O	-1.06043600	1.18672300	-1.37011200
C	-1.00167500	2.49713500	-0.99825400
O	0.03898700	2.97730400	-0.60204500

B3

N	3.22846300	0.47543000	-0.81051900
C	3.22269900	0.60854700	-2.33234000
H	3.02931300	-0.38285400	-2.72617700
H	4.24297700	0.88887400	-2.58854600
C	3.49842400	1.86648000	-0.22962300
H	2.57483300	2.43245000	-0.33410500
H	4.22688700	2.30735200	-0.90712100
C	4.36860600	-0.45461200	-0.41685100
H	4.23546100	-0.69655900	0.63398800
H	5.26334200	0.16004200	-0.49507800

C	4.01518600	1.96094200	1.19263500
H	4.96287900	1.44704200	1.33599400
H	4.18959400	3.02175500	1.37373800
H	3.30126400	1.63232100	1.94146000
C	4.56546800	-1.71735600	-1.23511100
H	4.88125000	-1.50594600	-2.25434300
H	5.37275500	-2.26724800	-0.75132300
H	3.70076200	-2.37438800	-1.26484300
C	2.22864000	1.59704500	-2.90573100
H	2.37537500	2.61483800	-2.54993900
H	2.38584300	1.60273800	-3.98409100
H	1.19368300	1.29947200	-2.74041300
C	1.68774800	-0.47484300	1.07937300
C	1.84474500	0.00809100	-0.37633200
O	1.46711500	-1.10119600	-1.12697100
H	2.56646300	-0.27293100	1.68509800
H	1.18917800	0.84056500	-0.61315900
C	-0.83198200	0.50557400	1.23905900
C	0.51097000	0.12433200	1.87179100
H	-1.55362000	0.56945400	2.04829400
H	0.34796300	-0.50147300	2.74482800
O	0.97177400	1.41824700	2.29828300
O	-0.56928800	1.85703300	0.78037900
C	0.39238500	2.37991600	1.54665300
O	0.73025800	3.52109900	1.55095000
C	1.40881600	-2.22438900	-0.33961700
O	1.30015500	-3.31678200	-0.76935900
O	1.59377600	-1.88230900	0.94097700
C	-2.88972000	-0.00426900	-0.06258800
C	-1.41713100	-0.30748500	0.08165600
H	-0.91338900	0.01360700	-0.83513900
O	-1.15490600	-1.68279900	0.16624900
O	-2.00551600	-1.69077800	2.27497500
C	-1.62469700	-2.40353000	1.33747400

O	-1.53813000	-3.61393400	1.19733000
H	-3.49770400	-0.24171900	0.80327300
C	-3.29471400	1.18082800	-0.89471500
C	-3.51085200	-0.19710000	-1.41322200
H	-2.60569700	1.91547000	-1.28093900
H	-3.00992000	-0.66055200	-2.24862300
O	-4.91307900	-0.36955800	-1.41965100
O	-4.58781100	1.68832300	-0.64307500
C	-5.50481200	0.74581300	-0.94843000
O	-6.67902300	0.88087400	-0.81054700

B4

N	-3.29058300	-0.38462400	-0.85854200
C	-3.26147200	-0.72890800	-2.33752600
H	-2.75062500	0.09300400	-2.82455500
H	-4.30446200	-0.73170100	-2.65349400
C	-3.98020800	-1.52656700	-0.13623800
H	-3.32113900	-2.38753500	-0.21750300
H	-4.87159500	-1.73565500	-0.72641500
C	-4.11535100	0.87937500	-0.68663300
H	-3.98061900	1.21154200	0.33737500
H	-5.15042600	0.55348300	-0.79025300
C	-4.36221000	-1.31772700	1.31671500
H	-4.98907000	-0.44173200	1.47368700
H	-4.94621700	-2.19037800	1.61029100
H	-3.49945200	-1.27750500	1.97636200
C	-3.82980000	2.02352900	-1.64015400
H	-4.13963700	1.79951400	-2.65960500
H	-4.42923100	2.86757400	-1.29634600
H	-2.78522600	2.32992700	-1.63423100
C	-2.58341900	-2.03561500	-2.69857600
H	-3.09369300	-2.91207200	-2.30338900
H	-2.60099800	-2.11045800	-3.78590300

H	-1.53802400	-2.05580000	-2.39250400
C	-1.63191400	0.49878800	0.95917400
C	-1.82090400	-0.25967900	-0.37279400
O	-1.08607400	0.42732400	-1.27941700
H	-2.54897500	0.57016300	1.53840100
H	-1.50687200	-1.30499800	-0.29410300
C	0.82505900	-0.45762900	1.37878600
C	-0.59538900	-0.13255200	1.89542000
H	1.55615900	-0.09524700	2.09937700
H	-0.52585300	0.51572600	2.76550700
O	-1.08413200	-1.40722600	2.33009700
O	0.86144000	-1.89593200	1.40781700
C	-0.23608900	-2.39016700	1.98750700
O	-0.44660500	-3.54869400	2.16805500
C	-0.46876900	1.71084100	-0.66056900
O	-0.52309200	2.70206800	-1.37690200
O	-1.24944300	1.77605700	0.57172600
C	2.71099100	-0.12403800	-0.20403600
C	1.21971200	-0.00580100	-0.03392700
H	0.72771200	-0.67087300	-0.74931200
O	0.88358100	1.33071900	-0.29792100
O	1.38038100	2.40627500	2.64087700
C	1.31294600	3.31882200	1.93028500
O	1.25934700	4.24994300	1.25181700
H	3.30916900	0.47633100	0.47438700
C	3.28620500	-1.44428600	-0.63666100
C	3.24218700	-0.30525900	-1.59391600
H	2.72292600	-2.36190900	-0.69451100
H	2.63645200	-0.22831800	-2.48303700
O	4.59191900	0.06662600	-1.78355400
O	4.65612000	-1.63126700	-0.34981500
C	5.38416800	-0.71913500	-1.02773800
O	6.56772500	-0.61647700	-0.95717600

B5

N	3.29010200	-1.05085400	0.63499200
C	3.29259000	-1.79885800	1.96673200
H	3.05589800	-1.06625200	2.73015100
H	4.32394400	-2.12030400	2.10453000
C	3.60233500	-2.06972800	-0.46499800
H	2.69727300	-2.65571400	-0.61214600
H	4.34740000	-2.72782200	-0.02251000
C	4.39758800	-0.00654400	0.66711400
H	4.25918400	0.63116300	-0.20160700
H	5.31266300	-0.57344100	0.50701100
C	4.11655600	-1.55298200	-1.79455800
H	5.04433100	-0.99292200	-1.70360500
H	4.32854100	-2.43879000	-2.39374900
H	3.38729700	-0.97103400	-2.34951300
C	4.54838500	0.82548600	1.92689500
H	4.85832000	0.22953400	2.78243700
H	5.34441800	1.54133000	1.72221800
H	3.66495200	1.39623900	2.19872700
C	2.34240800	-2.97513900	2.06288600
H	2.54821700	-3.75727800	1.33493400
H	2.48238100	-3.40635400	3.05390000
H	1.29527300	-2.68204200	1.99161400
C	1.70865000	0.53906700	-0.71495100
C	1.89065900	-0.49004300	0.41773800
O	1.47879800	0.20380700	1.55242300
H	2.58742200	0.62848000	-1.34624700
H	1.26274100	-1.36617400	0.28934900
C	-0.77841100	-0.37834900	-1.26682800
C	0.54205500	0.27322400	-1.68403500
H	-1.50422900	-0.11249200	-2.03166300
H	0.34164800	1.19359900	-2.22690000
O	1.04479200	-0.72502400	-2.59268500

O	-0.46554600	-1.79387200	-1.38866900
C	0.50586300	-1.92693200	-2.29522000
O	0.88386200	-2.95714600	-2.75872200
C	1.38419900	1.54850300	1.29052200
O	1.23367100	2.36457600	2.12849700
O	1.57981300	1.76467800	-0.01336400
C	-2.82936300	-0.52698000	0.13209900
C	-1.37586300	-0.11349300	0.11612600
H	-0.84080700	-0.73775700	0.83877900
O	-1.15426900	1.19917400	0.55554300
H	-3.45481900	-0.09043100	-0.63958100
C	-3.16169100	-1.92661100	0.56847100
C	-3.46531900	-0.78057700	1.46703700
H	-2.42846300	-2.70060400	0.73263200
H	-2.99354700	-0.55576300	2.41066900
O	-4.87475800	-0.69902500	1.49527100
O	-4.41942200	-2.41069200	0.15071300
C	-5.39499300	-1.65755700	0.70153700
O	-6.55768000	-1.81290500	0.50452200
C	-2.03858300	2.28529100	-1.50119300
C	-1.99766800	2.24013300	-0.02276200
H	-2.93682700	2.84386800	-1.78679200
H	-2.97117800	2.17925400	0.46331500
O	-1.33974400	3.42874200	0.41221400
O	-0.91439000	3.25173900	-1.74408900
C	-0.63864900	3.91244200	-0.63939900
O	0.13646900	4.82914300	-0.53792600

B6

N	-3.06671500	-1.04375800	0.08325400
C	-3.98186600	-0.04456000	-0.62081000
H	-3.94949100	0.86815300	-0.03578100
H	-4.97926400	-0.47262600	-0.53513300

C	-3.09038900	-2.33260300	-0.74541000
H	-2.49231900	-2.13492900	-1.63056200
H	-4.13450700	-2.44040800	-1.03386100
C	-3.64451400	-1.33862700	1.46043300
H	-2.87129300	-1.85049200	2.02774900
H	-4.43613900	-2.06197500	1.27533100
C	-2.61489900	-3.61121000	-0.08236200
H	-3.15837500	-3.85747800	0.82783400
H	-2.80903300	-4.40717200	-0.80152200
H	-1.54655900	-3.63059700	0.11542900
C	-4.21994400	-0.18244800	2.25991200
H	-5.10535600	0.24286000	1.79252700
H	-4.52739000	-0.60117600	3.21838700
H	-3.51621000	0.61907200	2.46502300
C	-3.64626600	0.25165800	-2.06832600
H	-3.69363600	-0.62637900	-2.70852200
H	-4.39540800	0.96025400	-2.42135000
H	-2.67495400	0.72888400	-2.19000200
C	-0.60054400	-1.18631700	0.93242600
C	-1.66622500	-0.44698800	0.10438100
O	-1.74762100	0.81641700	0.71256800
H	-0.97000300	-2.13029500	1.32188000
H	-1.36060500	-0.36569700	-0.93263300
C	1.61407700	-0.51706700	-0.46874000
C	0.78127100	-1.52699100	0.33928100
H	1.35451900	-1.74527200	1.24222400
O	0.73445300	-2.76552100	-0.33567500
O	-0.38154700	-1.84018500	-2.09074600
C	0.19240400	-2.85783800	-1.65867900
O	0.36631500	-3.96026900	-2.15718200
C	-1.08477800	0.82430200	1.89753400
O	-1.10912500	1.72548100	2.66733800
O	-0.41926500	-0.31714900	2.05915100
C	0.90613500	1.93997000	-0.32321600

C	1.91762800	0.88774500	0.08470000
H	2.05546200	0.87403100	1.17126900
O	3.16596600	1.23549300	-0.54035200
H	0.07594200	1.59422100	-0.92771900
C	0.61869700	3.13024500	0.56188300
C	1.39178100	3.32040700	-0.68444400
H	0.99073400	3.22720400	1.56970800
H	2.43320700	3.58119300	-0.76809600
O	0.53706500	4.04294600	-1.54454400
O	-0.61817100	3.76813600	0.33419000
C	-0.63592500	4.26986100	-0.91760500
O	-1.56697100	4.82493700	-1.40822900
C	3.01725400	-1.10723700	-0.68310600
C	3.93713500	0.11973400	-0.76383800
H	3.07499300	-1.77343600	-1.53771100
H	4.50305000	0.25327200	-1.68027500
O	4.87874800	-0.09273300	0.29413300
O	3.50158700	-1.81320500	0.46283800
C	4.56238900	-1.19079100	0.99652200
O	5.14718500	-1.56852300	1.96223800
H	1.17016200	-0.39898100	-1.45602900