

**Exposing the G-quadruplex to electric fields:
the role played by telomeres in the propagation
of DNA errors
(Electronic Supporting Information)**

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Optimized structures

SPT1 optimised at $E_{\text{ext}} = 80 \times 10^{-4}$ a.u.

N	0.01032200	-0.01162700	0.00914300
H	0.01821000	-0.01935100	1.03104200
C	1.25248200	-0.01643900	-0.60476100
C	-1.19786300	0.10582400	-0.66090500
C	1.16284000	0.08129400	-2.00184400
O	2.30272000	-0.09641400	0.14450700
N	-2.31107000	0.14932400	0.07467800
N	-1.29087400	0.18955200	-1.96779800
N	2.12753800	0.12232600	-2.98964100
C	-0.11863700	0.18963800	-2.59172300
H	-3.16003700	0.33485400	-0.44113400
H	-2.28164000	0.21501400	1.08771000
C	1.46778400	0.25504400	-4.10909600
N	0.10189700	0.32441500	-3.93360600
H	1.92519700	0.34681500	-5.07868600
N	-2.98899800	0.84589000	4.94789800
C	-3.14852700	0.68752300	3.58787300
C	-1.64483200	0.67276500	5.20880900
N	-2.03046400	0.44617800	2.96896500
H	-4.10385200	0.81766000	3.11208400
C	-1.07099000	0.43189400	3.95643300
N	-1.01000500	0.73002100	6.38980200
C	0.33005800	0.24058600	3.87522500
C	0.29689700	0.55344000	6.29334300

O	1.02412700	0.04425100	2.83766600
N	0.95298100	0.30790200	5.10514200
N	1.06237700	0.60834200	7.39250800
H	1.99033500	0.23090200	5.07065800
H	0.59143000	0.91457600	8.22921500
H	2.09266400	0.61729300	7.34994400
N	6.03743600	0.73174900	8.23481500
C	4.67347700	0.79275300	8.43346900
C	6.20025300	0.46487300	6.87065600
N	3.97673500	0.63218800	7.34241400
H	4.25289900	1.04649000	9.39079600
C	4.90830800	0.42423000	6.33462700
N	7.33399800	0.31426700	6.20496200
C	4.78008100	0.22353600	4.91373800
C	7.13937900	0.14233600	4.88480400
O	3.65578600	0.19808700	4.27566400
N	5.93664000	0.08213300	4.22348000
N	8.24648200	0.02898400	4.14574100
H	5.60655200	-0.06391200	2.51233100
H	9.12544500	0.14605800	4.62450500
H	8.21357400	0.00973900	3.12496400
N	9.07254800	0.19911500	-0.77474000
C	9.28611300	0.20171100	0.58457500
C	7.71644900	0.05844400	-0.95550900
N	8.20249100	0.10402800	1.29507600
H	10.26781900	0.32646700	1.00324600
C	7.18416200	0.01283900	0.36733200

N	7.04328700	0.00848300	-2.07818400
C	5.81697000	-0.08265200	0.48575100
C	5.71786000	-0.06632000	-1.93669000
O	5.08066600	-0.11106600	1.61078600
N	5.10996000	-0.13225700	-0.67902800
N	4.94857800	-0.06066400	-3.00117500
H	4.07718000	-0.15265700	-0.61539800
H	5.42573200	-0.00044300	-3.89558300
H	3.91065900	-0.04168000	-2.97639700
N	3.01191500	1.22381100	2.22945300
N	2.70986300	-1.35334100	2.02326600
C	-0.93290500	0.37549000	-4.96691800
O	-0.96855000	-0.85968100	-5.67222100
C	-0.67448800	1.43132900	-6.00438500
H	-1.89608100	0.55549600	-4.48942700
C	-1.15549000	-0.61025800	-7.10571000
C	-1.30483000	0.89963900	-7.25204000
H	-1.17457100	2.35476500	-5.71230400
H	0.40002500	1.53206800	-6.15733000
C	-0.00249600	-1.21527700	-7.86386000
H	-2.07988600	-1.08883200	-7.42907100
O	-2.72653600	1.14769900	-7.34579400
H	-0.78443500	1.26105600	-8.13899300
O	1.13904200	-0.38513300	-7.66891900
H	0.20363700	-2.21271200	-7.47569600
H	-0.24635800	-1.25343300	-8.92554100
P	-3.28894700	2.64768900	-7.45544700

P	2.30545500	-0.35851300	-8.78337400
O	-4.51230400	2.57106500	-8.28320300
O	-2.24870300	3.60164800	-7.92805500
O	-3.64387000	3.00545200	-5.93857300
O	3.03385500	-1.77490200	-8.59977000
O	1.70486400	-0.38872200	-10.14096000
O	3.19441600	0.77363000	-8.43859800
H	-5.27744300	2.46086200	-7.71397800
C	-4.71115600	2.28454100	-5.30608100
C	4.24875500	-1.92277800	-7.82146400
H	1.42662500	-1.28390000	-10.34793800
C	-4.94743300	2.86480400	-3.96329500
H	-4.43075300	1.23611700	-5.20434700
H	-5.61671400	2.37647500	-5.90580900
C	4.46409000	-3.41579700	-7.78104900
C	4.03291900	-1.56453600	-6.36071900
H	5.09293300	-1.39133100	-8.26093000
O	-3.80397400	2.55803300	-3.14074300
C	-5.09266500	4.38526800	-3.96295300
H	-5.83920200	2.41554400	-3.52625600
C	5.91690400	-3.81895400	-7.85119100
O	3.89789300	-3.91740100	-6.55222800
H	3.93497000	-3.86805600	-8.61985500
C	3.41079100	-2.82993300	-5.79707800
H	3.31241600	-0.74934300	-6.29351200
H	4.99939100	-1.39704000	-5.88537900
C	-3.61063800	3.67616700	-2.26019100

O	-6.40646900	4.63812700	-3.42741500
C	-3.96044100	4.91498500	-3.08521900
H	-5.00902000	4.77890700	-4.97599600
H	6.00900300	-4.86126600	-7.62757900
H	6.29214100	-3.63080800	-8.83541600
H	6.47949200	-3.25059300	-7.14030400
N	3.68454000	-3.07803000	-4.42532500
H	2.33032600	-2.77296000	-5.92956100
N	-2.20719100	3.58387900	-1.84235300
H	-4.27001300	3.59711700	-1.39587300
H	-6.56431200	5.58466700	-3.39916700
H	-4.35241800	5.68686800	-2.42293900
H	-3.11087200	5.17614500	-3.71621200
C	4.93941100	-3.20523700	-3.87788600
C	2.81330600	-3.19267700	-3.36735400
C	-1.08593600	3.48460500	-2.64655100
C	-1.74568800	3.48108600	-0.55034900
N	4.93415800	-3.35870200	-2.58310300
H	5.81176500	-3.17299600	-4.51373900
C	3.59424200	-3.34631200	-2.23895600
N	1.46305800	-3.20318400	-3.44216100
N	0.00377600	3.27297800	-1.99021700
H	-1.17925300	3.58400700	-3.71791700
N	-2.48713300	3.56451200	0.56611000
C	-0.37874600	3.29928700	-0.65765100
C	2.96083200	-3.45616400	-0.98663900
C	0.89899500	-3.29950600	-2.24600400

C	-1.72962800	3.48546100	1.68169000
C	0.37615400	3.18948700	0.53608700
O	3.49116500	-3.53288800	0.13835600
N	1.58349800	-3.39705100	-1.06946800
N	-0.42869300	-3.29787700	-2.14615500
N	-0.38379800	3.28577600	1.67385300
N	-2.32125400	3.68129300	2.86206300
O	1.59298700	2.97276100	0.62121500
H	1.02529400	-3.42557100	-0.22820400
H	-0.99759800	-3.22829600	-2.97778600
H	-0.86697400	-3.36615600	-1.23881400
H	0.05312800	3.20775800	2.58110200
H	-3.31879700	3.83300000	2.90797100
H	-1.77143800	3.67774600	3.70930300
N	-1.04423000	3.94455800	5.32662400
C	-1.67434600	4.22126800	6.43646800
C	0.28216200	3.84652900	5.73755100
N	-0.86705900	4.23054000	7.55337200
H	-2.72941700	4.43181800	6.53096900
C	1.47128100	3.56779900	4.99743900
C	0.39735800	3.98801600	7.09180100
C	-1.27208900	4.35077200	8.93949900
O	1.52948700	3.30198100	3.78533300
N	2.60285300	3.53448500	5.76115400
N	1.49729700	3.96679100	7.84871300
C	-2.19943400	5.51612800	9.22518500
O	-2.13805500	3.23904000	9.16190700

H	-0.41613400	4.33910100	9.61431900
C	2.59746500	3.74321400	7.11748200
H	3.49752000	3.34949300	5.33051900
C	-3.01968400	5.07991800	10.42250600
H	-1.60771200	6.39176600	9.49214700
H	-2.85957600	5.67027400	8.37164600
C	-3.04631200	3.56902700	10.23312300
N	3.78671200	3.75210200	7.73343100
O	-2.36147400	5.27587800	11.68632800
H	-4.02063800	5.51114700	10.41153000
C	-4.39190500	3.00029500	9.90027400
H	-2.68795400	3.09855000	11.14875600
H	3.83760500	3.90162900	8.73099800
H	4.63256200	3.60919300	7.20036800
H	-2.30647900	6.21517100	11.87677200
O	-4.87718200	3.73082900	8.75667000
H	-4.28578900	1.94732800	9.63934300
H	-5.06802700	3.15301200	10.74145300
P	-6.40201100	3.50386000	8.27726900
O	-6.37649400	2.01537200	7.67398100
O	-7.33927200	3.43232300	9.41251400
O	-6.74044600	4.51024000	7.22829600
C	-6.28834800	1.79221400	6.25529000
H	-6.84515500	3.42684700	10.23556900
C	-6.26761800	0.28305200	6.09440700
C	-4.95423400	2.23568100	5.62849500
H	-7.13668800	2.23374000	5.73234700

C	-7.09464800	-0.30626700	4.94245200
O	-4.87320400	-0.08955600	6.04243500
H	-6.67031500	-0.13632000	7.01632000
C	-4.03944800	1.05258500	5.92931800
H	-4.58609700	3.11683600	6.15397000
H	-5.07783900	2.32857900	4.54949700
O	-6.73159400	0.47663500	3.80570200
H	-6.79719900	-1.34182600	4.77749000
H	-8.15532500	-0.16808000	5.15207400
H	-3.56630000	1.22550500	6.89588200
P	-7.81112800	0.48557100	2.59043200
O	-7.73936900	-1.00721100	2.02586400
O	-9.20534800	0.63788600	3.05383500
O	-7.32021600	1.46477500	1.57079000
C	-6.98036700	-1.33136400	0.85715100
H	-9.22217300	0.66833100	4.01320500
C	-7.08442300	-2.84509200	0.72758400
C	-5.48515900	-1.11470700	1.07229200
H	-7.34831100	-0.81535400	-0.02972000
C	-7.14357100	-3.31546800	-0.71100300
O	-5.90283800	-3.40418000	1.37209000
H	-7.97519000	-3.18883900	1.25337100
C	-5.00581500	-2.38407400	1.76532000
H	-5.33542500	-0.26263900	1.73535100
H	-4.99076100	-1.02241200	0.10530500
H	-7.07851000	-4.38309200	-0.74013100
H	-8.06729400	-3.00229600	-1.15095700

H	-6.32669200	-2.89329900	-1.25816100
N	-3.67716300	-2.75444100	1.49333000
H	-5.10483300	-2.24128700	2.84142000
C	-3.13005300	-2.92508200	0.25631100
C	-2.63942300	-2.84383700	2.38436500
N	-1.85445800	-3.12834000	0.26589000
H	-3.75726200	-2.88390600	-0.62187600
C	-1.51104800	-3.06848600	1.61576800
N	-2.70814600	-2.72318400	3.72345800
C	-0.26165200	-3.17015800	2.26843900
C	-1.52820800	-2.86907100	4.30433400
O	0.85011200	-3.31252300	1.71536400
N	-0.36188200	-3.05029700	3.63649500
N	-1.44276800	-2.81566800	5.63982800
H	0.46848800	-3.09589900	4.20966500
H	-2.27640200	-2.68244700	6.19427800
H	-0.54474300	-2.90861200	6.09253800
N	0.97435000	-2.72901200	7.05104700
C	0.97825200	-2.44917200	8.31811800
C	2.32165200	-2.82504800	6.71458200
N	2.24640300	-2.41946000	8.86730300
H	0.11653400	-2.24980900	8.93789500
C	2.95930700	-3.05089100	5.47234900
C	3.11005100	-2.66753900	7.83184100
C	2.53909800	-2.13407800	10.23239900
O	2.39410800	-3.12519400	4.35943700
N	4.32457300	-3.09741600	5.55295900

N	4.44631000	-2.73795500	7.91711900
C	2.01770900	-0.79034000	10.68848500
O	1.91798200	-3.10166800	11.05036300
H	3.61772400	-2.17239900	10.38501300
C	5.00339000	-2.96787800	6.74477800
H	4.87558400	-3.23125400	4.71715400
C	1.79797700	-0.99314900	12.17406100
H	2.78951800	-0.03535300	10.53886100
H	1.05991900	-0.59376100	10.20675500
C	1.43402500	-2.45784000	12.25306700
N	6.33863900	-3.04079900	6.65051600
O	2.99102700	-0.81197100	12.94221900
H	0.98898000	-0.36350700	12.54439600
C	-0.06935900	-2.75884600	12.37954000
H	1.94713900	-2.89548800	13.10945400
H	6.90882100	-2.95510700	7.47971300
H	6.77441400	-3.18145100	5.75023300
P	3.75426100	0.61680300	13.01296700
H	-0.23954600	-3.80193300	12.21248700
H	-0.40450800	-2.49547500	13.36097300
H	-0.60964700	-2.18848700	11.65312600
O	4.24660000	0.70602400	14.39769700
O	2.90557100	1.71862400	12.49910400
O	4.96501400	0.39650700	11.96430500
H	4.95305000	0.06915700	14.52780400
C	5.96296000	-0.58279200	12.21310500
C	7.17750400	-0.24907400	11.42747900

H	5.59321600	-1.56275100	11.91125000
H	6.20806200	-0.58969500	13.27518000
O	6.96607700	-0.50382800	10.03070800
C	7.55997900	1.20796000	11.56170400
H	8.00540400	-0.86548800	11.77782300
C	7.08584100	0.67951300	9.25698900
O	9.00191400	1.22564700	11.54764900
C	7.03850300	1.79874700	10.26841500
H	7.13619900	1.68031100	12.44794800
H	8.04991800	0.68734600	8.74843200
P	9.83808700	2.55542100	11.85801100
H	7.69783800	2.60507400	9.94711100
H	6.00556800	2.11793500	10.40684900
O	11.01687600	2.12733200	12.59925200
O	8.98847600	3.60537200	12.49988200
O	10.19714500	3.10384300	10.38946100
H	10.91536600	2.36134700	13.52474200
C	11.15162600	2.30337900	9.67036600
C	11.33263200	3.01536100	8.34358400
H	10.73263500	1.31262600	9.49448600
H	12.09869900	2.29873100	10.21000200
O	10.18245100	2.74073400	7.52828300
C	11.50497800	4.53632500	8.29958700
H	12.19775700	2.57302600	7.84955400
C	9.86697600	3.90965700	6.79427800
O	12.77702100	4.55488300	7.63529400
C	10.13959800	5.00645600	7.81346300

H	11.64663000	4.89405200	9.31942400
N	8.53392000	3.77516500	6.37554900
H	10.52959900	4.01242900	5.93485800
H	13.06190200	5.46359700	7.51387800
H	10.25829600	5.95466300	7.28914100
H	9.42330500	4.91612000	8.63008600
C	7.41356500	3.77096900	7.16926600
C	8.07543800	3.62727600	5.09310100
N	6.30167900	3.64895500	6.49854500
H	7.51064700	3.86349200	8.24087100
C	6.70565500	3.51184100	5.18463200
N	8.86133400	3.55821700	3.99348600
C	5.97422500	3.30604100	3.98742800
C	8.12549600	3.32827000	2.90366700
O	4.75048000	3.15129300	3.88186700
N	6.76268300	3.23153100	2.85827100
N	8.77096500	3.31677000	1.72302600
H	6.33606600	3.10052900	1.95218000
H	9.77827400	3.38541200	1.69748000
H	8.24805900	3.23945300	0.86236100
N	7.43952300	3.21836800	-0.70914600
C	8.12134500	3.49389400	-1.78293900
C	6.11837200	3.23750900	-1.12557500
N	7.35419500	3.59879900	-2.89725500
H	9.18992300	3.63661200	-1.84757400
C	4.89694000	3.05046500	-0.41463000
C	6.04789500	3.48673000	-2.47885400

C	7.81701200	3.85933100	-4.22061100
O	4.79110200	2.87939800	0.81134100
N	3.77469900	3.11069500	-1.19404500
N	4.94651400	3.46912500	-3.24764700
O	8.31018200	2.62785900	-4.76654600
C	8.98842500	4.84679400	-4.29941900
H	6.99074500	4.22396900	-4.83083700
C	3.82817200	3.30670100	-2.54086800
H	2.86191400	3.00816500	-0.77393500
C	9.08609700	2.97091500	-5.93163400
C	9.38632500	4.45496500	-5.71329300
H	8.58517700	5.85920600	-4.32256600
H	9.76867700	4.51169900	-3.61600400
N	2.65385700	3.36337900	-3.17662300
C	10.35365700	2.13632300	-5.88762700
H	8.52605100	2.80443000	-6.85180800
O	8.60053600	5.12288400	-6.67138900
H	10.44410800	4.65765800	-5.88073400
H	2.62711100	3.50686300	-4.17603100
H	1.79320800	3.26271600	-2.65767700
O	11.20582900	2.69015500	-4.85831500
H	10.10132900	1.10656600	-5.63451900
H	10.86134800	2.19668300	-6.85023800
H	8.73767300	6.06995400	-6.59443900
P	12.62115800	2.01296100	-4.57550500
O	12.26724200	0.67202700	-3.80889400
O	13.33803700	1.60835400	-5.79348300

O	13.42701200	2.92059600	-3.67406100
C	12.35207400	0.61049000	-2.36450100
H	14.23027100	1.33784200	-5.56469900
C	12.18692900	-0.87536600	-2.11814400
C	11.15308500	1.21739400	-1.66593400
H	13.29798700	0.99564800	-1.98368100
C	13.07338000	-1.56753200	-1.11363400
O	10.78458800	-1.08354900	-1.79337800
H	12.35953600	-1.36861600	-3.07470300
C	10.08430700	0.16478900	-1.82129800
H	10.84804100	2.12093700	-2.19378500
H	11.38010700	1.34660300	-0.60772300
O	13.05399800	-0.73301900	0.00184000
H	12.63731200	-2.53139800	-0.85106100
H	14.08887200	-1.62245000	-1.50578900
H	9.59001500	0.28517200	-2.78526500
P	14.29230500	-0.92394500	1.04095200
O	13.84596900	-2.13975700	1.99337200
O	15.55073600	-1.31847800	0.42293600
O	14.16614000	0.27905500	1.84129900
C	13.10322600	-1.92944400	3.23639500
H	16.22076900	-1.42622800	1.10194000
C	13.00541100	-3.36663000	3.67658700
C	11.62374000	-1.52010300	3.09683200
H	13.64526600	-1.30802400	3.94923100
C	13.02145900	-3.61873200	5.17346700
O	11.76891600	-3.84946100	3.09566000

H	13.83175900	-3.91825900	3.22830100
C	10.98883900	-2.79153900	2.54592100
H	11.53971400	-0.72650900	2.35437600
H	11.21383300	-1.31394300	4.08553400
H	12.86625500	-4.66060700	5.36137100
H	13.96740300	-3.32089900	5.57519600
H	12.24203100	-3.05238400	5.63891600
N	9.63268400	-3.01296100	2.94639400
H	11.06173000	-2.80236200	1.45838800
C	9.07671600	-2.99151800	4.19511400
C	8.56950300	-3.19559100	2.07701500
N	7.79509800	-3.15179700	4.22152900
H	9.70348600	-2.84837300	5.06294500
N	8.63118000	-3.27186500	0.72739400
C	7.44316100	-3.26922400	2.87896300
C	7.43257400	-3.38724200	0.17300400
C	6.17700100	-3.38669900	2.24923300
N	6.25750000	-3.43738300	0.87976600
N	7.33630300	-3.52597400	-1.14145600
O	5.07602200	-3.40263900	2.82497500
H	5.41590600	-3.51665900	0.32706200
H	8.16753600	-3.49764700	-1.71443300
H	6.43166100	-3.65999100	-1.57017900

SPT1 optimised at $E_{\text{ext}} = 100 \times 10^{-4}$ a.u.

N	-0.13418400	0.07765800	-0.00276200
H	-0.33187500	0.07807300	0.99875200

C	1.20256900	0.12940000	-0.36553500
C	-1.19247600	0.13883900	-0.89907600
C	1.39076500	0.21549100	-1.74645400
O	2.09351800	0.10016700	0.58051100
N	-2.42980300	0.13937700	-0.40369000
N	-1.02461600	0.21393300	-2.19858300
N	2.52822400	0.29198500	-2.52896600
C	0.24373900	0.26525500	-2.57815400
H	-3.16775500	0.26700500	-1.08387500
H	-2.61281200	0.18248400	0.59263000
C	2.09054700	0.39200400	-3.75719400
N	0.71634700	0.40418700	-3.84877500
H	2.72043200	0.49505900	-4.62380300
N	-4.05901300	0.79988500	4.26248200
C	-3.94671600	0.63290800	2.89747900
C	-2.78816700	0.67857400	4.77860600
N	-2.72138800	0.43055800	2.50996200
H	-4.79581300	0.72707700	2.24422100
C	-1.97298900	0.45472600	3.66447200
N	-2.39609700	0.76422200	6.06134600
C	-0.57875500	0.31114400	3.86013600
C	-1.09299000	0.63687200	6.22065600
O	0.31269600	0.12988900	2.98299300
N	-0.20945000	0.41079500	5.18796200
N	-0.55946500	0.72025700	7.45330100
H	0.81580800	0.38075200	5.35576300
H	-1.19280200	1.05108400	8.16399600

H	0.45490100	0.79784100	7.60214600
N	4.15938500	1.06787700	9.24181500
C	2.77964400	1.07288200	9.17460400
C	4.59525800	0.80626600	7.93788400
N	2.31824300	0.88597500	7.97023900
H	2.17085400	1.31497500	10.02838200
C	3.43455300	0.71438400	7.16586600
N	5.84456100	0.70125000	7.50688500
C	3.58784400	0.51259900	5.74386400
C	5.90808900	0.51966900	6.17310300
O	2.61246000	0.45382800	4.91051400
N	4.86315800	0.41155100	5.29557900
N	7.14090000	0.44603700	5.65604000
H	4.87035800	0.24135200	3.49007800
H	7.90721000	0.62262600	6.28510700
H	7.29551400	0.43517600	4.64534900
N	8.89543100	0.65551600	0.98262700
C	8.83148100	0.66080300	2.35555600
C	7.60596300	0.46228300	0.53208500
N	7.63292100	0.51778000	2.83747500
H	9.70515000	0.82303800	2.96003100
C	6.82473800	0.39062600	1.72309800
N	7.17302000	0.38891600	-0.70034100
C	5.46647800	0.23662400	1.56478400
C	5.84670300	0.26133500	-0.82884000
O	4.52592600	0.16863500	2.52346500
N	5.00486300	0.16399100	0.28673500

N	5.30163500	0.24412900	-2.02001900
H	3.97922900	0.10820000	0.14802800
H	5.93761400	0.32955400	-2.80814700
H	4.27403200	0.21612500	-2.19591500
N	2.27241400	1.38182500	2.68786800
N	2.09821600	-1.24111000	2.37746300
C	-0.10214700	0.41175600	-5.05933500
O	0.05011700	-0.82411100	-5.74768000
C	0.30879800	1.47706300	-6.03614500
H	-1.14611100	0.55148800	-4.77875900
C	0.13425800	-0.58331300	-7.19232000
C	-0.04566700	0.91895100	-7.37761200
H	-0.27579600	2.37887900	-5.85419600
H	1.38754100	1.62262200	-5.97916600
C	1.43605200	-1.13985500	-7.70790400
H	-0.68961500	-1.10028700	-7.68433200
O	-1.43125200	1.10725400	-7.74675600
H	0.62138300	1.30147000	-8.15016700
O	2.48323100	-0.26258400	-7.30286000
H	1.60381200	-2.12763200	-7.27872700
H	1.40417900	-1.18861600	-8.79634300
P	-2.02277100	2.58234700	-7.97589800
P	3.84129400	-0.18762400	-8.17078000
O	-3.05848200	2.45425400	-9.02401400
O	-0.95068100	3.57881500	-8.24641600
O	-2.67908300	2.92555900	-6.55944700
O	4.57777000	-1.57221200	-7.83768500

O	3.51672800	-0.24349400	-9.61860500
O	4.59950100	0.98087200	-7.67017100
H	-3.91419900	2.31235700	-8.61265800
C	-3.81819300	2.16086900	-6.13928600
C	5.62396800	-1.66879600	-6.83780900
H	3.32076300	-1.14961700	-9.86788300
C	-4.33361300	2.73128100	-4.87256600
H	-3.52007400	1.12514100	-5.97631300
H	-4.59346000	2.21458000	-6.90364000
C	5.88840100	-3.15147800	-6.74380300
C	5.11484100	-1.31930800	-5.44952100
H	6.51476900	-1.10266300	-7.11015300
O	-3.35949900	2.47296900	-3.84175200
C	-4.53834700	4.24433500	-4.91325700
H	-5.27396000	2.24527000	-4.61250900
C	7.34257400	-3.49350800	-6.52811500
O	5.11599600	-3.67584000	-5.64352100
H	5.55072400	-3.62582700	-7.66525300
C	4.44772800	-2.60940400	-5.00615200
H	4.36217200	-0.53495600	-5.52991300
H	5.96327300	-1.11131600	-4.79762100
C	-3.38633400	3.59857300	-2.94997300
O	-5.94022800	4.44220500	-4.64418800
C	-3.62021200	4.82133000	-3.83759300
H	-4.27630800	4.64071800	-5.89428700
H	7.43226200	-4.53096100	-6.28205400
H	7.89327700	-3.29022200	-7.42271100

H	7.73307100	-2.90181000	-5.72667500
N	4.46058000	-2.84526900	-3.60529500
H	3.41196300	-2.59775400	-5.34564800
N	-2.08779100	3.56527300	-2.26773600
H	-4.19680300	3.49234700	-2.22891300
H	-6.13920800	5.38132100	-4.65506100
H	-4.16432000	5.57640100	-3.27024900
H	-2.67596100	5.11756100	-4.29449600
C	5.58982000	-2.91962300	-2.82435900
C	3.40640100	-2.99584800	-2.73493400
C	-0.82891700	3.51268500	-2.83893800
C	-1.88141100	3.48241000	-0.91003000
N	5.34021800	-3.07264700	-1.55379900
H	6.56672800	-2.85115900	-3.27967600
C	3.95966100	-3.11620600	-1.47550400
N	2.09778800	-3.06288700	-3.06946700
N	0.12080400	3.34711700	-1.98240400
H	-0.71698500	3.60765900	-3.90892200
N	-2.82781200	3.53518500	0.04113800
C	-0.51328600	3.35793500	-0.74929400
C	3.10076800	-3.25196200	-0.36850500
C	1.31719100	-3.18224500	-2.00426300
C	-2.29809400	3.48836000	1.28282500
C	0.00000300	3.28031100	0.56883000
O	3.40589000	-3.30596600	0.83844900
N	1.76430400	-3.25057900	-0.71674000
N	-0.00363000	-3.23614300	-2.16318500

N	-0.96919300	3.34517300	1.53721100
N	-3.11462500	3.65974000	2.32472700
O	1.18515500	3.11473600	0.88960800
H	1.05539900	-3.30209400	0.00084500
H	-0.40308000	-3.19077100	-3.08973000
H	-0.60615200	-3.32233600	-1.35723400
H	-0.71340900	3.28587800	2.51248000
H	-4.10753700	3.76958400	2.17548200
H	-2.73961500	3.67955100	3.26233100
N	-2.35093400	3.97722200	4.98745800
C	-3.19484900	4.22776900	5.95203200
C	-1.12634700	3.93495800	5.64805600
N	-2.62021000	4.27127400	7.20389800
H	-4.25597300	4.39401600	5.83883000
C	0.19399200	3.70593800	5.15438200
C	-1.28148700	4.08169300	6.99775300
C	-3.29058400	4.37501200	8.48440200
O	0.49667100	3.44229600	3.97874300
N	1.15664200	3.72032200	6.12284700
N	-0.34902200	4.10682900	7.95332100
C	-4.30266200	5.50065200	8.57535800
O	-4.13692600	3.22810300	8.54451600
H	-2.58177000	4.39944900	9.31214700
C	0.88014600	3.92919400	7.45068200
H	2.12458200	3.57276100	5.87502800
C	-5.32067300	5.03098200	9.59502900
H	-3.81023100	6.40039600	8.94430000

H	-4.79076600	5.62668800	7.60894900
C	-5.24818100	3.52022400	9.41692700
N	1.92621600	3.98809700	8.28497800
O	-4.92826400	5.25483200	10.96060300
H	-6.31736800	5.41993700	9.38694100
C	-6.47938500	2.89553900	8.83488500
H	-5.05495100	3.06552900	10.38855900
H	1.77679000	4.14002900	9.27223500
H	2.86441600	3.88049700	7.92686700
H	-4.94973000	6.19568100	11.15009500
O	-6.76353200	3.60465800	7.61283200
H	-6.28168600	1.84783000	8.60837700
H	-7.31128600	3.02016700	9.52803300
P	-8.15605000	3.31387600	6.84942900
O	-7.95320800	1.82751500	6.27515500
O	-9.29168000	3.20363700	7.78246000
O	-8.32589200	4.30478400	5.74627900
C	-7.58292400	1.60766500	4.90227200
H	-8.96650500	3.21918000	8.68557700
C	-7.46960100	0.10062800	4.76127800
C	-6.17199900	2.10632400	4.54168100
H	-8.33130100	2.01308700	4.22134600
C	-8.03303400	-0.52325600	3.47613600
O	-6.07744400	-0.21331600	4.98323400
H	-8.02567700	-0.33485600	5.59139500
C	-5.28508500	0.96267300	5.02385300
H	-5.94901800	3.00232800	5.12093900

H	-6.08801200	2.19352900	3.45840500
O	-7.48911000	0.27369200	2.42448800
H	-7.66708600	-1.54552600	3.38065000
H	-9.11898100	-0.42949600	3.47540700
H	-5.01556600	1.15563600	6.06218800
P	-8.31230600	0.23694600	1.02329100
O	-8.07146000	-1.25175400	0.49598800
O	-9.77492200	0.33096500	1.20688800
O	-7.67377700	1.23542300	0.10960100
C	-7.08786400	-1.54433300	-0.50100100
H	-9.97844800	0.36106900	2.14458300
C	-7.10273600	-3.06114200	-0.63537600
C	-5.67278300	-1.26520100	-0.00249900
H	-7.29792700	-1.04453400	-1.44665700
C	-6.86284700	-3.53416600	-2.05417300
O	-6.04643000	-3.57002600	0.23028400
H	-8.06361200	-3.44165400	-0.28895500
C	-5.28511300	-2.51311200	0.78094200
H	-5.68933600	-0.40734300	0.66973200
H	-5.00468800	-1.15268800	-0.85631400
H	-6.74968000	-4.59814300	-2.06108400
H	-7.69592700	-3.26010700	-2.66717300
H	-5.97347200	-3.07840100	-2.43652200
N	-3.91490000	-2.82765900	0.77430300
H	-5.59641600	-2.37415700	1.81630000
C	-3.13206700	-2.97575500	-0.33199900
C	-3.06658300	-2.87318300	1.85000100

N	-1.87523700	-3.12544500	-0.07408400
H	-3.57848700	-2.96122200	-1.31525700
C	-1.80248600	-3.05072300	1.31617000
N	-3.39821400	-2.75496700	3.14942300
C	-0.70003800	-3.09975100	2.19907000
C	-2.34813400	-2.85110800	3.94882500
O	0.50266800	-3.19568600	1.87276700
N	-1.06812800	-2.98363300	3.52081700
N	-2.52519900	-2.79363300	5.27511300
H	-0.36331700	-2.99421000	4.24417600
H	-3.45517000	-2.69519200	5.65665200
H	-1.72880400	-2.84872700	5.89378300
N	-0.43274900	-2.60531800	7.12651800
C	-0.68576800	-2.32504500	8.36797800
C	0.95698800	-2.64501900	7.05790000
N	0.44972100	-2.24206100	9.15186200
H	-1.65862800	-2.16166900	8.80761100
C	1.83184700	-2.84448200	5.96447000
C	1.50696900	-2.45419800	8.30520000
C	0.46057100	-1.94412400	10.54531700
O	1.49639700	-2.94282700	4.76390900
N	3.15639500	-2.83379500	6.30808600
N	2.80315900	-2.46859300	8.64798700
C	-0.19389300	-0.62319900	10.88047000
O	-0.26700600	-2.93652900	11.23585700
H	1.48987000	-1.93720700	10.90404800
C	3.58566900	-2.67547600	7.60757200

H	3.86384600	-2.94479400	5.59584500
C	-0.68865600	-0.83442300	12.29713600
H	0.56068000	0.16336700	10.87657900
H	-1.04749800	-0.46707400	10.22088500
C	-1.00068200	-2.31303000	12.31668800
N	4.91574100	-2.69248900	7.77404400
O	0.32460500	-0.60316000	13.28003000
H	-1.57916600	-0.23904000	12.49859100
C	-2.48647500	-2.67664100	12.15246800
H	-0.64562900	-2.72847200	13.25985600
H	5.31055100	-2.58267200	8.69712800
H	5.52300200	-2.81514500	6.97630900
P	1.00048400	0.85633400	13.48495200
H	-2.57819800	-3.72600400	11.96452100
H	-3.01584600	-2.42712800	13.04824200
H	-2.89877300	-2.12968900	11.33042600
O	1.21126400	0.96664500	14.93796200
O	0.22294500	1.92146100	12.80725200
O	2.39938700	0.68647700	12.69225800
H	1.90463900	0.35995500	15.20769800
C	3.36953800	-0.25009700	13.13774700
C	4.69851500	0.13384000	12.59913200
H	3.10572600	-1.24479500	12.77840500
H	3.40439700	-0.24630400	14.22719500
O	4.77220400	-0.13010700	11.19006500
C	4.98771800	1.60565900	12.79242400
H	5.46744900	-0.44724200	13.10825900

C	4.99093800	1.05689500	10.44410100
O	6.40311900	1.68367300	13.05745400
C	4.70280200	2.17357800	11.41770400
H	4.38134000	2.06022100	13.57588600
H	6.03410300	1.10486300	10.13162300
P	7.10814800	3.04740300	13.51240700
H	5.37826900	3.00666200	11.22318700
H	3.65041600	2.44931200	11.35096300
O	8.13761100	2.66932500	14.47131600
O	6.10801800	4.06113700	13.96882600
O	7.72201900	3.60977500	12.13646100
H	7.84929300	2.89926300	15.35765700
C	8.82967500	2.84966700	11.62244800
C	9.23486000	3.56806100	10.34974700
H	8.49363600	1.84217500	11.37726000
H	9.65369500	2.88487900	12.33513700
O	8.27657900	3.24520600	9.32969100
C	9.34998600	5.09488700	10.32699300
H	10.19666600	3.16212000	10.03620600
C	8.06158700	4.39960300	8.53860700
O	10.72474200	5.16639600	9.92121900
C	8.08649600	5.50726500	9.58191600
H	9.27667800	5.45864400	11.35188800
N	6.84150800	4.20926800	7.87104300
H	8.87331800	4.52966700	7.82277900
H	10.99025900	6.08618800	9.84949000
H	8.26552500	6.45939600	9.08242100

H	7.22993500	5.38736200	10.24526700
C	5.58978600	4.15850900	8.43301600
C	6.64651200	4.04179800	6.52542800
N	4.63478900	3.98979500	7.56091400
H	5.47363300	4.25545000	9.50233100
C	5.29083800	3.86917400	6.35119700
N	7.63263400	4.00524400	5.59926300
C	4.81415900	3.63245600	5.03689700
C	7.13182900	3.74425900	4.38966800
O	3.64141200	3.42658400	4.69789400
N	5.80873700	3.59055000	4.08229200
N	7.99363500	3.75930400	3.35635300
H	5.57139900	3.44144000	3.11193000
H	8.98314700	3.87003300	3.52559000
H	7.65091600	3.65982000	2.41147200
N	7.16357400	3.60427600	0.71346700
C	8.02855900	3.90765900	-0.21043000
C	5.94842300	3.56793800	0.04915700
N	7.48808300	3.97991300	-1.45296300
H	9.08266200	4.09494800	-0.06831800
C	4.62114600	3.33022800	0.51192400
C	6.13119700	3.81344100	-1.29425800
C	8.18734000	4.25904800	-2.66394200
O	4.28699700	3.15537900	1.69566600
N	3.66958000	3.34312000	-0.47036700
N	5.20121100	3.74944400	-2.26143100
O	8.82694200	3.04907300	-3.09365700

C	9.31036900	5.29464000	-2.52302300
H	7.48065300	4.58853800	-3.42557400
C	3.97478200	3.54064500	-1.78301500
H	2.69770100	3.20264900	-0.23393400
C	9.79907100	3.42382900	-4.08949100
C	9.99025800	4.91923200	-3.82981800
H	8.87809300	6.28927900	-2.63235600
H	9.95656800	4.99277100	-1.69874100
N	2.94449800	3.54786700	-2.63441100
C	11.06723100	2.64303600	-3.79398700
H	9.43512600	3.23367700	-5.09918200
O	9.37818600	5.55329000	-4.92748200
H	11.05123000	5.16595000	-3.79116500
H	3.10594200	3.68970000	-3.62129400
H	2.00450700	3.41148400	-2.29094100
O	11.68051300	3.23246600	-2.62400100
H	10.81308000	1.60372400	-3.58573200
H	11.74881700	2.72419900	-4.64066600
H	9.45889600	6.50530100	-4.83351000
P	13.04082100	2.61521400	-2.06696400
O	12.60040300	1.26095500	-1.37193400
O	13.99596500	2.24047000	-3.11975000
O	13.61896500	3.55614700	-1.03439500
C	12.40636300	1.20361000	0.06205100
H	14.83732500	2.00762900	-2.72037700
C	12.25766900	-0.28775600	0.28442900
C	11.07094600	1.76008600	0.51026600

H	13.24402800	1.62817300	0.61539200
C	12.96041700	-0.94180700	1.44731000
O	10.82871500	-0.55431500	0.33350800
H	12.63231800	-0.77373900	-0.61643400
C	10.09653900	0.66361000	0.16001800
H	10.83713000	2.64985600	-0.07429200
H	11.08325200	1.89911300	1.59126800
O	12.69120200	-0.10838300	2.53082100
H	12.52162900	-1.92297200	1.62874200
H	14.03401000	-0.95433600	1.25951200
H	9.79377100	0.76280800	-0.88235400
P	13.71160200	-0.24689400	3.79146000
O	13.13948100	-1.47993400	4.64983600
O	15.08098300	-0.58866500	3.43196600
O	13.38364200	0.95009700	4.54201700
C	12.16209800	-1.30038500	5.72384200
H	15.61068100	-0.66800200	4.22866300
C	12.03987000	-2.74022600	6.14899800
C	10.72213800	-0.95337800	5.29720600
H	12.52990100	-0.65653400	6.52276800
C	11.77605300	-2.99082700	7.62279000
O	10.96012700	-3.27462000	5.34395000
H	12.95928600	-3.25697000	5.87376100
C	10.25859100	-2.25049600	4.64470100
H	10.75103300	-0.16429800	4.54580000
H	10.12042500	-0.76415300	6.18613400
H	11.63022800	-4.03820800	7.78596900

H	12.61327700	-2.65350200	8.19739200
H	10.89870100	-2.45740700	7.92381700
N	8.86079000	-2.52831900	4.77710200
H	10.54109000	-2.25870100	3.59195000
C	8.07312300	-2.52965500	5.89443800
C	7.99449000	-2.75563800	3.72004100
N	6.81831600	-2.74342100	5.67376300
H	8.51356500	-2.36005200	6.86588400
N	8.31943400	-2.82981300	2.40855000
C	6.73815100	-2.87602000	4.28952200
C	7.25663300	-2.99547800	1.63374300
C	5.62380900	-3.04664000	3.42774900
N	5.96999700	-3.09446700	2.10021200
N	7.42250500	-3.13865200	0.32672100
O	4.43377200	-3.10841000	3.77972200
H	5.25533800	-3.20912100	1.39582200
H	8.34709000	-3.07579400	-0.07483300
H	6.62427900	-3.31058700	-0.26776700

SPT2 optimised at $E_{\text{ext}} = 80 \times 10^{-4}$ a.u.

N	-0.13358600	0.05605600	0.02056300
H	-0.08620600	0.12201100	1.03940900
C	1.08144000	0.10843300	-0.64136800
C	-1.36690900	0.02130300	-0.60990800
C	0.94635500	0.08744700	-2.03554800
O	2.15846700	0.17949400	0.05731400
N	-2.45718000	0.02767800	0.16288100

N	-1.50518800	-0.00627200	-1.91439700
N	1.87947100	0.13304300	-3.05425200
C	-0.35439500	0.04152600	-2.57934000
H	-3.33208200	0.12220000	-0.33394100
H	-2.39886600	0.19817900	1.16266000
C	1.17501400	0.12143000	-4.15447800
N	-0.18549700	0.08822900	-3.93231700
H	1.59121300	0.17690200	-5.14507700
N	-3.03442000	1.05812800	4.99401400
C	-3.22594100	0.78408200	3.65685900
C	-1.67331000	1.01497900	5.21178200
N	-2.11218800	0.58699100	3.01409700
H	-4.20287100	0.80348100	3.20845800
C	-1.12179300	0.72562200	3.96008600
N	-1.01464400	1.21673100	6.36453000
C	0.29121500	0.64063100	3.83732000
C	0.29668800	1.14057200	6.23241600
O	0.97224700	0.42195100	2.80030300
N	0.93262400	0.85307400	5.04508700
N	1.08716900	1.34482300	7.29885100
H	1.96722700	0.85915000	4.98483800
H	0.61562000	1.69888900	8.11622300
H	2.10699800	1.45184100	7.21834600
N	6.08545300	1.96999600	7.92989600
C	4.73193100	1.93022700	8.19812900
C	6.22917900	1.61278300	6.57396400
N	4.00063100	1.62710500	7.16824000

H	4.33820700	2.21631800	9.15766300
C	4.90060500	1.42191200	6.13701900
N	7.34261800	1.51712800	5.86295000
C	4.68259900	1.09259800	4.77311000
C	7.14690500	1.23004000	4.54411500
O	3.57972100	0.91607200	4.16352900
N	5.84676000	0.97936700	4.07142000
N	8.07607300	1.17796000	3.63191100
H	5.74345700	0.76210500	3.07676400
H	8.98163000	1.37123200	4.05160400
H	7.97767800	1.02798300	2.06079700
N	8.84913300	0.97121300	-1.10652400
C	9.09343100	1.09541600	0.21837500
C	7.48675300	0.70367300	-1.25143900
N	7.99967200	0.94740000	0.93713400
H	10.05213000	1.34265600	0.63457500
C	6.95518700	0.69767500	0.05048900
N	6.84255400	0.52650900	-2.38347400
C	5.56515300	0.47386000	0.21069800
C	5.52996700	0.35017600	-2.24682400
O	4.89365700	0.43924400	1.29255100
N	4.92102600	0.29771300	-0.99373500
N	4.76099600	0.23558200	-3.30734700
H	3.89710500	0.19608700	-0.93234400
H	5.21502400	0.30075900	-4.21275600
H	3.73371700	0.15347600	-3.24694800
N	2.85127200	1.65004600	1.91258800

N	2.95886100	-0.90162500	1.85984400
C	-1.25272000	-0.03119400	-4.92001200
O	-1.20289400	-1.31763800	-5.52579200
C	-1.12001300	0.95588800	-6.04516100
H	-2.21240900	0.10473500	-4.42137400
C	-1.45587000	-1.20084000	-6.96607300
C	-1.74063600	0.27443700	-7.22292000
H	-1.68914900	1.85434800	-5.80645400
H	-0.06369800	1.13424000	-6.24644300
C	-0.27902300	-1.76545000	-7.71871900
H	-2.34481100	-1.78006800	-7.21584200
O	-3.18078500	0.39342000	-7.28110900
H	-1.28186600	0.60600800	-8.15443000
O	0.79147300	-0.82905500	-7.63239000
H	0.02528700	-2.70753500	-7.26274900
H	-0.55194200	-1.90920300	-8.76415900
P	-3.87482800	1.82698000	-7.48484600
P	1.91547200	-0.79381900	-8.78938100
O	-5.11232000	1.58124000	-8.25677700
O	-2.93698700	2.82417700	-8.06927600
O	-4.21161800	2.27425500	-5.98771800
O	2.76984100	-2.12441200	-8.52478600
O	1.27734800	-0.98352500	-10.11658500
O	2.71290000	0.43326400	-8.56746700
H	-5.84665700	1.45301500	-7.65187400
C	-5.19164100	1.51908700	-5.26099000
C	4.01690100	-2.10633000	-7.78443300

H	1.07172700	-1.91269800	-10.24290900
C	-5.43514800	2.18336300	-3.95905100
H	-4.81795900	0.50960900	-5.08927800
H	-6.12019600	1.48587000	-5.83094200
C	4.36257300	-3.56779000	-7.63693600
C	3.81679200	-1.65136500	-6.34858500
H	4.79734800	-1.54263800	-8.29566600
O	-4.24399400	2.04116400	-3.15959300
C	-5.71212400	3.68126700	-4.07074800
H	-6.27021200	1.69709200	-3.45477200
C	5.84204000	-3.85136000	-7.73122700
O	3.88116800	-4.01499000	-6.35223900
H	3.84869300	-4.12897000	-8.41738900
C	3.32525300	-2.91531600	-5.66537400
H	3.03052500	-0.89706000	-6.31710800
H	4.77949600	-1.36534000	-5.92495500
C	-4.12111600	3.23873400	-2.37620300
O	-7.02544000	3.86467000	-3.50649300
C	-4.60324700	4.37334900	-3.28058100
H	-5.69500400	3.99788900	-5.11365800
H	6.03153200	-4.86085100	-7.43135800
H	6.16829800	-3.71193400	-8.74069000
H	6.37510900	-3.18232300	-7.08847700
N	3.66261500	-3.02843800	-4.29002300
H	2.24029800	-2.96046300	-5.76042500
N	-2.70250600	3.29896000	-2.00648700
H	-4.74356400	3.17407300	-1.48376300

H	-7.26412500	4.79373200	-3.54551800
H	-5.03989400	5.16014300	-2.66547100
H	-3.79993200	4.65366000	-3.96192700
C	4.94040700	-3.00500600	-3.78280500
C	2.83841200	-3.13075600	-3.19379400
C	-1.60274300	3.23027800	-2.84291100
C	-2.19335900	3.33957500	-0.72901100
N	4.98930200	-3.05384600	-2.48078100
H	5.78618800	-2.95052600	-4.45215900
C	3.66489700	-3.12685200	-2.08760500
N	1.49252400	-3.26103400	-3.21584400
N	-0.47862100	3.16469100	-2.21435500
H	-1.73804400	3.23506300	-3.91439900
N	-2.90373200	3.44962300	0.40520200
C	-0.81982900	3.26571500	-0.87416800
C	3.08319900	-3.18874300	-0.80722600
C	0.97692900	-3.30815200	-1.99511400
C	-2.10747600	3.52459800	1.49374900
C	-0.02079200	3.31971100	0.29736000
O	3.65335300	-3.12985200	0.29921400
N	1.70402600	-3.25280300	-0.84161500
N	-0.34205500	-3.41044300	-1.84496100
N	-0.75036900	3.43826300	1.44992200
N	-2.67644800	3.76405400	2.67721200
O	1.21368500	3.20471100	0.34844600
H	1.17718900	-3.26060000	0.02007600
H	-0.94075700	-3.45611200	-2.65710300

H	-0.74394300	-3.44230900	-0.91895300
H	-0.27988300	3.47133900	2.34306900
H	-3.68147000	3.83432000	2.74938600
H	-2.10201000	3.87495100	3.50052800
N	-1.35023700	4.33119200	5.06335500
C	-1.96679600	4.64206400	6.17176900
C	-0.00808500	4.37751300	5.42991300
N	-1.12862000	4.80906400	7.25289900
H	-3.03269200	4.76982600	6.29000500
C	1.17089800	4.13873000	4.66910000
C	0.13695000	4.63770400	6.76342500
C	-1.49873800	5.00569500	8.64005500
O	1.22905900	3.79108400	3.47871100
N	2.33062300	4.26713600	5.38818100
N	1.25784400	4.77016400	7.47706700
C	-2.51456700	6.10789500	8.87002900
O	-2.25719000	3.84639100	8.98075400
H	-0.62419700	5.12048000	9.28050800
C	2.34973000	4.58211000	6.72375900
H	3.22393800	4.12338000	4.93947100
C	-3.25561800	5.70169600	10.12800700
H	-1.99321700	7.04890800	9.04562900
H	-3.21216600	6.13676400	8.03301100
C	-3.15655000	4.18362500	10.05720400
N	3.55248700	4.74068200	7.29121700
O	-2.57750800	6.05335000	11.34677400
H	-4.29016400	6.04472300	10.12202200

C	-4.45732700	3.47858200	9.82107300
H	-2.72994200	3.82012300	10.99209900
H	3.62155100	4.97362900	8.27155100
H	4.39036400	4.62722900	6.73882900
H	-2.59853100	7.00618900	11.46175600
O	-5.04012700	4.07135500	8.64380200
H	-4.26820600	2.42076100	9.63849300
H	-5.11735800	3.64084000	10.67317400
P	-6.55374000	3.67886400	8.24209100
O	-6.41773100	2.15418700	7.75519800
O	-7.44500500	3.62000600	9.41449700
O	-7.01136700	4.56559000	7.13214400
C	-6.35520100	1.82599900	6.35568600
H	-6.92662200	3.72234800	10.21599800
C	-6.20823100	0.31592800	6.31133100
C	-5.08516300	2.32856100	5.64588000
H	-7.25480200	2.15098800	5.83300500
C	-7.01666800	-0.43165400	5.24089700
O	-4.78900300	0.05923700	6.23501400
H	-6.54366000	-0.06047300	7.27764900
C	-4.06182400	1.25480800	6.00208300
H	-4.77877800	3.27697600	6.08715900
H	-5.25029400	2.32372100	4.56845200
O	-6.75912500	0.28520100	4.03394400
H	-6.63552900	-1.44834400	5.14526100
H	-8.07822100	-0.36698500	5.47963600
H	-3.57533600	1.54409300	6.93356100

P	-7.87306100	0.10543000	2.86382400
O	-7.68941700	-1.41650300	2.41407100
O	-9.25996600	0.17639900	3.36706700
O	-7.50161400	1.03743800	1.75346600
C	-6.94224900	-1.76835900	1.24574500
H	-9.24916400	0.28229500	4.32114700
C	-6.91814500	-3.29097000	1.23771600
C	-5.46555100	-1.40983800	1.38611300
H	-7.38146000	-1.35813100	0.33635100
C	-6.98137800	-3.87870900	-0.15686200
O	-5.67266600	-3.69486000	1.87784700
H	-7.75860400	-3.66523100	1.82221300
C	-4.85593100	-2.57447800	2.15639000
H	-5.36977100	-0.49767300	1.97506900
H	-5.01175700	-1.35418000	0.39667700
H	-6.82456100	-4.93592300	-0.10579900
H	-7.94225000	-3.68088800	-0.58405100
H	-6.22198900	-3.43450500	-0.76588800
N	-3.50930300	-2.85216600	1.86321900
H	-4.93307600	-2.35455600	3.22122100
C	-2.98863200	-3.07490500	0.62307700
C	-2.44018300	-2.78188100	2.71813600
N	-1.70051700	-3.16847200	0.59953100
H	-3.64438000	-3.15744100	-0.23102000
C	-1.32129400	-2.97162400	1.92660500
N	-2.47695700	-2.56025800	4.04553300
C	-0.04786300	-2.91483800	2.53689800

C	-1.27109600	-2.55901000	4.59037600
O	1.05410800	-3.00694100	1.95435500
N	-0.11502700	-2.69433000	3.89441500
N	-1.14862700	-2.39147200	5.91348900
H	0.73379300	-2.62356900	4.43720100
H	-1.97282300	-2.28489100	6.48746600
H	-0.23211400	-2.37170400	6.33733600
N	1.29499600	-1.98825200	7.22025300
C	1.31440900	-1.60818900	8.46080500
C	2.63427900	-1.99708200	6.84091700
N	2.59181700	-1.42764600	8.95711900
H	0.45854800	-1.43303600	9.09582400
C	3.24974900	-2.26743300	5.59638500
C	3.44075400	-1.68441700	7.91165800
C	2.90138700	-1.00985600	10.28385200
O	2.65840700	-2.47829300	4.51499800
N	4.61574000	-2.19206800	5.62805100
N	4.78008900	-1.63485100	7.95093300
C	2.27960400	0.31742600	10.65425900
O	2.39293300	-1.95751100	11.19736600
H	3.98352100	-0.94472200	10.39758700
C	5.31788600	-1.91043100	6.77943200
H	5.14972200	-2.34569100	4.78463100
C	2.12524400	0.21682400	12.15838800
H	2.97765400	1.12032100	10.41726800
H	1.29364600	0.39321800	10.19577200
C	1.89286500	-1.26223600	12.36430700

N	6.65078100	-1.87786200	6.64006900
O	3.32158100	0.55906400	12.86401600
H	1.27656200	0.80373400	12.50960000
C	0.42612800	-1.67777600	12.57111500
H	2.46884200	-1.58484500	13.23171400
H	7.23716000	-1.67806500	7.43772800
H	7.06858600	-2.05314800	5.73734800
P	3.95936800	2.04814600	12.79479200
H	0.34222700	-2.74153400	12.49187100
H	0.10038700	-1.36560100	13.54134200
H	-0.18436900	-1.21520700	11.82397100
O	4.48542100	2.28951700	14.14861700
O	3.00221500	3.02963600	12.23010400
O	5.15108500	1.84717000	11.72075100
H	5.24838100	1.72699200	14.30046400
C	6.23784000	0.97865500	12.00617800
C	7.39337900	1.34937500	11.15119900
H	5.94550100	-0.05006000	11.79538800
H	6.51592900	1.07779000	13.05544700
O	7.16106500	0.96631200	9.78743100
C	7.65158100	2.83952400	11.15759800
H	8.28242100	0.83509900	11.51623100
C	7.15292700	2.08953700	8.92049300
O	9.08534100	2.97752300	11.08705200
C	7.04019200	3.27842400	9.84339400
H	7.21639800	3.34413700	12.02021900
H	8.09617000	2.13773500	8.37633800

P	9.81191800	4.39367800	11.26141500
H	7.61637500	4.10903500	9.43569700
H	5.98826100	3.51948000	9.99615000
O	11.04625300	4.12743100	11.98789400
O	8.89475000	5.41642700	11.85219600
O	10.07545000	4.85065300	9.74218700
H	10.95394200	4.42565100	12.89571800
C	11.07288500	4.07833000	9.05116100
C	11.14935200	4.69413200	7.66733600
H	10.73641400	3.04486500	8.96859600
H	12.03328300	4.19691100	9.55290400
O	10.00235200	4.25890600	6.92032600
C	11.18715200	6.21574200	7.49927300
H	12.03371900	4.28805000	7.17625600
C	9.56335200	5.33430900	6.11072500
O	12.43120000	6.28804300	6.78735000
C	9.77139900	6.52851000	7.03084800
H	11.32915700	6.66491200	8.48221900
N	8.23454700	5.05470800	5.75496700
H	10.18712300	5.42319500	5.22120700
H	12.63191800	7.20483600	6.58520400
H	9.79052400	7.43814900	6.43060300
H	9.09175700	6.44401100	7.87882000
C	7.14435900	5.01985600	6.58891700
C	7.75053500	4.76613900	4.50628500
N	6.02675500	4.75104900	5.97268100
H	7.26670700	5.20602900	7.64565600

C	6.39964300	4.54299900	4.65888200
N	8.50444800	4.67546000	3.38604100
C	5.65189100	4.17860300	3.51354800
C	7.75748000	4.29748600	2.34622700
O	4.44290500	3.91782100	3.45794800
N	6.40740700	4.08337500	2.36051800
N	8.36400600	4.24562700	1.14618100
H	5.96560600	3.84399300	1.48437400
H	9.36020800	4.39667000	1.07687600
H	7.82298000	4.05560500	0.31471400
N	6.97027700	3.84024400	-1.21836300
C	7.59137400	4.08510600	-2.33555000
C	5.64016500	3.71361800	-1.58419500
N	6.78330400	4.03509700	-3.42446800
H	8.64090200	4.31174600	-2.45186900
C	4.47013000	3.47555900	-0.81454100
C	5.50554300	3.84727800	-2.94897500
C	7.17978500	4.22655300	-4.78074700
O	4.39797300	3.41078000	0.42402400
N	3.31509300	3.38742300	-1.55280600
N	4.38622100	3.67517600	-3.67139600
O	7.76086600	3.00117600	-5.24827300
C	8.25771200	5.29972200	-4.98045800
H	6.30610800	4.47002700	-5.38528300
C	3.30907600	3.47635900	-2.91189800
H	2.42858800	3.24035100	-1.09149400
C	8.46690000	3.31370700	-6.46523800

C	8.64350500	4.83051200	-6.37397800
H	7.76732300	6.26939100	-5.06639000
H	9.08530400	5.08759200	-4.30353000
N	2.11485400	3.38257200	-3.50473200
C	9.80306400	2.59519100	-6.40534800
H	7.89478400	3.02721300	-7.34767300
O	7.77277400	5.35066600	-7.35009100
H	9.67382400	5.10754900	-6.59694700
H	2.04426600	3.44253200	-4.51048600
H	1.28300500	3.25173100	-2.94700300
O	10.63576500	3.29979300	-5.45531700
H	9.64944400	1.57150300	-6.06388600
H	10.27301300	2.62060300	-7.38846300
H	7.82928800	6.30903500	-7.35192300
P	12.11287800	2.76924600	-5.17534300
O	11.90136600	1.46919000	-4.29433800
O	12.82355800	2.32997500	-6.38491600
O	12.86462900	3.81106600	-4.37829500
C	12.03666400	1.53126900	-2.85382300
H	13.74271500	2.15490400	-6.17020400
C	12.00935100	0.06139300	-2.48713900
C	10.81198200	2.08908400	-2.15891600
H	12.95697200	2.02414500	-2.54040400
C	12.98388300	-0.47062900	-1.46676600
O	10.64137700	-0.23751200	-2.09384400
H	12.19404600	-0.49080100	-3.40859100
C	9.83454500	0.94108700	-2.19138700

H	10.41295900	2.91835600	-2.74301000
H	11.06009400	2.32157100	-1.12333500
O	12.92704800	0.44619100	-0.41925500
H	12.64187400	-1.44360400	-1.11394000
H	13.98744900	-0.47106800	-1.89206900
H	9.30154900	0.94148100	-3.14216800
P	14.20937400	0.44444300	0.58336600
O	13.90079500	-0.72420800	1.64334400
O	15.47729300	0.10903300	-0.04998500
O	14.00421000	1.69292100	1.29251200
C	13.18206600	-0.47807600	2.89388600
H	16.17520600	0.11305600	0.60918200
C	13.22365800	-1.87836400	3.44733400
C	11.66890200	-0.20746000	2.77979600
H	13.69011700	0.24208200	3.53526100
C	13.30871300	-2.00713600	4.95751500
O	12.01622100	-2.50882400	2.95323000
H	14.08037000	-2.39259100	3.01176400
C	11.13007900	-1.56803100	2.35356800
H	11.49276700	0.51400100	1.98194600
H	11.27393300	0.04217200	3.76455000
H	13.25080200	-3.03991000	5.23123700
H	14.23731100	-1.59930600	5.29851400
H	12.49797900	-1.47295700	5.40725000
N	9.81163500	-1.87010300	2.82156600
H	11.16936000	-1.66001000	1.26814000
C	9.29550300	-1.79535200	4.08524300

C	8.74155000	-2.21096800	2.01023600
N	8.03417500	-2.06046500	4.17299700
H	9.93444100	-1.53062000	4.91478300
N	8.76711200	-2.38995300	0.66918900
C	7.65170500	-2.31462700	2.85798700
C	7.56624400	-2.65013400	0.17165300
C	6.38138500	-2.58864000	2.28814000
N	6.42283500	-2.74221600	0.92462100
N	7.44108200	-2.90164400	-1.12349000
O	5.30464800	-2.65103200	2.90509600
H	5.57435600	-2.93630800	0.41231300
H	8.24823900	-2.84946600	-1.72832700
H	6.53849500	-3.14545800	-1.50563300

SPT2 optimised at $E_{\text{ext}} = 100 \times 10^{-4}$ a.u.

N	-0.13653500	0.05457700	0.01286100
H	-0.09058700	0.11747000	1.03090000
C	1.07830000	0.10977300	-0.65020400
C	-1.36858300	0.01812700	-0.61925300
C	0.94824200	0.08858800	-2.04114600
O	2.15650200	0.18269300	0.05176800
N	-2.46310600	0.01810900	0.15110800
N	-1.50405900	-0.00834200	-1.92208100
N	1.88193500	0.13545800	-3.05924600
C	-0.35301300	0.04095900	-2.58646100
H	-3.33388400	0.12124900	-0.35204600
H	-2.40855100	0.20895700	1.14557400

C	1.17653800	0.12324000	-4.15998000
N	-0.18371200	0.08813300	-3.93585700
H	1.59092200	0.17898300	-5.15181800
N	-3.03569100	1.05855800	4.99383600
C	-3.22706800	0.78636600	3.65510200
C	-1.67512400	1.01431800	5.21210600
N	-2.11229900	0.58919600	3.01497400
H	-4.20295700	0.80866300	3.20428800
C	-1.12428700	0.72545400	3.96213100
N	-1.01557800	1.21503400	6.36784000
C	0.29045600	0.63823600	3.83739200
C	0.29426900	1.13651800	6.23352900
O	0.96877400	0.42059200	2.80405200
N	0.93094300	0.84926000	5.04889400
N	1.08612500	1.33392600	7.30548800
H	1.96586100	0.85955700	4.98639200
H	0.61474300	1.72567900	8.10544800
H	2.10271000	1.46129800	7.21523000
N	6.08114600	1.97244200	7.93719400
C	4.72668200	1.93670200	8.20726000
C	6.22366100	1.61212100	6.58280400
N	3.99622900	1.63596000	7.17631400
H	4.33165900	2.23094200	9.16398200
C	4.89532200	1.42615600	6.14588400
N	7.33931100	1.50945000	5.88168900
C	4.67773600	1.09762800	4.77911600
C	7.14732800	1.22285900	4.55866900

O	3.57559200	0.92832500	4.17294100
N	5.84379900	0.97763100	4.08222800
N	8.07664500	1.16634700	3.65423500
H	5.74405600	0.76336500	3.08609500
H	8.97951300	1.35886300	4.08053500
H	7.96502100	1.01096100	2.00840000
N	8.84537400	0.96983600	-1.11417100
C	9.08720500	1.08692900	0.20687100
C	7.48117500	0.70514900	-1.26944300
N	7.98827800	0.93609600	0.91815000
H	10.04468300	1.32826000	0.62920000
C	6.94388400	0.69304900	0.03025700
N	6.84320200	0.53363400	-2.40222800
C	5.55647400	0.46631400	0.18593500
C	5.52760900	0.35833300	-2.27391000
O	4.88844100	0.42059200	1.27238500
N	4.91432100	0.29947100	-1.01998300
N	4.76473800	0.25151100	-3.33639500
H	3.88961000	0.20290200	-0.96480200
H	5.22033400	0.32019500	-4.24230300
H	3.73725400	0.16480300	-3.27867700
N	2.84213500	1.62261300	1.87415500
N	3.00519100	-0.95698600	1.76262400
C	-1.25272600	-0.03120300	-4.92001400
O	-1.20288800	-1.31763800	-5.52579300
C	-1.12001300	0.95588900	-6.04516100
H	-2.21240800	0.10474300	-4.42137300

C	-1.45587100	-1.20084000	-6.96607300
C	-1.74063500	0.27443700	-7.22292100
H	-1.68914900	1.85434700	-5.80645400
H	-0.06369800	1.13424000	-6.24644200
C	-0.27902300	-1.76545000	-7.71871900
H	-2.34481100	-1.78006800	-7.21584200
O	-3.18078500	0.39342000	-7.28110900
H	-1.28186600	0.60600800	-8.15443000
O	0.79147300	-0.82905500	-7.63239000
H	0.02528700	-2.70753500	-7.26274900
H	-0.55194200	-1.90920300	-8.76415900
P	-3.87482800	1.82698000	-7.48484600
P	1.91547200	-0.79381900	-8.78938100
O	-5.11232000	1.58124000	-8.25677700
O	-2.93698700	2.82417700	-8.06927600
O	-4.21161800	2.27425500	-5.98771800
O	2.76984100	-2.12441200	-8.52478600
O	1.27734800	-0.98352500	-10.11658500
O	2.71290000	0.43326400	-8.56746700
H	-5.84665700	1.45301500	-7.65187400
C	-5.19164100	1.51908700	-5.26099000
C	4.01690100	-2.10633000	-7.78443300
H	1.07172700	-1.91269800	-10.24290900
C	-5.43514800	2.18336300	-3.95905100
H	-4.81795900	0.50960900	-5.08927800
H	-6.12019600	1.48587000	-5.83094200
C	4.36257300	-3.56779000	-7.63693600

C	3.81679200	-1.65136500	-6.34858500
H	4.79734800	-1.54263800	-8.29566600
O	-4.24399400	2.04116400	-3.15959300
C	-5.71212400	3.68126700	-4.07074800
H	-6.27021200	1.69709200	-3.45477200
C	5.84204000	-3.85136000	-7.73122700
O	3.88116800	-4.01499000	-6.35223900
H	3.84869300	-4.12897000	-8.41738900
C	3.32525300	-2.91531600	-5.66537400
H	3.03052500	-0.89706000	-6.31710800
H	4.77949600	-1.36534000	-5.92495500
C	-4.12111600	3.23873400	-2.37620300
O	-7.02544000	3.86467000	-3.50649300
C	-4.60324700	4.37334900	-3.28058100
H	-5.69500400	3.99788900	-5.11365800
H	6.03153200	-4.86085100	-7.43135800
H	6.16829800	-3.71193400	-8.74069000
H	6.37510900	-3.18232300	-7.08847700
N	3.66261500	-3.02843800	-4.29002300
H	2.24029800	-2.96046300	-5.76042500
N	-2.70250600	3.29896000	-2.00648700
H	-4.74356400	3.17407300	-1.48376300
H	-7.26412500	4.79373200	-3.54551800
H	-5.03989400	5.16014300	-2.66547100
H	-3.79993200	4.65366000	-3.96192700
C	4.94040700	-3.00500600	-3.78280500
C	2.83841200	-3.13075600	-3.19379400

C	-1.60274300	3.23027800	-2.84291100
C	-2.19335900	3.33957500	-0.72901100
N	4.98930200	-3.05384600	-2.48078100
H	5.78618800	-2.95052600	-4.45215900
C	3.66489700	-3.12685200	-2.08760500
N	1.49252400	-3.26103400	-3.21584400
N	-0.47862100	3.16469100	-2.21435500
H	-1.73804400	3.23506300	-3.91439900
N	-2.90373200	3.44962300	0.40520200
C	-0.81983200	3.26569000	-0.87416400
C	3.08319900	-3.18874300	-0.80722600
C	0.97692900	-3.30815200	-1.99511400
C	-2.10747600	3.52459800	1.49374900
C	-0.02094000	3.31754000	0.29528200
O	3.65335300	-3.12985200	0.29921400
N	1.70402600	-3.25280300	-0.84161500
N	-0.34205500	-3.41044300	-1.84496100
N	-0.75029000	3.43906700	1.44989000
N	-2.67644800	3.76405400	2.67721200
O	1.21358000	3.20757900	0.35228500
H	1.17718900	-3.26060000	0.02007600
H	-0.94075700	-3.45611200	-2.65710300
H	-0.74394300	-3.44230900	-0.91895300
H	-0.27988300	3.47133900	2.34306900
H	-3.68147000	3.83432000	2.74938600
H	-2.10201000	3.87495100	3.50052800
N	-1.35023700	4.33119200	5.06335500

C	-1.96679600	4.64206400	6.17176900
C	-0.00807500	4.37772900	5.42985800
N	-1.12862000	4.80906400	7.25289900
H	-3.03269200	4.76982600	6.29000500
C	1.17453600	4.14120200	4.66862100
C	0.13695000	4.63770400	6.76342500
C	-1.49873800	5.00569500	8.64005500
O	1.22603100	3.78768400	3.47743600
N	2.33059300	4.26664300	5.38832000
N	1.25784400	4.77016400	7.47706700
C	-2.51456700	6.10789500	8.87002900
O	-2.25719000	3.84639100	8.98075400
H	-0.62419700	5.12048000	9.28050800
C	2.34973000	4.58211000	6.72375900
H	3.22393800	4.12338000	4.93947100
C	-3.25561800	5.70169600	10.12800700
H	-1.99321700	7.04890800	9.04562900
H	-3.21216600	6.13676400	8.03301100
C	-3.15655000	4.18362500	10.05720400
N	3.55248700	4.74068200	7.29121700
O	-2.57750800	6.05335000	11.34677400
H	-4.29016400	6.04472300	10.12202200
C	-4.45732700	3.47858200	9.82107300
H	-2.72994200	3.82012300	10.99209900
H	3.62155100	4.97362900	8.27155100
H	4.39036400	4.62722900	6.73882900
H	-2.59853100	7.00618900	11.46175600

O	-5.04012700	4.07135500	8.64380200
H	-4.26820600	2.42076100	9.63849300
H	-5.11735800	3.64084000	10.67317400
P	-6.55374000	3.67886400	8.24209100
O	-6.41773100	2.15418700	7.75519800
O	-7.44500500	3.62000600	9.41449700
O	-7.01136700	4.56559000	7.13214400
C	-6.35520100	1.82599900	6.35568600
H	-6.92662200	3.72234800	10.21599800
C	-6.20823100	0.31592800	6.31133000
C	-5.08516100	2.32856300	5.64588100
H	-7.25480200	2.15098800	5.83300500
C	-7.01666800	-0.43165400	5.24089700
O	-4.78900100	0.05923600	6.23501500
H	-6.54366000	-0.06047300	7.27764900
C	-4.06182700	1.25480600	6.00208100
H	-4.77877800	3.27697600	6.08715900
H	-5.25029500	2.32372000	4.56845200
O	-6.75912500	0.28520100	4.03394400
H	-6.63552900	-1.44834400	5.14526100
H	-8.07822100	-0.36698500	5.47963600
H	-3.57533600	1.54409400	6.93356100
P	-7.87306100	0.10543000	2.86382400
O	-7.68941700	-1.41650300	2.41407100
O	-9.25996600	0.17639900	3.36706700
O	-7.50161400	1.03743800	1.75346600
C	-6.94224900	-1.76835900	1.24574500

H	-9.24916400	0.28229500	4.32114700
C	-6.91814500	-3.29097000	1.23771600
C	-5.46555100	-1.40983800	1.38611300
H	-7.38146000	-1.35813100	0.33635100
C	-6.98137800	-3.87870900	-0.15686200
O	-5.67266600	-3.69486000	1.87784700
H	-7.75860400	-3.66523100	1.82221300
C	-4.85593100	-2.57447800	2.15639000
H	-5.36977100	-0.49767300	1.97506900
H	-5.01175700	-1.35418000	0.39667700
H	-6.82456100	-4.93592300	-0.10579900
H	-7.94225000	-3.68088800	-0.58405100
H	-6.22198900	-3.43450500	-0.76588800
N	-3.50930300	-2.85216600	1.86321900
H	-4.93307600	-2.35455600	3.22122100
C	-2.98863200	-3.07490500	0.62307700
C	-2.44018300	-2.78188100	2.71813600
N	-1.70051700	-3.16847200	0.59953100
H	-3.64438000	-3.15744100	-0.23102000
C	-1.32129400	-2.97162400	1.92660500
N	-2.47695700	-2.56025800	4.04553300
C	-0.04786300	-2.91483800	2.53689800
C	-1.27109600	-2.55901000	4.59037600
O	1.05410800	-3.00694100	1.95435500
N	-0.11502700	-2.69433000	3.89441500
N	-1.14862700	-2.39147200	5.91348900
H	0.73379300	-2.62356900	4.43720100

H	-1.97282300	-2.28489100	6.48746600
H	-0.23211400	-2.37170400	6.33733600
N	1.29499600	-1.98825200	7.22025300
C	1.31440900	-1.60818900	8.46080500
C	2.63427900	-1.99708200	6.84091700
N	2.59181700	-1.42764600	8.95711900
H	0.45854800	-1.43303600	9.09582400
C	3.24974900	-2.26743300	5.59638500
C	3.44075400	-1.68441700	7.91165800
C	2.90138700	-1.00985600	10.28385200
O	2.65840700	-2.47829300	4.51499800
N	4.61574000	-2.19206800	5.62805100
N	4.78008900	-1.63485100	7.95093300
C	2.27960400	0.31742600	10.65425900
O	2.39293300	-1.95751100	11.19736600
H	3.98352100	-0.94472200	10.39758700
C	5.31788600	-1.91043100	6.77943200
H	5.14972200	-2.34569100	4.78463100
C	2.12524400	0.21682400	12.15838800
H	2.97765400	1.12032100	10.41726800
H	1.29364600	0.39321800	10.19577200
C	1.89286500	-1.26223600	12.36430700
N	6.65078100	-1.87786200	6.64006900
O	3.32158100	0.55906400	12.86401600
H	1.27656200	0.80373400	12.50960000
C	0.42612800	-1.67777600	12.57111500
H	2.46884200	-1.58484500	13.23171400

H	7.23716000	-1.67806500	7.43772800
H	7.06858600	-2.05314800	5.73734800
P	3.95936800	2.04814600	12.79479200
H	0.34222700	-2.74153400	12.49187100
H	0.10038700	-1.36560100	13.54134200
H	-0.18436900	-1.21520700	11.82397100
O	4.48542100	2.28951700	14.14861700
O	3.00221500	3.02963600	12.23010400
O	5.15108500	1.84717000	11.72075100
H	5.24838100	1.72699200	14.30046400
C	6.23784000	0.97865500	12.00617800
C	7.39337900	1.34937500	11.15119900
H	5.94550100	-0.05006000	11.79538800
H	6.51592900	1.07779000	13.05544700
O	7.16106400	0.96631300	9.78743200
C	7.65158100	2.83952400	11.15759800
H	8.28242100	0.83509900	11.51623100
C	7.15292700	2.08953300	8.92049300
O	9.08534100	2.97752300	11.08705200
C	7.04019300	3.27842400	9.84339400
H	7.21639800	3.34413700	12.02021900
H	8.09617000	2.13773900	8.37633700
P	9.81191800	4.39367800	11.26141500
H	7.61637500	4.10903500	9.43569700
H	5.98826100	3.51948000	9.99615000
O	11.04625300	4.12743100	11.98789400
O	8.89475000	5.41642700	11.85219600

O	10.07545000	4.85065300	9.74218700
H	10.95394200	4.42565100	12.89571800
C	11.07288500	4.07833000	9.05116100
C	11.14935200	4.69413200	7.66733600
H	10.73641400	3.04486500	8.96859600
H	12.03328300	4.19691100	9.55290400
O	10.00235200	4.25890600	6.92032600
C	11.18715200	6.21574200	7.49927300
H	12.03371900	4.28805000	7.17625600
C	9.56335200	5.33430900	6.11072500
O	12.43120000	6.28804300	6.78735000
C	9.77139900	6.52851000	7.03084800
H	11.32915700	6.66491200	8.48221900
N	8.23454700	5.05470800	5.75496700
H	10.18712300	5.42319500	5.22120700
H	12.63191800	7.20483600	6.58520400
H	9.79052400	7.43814900	6.43060300
H	9.09175700	6.44401100	7.87882000
C	7.14435900	5.01985600	6.58891700
C	7.75053500	4.76613900	4.50628500
N	6.02675500	4.75104900	5.97268100
H	7.26670700	5.20602900	7.64565600
C	6.39980500	4.54224400	4.65901400
N	8.50444800	4.67546000	3.38604100
C	5.65192000	4.17864200	3.51329300
C	7.75748000	4.29748600	2.34622700
O	4.43957900	3.91925700	3.45728500

N	6.40743200	4.08324600	2.36054400
N	8.36400600	4.24562700	1.14618100
H	5.96560600	3.84399300	1.48437400
H	9.36020800	4.39667000	1.07687600
H	7.82298000	4.05560500	0.31471400
N	6.97027700	3.84024400	-1.21836300
C	7.59137400	4.08510600	-2.33555000
C	5.64017900	3.71342900	-1.58422300
N	6.78330400	4.03509700	-3.42446800
H	8.64090200	4.31174600	-2.45186900
C	4.46517700	3.48066500	-0.81469500
C	5.50554300	3.84727800	-2.94897500
C	7.17978500	4.22655300	-4.78074700
O	4.40543300	3.40678100	0.42497300
N	3.31526900	3.38564100	-1.55287800
N	4.38622100	3.67517600	-3.67139600
O	7.76086600	3.00117600	-5.24827300
C	8.25771200	5.29972200	-4.98045800
H	6.30610800	4.47002700	-5.38528300
C	3.30907600	3.47635900	-2.91189800
H	2.42858800	3.24035100	-1.09149400
C	8.46690000	3.31370700	-6.46523800
C	8.64350500	4.83051200	-6.37397800
H	7.76732300	6.26939100	-5.06639000
H	9.08530400	5.08759200	-4.30353000
N	2.11485400	3.38257200	-3.50473200
C	9.80306400	2.59519100	-6.40534800

H	7.89478400	3.02721300	-7.34767300
O	7.77277400	5.35066600	-7.35009100
H	9.67382400	5.10754900	-6.59694700
H	2.04426600	3.44253200	-4.51048600
H	1.28300500	3.25173100	-2.94700300
O	10.63576500	3.29979300	-5.45531700
H	9.64944400	1.57150300	-6.06388600
H	10.27301300	2.62060300	-7.38846300
H	7.82928800	6.30903500	-7.35192300
P	12.11287800	2.76924600	-5.17534300
O	11.90136600	1.46919000	-4.29433800
O	12.82355800	2.32997500	-6.38491600
O	12.86462900	3.81106600	-4.37829500
C	12.03666400	1.53126800	-2.85382100
H	13.74271500	2.15490400	-6.17020400
C	12.00935000	0.06139200	-2.48714400
C	10.81198000	2.08908600	-2.15892000
H	12.95697200	2.02414500	-2.54040400
C	12.98388300	-0.47062900	-1.46676600
O	10.64138400	-0.23750600	-2.09382800
H	12.19404600	-0.49080100	-3.40859100
C	9.83454500	0.94105700	-2.19139700
H	10.41296000	2.91835600	-2.74301100
H	11.06009400	2.32157200	-1.12333500
O	12.92704800	0.44619100	-0.41925500
H	12.64187400	-1.44360400	-1.11394000
H	13.98744900	-0.47106800	-1.89206900

H	9.30154600	0.94150400	-3.14216600
P	14.20937400	0.44444300	0.58336600
O	13.90079500	-0.72420800	1.64334400
O	15.47729300	0.10903300	-0.04998500
O	14.00421000	1.69292100	1.29251200
C	13.18206600	-0.47807600	2.89388600
H	16.17520600	0.11305600	0.60918200
C	13.22365800	-1.87836400	3.44733400
C	11.66890200	-0.20746000	2.77979600
H	13.69011700	0.24208200	3.53526100
C	13.30871300	-2.00713600	4.95751500
O	12.01622100	-2.50882400	2.95323000
H	14.08037000	-2.39259100	3.01176400
C	11.13007900	-1.56803100	2.35356800
H	11.49276700	0.51400100	1.98194600
H	11.27393300	0.04217200	3.76455000
H	13.25080200	-3.03991000	5.23123700
H	14.23731100	-1.59930600	5.29851400
H	12.49797900	-1.47295700	5.40725000
N	9.81163500	-1.87010300	2.82156600
H	11.16936000	-1.66001000	1.26814000
C	9.29550300	-1.79535200	4.08524300
C	8.74155000	-2.21096800	2.01023600
N	8.03417500	-2.06046500	4.17299700
H	9.93444100	-1.53062000	4.91478300
N	8.76711200	-2.38995300	0.66918900
C	7.65170500	-2.31462700	2.85798700

C	7.56624400	-2.65013400	0.17165300
C	6.38138500	-2.58864000	2.28814000
N	6.42283500	-2.74221600	0.92462100
N	7.44108200	-2.90164400	-1.12349000
O	5.30464800	-2.65103200	2.90509600
H	5.57435600	-2.93630800	0.41231300
H	8.24823900	-2.84946600	-1.72832700
H	6.53849500	-3.14545800	-1.50563300

QPT1 optimised at $E_{\text{ext}} = 80 \times 10^{-4}$ a.u.

N	-0.03665700	0.08822100	0.10874000
H	-0.07480400	0.17894700	1.82913000
C	1.19233500	0.14561900	-0.40693800
C	-1.08461500	0.11558200	-0.79508700
C	1.41884000	0.22312200	-1.76419000
O	2.22218200	0.14086700	0.52598600
N	-2.32985800	0.07276900	-0.32278300
N	-0.97804600	0.19868200	-2.12516500
N	2.54794900	0.30071400	-2.55291600
C	0.25428400	0.26389800	-2.56923500
H	-3.06052700	0.17638500	-1.01268300
H	-2.52457500	0.13939500	0.66946300
C	2.09003200	0.39549700	-3.77206900
N	0.71518600	0.40546600	-3.85209100
H	2.71348400	0.49487900	-4.64316900
N	-4.06972600	0.79991600	4.24324200
C	-3.98348200	0.65010100	2.87495300

C	-2.78405400	0.67949900	4.72688300
N	-2.76963900	0.46402900	2.45346900
H	-4.84469800	0.74421200	2.23893300
C	-1.98726300	0.48001000	3.58386800
N	-2.34303900	0.73884100	5.97413100
C	-0.61038400	0.37152400	3.79453700
C	-1.01545200	0.60815100	6.06606100
O	0.30498000	0.22971500	2.80026200
N	-0.12771000	0.43442700	5.03658400
N	-0.50486600	0.65212600	7.31335100
H	1.68985000	0.41588400	5.21752900
H	-1.15519900	0.92778900	8.03188800
H	0.49463600	0.74502800	7.48388500
N	4.16478200	1.06722900	9.24344500
C	2.78611500	1.07604300	9.17738100
C	4.60624300	0.80693600	7.94774200
N	2.31861500	0.88579000	7.97960000
H	2.17859200	1.31024800	10.03374300
C	3.43236500	0.71310500	7.17925600
N	5.84598900	0.70646900	7.50804200
C	3.62544300	0.49971100	5.79912300
C	5.91704700	0.52524400	6.17382900
O	2.63864800	0.41379500	4.87451100
N	4.85012200	0.40133800	5.31546800
N	7.12888100	0.47462700	5.62772800
H	4.89807700	0.19229200	3.35432900
H	7.91552500	0.62301500	6.24068100

H	7.26599800	0.44029900	4.60502900
N	8.89142000	0.65564300	0.98100900
C	8.80709500	0.65358100	2.34933700
C	7.60155200	0.45845500	0.51401100
N	7.59475100	0.50229400	2.81194300
H	9.66933300	0.81969800	2.96949300
C	6.80389600	0.37714400	1.68039900
N	7.18173000	0.38697100	-0.72220600
C	5.44540700	0.20857600	1.43805600
C	5.84865900	0.24665600	-0.84665300
O	4.49088400	0.12135200	2.44896300
N	4.95808500	0.14131900	0.21285100
N	5.35700600	0.22600800	-2.07204300
H	3.14132100	0.17095200	0.10096700
H	6.01479000	0.33085300	-2.83461100
H	4.34842200	0.19128100	-2.25904200
N	2.38619700	1.45946800	2.52808300
N	2.53952500	-1.35441200	2.20528800
C	-0.10214600	0.41176200	-5.05932400
O	0.05011800	-0.82411000	-5.74768100
C	0.30879900	1.47706000	-6.03614800
H	-1.14611200	0.55148400	-4.77876100
C	0.13425700	-0.58331400	-7.19232100
C	-0.04566700	0.91895100	-7.37761200
H	-0.27579700	2.37887900	-5.85419600
H	1.38754100	1.62262300	-5.97916500
C	1.43605200	-1.13985500	-7.70790400

H	-0.68961500	-1.10028700	-7.68433200
O	-1.43125200	1.10725400	-7.74675600
H	0.62138300	1.30147000	-8.15016700
O	2.48323100	-0.26258400	-7.30286000
H	1.60381200	-2.12763200	-7.27872700
H	1.40417900	-1.18861600	-8.79634300
P	-2.02277100	2.58234700	-7.97589800
P	3.84129400	-0.18762400	-8.17078000
O	-3.05848200	2.45425400	-9.02401400
O	-0.95068100	3.57881500	-8.24641600
O	-2.67908300	2.92555900	-6.55944700
O	4.57777000	-1.57221200	-7.83768500
O	3.51672800	-0.24349400	-9.61860500
O	4.59950100	0.98087200	-7.67017100
H	-3.91419900	2.31235700	-8.61265800
C	-3.81819300	2.16086900	-6.13928600
C	5.62396800	-1.66879600	-6.83780900
H	3.32076300	-1.14961700	-9.86788300
C	-4.33361300	2.73128100	-4.87256600
H	-3.52007400	1.12514100	-5.97631300
H	-4.59346000	2.21458000	-6.90364000
C	5.88840100	-3.15147800	-6.74380300
C	5.11484100	-1.31930800	-5.44952000
H	6.51476900	-1.10266300	-7.11015300
O	-3.35949900	2.47296900	-3.84175200
C	-4.53834700	4.24433500	-4.91325700
H	-5.27396000	2.24527000	-4.61250900

C	7.34257400	-3.49350800	-6.52811500
O	5.11599600	-3.67584000	-5.64352100
H	5.55072400	-3.62582700	-7.66525300
C	4.44772800	-2.60940400	-5.00615200
H	4.36217200	-0.53495600	-5.52991300
H	5.96327300	-1.11131600	-4.79762100
C	-3.38633400	3.59857300	-2.94997300
O	-5.94022800	4.44220500	-4.64418800
C	-3.62021200	4.82133000	-3.83759300
H	-4.27630800	4.64071800	-5.89428700
H	7.43226200	-4.53096100	-6.28205400
H	7.89327700	-3.29022200	-7.42271100
H	7.73307100	-2.90181000	-5.72667500
N	4.46058000	-2.84526900	-3.60529500
H	3.41196300	-2.59775400	-5.34564800
N	-2.08779100	3.56527300	-2.26773600
H	-4.19680300	3.49234700	-2.22891300
H	-6.13920800	5.38132100	-4.65506100
H	-4.16432000	5.57640100	-3.27024900
H	-2.67596100	5.11756100	-4.29449600
C	5.58982000	-2.91962300	-2.82435900
C	3.40640100	-2.99584800	-2.73493400
C	-0.82891700	3.51268500	-2.83893800
C	-1.88141100	3.48241000	-0.91003000
N	5.34021800	-3.07264700	-1.55379900
H	6.56672800	-2.85115900	-3.27967600
C	3.95966100	-3.11620600	-1.47550400

N	2.09778800	-3.06288700	-3.06946700
N	0.12080400	3.34711700	-1.98240400
H	-0.71698500	3.60765900	-3.90892200
N	-2.82781200	3.53518500	0.04113800
C	-0.51330300	3.35781200	-0.74929500
C	3.10076800	-3.25196200	-0.36850500
C	1.31719100	-3.18224500	-2.00426300
C	-2.29809400	3.48836000	1.28282500
C	0.00005600	3.28024900	0.56860000
O	3.40589000	-3.30596600	0.83844900
N	1.76430400	-3.25057900	-0.71674000
N	-0.00363000	-3.23614300	-2.16318500
N	-0.96927700	3.34547100	1.53725200
N	-3.11462500	3.65974000	2.32472700
O	1.18542300	3.11489400	0.89078700
H	1.05539900	-3.30209400	0.00084500
H	-0.40308000	-3.19077100	-3.08973000
H	-0.60615200	-3.32233600	-1.35723400
H	-0.71338200	3.28531700	2.51251700
H	-4.10753700	3.76958400	2.17548200
H	-2.73961500	3.67955100	3.26233100
N	-2.35093400	3.97722200	4.98745800
C	-3.19484900	4.22776900	5.95203200
C	-1.12636600	3.93476900	5.64809300
N	-2.62021000	4.27127400	7.20389800
H	-4.25597300	4.39401600	5.83883000
C	0.19365300	3.70585600	5.15431300

C	-1.28148700	4.08169300	6.99775300
C	-3.29058400	4.37501200	8.48440200
O	0.49847200	3.44241600	3.97837800
N	1.15664900	3.72036300	6.12283900
N	-0.34902200	4.10682900	7.95332100
C	-4.30266200	5.50065200	8.57535800
O	-4.13692600	3.22810300	8.54451600
H	-2.58177000	4.39944900	9.31214700
C	0.88014600	3.92919400	7.45068200
H	2.12458200	3.57276100	5.87502800
C	-5.32067300	5.03098200	9.59502900
H	-3.81023100	6.40039600	8.94430000
H	-4.79076600	5.62668800	7.60894900
C	-5.24818100	3.52022400	9.41692700
N	1.92621600	3.98809700	8.28497800
O	-4.92826400	5.25483200	10.96060300
H	-6.31736800	5.41993700	9.38694100
C	-6.47938500	2.89553900	8.83488500
H	-5.05495100	3.06552900	10.38855900
H	1.77679000	4.14002900	9.27223500
H	2.86441600	3.88049700	7.92686700
H	-4.94973000	6.19568100	11.15009500
O	-6.76353200	3.60465800	7.61283200
H	-6.28168600	1.84783000	8.60837700
H	-7.31128600	3.02016700	9.52803300
P	-8.15605000	3.31387600	6.84942900
O	-7.95320700	1.82751500	6.27515500

O	-9.29168000	3.20363700	7.78246000
O	-8.32589200	4.30478400	5.74627900
C	-7.58292400	1.60766500	4.90227100
H	-8.96650500	3.21918000	8.68557700
C	-7.46960100	0.10062800	4.76127800
C	-6.17200100	2.10632100	4.54167900
H	-8.33130100	2.01308700	4.22134600
C	-8.03303400	-0.52325600	3.47613600
O	-6.07744600	-0.21331400	4.98323300
H	-8.02567700	-0.33485600	5.59139500
C	-5.28506900	0.96267600	5.02385400
H	-5.94901900	3.00232800	5.12094000
H	-6.08801200	2.19352900	3.45840500
O	-7.48911000	0.27369200	2.42448800
H	-7.66708600	-1.54552600	3.38065000
H	-9.11898100	-0.42949600	3.47540700
H	-5.01557000	1.15563400	6.06218900
P	-8.31230600	0.23694600	1.02329100
O	-8.07146000	-1.25175400	0.49598800
O	-9.77492200	0.33096500	1.20688800
O	-7.67377700	1.23542300	0.10960100
C	-7.08786400	-1.54433300	-0.50100100
H	-9.97844800	0.36106900	2.14458300
C	-7.10273600	-3.06114200	-0.63537600
C	-5.67278300	-1.26520100	-0.00249900
H	-7.29792700	-1.04453400	-1.44665700
C	-6.86284700	-3.53416600	-2.05417300

O	-6.04643000	-3.57002600	0.23028400
H	-8.06361200	-3.44165400	-0.28895500
C	-5.28511300	-2.51311200	0.78094200
H	-5.68933600	-0.40734300	0.66973200
H	-5.00468800	-1.15268800	-0.85631400
H	-6.74968000	-4.59814300	-2.06108400
H	-7.69592700	-3.26010700	-2.66717400
H	-5.97347200	-3.07840100	-2.43652200
N	-3.91490000	-2.82765900	0.77430300
H	-5.59641600	-2.37415700	1.81630000
C	-3.13206700	-2.97575500	-0.33199900
C	-3.06658300	-2.87318300	1.85000100
N	-1.87523700	-3.12544500	-0.07408400
H	-3.57848700	-2.96122200	-1.31525700
C	-1.80248600	-3.05072300	1.31617000
N	-3.39821400	-2.75496700	3.14942300
C	-0.70003800	-3.09975100	2.19907000
C	-2.34813400	-2.85110800	3.94882500
O	0.50266800	-3.19568600	1.87276700
N	-1.06812800	-2.98363300	3.52081700
N	-2.52519900	-2.79363300	5.27511300
H	-0.36331700	-2.99421000	4.24417600
H	-3.45517000	-2.69519200	5.65665200
H	-1.72880400	-2.84872700	5.89378300
N	-0.43274900	-2.60531800	7.12651800
C	-0.68576800	-2.32504500	8.36797800
C	0.95698800	-2.64501900	7.05790000

N	0.44972100	-2.24206100	9.15186200
H	-1.65862800	-2.16166900	8.80761100
C	1.83184700	-2.84448200	5.96447000
C	1.50696900	-2.45419800	8.30520000
C	0.46057100	-1.94412400	10.54531700
O	1.49639700	-2.94282700	4.76390900
N	3.15639500	-2.83379500	6.30808600
N	2.80315900	-2.46859300	8.64798700
C	-0.19389300	-0.62319900	10.88047000
O	-0.26700600	-2.93652900	11.23585700
H	1.48987000	-1.93720700	10.90404800
C	3.58566900	-2.67547600	7.60757200
H	3.86384600	-2.94479400	5.59584500
C	-0.68865600	-0.83442300	12.29713600
H	0.56068000	0.16336700	10.87657900
H	-1.04749800	-0.46707400	10.22088500
C	-1.00068200	-2.31303000	12.31668800
N	4.91574100	-2.69248900	7.77404400
O	0.32460500	-0.60316000	13.28003000
H	-1.57916600	-0.23904000	12.49859100
C	-2.48647500	-2.67664100	12.15246800
H	-0.64562900	-2.72847200	13.25985600
H	5.31055100	-2.58267200	8.69712800
H	5.52300200	-2.81514500	6.97630900
P	1.00048400	0.85633400	13.48495200
H	-2.57819800	-3.72600400	11.96452100
H	-3.01584600	-2.42712800	13.04824200

H	-2.89877300	-2.12968900	11.33042600
O	1.21126400	0.96664500	14.93796200
O	0.22294500	1.92146100	12.80725200
O	2.39938700	0.68647700	12.69225800
H	1.90463900	0.35995500	15.20769800
C	3.36953800	-0.25009700	13.13774700
C	4.69851500	0.13384000	12.59913200
H	3.10572600	-1.24479500	12.77840500
H	3.40439700	-0.24630400	14.22719500
O	4.77220600	-0.13010700	11.19006600
C	4.98771800	1.60566000	12.79242400
H	5.46744900	-0.44724200	13.10825900
C	4.99093100	1.05689600	10.44409200
O	6.40312000	1.68367300	13.05745400
C	4.70280100	2.17357600	11.41770600
H	4.38134000	2.06022100	13.57588600
H	6.03410300	1.10486300	10.13162500
P	7.10814800	3.04740300	13.51240700
H	5.37826900	3.00666200	11.22318800
H	3.65041600	2.44931300	11.35096200
O	8.13761100	2.66932500	14.47131600
O	6.10801800	4.06113700	13.96882600
O	7.72201900	3.60977500	12.13646100
H	7.84929300	2.89926300	15.35765700
C	8.82967500	2.84966700	11.62244800
C	9.23486000	3.56806100	10.34974700
H	8.49363600	1.84217500	11.37726000

H	9.65369500	2.88487900	12.33513700
O	8.27657900	3.24520600	9.32969100
C	9.34998600	5.09488700	10.32699300
H	10.19666600	3.16212000	10.03620600
C	8.06158700	4.39960300	8.53860700
O	10.72474200	5.16639600	9.92121900
C	8.08649600	5.50726500	9.58191600
H	9.27667800	5.45864400	11.35188800
N	6.84150800	4.20926800	7.87104200
H	8.87331800	4.52966700	7.82277900
H	10.99025900	6.08618800	9.84949000
H	8.26552500	6.45939600	9.08242100
H	7.22993500	5.38736200	10.24526700
C	5.58978600	4.15850900	8.43301600
C	6.64651200	4.04179800	6.52542800
N	4.63478900	3.98979500	7.56091400
H	5.47363300	4.25545000	9.50233100
C	5.29088700	3.86881300	6.35124400
N	7.63263400	4.00524400	5.59926300
C	4.81406200	3.63175900	5.03765700
C	7.13182900	3.74425900	4.38966800
O	3.64088600	3.42756300	4.69578200
N	5.80872300	3.59065700	4.08227300
N	7.99363500	3.75930400	3.35635300
H	5.57139900	3.44144000	3.11193000
H	8.98314700	3.87003300	3.52559000
H	7.65091600	3.65982000	2.41147200

N	7.16357400	3.60427600	0.71346700
C	8.02855900	3.90765900	-0.21043000
C	5.94847200	3.56759300	0.04912000
N	7.48808300	3.97991300	-1.45296300
H	9.08266200	4.09494800	-0.06831800
C	4.62180500	3.32943800	0.51199400
C	6.13119700	3.81344100	-1.29425800
C	8.18734000	4.25904800	-2.66394200
O	4.28518900	3.15678100	1.69632300
N	3.66956900	3.34322300	-0.47035500
N	5.20121100	3.74944400	-2.26143100
O	8.82694200	3.04907300	-3.09365700
C	9.31036900	5.29464000	-2.52302300
H	7.48065300	4.58853800	-3.42557400
C	3.97478200	3.54064500	-1.78301500
H	2.69770100	3.20264900	-0.23393400
C	9.79907100	3.42382900	-4.08949100
C	9.99025800	4.91923200	-3.82981800
H	8.87809300	6.28927900	-2.63235700
H	9.95656800	4.99277100	-1.69874100
N	2.94449800	3.54786700	-2.63441100
C	11.06723100	2.64303600	-3.79398700
H	9.43512600	3.23367700	-5.09918200
O	9.37818600	5.55328900	-4.92748200
H	11.05123000	5.16595000	-3.79116500
H	3.10594200	3.68970000	-3.62129400
H	2.00450700	3.41148400	-2.29094100

O	11.68051400	3.23246600	-2.62400100
H	10.81308000	1.60372400	-3.58573200
H	11.74881700	2.72419900	-4.64066600
H	9.45889600	6.50530000	-4.83351000
P	13.04082100	2.61521400	-2.06696400
O	12.60040300	1.26095500	-1.37193400
O	13.99596500	2.24047000	-3.11975000
O	13.61896500	3.55614700	-1.03439500
C	12.40636300	1.20361000	0.06205100
H	14.83732500	2.00762900	-2.72037800
C	12.25766900	-0.28775600	0.28442900
C	11.07095000	1.76008100	0.51027000
H	13.24402800	1.62817300	0.61539200
C	12.96041700	-0.94180700	1.44731000
O	10.82871500	-0.55431500	0.33350700
H	12.63231800	-0.77373900	-0.61643400
C	10.09652900	0.66361200	0.16001600
H	10.83713100	2.64985500	-0.07429300
H	11.08325000	1.89911500	1.59126800
O	12.69120200	-0.10838300	2.53082100
H	12.52162900	-1.92297200	1.62874200
H	14.03401000	-0.95433600	1.25951200
H	9.79377400	0.76280900	-0.88235500
P	13.71160200	-0.24689400	3.79146000
O	13.13948100	-1.47993400	4.64983600
O	15.08098300	-0.58866500	3.43196600
O	13.38364200	0.95009700	4.54201700

C	12.16209800	-1.30038500	5.72384200
H	15.61068100	-0.66800200	4.22866300
C	12.03987000	-2.74022600	6.14899800
C	10.72213800	-0.95337800	5.29720600
H	12.52990100	-0.65653400	6.52276800
C	11.77605300	-2.99082700	7.62279000
O	10.96012700	-3.27462000	5.34395000
H	12.95928600	-3.25697000	5.87376100
C	10.25859100	-2.25049600	4.64470100
H	10.75103300	-0.16429800	4.54580000
H	10.12042500	-0.76415300	6.18613400
H	11.63022800	-4.03820800	7.78596900
H	12.61327700	-2.65350200	8.19739200
H	10.89870100	-2.45740700	7.92381700
N	8.86079000	-2.52831900	4.77710200
H	10.54109000	-2.25870100	3.59195000
C	8.07312300	-2.52965500	5.89443800
C	7.99449000	-2.75563800	3.72004100
N	6.81831600	-2.74342100	5.67376300
H	8.51356500	-2.36005200	6.86588400
N	8.31943400	-2.82981300	2.40855000
C	6.73815100	-2.87602000	4.28952200
C	7.25663300	-2.99547800	1.63374300
C	5.62380900	-3.04664000	3.42774900
N	5.96999700	-3.09446700	2.10021200
N	7.42250500	-3.13865200	0.32672100
O	4.43377200	-3.10841000	3.77972200

H	5.25533800	-3.20912100	1.39582200
H	8.34709000	-3.07579400	-0.07483300
H	6.62427900	-3.31058700	-0.26776700

QPT1 optimised at $E_{\text{ext}} = 100 \times 10^{-4}$ a.u.

N	-0.03103600	0.10038400	0.11151300
H	-0.07315300	0.18555700	1.73638500
C	1.20021600	0.16139800	-0.41307200
C	-1.08086800	0.11768800	-0.79446000
C	1.42378800	0.23020800	-1.76717800
O	2.23353100	0.16608100	0.51537900
N	-2.32808900	0.06682100	-0.32974100
N	-0.97223200	0.19775000	-2.12354400
N	2.55238300	0.30673700	-2.55662200
C	0.25731800	0.26596400	-2.57262100
H	-3.05256800	0.15925500	-1.02863000
H	-2.53477400	0.13649800	0.65873800
C	2.09164100	0.39731600	-3.77595100
N	0.71639900	0.40520900	-3.85334700
H	2.71240600	0.49359800	-4.64987600
N	-4.07372400	0.80023600	4.23543500
C	-3.99809600	0.65460500	2.86447300
C	-2.78428200	0.67746600	4.70634800
N	-2.78805900	0.46875600	2.43509700
H	-4.86253000	0.75377600	2.23380600
C	-1.99604200	0.48040700	3.55738400
N	-2.33250100	0.73167500	5.95173300

C	-0.61368200	0.37037900	3.74719700
C	-1.00583700	0.59642400	6.02714300
O	0.28869600	0.23356000	2.74964200
N	-0.12577300	0.42813600	4.99299600
N	-0.48765800	0.62382200	7.27750300
H	1.68059200	0.41789800	5.20031600
H	-1.13212200	0.93344300	7.98766000
H	0.50878500	0.74906000	7.43860900
N	4.16571500	1.06798500	9.24362800
C	2.78621400	1.07950600	9.17823000
C	4.60676600	0.80711400	7.94537800
N	2.31989300	0.89252700	7.98058100
H	2.17807500	1.31612600	10.03371500
C	3.43177200	0.71687000	7.17961100
N	5.84695900	0.70469600	7.50575400
C	3.61984900	0.50266100	5.79580500
C	5.91353400	0.52512800	6.16867500
O	2.63665300	0.42057200	4.87326900
N	4.84405300	0.40150600	5.31468400
N	7.12078500	0.47578800	5.61455400
H	4.89216100	0.17895200	3.32736500
H	7.91233600	0.62507600	6.22073300
H	7.25238100	0.44101800	4.58737900
N	8.88918200	0.65497400	0.97821300
C	8.80031600	0.64864200	2.34447900
C	7.59962400	0.45949300	0.50515700
N	7.58599100	0.49613000	2.80489700

H	9.66144400	0.81225400	2.96693500
C	6.79784400	0.37445900	1.66926900
N	7.18636000	0.39197400	-0.73167800
C	5.44121000	0.20552300	1.41785000
C	5.85296000	0.25329200	-0.86643500
O	4.48157100	0.11224700	2.42673300
N	4.95800100	0.14376300	0.19188900
N	5.36737200	0.23916100	-2.09178900
H	3.15301900	0.19134200	0.08557000
H	6.02680600	0.34397100	-2.85424900
H	4.35900700	0.20039500	-2.28184400
N	2.38135600	1.45254000	2.49371200
N	2.50852600	-1.36856000	2.12982700
C	-0.10214700	0.41175600	-5.05933500
O	0.05011700	-0.82411100	-5.74768000
C	0.30879800	1.47706300	-6.03614500
H	-1.14611100	0.55148800	-4.77875900
C	0.13425800	-0.58331300	-7.19232100
C	-0.04566700	0.91895100	-7.37761200
H	-0.27579600	2.37887900	-5.85419600
H	1.38754100	1.62262200	-5.97916600
C	1.43605200	-1.13985500	-7.70790400
H	-0.68961500	-1.10028700	-7.68433200
O	-1.43125200	1.10725400	-7.74675600
H	0.62138300	1.30147000	-8.15016700
O	2.48323100	-0.26258400	-7.30286000
H	1.60381200	-2.12763200	-7.27872700

H	1.40417900	-1.18861600	-8.79634300
P	-2.02277100	2.58234700	-7.97589800
P	3.84129400	-0.18762400	-8.17078000
O	-3.05848200	2.45425400	-9.02401400
O	-0.95068100	3.57881500	-8.24641600
O	-2.67908300	2.92555900	-6.55944700
O	4.57777000	-1.57221200	-7.83768500
O	3.51672800	-0.24349400	-9.61860500
O	4.59950100	0.98087200	-7.67017100
H	-3.91419900	2.31235700	-8.61265800
C	-3.81819300	2.16086900	-6.13928600
C	5.62396800	-1.66879600	-6.83780900
H	3.32076300	-1.14961700	-9.86788300
C	-4.33361300	2.73128100	-4.87256600
H	-3.52007400	1.12514100	-5.97631300
H	-4.59346000	2.21458000	-6.90364000
C	5.88840100	-3.15147800	-6.74380300
C	5.11484100	-1.31930800	-5.44952000
H	6.51476900	-1.10266300	-7.11015300
O	-3.35949900	2.47296900	-3.84175200
C	-4.53834700	4.24433500	-4.91325700
H	-5.27396000	2.24527000	-4.61250900
C	7.34257400	-3.49350800	-6.52811500
O	5.11599600	-3.67584000	-5.64352100
H	5.55072400	-3.62582700	-7.66525300
C	4.44772800	-2.60940400	-5.00615200
H	4.36217200	-0.53495600	-5.52991300

H	5.96327300	-1.11131600	-4.79762100
C	-3.38633400	3.59857300	-2.94997300
O	-5.94022800	4.44220500	-4.64418800
C	-3.62021200	4.82133000	-3.83759300
H	-4.27630800	4.64071800	-5.89428700
H	7.43226200	-4.53096100	-6.28205400
H	7.89327700	-3.29022200	-7.42271100
H	7.73307100	-2.90181000	-5.72667500
N	4.46058000	-2.84526900	-3.60529500
H	3.41196300	-2.59775400	-5.34564800
N	-2.08779100	3.56527300	-2.26773600
H	-4.19680300	3.49234700	-2.22891300
H	-6.13920800	5.38132100	-4.65506100
H	-4.16432000	5.57640100	-3.27024900
H	-2.67596100	5.11756100	-4.29449600
C	5.58982000	-2.91962300	-2.82435900
C	3.40640100	-2.99584800	-2.73493400
C	-0.82891700	3.51268500	-2.83893800
C	-1.88141100	3.48241000	-0.91003000
N	5.34021800	-3.07264700	-1.55379900
H	6.56672800	-2.85115900	-3.27967600
C	3.95966100	-3.11620600	-1.47550400
N	2.09778800	-3.06288700	-3.06946700
N	0.12080400	3.34711700	-1.98240400
H	-0.71698500	3.60765900	-3.90892200
N	-2.82781200	3.53518500	0.04113800
C	-0.51328600	3.35793500	-0.74929400

C	3.10076800	-3.25196200	-0.36850500
C	1.31719100	-3.18224500	-2.00426300
C	-2.29809400	3.48836000	1.28282500
C	0.00000300	3.28031100	0.56883000
O	3.40589000	-3.30596600	0.83844900
N	1.76430400	-3.25057900	-0.71674000
N	-0.00363000	-3.23614300	-2.16318500
N	-0.96919300	3.34517300	1.53721100
N	-3.11462500	3.65974000	2.32472700
O	1.18515500	3.11473600	0.88960800
H	1.05539900	-3.30209400	0.00084500
H	-0.40308000	-3.19077100	-3.08973000
H	-0.60615200	-3.32233600	-1.35723400
H	-0.71340900	3.28587800	2.51248000
H	-4.10753700	3.76958400	2.17548200
H	-2.73961500	3.67955100	3.26233100
N	-2.35093400	3.97722200	4.98745800
C	-3.19484900	4.22776900	5.95203200
C	-1.12634700	3.93495800	5.64805600
N	-2.62021000	4.27127400	7.20389800
H	-4.25597300	4.39401600	5.83883000
C	0.19399200	3.70593800	5.15438200
C	-1.28148700	4.08169300	6.99775300
C	-3.29058400	4.37501200	8.48440200
O	0.49667100	3.44229600	3.97874300
N	1.15664200	3.72032200	6.12284700
N	-0.34902200	4.10682900	7.95332100

C	-4.30266200	5.50065200	8.57535800
O	-4.13692600	3.22810300	8.54451600
H	-2.58177000	4.39944900	9.31214700
C	0.88014600	3.92919400	7.45068200
H	2.12458200	3.57276100	5.87502800
C	-5.32067300	5.03098200	9.59502900
H	-3.81023100	6.40039600	8.94430000
H	-4.79076600	5.62668800	7.60894900
C	-5.24818100	3.52022400	9.41692700
N	1.92621600	3.98809700	8.28497800
O	-4.92826400	5.25483200	10.96060300
H	-6.31736800	5.41993700	9.38694100
C	-6.47938500	2.89553900	8.83488500
H	-5.05495100	3.06552900	10.38855900
H	1.77679000	4.14002900	9.27223500
H	2.86441600	3.88049700	7.92686700
H	-4.94973000	6.19568100	11.15009500
O	-6.76353200	3.60465800	7.61283200
H	-6.28168600	1.84783000	8.60837700
H	-7.31128600	3.02016700	9.52803300
P	-8.15605000	3.31387600	6.84942900
O	-7.95320700	1.82751500	6.27515500
O	-9.29168000	3.20363700	7.78246000
O	-8.32589200	4.30478400	5.74627900
C	-7.58292400	1.60766500	4.90227200
H	-8.96650500	3.21918000	8.68557700
C	-7.46960100	0.10062800	4.76127800

C	-6.17199900	2.10632400	4.54168100
H	-8.33130100	2.01308700	4.22134600
C	-8.03303400	-0.52325600	3.47613600
O	-6.07744400	-0.21331600	4.98323400
H	-8.02567700	-0.33485600	5.59139500
C	-5.28508500	0.96267300	5.02385300
H	-5.94901800	3.00232800	5.12093900
H	-6.08801200	2.19352900	3.45840500
O	-7.48911000	0.27369200	2.42448800
H	-7.66708600	-1.54552600	3.38065000
H	-9.11898100	-0.42949600	3.47540700
H	-5.01556600	1.15563600	6.06218800
P	-8.31230600	0.23694600	1.02329100
O	-8.07146000	-1.25175400	0.49598800
O	-9.77492200	0.33096500	1.20688800
O	-7.67377700	1.23542300	0.10960100
C	-7.08786400	-1.54433300	-0.50100100
H	-9.97844800	0.36106900	2.14458300
C	-7.10273600	-3.06114200	-0.63537600
C	-5.67278300	-1.26520100	-0.00249900
H	-7.29792700	-1.04453400	-1.44665700
C	-6.86284700	-3.53416600	-2.05417300
O	-6.04643000	-3.57002600	0.23028400
H	-8.06361200	-3.44165400	-0.28895500
C	-5.28511300	-2.51311200	0.78094200
H	-5.68933600	-0.40734300	0.66973200
H	-5.00468800	-1.15268800	-0.85631400

H	-6.74968000	-4.59814300	-2.06108400
H	-7.69592700	-3.26010700	-2.66717400
H	-5.97347200	-3.07840100	-2.43652200
N	-3.91490000	-2.82765900	0.77430300
H	-5.59641600	-2.37415700	1.81630000
C	-3.13206700	-2.97575500	-0.33199900
C	-3.06658300	-2.87318300	1.85000100
N	-1.87523700	-3.12544500	-0.07408400
H	-3.57848700	-2.96122200	-1.31525700
C	-1.80248600	-3.05072300	1.31617000
N	-3.39821400	-2.75496700	3.14942300
C	-0.70003800	-3.09975100	2.19907000
C	-2.34813400	-2.85110800	3.94882500
O	0.50266800	-3.19568600	1.87276700
N	-1.06812800	-2.98363300	3.52081700
N	-2.52519900	-2.79363300	5.27511300
H	-0.36331700	-2.99421000	4.24417600
H	-3.45517000	-2.69519200	5.65665200
H	-1.72880400	-2.84872700	5.89378300
N	-0.43274900	-2.60531800	7.12651800
C	-0.68576800	-2.32504500	8.36797800
C	0.95698800	-2.64501900	7.05790000
N	0.44972100	-2.24206100	9.15186200
H	-1.65862800	-2.16166900	8.80761100
C	1.83184700	-2.84448200	5.96447000
C	1.50696900	-2.45419800	8.30520000
C	0.46057100	-1.94412400	10.54531700

O	1.49639700	-2.94282700	4.76390900
N	3.15639500	-2.83379500	6.30808600
N	2.80315900	-2.46859300	8.64798700
C	-0.19389300	-0.62319900	10.88047000
O	-0.26700600	-2.93652900	11.23585700
H	1.48987000	-1.93720700	10.90404800
C	3.58566900	-2.67547600	7.60757200
H	3.86384600	-2.94479400	5.59584500
C	-0.68865600	-0.83442300	12.29713600
H	0.56068000	0.16336700	10.87657900
H	-1.04749800	-0.46707400	10.22088500
C	-1.00068200	-2.31303000	12.31668800
N	4.91574100	-2.69248900	7.77404400
O	0.32460500	-0.60316000	13.28003000
H	-1.57916600	-0.23904000	12.49859100
C	-2.48647500	-2.67664100	12.15246800
H	-0.64562900	-2.72847200	13.25985600
H	5.31055100	-2.58267200	8.69712800
H	5.52300200	-2.81514500	6.97630900
P	1.00048400	0.85633400	13.48495200
H	-2.57819800	-3.72600400	11.96452100
H	-3.01584600	-2.42712800	13.04824200
H	-2.89877300	-2.12968900	11.33042600
O	1.21126400	0.96664500	14.93796200
O	0.22294500	1.92146100	12.80725200
O	2.39938700	0.68647700	12.69225800
H	1.90463900	0.35995500	15.20769800

C	3.36953800	-0.25009700	13.13774700
C	4.69851500	0.13384000	12.59913200
H	3.10572600	-1.24479500	12.77840500
H	3.40439700	-0.24630400	14.22719500
O	4.77220400	-0.13010700	11.19006500
C	4.98771800	1.60565900	12.79242400
H	5.46744900	-0.44724200	13.10825900
C	4.99093800	1.05689500	10.44410200
O	6.40312000	1.68367300	13.05745400
C	4.70280200	2.17357800	11.41770400
H	4.38134000	2.06022100	13.57588600
H	6.03410300	1.10486300	10.13162300
P	7.10814800	3.04740300	13.51240700
H	5.37826900	3.00666200	11.22318700
H	3.65041600	2.44931200	11.35096300
O	8.13761100	2.66932500	14.47131600
O	6.10801800	4.06113700	13.96882600
O	7.72201900	3.60977500	12.13646100
H	7.84929300	2.89926300	15.35765700
C	8.82967500	2.84966700	11.62244800
C	9.23486000	3.56806100	10.34974700
H	8.49363600	1.84217500	11.37726000
H	9.65369500	2.88487900	12.33513700
O	8.27657900	3.24520600	9.32969100
C	9.34998600	5.09488700	10.32699300
H	10.19666600	3.16212000	10.03620600
C	8.06158700	4.39960300	8.53860700

O	10.72474200	5.16639600	9.92121900
C	8.08649600	5.50726500	9.58191600
H	9.27667800	5.45864400	11.35188800
N	6.84150800	4.20926800	7.87104200
H	8.87331800	4.52966700	7.82277900
H	10.99025900	6.08618800	9.84949000
H	8.26552500	6.45939600	9.08242100
H	7.22993500	5.38736200	10.24526700
C	5.58978600	4.15850900	8.43301600
C	6.64651200	4.04179800	6.52542800
N	4.63478900	3.98979500	7.56091400
H	5.47363300	4.25545000	9.50233100
C	5.29083800	3.86917400	6.35119700
N	7.63263400	4.00524400	5.59926300
C	4.81415900	3.63245600	5.03689700
C	7.13182900	3.74425900	4.38966800
O	3.64141200	3.42658400	4.69789400
N	5.80873700	3.59055000	4.08229200
N	7.99363500	3.75930400	3.35635300
H	5.57139900	3.44144000	3.11193000
H	8.98314700	3.87003300	3.52559000
H	7.65091600	3.65982000	2.41147200
N	7.16357400	3.60427600	0.71346700
C	8.02855900	3.90765900	-0.21043000
C	5.94842300	3.56793800	0.04915700
N	7.48808300	3.97991300	-1.45296300
H	9.08266200	4.09494800	-0.06831800

C	4.62114600	3.33022800	0.51192400
C	6.13119700	3.81344100	-1.29425800
C	8.18734000	4.25904800	-2.66394200
O	4.28699700	3.15537900	1.69566600
N	3.66958000	3.34312000	-0.47036700
N	5.20121100	3.74944400	-2.26143100
O	8.82694200	3.04907300	-3.09365700
C	9.31036900	5.29464000	-2.52302300
H	7.48065300	4.58853800	-3.42557400
C	3.97478200	3.54064500	-1.78301500
H	2.69770100	3.20264900	-0.23393400
C	9.79907100	3.42382900	-4.08949100
C	9.99025800	4.91923200	-3.82981800
H	8.87809300	6.28927900	-2.63235700
H	9.95656800	4.99277100	-1.69874100
N	2.94449800	3.54786700	-2.63441100
C	11.06723100	2.64303600	-3.79398700
H	9.43512600	3.23367700	-5.09918200
O	9.37818600	5.55328900	-4.92748200
H	11.05123000	5.16595000	-3.79116500
H	3.10594200	3.68970000	-3.62129400
H	2.00450700	3.41148400	-2.29094100
O	11.68051400	3.23246600	-2.62400100
H	10.81308000	1.60372400	-3.58573200
H	11.74881700	2.72419900	-4.64066600
H	9.45889600	6.50530000	-4.83351000
P	13.04082100	2.61521400	-2.06696400

O	12.60040300	1.26095500	-1.37193400
O	13.99596500	2.24047000	-3.11975000
O	13.61896500	3.55614700	-1.03439500
C	12.40636300	1.20361000	0.06205100
H	14.83732500	2.00762900	-2.72037800
C	12.25766900	-0.28775600	0.28442900
C	11.07094600	1.76008600	0.51026600
H	13.24402800	1.62817300	0.61539200
C	12.96041700	-0.94180700	1.44731000
O	10.82871500	-0.55431500	0.33350800
H	12.63231800	-0.77373900	-0.61643400
C	10.09653900	0.66361000	0.16001800
H	10.83713000	2.64985600	-0.07429200
H	11.08325200	1.89911300	1.59126800
O	12.69120200	-0.10838300	2.53082100
H	12.52162900	-1.92297200	1.62874200
H	14.03401000	-0.95433600	1.25951200
H	9.79377200	0.76280800	-0.88235400
P	13.71160200	-0.24689400	3.79146000
O	13.13948100	-1.47993400	4.64983600
O	15.08098300	-0.58866500	3.43196600
O	13.38364200	0.95009700	4.54201700
C	12.16209800	-1.30038500	5.72384200
H	15.61068100	-0.66800200	4.22866300
C	12.03987000	-2.74022600	6.14899800
C	10.72213800	-0.95337800	5.29720600
H	12.52990100	-0.65653400	6.52276800

C	11.77605300	-2.99082700	7.62279000
O	10.96012700	-3.27462000	5.34395000
H	12.95928600	-3.25697000	5.87376100
C	10.25859100	-2.25049600	4.64470100
H	10.75103300	-0.16429800	4.54580000
H	10.12042500	-0.76415300	6.18613400
H	11.63022800	-4.03820800	7.78596900
H	12.61327700	-2.65350200	8.19739200
H	10.89870100	-2.45740700	7.92381700
N	8.86079000	-2.52831900	4.77710200
H	10.54109000	-2.25870100	3.59195000
C	8.07312300	-2.52965500	5.89443800
C	7.99449000	-2.75563800	3.72004100
N	6.81831600	-2.74342100	5.67376300
H	8.51356500	-2.36005200	6.86588400
N	8.31943400	-2.82981300	2.40855000
C	6.73815100	-2.87602000	4.28952200
C	7.25663300	-2.99547800	1.63374300
C	5.62380900	-3.04664000	3.42774900
N	5.96999700	-3.09446700	2.10021200
N	7.42250500	-3.13865200	0.32672100
O	4.43377200	-3.10841000	3.77972200
H	5.25533800	-3.20912100	1.39582200
H	8.34709000	-3.07579400	-0.07483300
H	6.62427900	-3.31058700	-0.26776700