

Supplementary Information

Theoretical insight into the Zinc(II)-catalyzed synthesis of 2-indolyltetrahydroquinolines from *N*-propargylanilines and indoles: a cross-dehydrogenative coupling with temporally separated catalytic activity

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1. Additional computational results.

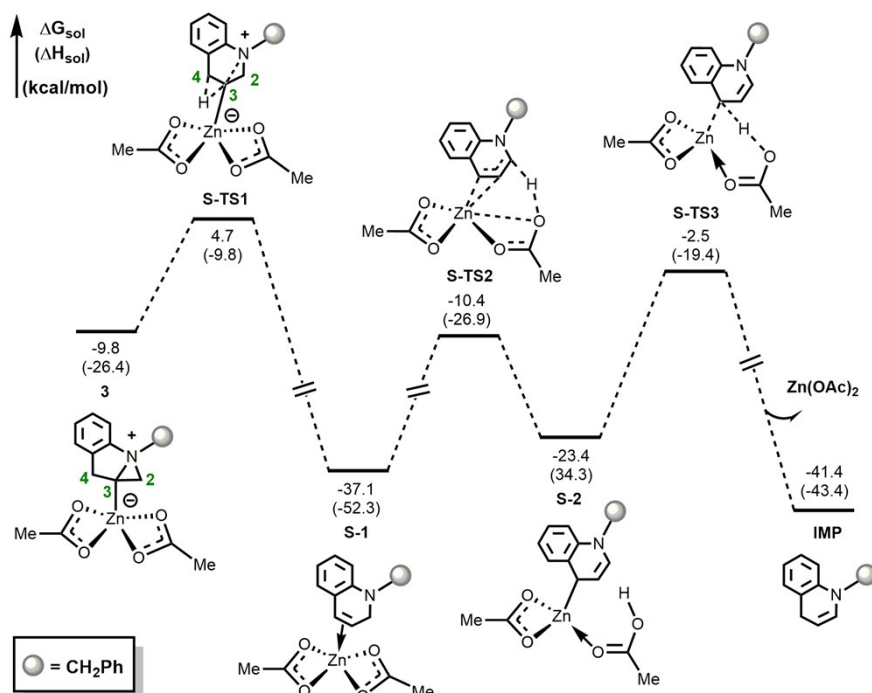


Fig. S1 Gibbs free energy profile for the formation of **IMP** from intermediate **3**.

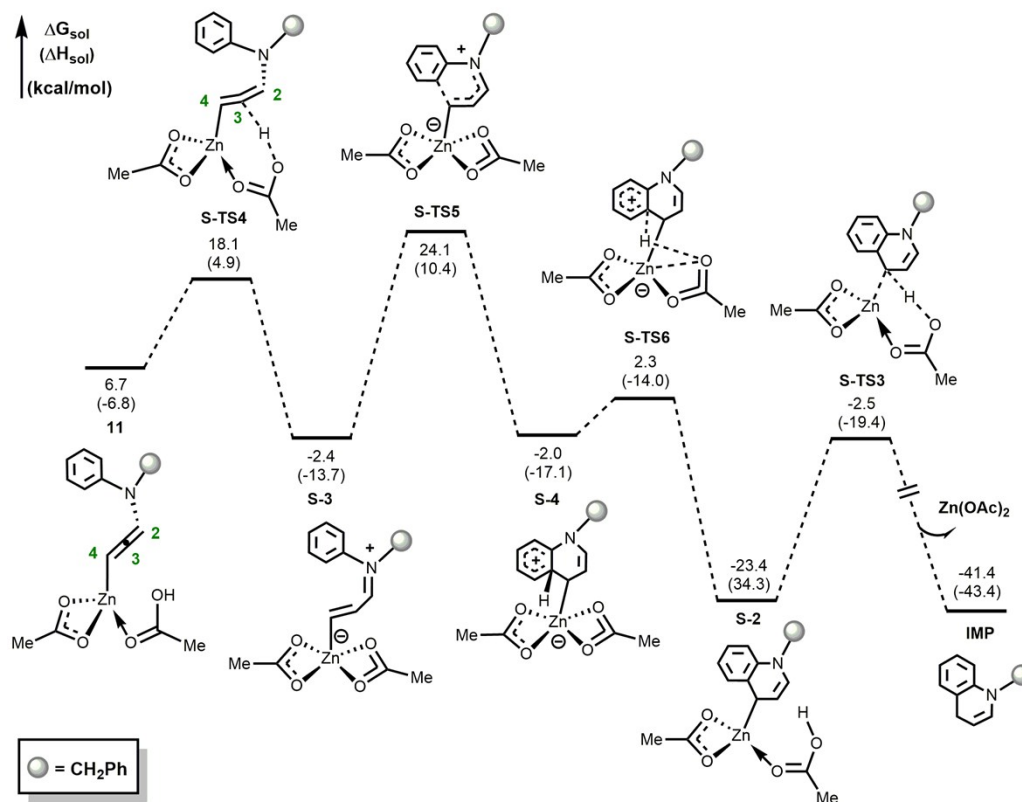


Fig. S2 Gibbs free energy profile for the formation of **IMP** from intermediate **11**.

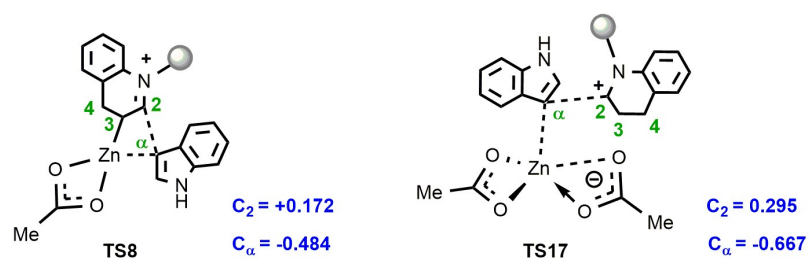


Fig. S3 Calculated NBO charges on transition states **TS8** and **TS17**.

2. Cartesian coordinates as well as electron energies

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Zn(OAc) ₂	Eelec= -2236.18521414 a. u.		
Zn	-0.00002700	-0.00172600	0.00436300
O	-1.68272800	-0.78404000	0.76140700
C	-2.33012800	0.01126200	-0.00212800
O	-1.67417500	0.79993900	-0.76241600
C	-3.83263700	0.00069200	-0.00852000
H	-4.17885200	-0.94255100	-0.44292600
H	-4.20423800	0.04129100	1.01827600
H	-4.22407000	0.83449800	-0.59042600
O	1.67510500	-0.77210800	-0.78685200
C	2.33018400	-0.01015300	0.00158100
O	1.68189700	0.75582300	0.79315800
C	3.83262300	0.00418500	-0.01138600
H	4.22272900	-0.83314100	-0.58923300
H	4.17305700	0.94347800	-0.45924700
H	4.21113100	-0.02462600	1.01299400

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R1	Eelec= -673.40162957 a. u.		
C	1.15890700	2.58563100	-1.05213700
C	0.81907500	1.23989200	-1.20214500
C	1.06349500	0.32680600	-0.16715600
C	1.65572800	0.78652800	1.01651700
C	2.00776200	2.12799900	1.15775600
C	1.75834100	3.03436100	0.12495400
H	0.95588900	3.28296000	-1.86034000
H	0.35780600	0.90827500	-2.12682300
H	1.82899600	0.07800500	1.81858700
H	2.46523500	2.46841400	2.08255300
H	2.02177200	4.08184600	0.23964100
N	0.73512800	-1.07342700	-0.26801700
C	-0.50719900	-1.38671100	-0.98521400
H	-0.47807500	-1.10480000	-2.05319200
H	-0.60040300	-2.48095200	-0.97176400
C	-1.73874500	-0.78586700	-0.33696100
C	-1.93113000	-0.87956400	1.04794200
C	-2.72807500	-0.17699400	-1.11570000
C	-3.08932200	-0.37566700	1.63763700
H	-1.15852100	-1.34055600	1.65574900
C	-3.89202900	0.32406800	-0.52829500
H	-2.58738300	-0.09342500	-2.19098500

C	-4.07521600	0.22642900	0.85098500
H	-3.22430300	-0.45251100	2.71305300
H	-4.64990500	0.79564900	-1.14769600
H	-4.97725700	0.61925100	1.31160000
C	1.85045800	-1.90775500	-0.75904400
H	1.47222900	-2.93406100	-0.84779000
H	2.16975700	-1.60496200	-1.77389300
C	3.02559300	-1.92856000	0.11405600
C	4.01740800	-1.99045900	0.79935300
H	4.88796300	-2.02997200	1.41213400

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l Eelec= -2909.60812691 a. u.

Zn	-2.26940500	-0.25756400	0.05955200
O	-3.99051300	0.73412700	-0.39576600
C	-3.30626900	1.66314900	-0.93562500
O	-2.03814900	1.56041700	-0.98722500
C	-3.99047600	2.88844300	-1.48532100
H	-5.05251900	2.70082900	-1.64491900
H	-3.88112000	3.70541100	-0.76404800
H	-3.51026700	3.20356200	-2.41418100
O	-2.79008000	-1.77485800	1.45318100
C	-1.95494900	-1.22507000	2.23096700
O	-1.28995500	-0.20638300	1.82850900
C	-1.75508800	-1.74011100	3.63341800
H	-2.50421800	-1.27828800	4.28582900
H	-1.90327700	-2.82088000	3.66605200
H	-0.76548700	-1.47236900	4.00619900
C	3.64106200	-2.59964200	-1.51471200
C	2.78726300	-1.54804300	-1.84853800
C	1.83649700	-1.09062200	-0.92604900
C	1.75129200	-1.69351700	0.33214400
C	2.60683400	-2.74631900	0.66364700
C	3.55157200	-3.20149700	-0.25732000
H	4.37641400	-2.94822200	-2.23458100
H	2.86318700	-1.08163300	-2.82775600
H	1.01623200	-1.31767600	1.03616100
H	2.53615300	-3.20911200	1.64391700
H	4.21680200	-4.02005900	0.00219800
N	0.92731600	-0.00978900	-1.23987600
C	1.56615100	1.30517900	-1.43845700
H	2.26430800	1.30791200	-2.29395900
H	0.75600200	2.00341400	-1.68053000
C	2.29095000	1.79919700	-0.20273200

C	1.64079200	1.83640000	1.03934300
C	3.60546500	2.26774900	-0.29393600
C	2.29795800	2.33894500	2.16161500
H	0.62768100	1.45651100	1.12641400
C	4.26256900	2.77625500	0.82905800
H	4.12061600	2.23454500	-1.25123800
C	3.60912300	2.81300000	2.06055700
H	1.78367100	2.36083400	3.11846700
H	5.28399700	3.13610500	0.74094400
H	4.11765900	3.20472300	2.93718600
C	-0.02687400	-0.33886700	-2.30196600
H	-0.54351100	0.58031200	-2.59398100
H	0.43450500	-0.76960300	-3.20810600
C	-1.04834400	-1.27742400	-1.81795600
C	-1.89700000	-2.04322600	-1.40572100
H	-2.58746700	-2.79116700	-1.08159100

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TS1 Eelec= -2909.59099517 a.u.

Zn	-2.11883700	-0.38698800	0.28743600
O	-3.80870300	-1.14076300	-0.51121600
C	-3.60266300	-0.54300600	-1.62368600
O	-2.56453100	0.16048600	-1.79118500
C	-4.63519900	-0.66207200	-2.72027400
H	-4.17689900	-0.50544900	-3.69803900
H	-5.13238100	-1.63276700	-2.67592100
H	-5.39552500	0.11236000	-2.57097900
O	-2.24752100	-0.44593700	2.42372800
C	-2.13775500	0.81369200	2.38393200
O	-2.02324700	1.41407100	1.25915100
C	-2.13839100	1.63170200	3.65366600
H	-1.19711800	2.18425600	3.73296100
H	-2.94390800	2.37045200	3.60971600
H	-2.26760700	0.99399200	4.52823600
C	2.90709200	-3.31076200	1.01953200
C	2.09229500	-2.68302400	0.04262500
C	2.50499400	-1.43742200	-0.53474500
C	3.70748300	-0.85043600	-0.06411300
C	4.45636500	-1.47756200	0.91430000
C	4.05938400	-2.70867600	1.47750900
H	2.60126100	-4.28048300	1.40198500
H	1.39408100	-3.31046600	-0.50138000
H	4.02647600	0.11127400	-0.44263400
H	5.36677900	-0.99852700	1.26338200

H	4.66649800	-3.17969900	2.24360100
N	1.69989800	-0.83078000	-1.46419200
C	2.08265400	0.44711300	-2.09033500
H	3.10284900	0.33961400	-2.47203000
H	1.43976900	0.55384600	-2.97024500
C	1.99012300	1.70149200	-1.23136300
C	0.85037000	1.98998400	-0.46976100
C	3.04341600	2.62464700	-1.24390600
C	0.77054900	3.16872500	0.27109900
H	0.00839400	1.30983500	-0.44268700
C	2.96351600	3.80959200	-0.50932400
H	3.93267500	2.41871500	-1.83679200
C	1.82666400	4.08251400	0.25273800
H	-0.12742200	3.35460300	0.85168200
H	3.79001700	4.51443000	-0.53088300
H	1.76369300	5.00235900	0.82720200
C	0.29393800	-1.21748100	-1.51942600
H	-0.25215900	-0.50925700	-2.14031300
H	0.17944400	-2.20792700	-1.98366500
C	-0.30645600	-1.32322000	-0.12927000
C	0.23739200	-1.88282500	0.86814600
H	0.24427100	-2.15679600	1.90518800

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2 Eelec= -2909.60798328 a. u.

Zn	-2.04099300	-0.63042000	0.19357400
O	-3.74841300	-0.89490100	-0.80605400
C	-3.48171700	-0.05786200	-1.74154500
O	-2.39371500	0.57324400	-1.77422000
C	-4.54108000	0.17706100	-2.79965900
H	-4.09643900	0.59582300	-3.70400500
H	-5.07251600	-0.75023800	-3.02465500
H	-5.27394000	0.89286000	-2.41129400
O	-2.35871000	-1.04314800	2.27075000
C	-2.21542100	0.19845000	2.46899800
O	-1.99114900	0.99369100	1.49555600
C	-2.33439500	0.76650700	3.86688400
H	-1.52541600	1.47737300	4.05489700
H	-3.27753200	1.31711700	3.94782900
H	-2.32202000	-0.02880300	4.61300600
C	2.85143100	-3.24218900	0.72451600
C	1.95696600	-2.49494100	-0.19315300
C	2.51083900	-1.19551000	-0.70306000
C	3.79726500	-0.74570900	-0.27253200

C	4.52933100	-1.51085700	0.59183700
C	4.05992900	-2.77151600	1.10380900
H	2.47895200	-4.19259800	1.09692200
H	1.74503300	-3.13986100	-1.06730000
H	4.17176200	0.21720400	-0.59409200
H	5.49916900	-1.14623600	0.91896000
H	4.68808300	-3.32959200	1.79032300
N	1.71505700	-0.50121700	-1.50167800
C	2.04843600	0.85465900	-1.99855600
H	3.06630400	0.83679200	-2.39772400
H	1.37858600	1.03186700	-2.84421900
C	1.90577600	1.94909200	-0.95392000
C	0.73391600	2.07319700	-0.19504800
C	2.94755300	2.86400500	-0.75957700
C	0.61699600	3.08629500	0.75558000
H	-0.09911200	1.39323300	-0.32754800
C	2.82372400	3.88821100	0.18170900
H	3.85801200	2.78230300	-1.35062200
C	1.65968800	3.99681800	0.94412700
H	-0.29664000	3.14076100	1.33861000
H	3.63771100	4.59403800	0.32091800
H	1.56581900	4.78859500	1.68193200
C	0.32172700	-0.97944000	-1.67182700
H	-0.26000800	-0.19181700	-2.14965700
H	0.34612400	-1.84087700	-2.36130500
C	-0.27710800	-1.42448000	-0.35091700
C	0.52771500	-2.17980800	0.38766500
H	0.29893900	-2.56979200	1.37329700

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TS2 Eelec= -2909.57008000 a. u.

Zn	-2.08843200	-0.54545200	0.18654300
O	-3.81219200	-0.89309400	-0.76569100
C	-3.54499300	-0.10131100	-1.73929900
O	-2.45199400	0.52423200	-1.79231200
C	-4.59623800	0.08958100	-2.81148300
H	-4.14116500	0.44518500	-3.73732300
H	-5.14558900	-0.83860700	-2.98216200
H	-5.31420500	0.84287500	-2.46897800
O	-2.28822300	-1.00869800	2.29882000
C	-2.18591200	0.23789500	2.48311100
O	-2.04111600	1.03464700	1.49230900
C	-2.25594300	0.81791300	3.87831300
H	-1.45771600	1.55078500	4.02234300

H	-3.20778700	1.34628600	3.99604100
H	-2.18977800	0.03111400	4.63050500
C	2.85680600	-2.97269600	1.04167800
C	1.97908700	-2.22763700	0.21245200
C	2.48277000	-1.21038600	-0.67061400
C	3.86560300	-0.91326900	-0.58588900
C	4.69780000	-1.65401700	0.23272100
C	4.20597700	-2.69788100	1.04561700
H	2.43925900	-3.74196500	1.68517400
H	1.01854300	-3.02706900	-0.18502500
H	4.27769600	-0.10979700	-1.18269000
H	5.75905900	-1.42402100	0.24488000
H	4.88041000	-3.26297200	1.67949200
N	1.61090100	-0.55042100	-1.47825700
C	1.89982800	0.78659000	-2.02960800
H	2.86409400	0.76182900	-2.54889200
H	1.14099300	0.96761100	-2.79513200
C	1.88489600	1.89804700	-0.99391200
C	0.73498600	2.12731900	-0.22601600
C	3.00677300	2.71041300	-0.79991900
C	0.71550900	3.13974400	0.73100100
H	-0.15529500	1.52402500	-0.36815700
C	2.98549000	3.73374700	0.15132200
H	3.90177200	2.54884200	-1.39748500
C	1.84155400	3.94589600	0.92145200
H	-0.18510500	3.28289400	1.31951900
H	3.86327200	4.35817100	0.29221300
H	1.82634100	4.73713000	1.66571300
C	0.28735500	-1.15844000	-1.68171200
H	-0.32656500	-0.48386600	-2.27707900
H	0.40594800	-2.10276300	-2.24385800
C	-0.35093400	-1.41626700	-0.33306000
C	0.44268200	-2.13092000	0.51324000
H	0.15210900	-2.47178500	1.50103900

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3 Eelec= -2909.63626653 a. u.

Zn	-1.94519400	-0.30177000	0.25150900
O	-3.61721800	-1.06332300	-0.56688100
C	-3.35335000	-0.64909300	-1.74838800
O	-2.28719200	-0.02031100	-1.99869400
C	-4.36844900	-0.90099700	-2.84231500
H	-3.88703400	-0.90293300	-3.82174900
H	-4.89852600	-1.83960500	-2.66913800

H	-5.10703800	-0.09201000	-2.82650300
O	-2.35320800	-0.12500500	2.38854100
C	-2.32433700	1.11990700	2.18773700
O	-2.08029600	1.58712700	1.01774200
C	-2.60382600	2.09206200	3.31138500
H	-1.90510600	2.93131800	3.27032900
H	-3.61175000	2.50041600	3.18200000
H	-2.54670500	1.59277000	4.27925500
C	3.00659900	-2.40223000	1.85263700
C	1.94436900	-1.90924200	1.09733300
C	2.20910500	-1.34717100	-0.15112300
C	3.48935500	-1.25078100	-0.68076200
C	4.54650400	-1.73724000	0.09463200
C	4.30729400	-2.30759600	1.34798500
H	2.82650900	-2.84526100	2.82788000
H	0.06486500	-2.85370400	1.66395100
H	3.67167700	-0.81593300	-1.65614400
H	5.56078500	-1.67207200	-0.28650500
H	5.14080100	-2.67889300	1.93656200
N	0.96860800	-0.94827500	-0.80505100
C	0.93955800	0.22186700	-1.74627200
H	1.46524500	-0.09660000	-2.65275600
H	-0.11494900	0.35992300	-1.99588300
C	1.56307100	1.47992400	-1.18867300
C	0.95291700	2.18777700	-0.14318900
C	2.74305300	1.98246500	-1.75290000
C	1.53377900	3.36137200	0.33796900
H	0.01362500	1.84806800	0.28303000
C	3.31779100	3.16112200	-1.27629300
H	3.20983000	1.45546700	-2.58225400
C	2.71593200	3.84980100	-0.22257900
H	1.04833900	3.90299100	1.14445500
H	4.23010400	3.53960500	-1.72822200
H	3.15954400	4.76791400	0.15201000
C	0.07670100	-2.11485000	-1.09367600
H	-0.57597800	-1.95297100	-1.94794800
H	0.60704300	-3.06589200	-1.08112900
C	-0.21506600	-1.34013300	0.14295300
C	0.46528000	-1.86440100	1.40846900
H	0.24993000	-1.21486200	2.26360100

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TS3 Eelec= -2909.60600922 a. u.

Zn	2.60565400	-0.12303800	0.08118300
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O	4.16373500	-0.16480600	-1.18113400
C	3.78226100	-1.27472300	-1.69980500
O	2.71843700	-1.83319900	-1.31124600
C	4.64947800	-1.91691100	-2.75736800
H	4.04576500	-2.53908000	-3.42025800
H	5.19388800	-1.15988800	-3.32460300
H	5.38425500	-2.56140600	-2.26248400
O	3.00847000	1.38534700	1.66896400
C	3.02301500	0.37562900	2.42563100
O	2.81149000	-0.79940100	1.95335300
C	3.32172100	0.51531000	3.90038800
H	2.74914200	-0.21208300	4.47945100
H	4.38476500	0.30703900	4.06336600
H	3.11360200	1.53093000	4.23999500
C	-1.54132600	3.61122300	-0.22138300
C	-1.07982700	2.30710400	-0.40929600
C	-1.97517700	1.28906400	-0.81266600
C	-3.33443900	1.60979000	-0.97860800
C	-3.77317300	2.91756600	-0.78293100
C	-2.88391300	3.92920700	-0.41318400
H	-0.83819800	4.37915000	0.09262600
H	1.05830800	2.48568500	-0.77485300
H	-4.04854300	0.84286800	-1.24972200
H	-4.82553000	3.14596200	-0.92541900
H	-3.23459900	4.94520100	-0.26407900
N	-1.46285000	-0.00303500	-0.99068500
C	-2.34818000	-1.10885600	-1.34831800
H	-2.92050300	-0.87705800	-2.26125400
H	-1.70106500	-1.95461100	-1.60494200
C	-3.30007100	-1.54103500	-0.24362800
C	-2.88453100	-1.58092000	1.09239700
C	-4.59312100	-1.96939900	-0.56459900
C	-3.74791300	-2.03797400	2.08778600
H	-1.88394500	-1.24560700	1.34843400
C	-5.45714200	-2.43233800	0.42959300
H	-4.92721100	-1.94153100	-1.59972800
C	-5.03633000	-2.46618600	1.75961500
H	-3.41334600	-2.06155100	3.12096500
H	-6.45853700	-2.75992600	0.16518600
H	-5.70781000	-2.82149400	2.53584000
C	-0.07662300	-0.09372800	-1.45719300
H	0.21972600	-1.14110900	-1.54902700
H	0.08953100	0.36290900	-2.46202900
C	0.82265000	0.61977900	-0.51688300

C	0.34114200	1.92580900	-0.11638800
H	0.72258700	2.21400800	0.87336900
47			
4	Eelec= -2909.61283360 a. u.		
Zn	2.79034300	-0.22058900	0.09012400
O	3.91388300	-0.76233800	-1.46819800
C	3.41546300	-1.94497100	-1.51402100
O	2.50886000	-2.29373400	-0.70946300
C	3.96335100	-2.91618000	-2.53425400
H	3.23773100	-3.70369200	-2.74315700
H	4.24403300	-2.39412300	-3.45117100
H	4.86739700	-3.38050200	-2.12538900
O	3.57867900	1.63173400	0.95921500
C	3.84961500	0.90258900	1.95450600
O	3.53997700	-0.34209900	1.95342800
C	4.57446700	1.46972600	3.15263000
H	4.27553900	0.95177600	4.06582400
H	5.65028000	1.31487400	3.01556200
H	4.39306500	2.54234300	3.23753800
C	-1.15281100	3.35403400	-1.11348500
C	-0.90932600	2.06560800	-0.64463600
C	-1.88195800	1.05618800	-0.81166900
C	-3.10404000	1.38398200	-1.41774400
C	-3.33973300	2.68719300	-1.85960200
C	-2.36733100	3.67588000	-1.72302400
H	-0.38610400	4.11419700	-0.98698900
H	1.17270900	2.46446500	-0.04397000
H	-3.87947900	0.63722300	-1.53045700
H	-4.29457000	2.92224200	-2.32074600
H	-2.55229300	4.68593600	-2.07410700
N	-1.57029500	-0.24355400	-0.35072600
C	-2.51972000	-1.33116500	-0.59344700
H	-2.82122200	-1.36982600	-1.65235100
H	-1.98073300	-2.26532100	-0.39792700
C	-3.75744400	-1.29345600	0.28905300
C	-3.69487600	-0.83915800	1.61110600
C	-4.97412900	-1.78061600	-0.20317800
C	-4.82826000	-0.87032600	2.42392800
H	-2.75574300	-0.45288000	1.99502700
C	-6.10771900	-1.81794100	0.61044100
H	-5.03578800	-2.13358700	-1.23045600
C	-6.03767600	-1.36124600	1.92733000
H	-4.76650300	-0.51096400	3.44723700

H	-7.04477400	-2.19765200	0.21329100
H	-6.91935100	-1.38450200	2.56110500
C	-0.17500300	-0.61758700	-0.44770700
H	0.02426400	-1.60118900	-0.00879800
H	0.18275800	-0.76746400	-1.51144900
C	0.85537500	0.34725400	-0.12486200
C	0.37968900	1.71853100	0.05959800
H	0.21178500	1.65267800	1.16711700

8

HOAc Eelec= -229.07765992 a. u.

O	0.69913500	1.20029400	-0.00014100
C	0.13348900	0.13786400	0.00001900
O	0.85512300	-1.01906300	0.00007600
C	-1.37487000	-0.03949400	0.00002300
H	-1.69855500	-0.59741100	0.88592400
H	-1.85163100	0.93979800	-0.00050200
H	-1.69853400	-0.59838000	-0.88527200
H	0.26294300	-1.78408200	0.00011900

47

TS4 Eelec= -2909.60493275 a. u.

Zn	-2.68500900	-0.63150600	-0.05670100
O	-2.34455200	-2.58497600	0.63825900
C	-2.72675200	-2.97245500	-0.51025500
O	-3.06697100	-2.11248900	-1.39301100
C	-2.81430700	-4.44258100	-0.83437900
H	-2.56560600	-4.61787400	-1.88280300
H	-2.16215800	-5.02104100	-0.17874300
H	-3.84633000	-4.77420000	-0.67643200
O	-3.38760600	2.26835500	-0.02375700
C	-4.23858600	1.56908300	0.54924200
O	-4.17570000	0.27746800	0.69429900
C	-5.48330300	2.20249100	1.14538200
H	-6.37273200	1.78096800	0.66723900
H	-5.54778900	1.95944600	2.21030600
H	-5.46646500	3.28400700	1.00905700
C	0.89540800	3.42567700	-1.22043300
C	0.69012400	2.16590600	-0.65873600
C	1.73363000	1.53097400	0.05442900
C	2.96993600	2.19032300	0.16293900
C	3.15388300	3.44950300	-0.41020300
C	2.12166000	4.08039100	-1.10159500
H	0.07626700	3.89745000	-1.75808700

H	-1.51707100	2.02237000	-0.30991700
H	3.79988100	1.71704500	0.67158100
H	4.12031800	3.93540200	-0.31054300
H	2.26741200	5.06013100	-1.54466000
N	1.52195200	0.24800300	0.59050500
C	2.53433800	-0.34943700	1.45614100
H	2.85569000	0.36088500	2.23436800
H	2.04777100	-1.17532300	1.98814900
C	3.75710000	-0.89994300	0.73455300
C	3.67170600	-1.40172900	-0.56835800
C	4.98395300	-0.96398300	1.40640600
C	4.79193100	-1.95802000	-1.18715600
H	2.72575200	-1.34250400	-1.09778900
C	6.10408000	-1.52486300	0.79122100
H	5.06401100	-0.57167500	2.41811500
C	6.01077400	-2.02372000	-0.50926100
H	4.71242400	-2.33953000	-2.20122800
H	7.04927500	-1.56590700	1.32510500
H	6.88234300	-2.45580000	-0.99228000
C	0.15498000	-0.17470300	0.86053900
H	0.10679000	-1.26620100	0.96223500
H	-0.24653600	0.19760700	1.83910100
C	-0.88153000	0.26286900	-0.08456500
C	-0.63340500	1.47833700	-0.79617000
H	-1.06173300	1.47229100	-1.81005500

39

5 Eelec= -2680.52849955 a. u.

Zn	3.01963500	-0.08983000	-0.13986600
O	4.86930400	0.22249100	0.57742100
C	5.16331300	-0.97671200	0.24221300
O	4.27011000	-1.68749400	-0.32343500
C	6.53571700	-1.52328000	0.52090900
H	6.64392600	-2.52841600	0.11464300
H	7.28719000	-0.85649600	0.08935300
H	6.70215000	-1.54022100	1.60231800
C	-0.83881500	3.47478900	0.68822500
C	-0.50020500	2.20722900	0.20176700
C	-1.51345100	1.37118800	-0.34651200
C	-2.83689000	1.84325500	-0.36764600
C	-3.14234600	3.11621100	0.11733600
C	-2.14995800	3.94456800	0.64257500
H	-0.05067600	4.09466600	1.10968800
H	-3.63635200	1.21751600	-0.74380800

H	-4.17332500	3.45767500	0.08222500
H	-2.39544400	4.93241000	1.01947300
N	-1.15329300	0.09353600	-0.78259400
C	-2.15747300	-0.75240100	-1.41414600
H	-2.69522200	-0.21208600	-2.21058600
H	-1.61644400	-1.56157900	-1.91810500
C	-3.16527300	-1.37780300	-0.45868500
C	-2.82523700	-1.67552200	0.86536200
C	-4.44005800	-1.72348200	-0.92347100
C	-3.74177600	-2.30782700	1.70646400
H	-1.84208700	-1.39553200	1.23119700
C	-5.35644500	-2.36067500	-0.08551100
H	-4.71861600	-1.49118600	-1.94945400
C	-5.00918700	-2.65492300	1.23422600
H	-3.46565500	-2.52829400	2.73400500
H	-6.34216000	-2.62055400	-0.46149600
H	-5.72214600	-3.14585700	1.89047900
C	0.22402000	-0.09456000	-1.26067800
H	0.39851900	-1.17364700	-1.31926300
H	0.34232100	0.29254200	-2.29483600
C	1.24658700	0.56590700	-0.35918200
C	0.85794700	1.68626700	0.28827300
H	1.54990400	2.24586800	0.91730200

47

TS5 Eelec= -2909.55741934 a. u.

Zn	-2.63491400	-0.62461100	-0.45945000
O	-4.40834500	-0.98733100	0.40627500
C	-4.70502100	-1.70002000	-0.61155400
O	-3.83651500	-1.81051500	-1.54402200
C	-6.02315200	-2.41190200	-0.70381100
H	-5.86434200	-3.47239400	-0.48071500
H	-6.73438400	-2.00119600	0.01248100
H	-6.41246900	-2.34494400	-1.72177600
C	0.67050200	3.16548200	-2.16215700
C	0.50739900	2.11987900	-1.26067600
C	1.64197800	1.41349700	-0.79631500
C	2.91144100	1.78000600	-1.26445700
C	3.05692900	2.85793700	-2.14529900
C	1.94304800	3.55465400	-2.60081400
H	-0.21050300	3.69988100	-2.51020700
H	3.78733500	1.22000500	-0.95435000
H	4.05244400	3.13740600	-2.47862400
H	2.05295500	4.39080300	-3.28427900

N	1.44988500	0.36454200	0.11258100
C	2.49249100	-0.09699800	1.01000100
H	3.22681600	0.70955900	1.11973300
H	2.05029500	-0.23527000	2.00542700
C	3.20242600	-1.38254100	0.59572500
C	3.19839800	-1.83383700	-0.72857200
C	3.89833200	-2.12586900	1.55879200
C	3.88150600	-2.99969300	-1.08414000
H	2.65671600	-1.26829000	-1.48077500
C	4.58486200	-3.28697500	1.20552200
H	3.89955500	-1.79243500	2.59453400
C	4.57819500	-3.72868600	-0.12006800
H	3.86822800	-3.33693100	-2.11701700
H	5.11863600	-3.85138600	1.96523800
H	5.10854500	-4.63544500	-0.39662400
C	0.15439400	-0.25526300	0.26054300
H	0.20964000	-1.34948300	0.30230700
H	-0.25422300	0.10339900	1.39065300
C	-0.95870400	0.31521400	-0.40780300
C	-0.84738800	1.69024300	-0.76030400
H	-1.68299200	2.13211500	-1.30757500
O	-0.46760500	0.70794700	2.69268100
C	-0.75328200	1.94308000	2.71036700
O	-0.93522700	2.70362800	1.70737700
C	-0.92163700	2.59794900	4.07243100
H	-1.97840100	2.84288400	4.21957200
H	-0.59040300	1.93231900	4.86964400
H	-0.36364000	3.53712000	4.10125900
H	-0.93634100	2.16203700	0.44359000

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6 Eelec= -2680.53283304 a. u.

Zn	2.86854800	0.05721700	-0.09263900
O	4.75201400	0.18723700	0.59700100
C	4.94320600	-1.01588100	0.20664400
O	3.98463100	-1.63408000	-0.35882000
C	6.28121200	-1.67131600	0.41209400
H	6.25862600	-2.71100600	0.08698200
H	7.04041200	-1.12221800	-0.15319800
H	6.55831700	-1.61040600	1.46809100
C	-1.17231800	3.62791300	0.67994200
C	-0.70169200	2.46773000	0.06417600
C	-1.63826600	1.51690700	-0.39930200
C	-3.01254100	1.77116500	-0.25402100

C	-3.45345100	2.95305500	0.33986800
C	-2.53692700	3.88747200	0.81797300
H	-0.44621200	4.35173600	1.04374800
H	-3.74228000	1.03802200	-0.57532100
H	-4.52066400	3.12940000	0.44000600
H	-2.87617000	4.80433600	1.29029000
N	-1.16620300	0.31989400	-0.97305400
C	-2.08374500	-0.66009300	-1.53318100
H	-2.79398600	-0.14534500	-2.19084600
H	-1.49178200	-1.30978200	-2.18840500
C	-2.84861200	-1.52519600	-0.53535000
C	-2.42092200	-1.68629200	0.78636200
C	-3.99053600	-2.21382900	-0.96578800
C	-3.11973500	-2.52329600	1.65913200
H	-1.54612700	-1.14730200	1.13649700
C	-4.68709200	-3.05308500	-0.09660900
H	-4.33744200	-2.09159200	-1.99000700
C	-4.25232100	-3.21053300	1.22136000
H	-2.77829500	-2.63485700	2.68443900
H	-5.57138600	-3.57881900	-0.44596700
H	-4.79531100	-3.86012200	1.90177100
C	0.17205400	-0.03692400	-0.79393700
H	0.36271300	-1.08138700	-1.02944500
C	1.14412600	0.79365700	-0.35746200
C	0.78556300	2.25551200	-0.15723500
H	1.34091500	2.69471300	0.68100900
H	1.10447900	2.83182200	-1.04253000

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TS6 Eelec= -2909.60433316 a. u.

Zn	-2.31961700	0.61053000	0.42307100
O	-3.14393400	2.29276600	-0.28342900
C	-4.09467100	2.12792900	0.55657700
O	-4.02711700	1.14332300	1.36566400
C	-5.27285800	3.05918800	0.56857300
H	-5.75311300	3.05577800	1.54747000
H	-4.96148000	4.06668600	0.28832200
H	-5.99831300	2.71142000	-0.17503100
C	0.72713000	-1.98125500	3.32537300
C	0.49061000	-1.64167000	1.99262500
C	1.56259800	-1.13593500	1.23250300
C	2.83546000	-0.99640100	1.79549000
C	3.04841200	-1.36206700	3.12502500
C	1.99462800	-1.84973300	3.89594700

H	-0.09657300	-2.37167800	3.91766600
H	-1.76555100	-1.32897800	-0.68935700
H	3.65121900	-0.58262100	1.21487000
H	4.03913600	-1.25196900	3.55516400
H	2.15621500	-2.12906000	4.93256900
N	1.31101900	-0.72598900	-0.11378200
C	2.40828000	-0.56351500	-1.08003000
H	3.10961500	-1.38801700	-0.92169300
H	1.96132200	-0.73145000	-2.06481500
C	3.14244500	0.76658900	-1.02698800
C	2.55166900	1.93019800	-0.52312800
C	4.44044900	0.84028000	-1.55055000
C	3.24268000	3.14336500	-0.54496300
H	1.55168400	1.89075100	-0.10161200
C	5.12981500	2.05221900	-1.57787300
H	4.91282100	-0.05757100	-1.94268800
C	4.53199800	3.20926700	-1.07392500
H	2.77086900	4.03710100	-0.14691300
H	6.13494800	2.09127500	-1.98773700
H	5.06849800	4.15329700	-1.09042900
C	0.05975400	-0.51420100	-0.52689700
C	-1.10243000	-0.87199800	0.19191300
C	-0.84792600	-1.86748600	1.32586100
H	-0.85915100	-2.87844500	0.88854900
H	-1.64465000	-1.85796600	2.07578000
H	-0.03423200	-0.05070800	-1.49950100
O	-0.18430500	-2.06065400	-2.54722300
C	-1.40683900	-2.29243300	-2.72998100
O	-2.36317700	-1.92764000	-1.96095900
C	-1.82029100	-3.09891100	-3.96249100
H	-2.18234000	-4.08365100	-3.64664700
H	-2.64910400	-2.60225100	-4.47595200
H	-0.97767000	-3.22886300	-4.64445900

40

7 Eelec= -2680.94391230 a. u.

Zn	1.83213100	-0.60592400	-0.72989700
O	1.51655500	-2.46541200	-0.13954200
C	2.47623900	-2.31309600	0.70491800
O	3.07012000	-1.18034400	0.72187600
C	2.88020900	-3.42739900	1.61666100
H	3.53886000	-3.06254000	2.40369600
H	1.99176500	-3.90122900	2.03966500
H	3.40645600	-4.18724800	1.02881100

C	1.32730100	3.03478200	1.25948600
C	0.89892700	2.40179900	0.09095100
C	-0.43741500	1.95402400	0.02180900
C	-1.31463700	2.14177000	1.09716000
C	-0.86114700	2.78206000	2.24833600
C	0.45820900	3.22821900	2.33336200
H	2.35293800	3.38688500	1.32034900
H	1.95410700	0.81709800	-2.81153600
H	-2.33073300	1.77091100	1.06030500
H	-1.54220100	2.92330000	3.08079100
H	0.81011200	3.72468500	3.23162600
N	-0.88033300	1.29212400	-1.17777500
C	-2.31048900	0.94710400	-1.36269400
H	-2.90107500	1.82758100	-1.10047400
H	-2.44902900	0.78658400	-2.43650400
C	-2.75159900	-0.27296800	-0.57069000
C	-1.85858500	-1.28655700	-0.20603600
C	-4.10937300	-0.41120100	-0.25555400
C	-2.31573100	-2.42567500	0.45764400
H	-0.79628700	-1.20139900	-0.41467100
C	-4.56648500	-1.55301700	0.40260100
H	-4.81360600	0.37008800	-0.53120200
C	-3.67095300	-2.56333700	0.75965100
H	-1.60780400	-3.20086400	0.73267200
H	-5.62142800	-1.65069300	0.63871200
H	-4.02745500	-3.45025300	1.27366700
C	0.00443900	0.82027200	-2.03582500
C	1.41629300	0.98143900	-1.87595400
C	1.80172200	2.25191100	-1.11552200
H	1.68754900	3.12274200	-1.77878000
H	2.85019600	2.23396800	-0.80821300
H	-0.39893300	0.24851200	-2.86807700

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8 Eelec= -3044.80753642 a. u.

Zn	-1.16761500	-0.58951000	-0.57676600
O	-0.70481600	1.28882000	0.07138500
C	-0.76363600	0.83777700	1.26815100
O	-1.06790400	-0.38985400	1.44530200
C	-0.46378600	1.73734000	2.43197500
H	-0.67227500	1.23647500	3.37671300
H	0.59253400	2.02286200	2.39495300
H	-1.05237300	2.65452500	2.34812300
C	1.79232300	-3.47012400	1.21554200

C	1. 63145600	-2. 66921600	0. 08476300
C	2. 52448200	-1. 59705700	-0. 10795100
C	3. 54889400	-1. 34631900	0. 81129300
C	3. 69175400	-2. 16818300	1. 92853700
C	2. 81316300	-3. 22986200	2. 13585400
H	1. 11073800	-4. 30219700	1. 36921800
H	-0. 42767200	-1. 88483600	-2. 60549700
H	4. 21644100	-0. 50521900	0. 67873400
H	4. 48829000	-1. 96754600	2. 63744800
H	2. 92005800	-3. 86806900	3. 00691600
N	2. 35780900	-0. 75518100	-1. 26295300
C	3. 43682300	0. 17328100	-1. 68334800
H	4. 36700200	-0. 40138100	-1. 69252300
H	3. 21938400	0. 43232900	-2. 72431400
C	3. 60360400	1. 43347800	-0. 85313000
C	2. 50347500	2. 17819500	-0. 41168700
C	4. 89840800	1. 90132000	-0. 59426800
C	2. 70279900	3. 37376100	0. 28105600
H	1. 48837100	1. 83531600	-0. 58790400
C	5. 09426600	3. 09927700	0. 09459400
H	5. 75909900	1. 33139600	-0. 93698700
C	3. 99533300	3. 83810600	0. 53472600
H	1. 84256800	3. 94668400	0. 61442600
H	6. 10290900	3. 45143000	0. 28736900
H	4. 14503400	4. 77008000	1. 07103100
C	1. 23485400	-0. 81941300	-1. 96862800
C	0. 17463900	-1. 71614100	-1. 71080200
C	0. 58042300	-2. 98544700	-0. 95998500
H	0. 98342900	-3. 71982200	-1. 67481300
H	-0. 27745700	-3. 47280900	-0. 48518400
H	1. 15960100	-0. 10549500	-2. 78507600
C	-3. 91621600	0. 34776500	-0. 78885300
C	-4. 40760000	-0. 02039900	0. 48783700
C	-5. 09656700	0. 86887600	1. 31834700
C	-5. 30411400	2. 15091400	0. 82700400
C	-4. 83665000	2. 53605700	-0. 44811100
C	-4. 13962600	1. 65251500	-1. 25956400
H	-5. 46114900	0. 57027800	2. 29593100
H	-5. 84281500	2. 87143800	1. 43389000
H	-5. 02898500	3. 54517500	-0. 79769900
H	-3. 78149300	1. 95980600	-2. 23705000
C	-3. 23529000	-0. 81881800	-1. 32815500
H	-3. 01565800	-0. 99605300	-2. 37475600
H	-3. 14458400	-2. 88976500	-0. 45025900

N	-4.08903400	-1.36034400	0.68421200
C	-3.41558000	-1.84460400	-0.38577000
H	-4.24797700	-1.87084800	1.54141500

63

TS7 Eelec= -3273.46613699 a. u.

Zn	-1.03835400	-0.68983200	-0.22661600
O	-0.08981100	-0.85106400	1.58551000
C	-0.52268800	-2.04843400	1.67367900
O	-1.24856900	-2.52667600	0.74424700
C	-0.14039600	-2.89976500	2.85714100
H	-0.87801100	-3.68672700	3.01993900
H	0.82758200	-3.36848000	2.64790500
H	-0.02831700	-2.28221000	3.74995300
C	2.74816300	-3.73524900	-0.65745200
C	2.13527700	-2.56299000	-1.10489800
C	2.81873700	-1.33999100	-0.93425600
C	4.09172700	-1.32698800	-0.34762600
C	4.68470400	-2.51477000	0.07764800
C	4.01293200	-3.72623800	-0.06906800
H	2.21835600	-4.67608500	-0.78583200
H	-0.69548600	-1.17790400	-2.61110900
H	4.61402200	-0.39170400	-0.19588600
H	5.66991200	-2.48259400	0.53286300
H	4.46523100	-4.65366000	0.26864200
N	2.20455400	-0.12507900	-1.36022900
C	2.93041100	1.15555100	-1.31968500
H	3.85965700	1.04071300	-1.89017800
H	2.30503000	1.86954700	-1.86404100
C	3.24498700	1.71472600	0.06002300
C	2.39763900	1.51926500	1.15627100
C	4.39272100	2.50390600	0.21553100
C	2.69766800	2.10934800	2.38558500
H	1.50925300	0.90513300	1.06791800
C	4.68731200	3.09799000	1.44304600
H	5.05921300	2.65716600	-0.63092400
C	3.83809000	2.90041600	2.53354700
H	2.03037300	1.94759000	3.22671800
H	5.57997500	3.70833700	1.54752800
H	4.06556900	3.35811700	3.49209800
C	0.94186400	-0.13653200	-1.84020800
C	0.15708900	-1.27168200	-1.93959500
C	0.79442600	-2.64062500	-1.81456900
H	0.94257900	-3.06855800	-2.81916100

H	0.13607800	-3.33383400	-1.28085600
H	0.52597800	0.84045300	-2.10625500
C	-3.79009100	0.29049100	0.32731200
C	-4.90556700	0.29523200	-0.54615100
C	-6.21047600	0.03720500	-0.12085700
C	-6.39308600	-0.22187800	1.23399300
C	-5.30474300	-0.22324700	2.12817300
C	-4.00941900	0.02794900	1.68846400
H	-7.04843000	0.04255400	-0.81221200
H	-7.39239900	-0.42377400	1.60807600
H	-5.48484000	-0.42312000	3.18036600
H	-3.17567400	0.02793700	2.38463700
C	-2.59269000	0.59743200	-0.45599200
H	-1.71267800	1.45456000	-0.12645200
H	-2.51488000	1.12484500	-2.61887500
N	-4.41936100	0.60318000	-1.81487600
C	-3.07287800	0.78787100	-1.75478700
H	-4.98707500	0.71941900	-2.64078600
O	-0.87417200	2.49375600	0.18121100
C	-0.39802600	3.07416800	-0.86239200
O	-0.33984800	2.57387500	-2.01078600
C	0.15188500	4.47801900	-0.62532400
H	0.43416900	4.94849500	-1.56883400
H	-0.59280800	5.08917200	-0.10721100
H	1.02769200	4.41666600	0.02942500

55

9 Eelec= -3044.38110990 a. u.

Zn	-0.81461500	-1.60310100	0.37620000
O	0.55161100	-1.01201100	1.80956300
C	0.82940800	-2.24133400	1.99750700
O	0.26094200	-3.13040000	1.28462300
C	1.85350300	-2.63117300	3.03264700
H	1.77613100	-3.69129300	3.27574500
H	2.85169200	-2.43033700	2.62850700
H	1.73195300	-2.02090900	3.93015400
C	4.10032400	-1.98231300	-0.97428000
C	2.83497000	-1.45410000	-1.23838200
C	2.67091200	-0.05182400	-1.20541700
C	3.77201200	0.77048000	-0.92116100
C	5.02559200	0.21451300	-0.67224300
C	5.19742300	-1.16763800	-0.69390500
H	4.22324400	-3.06263600	-0.99883100
H	-0.50251900	-2.19902700	-2.01270600

H	3.65205800	1.84495400	-0.86516600
H	5.86237600	0.87050100	-0.45181700
H	6.16931300	-1.60803100	-0.49376400
N	1.39331700	0.51584400	-1.45452200
C	1.21638200	1.96359700	-1.56458200
H	1.96370500	2.35308100	-2.26719100
H	0.24355900	2.12254000	-2.04160300
C	1.26900300	2.76310100	-0.26837500
C	1.13856400	2.16889700	0.99079400
C	1.41370600	4.15491600	-0.35618600
C	1.14261100	2.96195700	2.14212300
H	1.05262900	1.09197400	1.09062100
C	1.41410300	4.94343400	0.79335300
H	1.52344100	4.62537700	-1.33145800
C	1.27686300	4.34688200	2.04934000
H	1.04100200	2.48521300	3.11261700
H	1.52508100	6.02087600	0.70904100
H	1.27855900	4.95857800	2.94693200
C	0.31886900	-0.30692900	-1.66002900
C	0.37205000	-1.66799900	-1.64641300
C	1.69318700	-2.39403600	-1.59201300
H	1.89323900	-2.86071300	-2.56994400
H	1.65194800	-3.21723300	-0.86910700
H	-0.62340900	0.20406700	-1.83518200
C	-3.36274600	0.01444200	-0.11256200
C	-4.74384500	-0.22815200	-0.36857800
C	-5.65692700	0.79818000	-0.63199900
C	-5.17446500	2.10309700	-0.63663300
C	-3.81653100	2.37670900	-0.37662500
C	-2.91683800	1.34932500	-0.11372100
H	-6.70594100	0.58770900	-0.82424900
H	-5.85727500	2.92413400	-0.83656500
H	-3.47302600	3.40748000	-0.37208200
H	-1.87867000	1.58114700	0.11554400
C	-2.70374100	-1.25793800	0.11703800
H	-3.66416300	-3.26922400	0.09181700
N	-4.92629200	-1.59277400	-0.29562200
C	-3.70800100	-2.19201500	-0.00775400
H	-5.80442400	-2.07188200	-0.41145700

16

R2 Eelec= -363.82233437 a. u.

C	0.25002800	0.75163800	-0.00000100
C	0.24798600	-0.67175500	-0.00003300

C	-0.93552000	-1.41917000	-0.00000500
C	-2.13587100	-0.71888300	0.00003500
C	-2.15918500	0.69211700	0.00001000
C	-0.98264700	1.42952600	-0.00001900
H	-0.91785200	-2.50572500	-0.00002100
H	-3.07338700	-1.26741300	0.00006700
H	-3.11628000	1.20577600	0.00001400
H	-1.01084500	2.51583100	-0.00003700
C	1.62636400	1.16711700	0.00005400
H	1.99894100	2.18160900	-0.00000300
H	3.46491000	-0.08511000	0.00001500
N	1.56656000	-1.08146800	-0.00021500
C	2.39025100	0.02995800	0.00005600
H	1.88015300	-2.03797100	0.00088700

55

TS8 Eelec= -3044.32597706 a. u.

Zn	1.67173800	0.08145100	-1.30659500
O	3.45013900	0.02024300	-0.28605000
C	3.94942200	-0.61636000	-1.27104100
O	3.22540400	-0.88682800	-2.28162600
C	5.39543900	-1.04753700	-1.22460100
H	5.69169600	-1.52023400	-2.16113000
H	6.03008700	-0.17974800	-1.02407700
H	5.53525000	-1.74913700	-0.39649800
C	1.46721000	3.87048300	0.82844000
C	0.59904600	2.99488600	0.17811100
C	-0.20861200	2.13625500	0.95343500
C	-0.13033900	2.17061900	2.35255800
C	0.73582200	3.06818900	2.98016200
C	1.53836800	3.91894400	2.22267300
H	2.09143300	4.52809600	0.22888400
H	0.01762500	1.39953100	-2.81625100
H	-0.71835000	1.49021700	2.95738700
H	0.78873300	3.08577800	4.06476900
H	2.21910600	4.61014400	2.71017900
N	-1.09700500	1.26865800	0.26000000
C	-2.20064600	0.62590500	0.99335500
H	-1.84593400	-0.29557000	1.47110800
H	-2.49734800	1.32019300	1.78382800
C	-3.40723700	0.32823900	0.12561500
C	-3.87001500	-0.98368500	-0.02365700
C	-4.10473300	1.36929900	-0.50472600
C	-5.01201900	-1.25285300	-0.78287000

H	-3.33266900	-1.79646700	0.45776800
C	-5.23998700	1.10217500	-1.26756400
H	-3.74945500	2.39091200	-0.39741100
C	-5.69848900	-0.21127500	-1.40655900
H	-5.36238400	-2.27590500	-0.88691100
H	-5.77133200	1.91781100	-1.74973500
H	-6.58582400	-0.41873000	-1.99771600
C	-0.69934400	0.72689500	-0.94070100
C	0.30844600	1.47090200	-1.76392400
C	0.44382800	2.92844100	-1.31988500
H	-0.44771000	3.51920200	-1.60060400
H	1.29809500	3.40835700	-1.80681000
H	-1.51456400	0.22914000	-1.45023300
C	0.31726300	-1.82094300	0.77639800
C	-0.12795400	-3.16780700	0.66517000
C	-0.08086200	-4.07819200	1.72465400
C	0.43013500	-3.62002400	2.93492300
C	0.89137200	-2.29621800	3.07379600
C	0.84724700	-1.40078400	2.00996800
H	-0.42128500	-5.10381100	1.60946000
H	0.48316400	-4.29737100	3.78238200
H	1.29997400	-1.97490700	4.02758900
H	1.22898000	-0.39097300	2.12572700
C	0.14995900	-1.16759700	-0.52044600
H	-0.72167600	-2.09498900	-2.35599200
N	-0.57114100	-3.33615100	-0.63763900
C	-0.40741000	-2.15446200	-1.32043200
H	-0.91053200	-4.20089800	-1.03010100

55

10 Eelec= -3044.37511170 a. u.

Zn	1.89625500	0.11958100	-0.98228500
O	3.80210900	0.79164200	-0.64954500
C	4.23056800	-0.28060700	-1.19018900
O	3.39597200	-1.15357500	-1.59412100
C	5.71246200	-0.52629700	-1.31588900
H	5.92120600	-1.18300800	-2.16177200
H	6.24950700	0.41825300	-1.41594100
H	6.06254600	-1.02163400	-0.40356900
C	0.58567900	3.89790500	0.01891600
C	-0.11962200	2.75390800	-0.34347800
C	-0.88029900	2.05909900	0.62993200
C	-0.90359400	2.54997300	1.94827200
C	-0.20892000	3.71643600	2.28185400

C	0.54161400	4.39614800	1.32598300
H	1.16829100	4.41466300	-0.74045700
H	0.02962300	0.20975800	-2.62862100
H	-1.44660200	2.02154100	2.72407400
H	-0.24702300	4.07907500	3.30564400
H	1.08954200	5.29565400	1.58926300
N	-1.60820000	0.93728600	0.20411500
C	-2.65675300	0.38854900	1.05428800
H	-2.27467900	-0.37837500	1.74735000
H	-3.03861900	1.20916400	1.66916000
C	-3.82741200	-0.18795800	0.27120500
C	-4.34302800	-1.45032600	0.58267100
C	-4.44705600	0.56185100	-0.73832900
C	-5.45797200	-1.95430200	-0.09242500
H	-3.86732500	-2.04272500	1.36049800
C	-5.55561900	0.05972600	-1.41862600
H	-4.04435100	1.53908600	-0.99026700
C	-6.06685500	-1.20071800	-1.09613600
H	-5.84725600	-2.93582400	0.16441800
H	-6.02433100	0.65291300	-2.19909500
H	-6.93201200	-1.59093800	-1.62468100
C	-1.01961800	-0.01100800	-0.77953800
C	0.10669000	0.65009200	-1.62598400
C	-0.12061400	2.16746200	-1.72784700
H	-1.09371100	2.37415000	-2.20719600
H	0.64487200	2.64430400	-2.34935700
H	-1.84687300	-0.30341900	-1.43936800
C	0.61567000	-1.39400800	0.78044800
C	0.86429500	-2.78501200	0.97000000
C	1.89034000	-3.25571100	1.79178200
C	2.68748400	-2.31349000	2.43622800
C	2.45133000	-0.93496800	2.28603800
C	1.42120500	-0.46107400	1.47514700
H	2.06283100	-4.32008100	1.92424100
H	3.49636600	-2.65030600	3.07744000
H	3.07384100	-0.22483300	2.82096300
H	1.19302900	0.60107000	1.45584200
C	-0.50088200	-1.27940900	-0.13538500
H	-1.66451200	-2.90471100	-1.09568500
N	-0.07074600	-3.47099100	0.22510300
C	-0.87663700	-2.56422800	-0.43842800
H	-0.11878400	-4.47200100	0.12742400

TS9	Eelec= -3273.46889744 a. u.		
Zn	2.05541200	1.00946200	0.23736000
O	3.50326600	0.63514900	1.72936300
C	4.12231000	-0.03189700	0.84815100
O	3.62704200	-0.14466800	-0.32694900
C	5.43311500	-0.70762000	1.16147400
H	6.18892200	-0.39518800	0.43555000
H	5.76246700	-0.46870200	2.17251900
H	5.31325900	-1.79043500	1.05800100
C	-1.02982300	-1.87444100	3.54216600
C	-0.85763600	-1.22912600	2.31765000
C	-1.91876400	-1.23445400	1.37303500
C	-3.12145900	-1.88534700	1.71988000
C	-3.2554600	-2.53741100	2.94454900
C	-2.21180700	-2.54142700	3.86811000
H	-0.20745600	-1.85147400	4.25410300
H	-0.63935900	1.30142600	1.72430300
H	-3.96861600	-1.86204300	1.04442400
H	-4.19527100	-3.03107200	3.17733100
H	-2.31752600	-3.04110400	4.82598100
N	-1.76125900	-0.61497800	0.12871600
C	-2.72595100	-0.78387900	-0.94159100
H	-2.17495000	-0.77180000	-1.89051800
H	-3.16180500	-1.78732100	-0.87341000
C	-3.84028100	0.25803700	-1.01688300
C	-4.60229500	0.35838800	-2.18960500
C	-4.13533100	1.11214300	0.05056900
C	-5.63882500	1.28496800	-2.29165600
H	-4.37903300	-0.29492700	-3.03092300
C	-5.17124800	2.04482500	-0.05067900
H	-3.55271000	1.04391700	0.96378400
C	-5.92673400	2.13399000	-1.21962000
H	-6.21830900	1.34923000	-3.20863600
H	-5.38657100	2.70106100	0.78811200
H	-6.73161200	2.85929700	-1.29779900
C	-0.65420900	0.30613400	-0.15803500
C	0.08782200	0.73619800	1.11950100
C	0.42242500	-0.50086300	1.97915800
H	0.94772000	-0.20533200	2.89242400
H	1.10688400	-1.17692900	1.44660000
H	-1.09522200	1.21471400	-0.59594900
C	0.74224100	-1.62480300	-1.41500900
C	1.64318300	-1.60461500	-2.51450800
C	2.26752100	-2.75887500	-2.99996900

C	1.96430600	-3.95955600	-2.37336600
C	1.06163100	-4.00965100	-1.29037600
C	0.45046600	-2.86164600	-0.80552400
H	2.96132900	-2.71574700	-3.83444700
H	2.42827400	-4.87666100	-2.72434900
H	0.84296400	-4.96679200	-0.82634200
H	-0.23668800	-2.91772200	0.03110300
C	0.31357800	-0.25729100	-1.19588000
H	0.84600400	1.55837700	-2.38110300
N	1.73378400	-0.30125500	-2.95664200
C	0.94636400	0.50316200	-2.16619500
H	2.39812000	0.03489200	-3.63534600
O	2.30152700	2.91328200	-0.35025000
C	1.59701500	3.71839300	0.32902300
O	0.70760000	3.33128100	1.16352900
C	1.81302200	5.20180700	0.17964100
H	2.43947000	5.54643000	1.00959100
H	2.32442500	5.42081900	-0.75806400
H	0.86044600	5.73163700	0.24004500
H	0.60878300	2.11003200	1.11809800

48

P Eelec= -1037.32732295 a. u.

C	3.22822800	-3.48320600	-0.79591800
C	3.09777500	-2.40334800	-1.66722800
C	2.19330100	-1.37802000	-1.40232900
C	1.37758100	-1.39970300	-0.24976600
C	1.53306100	-2.48534300	0.65020800
C	2.43916300	-3.50437600	0.35324700
H	3.92957600	-4.28588200	-1.00118900
H	3.70552600	-2.34761000	-2.56640100
H	2.13745900	-0.55001400	-2.09715700
H	2.52773800	-4.33204800	1.05418500
C	0.72095100	-2.52527900	1.92266500
H	0.56106000	-3.56301400	2.23635400
H	1.27214300	-2.03919200	2.74195500
C	-0.61354700	-1.81390600	1.72123300
H	-1.22757500	-2.36659900	1.00197100
H	-1.18129900	-1.75876900	2.65512200
N	0.43634300	-0.38354300	-0.01332900
C	0.52608600	0.86369700	-0.75620800
H	-0.40549800	1.40664900	-0.57783000
H	0.53162700	0.65285300	-1.83267600
C	1.69140700	1.79296500	-0.41993700

C	2.57180400	1.55291900	0.63895900
C	1.86497300	2.95547700	-1.18495800
C	3.59871900	2.45484100	0.93077100
H	2.46357400	0.64937600	1.22945000
C	2.88736600	3.85785400	-0.89616800
H	1.18970700	3.15482900	-2.01496800
C	3.76005100	3.61027500	0.16684600
H	4.27579000	2.24868000	1.75532400
H	3.00513800	4.75289000	-1.50111000
H	4.55942000	4.31015700	0.39308800
C	-0.40122000	-0.37871900	1.20795200
H	0.11435300	0.18262500	2.00737100
C	-2.74542700	-0.02729900	0.00041900
C	-3.85793700	0.82159100	0.25705400
C	-5.02501700	0.78314600	-0.51368900
C	-5.06996900	-0.12627500	-1.56379300
C	-3.97722200	-0.97263600	-1.84314700
C	-2.81936700	-0.93025400	-1.07664900
H	-5.86414700	1.43987900	-0.30120700
H	-5.96106100	-0.18287500	-2.18216400
H	-4.04371700	-1.66708000	-2.67556100
H	-1.97856700	-1.57582600	-1.30913700
C	-1.73208200	0.29436800	0.98238700
C	-2.25382800	1.29611100	1.76323100
H	-1.80820200	1.81130300	2.60311900
N	-3.52991600	1.61304200	1.33998000
H	-4.11715000	2.32390400	1.74381300

7

OAc- Eelec= -228.49744387 a. u.

O	0.69808300	1.16515100	0.00027700
C	0.22047500	0.00178400	-0.00125500
O	0.80608600	-1.10997200	0.00030000
C	-1.35395700	-0.05323400	-0.00043300
H	-1.73431800	-1.08140900	-0.02949000
H	-1.74638500	0.44672900	0.89640400
H	-1.75176400	0.50194300	-0.86140800

47

TS10 Eelec= -2909.58318851 a. u.

Zn	-2.00448400	-1.14157700	-0.41168200
O	-2.33404300	0.53289500	-1.31257800
C	-1.71661200	1.40504300	-1.99063300
O	-0.51363000	1.33069600	-2.39908600

C	-2.46454200	2.67384500	-2.33109400
H	-3.53408900	2.47701300	-2.41416600
H	-2.30812400	3.38358400	-1.51092600
H	-2.07453600	3.11775900	-3.24782000
O	-3.72724800	-2.15992000	-0.00916000
C	-3.58789600	-1.81840600	1.21203200
O	-2.58405800	-1.11308900	1.55688600
C	-4.62058900	-2.22911700	2.22905500
H	-5.50909200	-1.60165900	2.10176400
H	-4.92324800	-3.26448200	2.05783300
H	-4.23923300	-2.10189500	3.24240500
C	4.80257600	-2.40812500	-0.20094800
C	3.71810000	-1.72524600	-0.74845800
C	3.30636900	-0.48520600	-0.21946800
C	4.01624100	0.02826900	0.88640100
C	5.10314400	-0.66277600	1.41733500
C	5.51101500	-1.88512500	0.88131500
H	5.09828200	-3.35888900	-0.63669700
H	3.19852900	-2.15360000	-1.59783100
H	3.69641500	0.95167600	1.35597900
H	5.62553600	-0.24174200	2.27225500
H	6.35521000	-2.42157000	1.30276500
N	2.22004700	0.21734500	-0.76279400
C	2.09210500	1.65893600	-0.58433400
H	3.08051500	2.06797400	-0.34831300
H	1.80597400	2.10250800	-1.54586800
C	1.08069600	2.10924000	0.46537100
C	0.43638900	1.20403800	1.31374300
C	0.77098300	3.47269900	0.57484600
C	-0.50999100	1.64543000	2.24444700
H	0.67739100	0.14791000	1.24353200
C	-0.16186200	3.91836800	1.51052700
H	1.26195400	4.18939200	-0.08069400
C	-0.81028100	3.00357500	2.34590700
H	-1.01920900	0.92053500	2.87181400
H	-0.38773400	4.97883100	1.58456500
H	-1.54557900	3.34872600	3.06704500
C	1.33166900	-0.40290600	-1.71839200
H	0.29232100	0.43081000	-2.00225000
H	1.72088300	-0.51310200	-2.74141800
C	0.55882900	-1.46517600	-1.28283000
C	-0.36267400	-2.23251900	-0.89095800
H	-0.36817300	-3.28760100	-0.65564600

47

11 Eelec= -2909.60026852 a. u.

Zn	-1.85077200	-1.33200900	-0.58843900
O	-2.69659300	0.49945400	-0.92539900
C	-2.35124700	1.60043300	-1.36585400
O	-1.15345700	1.87502800	-1.83727200
C	-3.28208700	2.77773300	-1.38349600
H	-4.31203800	2.44103100	-1.27349900
H	-3.02071800	3.42469100	-0.53894700
H	-3.15338000	3.35663500	-2.30018300
O	-3.40477800	-2.51575300	-0.03376700
C	-3.10480000	-2.28096400	1.18525100
O	-2.13213400	-1.50611100	1.45369000
C	-3.90102900	-2.93191700	2.28678800
H	-4.96594700	-2.73834300	2.13229800
H	-3.75943400	-4.01616500	2.23990300
H	-3.58772800	-2.56429700	3.26381400
C	4.46704500	-2.50177100	-0.42202600
C	3.62597100	-1.56078600	-1.00591500
C	3.29870300	-0.36902800	-0.32668900
C	3.83828800	-0.16986200	0.95888500
C	4.68989900	-1.11846100	1.52698400
C	5.01331500	-2.29128300	0.84743800
H	4.70589000	-3.40761600	-0.97309500
H	3.22620200	-1.73484600	-1.99826400
H	3.57481300	0.71119400	1.53325800
H	5.08898400	-0.93644500	2.52130300
H	5.66998600	-3.02946200	1.29707500
N	2.49162400	0.60409100	-0.94162600
C	2.43106300	1.96976500	-0.44488800
H	3.39264600	2.21218300	0.02076700
H	2.34149300	2.63759500	-1.31373400
C	1.28270000	2.28069500	0.51363900
C	0.56603500	1.26804800	1.16279500
C	0.91902300	3.61457400	0.74332200
C	-0.49938800	1.57771400	2.01419900
H	0.83675600	0.23020800	0.99867500
C	-0.13347400	3.92974600	1.60289900
H	1.46060500	4.41333900	0.24034100
C	-0.85102400	2.91065100	2.23673900
H	-1.05321000	0.77126400	2.48579700
H	-0.39780000	4.97009200	1.77342100
H	-1.67489900	3.15488900	2.90161900
C	1.52288700	0.27844000	-1.93530600

H	-0.51535700	1.12435700	-1.73007900
H	1.55040400	0.89797300	-2.83398800
C	0.64553600	-0.71191000	-1.82046000
C	-0.22210600	-1.66055800	-1.62780600
H	0.03834500	-2.67512700	-1.93892100

39

12 Eelec= -2680.47549959 a. u.

Zn	-2.74182200	-0.94736600	-0.39974100
O	-4.66253500	-0.34568000	-0.49473400
C	-4.49326100	0.22752200	0.63555500
O	-3.35076700	0.14508000	1.19564600
C	-5.62378400	0.98011800	1.27964100
H	-5.94489700	1.78635400	0.61358100
H	-6.47780100	0.30907700	1.40845700
H	-5.31983400	1.39009500	2.24213600
C	2.71011000	-3.61147300	0.63491400
C	2.23048400	-2.68649200	-0.28685000
C	2.52384800	-1.31493500	-0.14487600
C	3.30549500	-0.91346900	0.95593600
C	3.78764600	-1.85416200	1.86654700
C	3.49518300	-3.20894600	1.71906200
H	2.47514200	-4.66341800	0.49539900
H	1.64208200	-3.02165800	-1.13220900
H	3.51665300	0.13735300	1.11977100
H	4.38681000	-1.51340400	2.70669400
H	3.86547900	-3.93675500	2.43435600
N	2.08790500	-0.37865600	-1.10073400
C	2.76910100	0.89746800	-1.26101700
H	3.81444900	0.76235700	-0.96261300
H	2.79038800	1.13304900	-2.33452800
C	2.16631800	2.08730500	-0.52018100
C	1.21082800	1.92823600	0.48885900
C	2.58926800	3.38210000	-0.85086000
C	0.69072800	3.04091800	1.15572900
H	0.87285600	0.93121100	0.75209800
C	2.07467700	4.49319800	-0.18431600
H	3.32638400	3.52125200	-1.63942600
C	1.12064300	4.32542900	0.82285200
H	-0.05217200	2.89890800	1.93566600
H	2.41374700	5.48979300	-0.45355000
H	0.71534100	5.19003000	1.34068800
C	0.91849700	-0.54401000	-1.87789300
H	0.96489600	-0.05089900	-2.84869100

C	-0.18252900	-1.19013500	-1.54472200
C	-1.27578300	-1.83607800	-1.24121900
H	-1.34859300	-2.90252600	-1.47071700

47

TS11 Eelec= -2909.58988475 a. u.

Zn	-2.10042800	-0.54757600	0.18959000
O	-3.64685600	0.60360200	0.54739900
C	-4.15692400	1.25659200	-0.41602600
O	-3.72335700	1.21460700	-1.61608600
C	-5.33380500	2.15167600	-0.12411700
H	-4.98605700	3.00931400	0.46103200
H	-5.79146800	2.50497900	-1.04789500
H	-6.06145300	1.61280500	0.48740500
O	-1.87710900	-2.25871600	1.25096100
C	-0.91431700	-1.69390200	1.86943400
O	-0.63196900	-0.47796200	1.59879300
C	-0.09952700	-2.45631900	2.87676700
H	0.18016600	-1.80383100	3.70628700
H	-0.64852700	-3.32684700	3.23673300
H	0.82107600	-2.79335500	2.38776700
C	1.75389900	-3.63505600	-0.97509500
C	1.48217800	-2.38328400	-1.51948400
C	2.12178200	-1.23009100	-1.02097900
C	3.03762900	-1.38267500	0.03764900
C	3.31127500	-2.64569500	0.56355500
C	2.67243100	-3.78262800	0.06836800
H	1.24956600	-4.50672700	-1.38288300
H	0.78757900	-2.29652300	-2.34626400
H	3.51632700	-0.51350700	0.47373000
H	4.02518600	-2.73196100	1.37832700
H	2.88424200	-4.76285800	0.48392200
N	1.89043800	0.03381300	-1.59664900
C	2.86126800	1.11267100	-1.45186000
H	3.85134200	0.65635200	-1.34379000
H	2.88772000	1.66583700	-2.40098100
C	2.61375700	2.10270500	-0.31876100
C	1.74512500	1.81894100	0.74061300
C	3.29373300	3.32849100	-0.33036400
C	1.56467100	2.74677600	1.77051100
H	1.20120600	0.88074700	0.77185100
C	3.11660500	4.25158400	0.69929200
H	3.96554600	3.56346800	-1.15391600
C	2.24824300	3.96243100	1.75539800

H	0.88410300	2.50881700	2.58301900
H	3.65054300	5.19764300	0.67486400
H	2.10491800	4.68213900	2.55647700
C	0.68716900	0.38487100	-2.23810000
H	-2.78721200	0.42725600	-1.68606900
H	0.79328000	1.15598900	-3.00097800
C	-0.52574500	-0.08111100	-2.01332500
C	-1.75507100	-0.52340200	-1.83779900
H	-2.06022800	-1.40686100	-2.41236700

47

13 Eelec= -2909.63453817 a. u.

Zn	2.23301500	-0.25805700	-0.05285500
O	3.99755900	-0.94910000	-0.79389900
C	4.63371200	-0.08262200	-0.10307200
O	4.00664900	0.73546600	0.63347900
C	6.14382400	-0.06781300	-0.14771000
H	6.50119100	-0.38064700	-1.13058700
H	6.52536300	0.92249600	0.10568400
H	6.52429300	-0.78137100	0.59139100
O	1.40366300	-1.07080000	1.59957000
C	0.86226500	-2.03533100	0.95035500
O	0.91415500	-2.07361200	-0.30960600
C	0.13808100	-3.10729300	1.73432400
H	0.10221700	-4.03803500	1.16545000
H	0.62595000	-3.26715300	2.69761200
H	-0.88836100	-2.77702700	1.92711800
C	-2.72077100	3.66028600	0.71387100
C	-2.32564500	2.86790500	-0.36429300
C	-1.53273000	1.74082900	-0.13667600
C	-1.12877800	1.39765500	1.15574800
C	-1.52434000	2.20206600	2.22508600
C	-2.32129000	3.32783600	2.00937000
H	-3.33348400	4.53934300	0.53824300
H	-2.61873700	3.13258400	-1.37594200
H	-0.50069000	0.52971300	1.32887800
H	-1.20592800	1.94181900	3.22965900
H	-2.62697200	3.94679400	2.84752100
N	-1.15521100	0.90954700	-1.25989700
C	-2.24254800	0.19966800	-1.98361000
H	-2.90799500	0.95758000	-2.40918500
H	-1.76806400	-0.32411800	-2.81784000
C	-3.04375200	-0.76454200	-1.13626200
C	-2.47789600	-1.97107000	-0.69977200

C	-4.37584000	-0.47648300	-0.81905500
C	-3.24615300	-2.87342600	0.03658700
H	-1.43762900	-2.20001800	-0.92017000
C	-5.14148400	-1.37966200	-0.07960300
H	-4.81847700	0.45808500	-1.15450300
C	-4.57727900	-2.58179500	0.34690600
H	-2.80545600	-3.81071300	0.36285300
H	-6.17462100	-1.14473900	0.15905000
H	-5.17104500	-3.29027600	0.91728000
C	0.11024900	0.79341500	-1.65758600
H	2.76028700	2.64456700	-0.45811700
H	0.24408000	0.11989600	-2.50535200
C	1.25497300	1.28990900	-1.03479400
C	1.85163600	2.48262900	-1.03006300
H	1.47646700	3.32751300	-1.60895900

47

TS12 Eelec= -2909.59525654 a. u.

Zn	-2.73937300	-0.28627300	-0.02423000
O	-3.39551900	0.36042300	1.78655500
C	-3.83824900	1.44372900	1.27143300
O	-3.70268000	1.67027700	0.03429100
C	-4.55728200	2.43606400	2.15734800
H	-4.47639500	3.44471200	1.74848300
H	-5.61883600	2.16780200	2.19441700
H	-4.16595600	2.39840600	3.17571500
O	-3.86946800	-1.55001100	-1.12173500
C	-3.29024100	-2.57657500	-0.62333900
O	-2.35843400	-2.44795700	0.22010300
C	-3.76754400	-3.95124600	-1.03545500
H	-4.60772800	-4.23810700	-0.39357000
H	-4.12334000	-3.94129800	-2.06747900
H	-2.97294500	-4.68809000	-0.90719700
C	2.83090900	3.26127100	0.10942300
C	2.62227200	1.93077700	0.42694400
C	1.81679300	1.12462600	-0.40754800
C	1.23506300	1.70121400	-1.59239500
C	1.52278600	3.06907000	-1.90274300
C	2.26609500	3.84686600	-1.04756300
H	3.43807800	3.87057100	0.77258100
H	3.07380100	1.51897200	1.31988200
H	1.12798600	1.00996900	-2.42313400
H	1.12991000	3.48369900	-2.82684300
H	2.45025600	4.89307600	-1.26908700

N	1.46202100	-0.16626600	-0.10204800
C	2.15950100	-0.88555900	0.98340700
H	2.03423500	-0.35445500	1.93576800
H	1.63692300	-1.83928600	1.09802500
C	3.62897800	-1.14248100	0.70778200
C	4.06332500	-1.57361000	-0.55215200
C	4.56509600	-1.01374800	1.73977700
C	5.40888300	-1.86381700	-0.77452500
H	3.34456800	-1.67701800	-1.35999400
C	5.91195900	-1.31024800	1.52050600
H	4.23890000	-0.68306300	2.72344300
C	6.33730300	-1.73409800	0.26140000
H	5.73292300	-2.19519700	-1.75690400
H	6.62646700	-1.20483000	2.33170300
H	7.38479000	-1.96151100	0.08682800
C	0.12462200	-0.60326700	-0.35642400
H	-0.87876100	1.52343700	-2.41568300
H	-0.07133100	-1.61737200	-0.02813200
C	-0.86583100	0.22820800	-0.71731000
C	-0.75932400	1.48631300	-1.33561200
H	-1.23835900	2.33885700	-0.84902400

47

14 Eelec= -2909.61312224 a. u.

Zn	-2.65453400	-0.39584400	0.01607500
O	-4.07587100	0.16384600	1.33864200
C	-4.47716300	1.12176200	0.58875700
O	-3.93071300	1.35406700	-0.52341600
C	-5.65326000	1.95471400	1.05558100
H	-5.65077400	2.93149700	0.56872200
H	-6.58034600	1.43767400	0.78443400
H	-5.64059500	2.06467300	2.14212100
O	-3.17056400	-1.87305700	-1.26364700
C	-2.65072200	-2.78710200	-0.53306000
O	-2.07345200	-2.51115000	0.55304000
C	-2.77757700	-4.22658000	-0.98995700
H	-3.74820200	-4.61516900	-0.66255000
H	-2.74516300	-4.28998500	-2.07976000
H	-1.99465000	-4.84246400	-0.54383700
C	3.22105600	3.47475000	-0.15246900
C	3.03023700	2.21918700	0.35563200
C	1.83719700	1.50112000	0.04203000
C	0.84143700	2.07105500	-0.93462200
C	1.13178000	3.46838600	-1.36554000

C	2.25366300	4.12495700	-0.99973900
H	4.13057500	4.01027200	0.10487300
H	3.78452200	1.77512900	0.99182200
H	0.89906200	1.41250400	-1.82702400
H	0.39104200	3.94011200	-2.00575800
H	2.44178800	5.14098300	-1.33135400
N	1.54030700	0.31015400	0.55213300
C	2.46900900	-0.41119800	1.45292200
H	2.77969000	0.26139000	2.25756700
H	1.87497500	-1.20108300	1.91865600
C	3.67744700	-0.99782800	0.74678800
C	3.54576300	-1.65605200	-0.48291700
C	4.93675900	-0.93074100	1.35341100
C	4.65870300	-2.23185000	-1.09479300
H	2.57282700	-1.71870300	-0.96243900
C	6.04986100	-1.51269200	0.74343900
H	5.04833100	-0.42646500	2.31085300
C	5.91294300	-2.16252700	-0.48333900
H	4.54518100	-2.73919600	-2.04822000
H	7.02132300	-1.45365000	1.22529400
H	6.77767200	-2.61307000	-0.96125100
C	0.24820200	-0.28248700	0.34004800
H	-1.30476100	2.16890600	-1.21156900
H	0.19532200	-1.32555300	0.63093000
C	-0.82901500	0.43143500	-0.03818800
C	-0.61000600	1.86457800	-0.42389400
H	-0.83704200	2.51946500	0.43382200

47

TS13 Eelec= -2909.60480612 a. u.

Zn	2.56183300	-0.10111900	-0.28258300
O	3.47261300	-1.96238500	-0.25733000
C	4.54802900	-1.37071900	-0.59232000
O	4.56030300	-0.10508300	-0.74156900
C	5.82126600	-2.15902500	-0.78263900
H	6.42472700	-1.71910100	-1.57910300
H	6.40491000	-2.11241100	0.14327400
H	5.59902000	-3.20487700	-0.99895200
O	2.30744300	0.56910800	1.55665900
C	1.30873400	0.83584900	2.30277100
O	0.15722000	1.20634200	1.94197500
C	1.55633400	0.69400600	3.79915900
H	0.67713400	0.98722300	4.37386900
H	1.81990000	-0.34413700	4.02425500

H	2.41415100	1.31050300	4.08392400
C	-3.37682400	2.99471000	-0.32474100
C	-3.12892800	1.72584200	-0.79206700
C	-1.78582900	1.28019200	-0.94684700
C	-0.67885400	2.14870300	-0.50892100
C	-1.04056600	3.51127700	-0.12536500
C	-2.33552000	3.91039100	0.01100300
H	-4.41019000	3.31188400	-0.21065200
H	-3.95724400	1.07177800	-1.03250900
H	-0.33824300	1.67391600	0.56352700
H	-0.22271000	4.18589200	0.11451200
H	-2.58588500	4.90841200	0.35436600
N	-1.46801400	0.06534300	-1.42733600
C	-2.48926900	-0.92231800	-1.78671300
H	-3.23145700	-0.44790800	-2.43728600
H	-1.98220200	-1.67109300	-2.40334800
C	-3.17773900	-1.59887600	-0.60773000
C	-2.65505300	-1.55595100	0.68963200
C	-4.35839800	-2.31583700	-0.84501100
C	-3.30550500	-2.22464800	1.72981600
H	-1.74875100	-0.99618600	0.90060100
C	-5.00342600	-2.98568400	0.19358900
H	-4.77509700	-2.35137300	-1.84955500
C	-4.47682100	-2.94166500	1.48665800
H	-2.89117800	-2.18071200	2.73267800
H	-5.91787400	-3.53711300	-0.00555400
H	-4.97895200	-3.46013100	2.29815300
C	-0.09996200	-0.38218500	-1.35619000
H	1.40298500	2.54382300	-0.86487900
H	-0.02826800	-1.46528600	-1.32335100
C	0.94592400	0.44755200	-1.24898100
C	0.61000600	1.93174000	-1.30586000
H	0.50010600	2.26907100	-2.34846400

47

15 Eelec= -2909.65564626 a. u.

Zn	2.64345300	-0.05853100	-0.16922300
O	3.80235700	-0.86885600	-1.66112600
C	4.68816300	-0.00441000	-1.36077200
O	4.47844900	0.80388200	-0.39627700
C	5.99109400	0.04912400	-2.11681900
H	6.30935700	1.08563900	-2.24598800
H	6.76018300	-0.46317200	-1.52871300
H	5.89861600	-0.44963200	-3.08214100

O	2.85297800	-1.39120400	1.41339500
C	1.90680300	-1.70609100	2.15056500
O	0.68384200	-1.24504800	2.01188600
C	2.07489900	-2.66603500	3.29409400
H	1.77344600	-2.18016800	4.22657300
H	1.41470300	-3.52603300	3.14755600
H	3.11132400	-2.99414900	3.35631200
C	-3.59224900	3.14111000	0.76757200
C	-3.21645000	2.09824600	-0.07830600
C	-1.86477400	1.73716900	-0.20404800
C	-0.88353800	2.43625400	0.53376800
C	-1.29295200	3.45677700	1.39275200
C	-2.63436300	3.82325800	1.51517400
H	-4.64283300	3.40513800	0.84870900
H	-3.98242500	1.55161900	-0.61472400
H	0.64164600	-0.60190800	1.22702500
H	-0.53484900	3.98643400	1.96569400
H	-2.92404500	4.62943600	2.18230200
N	-1.45969100	0.66818100	-1.02916200
C	-2.41475500	-0.03867700	-1.86955500
H	-3.00496000	0.69661100	-2.42880200
H	-1.83050900	-0.58226900	-2.62122200
C	-3.35436500	-1.01632700	-1.16936400
C	-3.05320000	-1.57568100	0.07675300
C	-4.53544300	-1.40357400	-1.81626800
C	-3.91460600	-2.50676100	0.66120700
H	-2.14922300	-1.27687400	0.59782800
C	-5.39447300	-2.33668600	-1.23614800
H	-4.78462300	-0.97000900	-2.78273500
C	-5.08543600	-2.89225400	0.00730000
H	-3.66988900	-2.92830100	1.63215700
H	-6.30677300	-2.62464100	-1.75106500
H	-5.75474800	-3.61544500	0.46423400
C	-0.18282200	0.13017200	-0.86201700
H	1.12087900	2.29571900	1.28906200
H	-0.07350800	-0.83923900	-1.34517300
C	0.83284500	0.70215200	-0.17099100
C	0.58774500	2.11501400	0.34620500
H	1.02872300	2.83302100	-0.36572100

47

TS14 Eelec= -2909.65137377 a. u.

Zn	2.67710300	-0.21145400	-0.18062600
O	3.56592400	-0.26634100	-2.02534800

C	4. 29867700	0. 70366800	-1. 64084100
O	4. 16233700	1. 16810600	-0. 46141500
C	5. 34302500	1. 27786900	-2. 56362400
H	6. 29272800	0. 76332100	-2. 38080400
H	5. 06312500	1. 11936600	-3. 60600900
H	5. 49026400	2. 33944300	-2. 35790200
O	3. 24130100	-1. 75234700	0. 95696200
C	2. 39648100	-2. 23222300	1. 76465500
O	1. 18611800	-1. 81905500	1. 87614900
C	2. 81822600	-3. 34757200	2. 68841900
H	3. 07890100	-2. 91622400	3. 66120700
H	1. 99266200	-4. 04469900	2. 84349800
H	3. 69345900	-3. 85992200	2. 28813700
C	-3. 42436000	3. 14069200	1. 08252600
C	-3. 06893600	2. 14935800	0. 16841600
C	-1. 76895200	1. 62153000	0. 16374600
C	-0. 81663600	2. 09101600	1. 09272700
C	-1. 20728800	3. 06893400	2. 00849400
C	-2. 49628200	3. 60399600	2. 01211200
H	-4. 43543300	3. 53694900	1. 06912600
H	-3. 81771000	1. 77452000	-0. 51797300
H	0. 99036300	-0. 90184100	1. 13325500
H	-0. 47338200	3. 42540500	2. 72769900
H	-2. 76922800	4. 37012400	2. 73140100
N	-1. 39978500	0. 59494200	-0. 74343000
C	-2. 34512600	0. 09777000	-1. 73845100
H	-2. 77451300	0. 95036900	-2. 27642200
H	-1. 75661200	-0. 45551100	-2. 47863600
C	-3. 46245100	-0. 79615000	-1. 21339900
C	-3. 31802800	-1. 54942800	-0. 04340300
C	-4. 64889000	-0. 90773100	-1. 94969200
C	-4. 34071700	-2. 40075700	0. 37911900
H	-2. 41031000	-1. 46339600	0. 54594200
C	-5. 66936300	-1. 76174800	-1. 53105500
H	-4. 77507500	-0. 32127300	-2. 85749100
C	-5. 51740600	-2. 51170100	-0. 36311600
H	-4. 21687400	-2. 97593400	1. 29224100
H	-6. 58396700	-1. 83620100	-2. 11252200
H	-6. 31228600	-3. 17359000	-0. 03190900
C	-0. 20380000	-0. 06179300	-0. 57159700
H	0. 98186400	1. 48188500	2. 09556500
H	-0. 12137900	-0. 95483000	-1. 18885200
C	0. 79072000	0. 27864600	0. 29909600
C	0. 61553300	1. 58804900	1. 06504000

H	1.25678900	2.36360700	0.61742300
47			
16	Eelec= -2909.69317691 a. u.		
Zn	2.06372200	0.07042600	0.15681600
O	0.94048000	-0.41065800	1.78394300
C	1.15894600	0.75023800	2.28214900
O	1.85259100	1.59117800	1.64080200
C	0.57641000	1.08937100	3.63127800
H	0.86706900	2.09345000	3.93971900
H	-0.51428300	1.01648800	3.58277900
H	0.91784400	0.35807500	4.36952700
O	2.57942000	-1.78438600	-0.82899800
C	3.78060000	-1.43435600	-0.63257400
O	4.03777000	-0.31534900	-0.06803400
C	4.92002500	-2.33984600	-1.03244400
H	5.81320000	-1.75687600	-1.26286600
H	5.15417400	-3.00029600	-0.19029800
H	4.63372100	-2.96330300	-1.88111600
C	-1.33444800	3.65797400	-0.20926700
C	-0.77204900	2.51314200	-0.77729500
C	-1.59630600	1.38310400	-0.96256600
C	-2.94698600	1.43231600	-0.58870700
C	-3.48316800	2.59367100	-0.03496600
C	-2.67768400	3.71308700	0.16150400
H	-0.69711200	4.52608100	-0.06082100
H	2.13697200	1.05807900	-2.06863000
H	-3.57860500	0.56073700	-0.70122500
H	-4.53060300	2.61114800	0.25049200
H	-3.08625600	4.61771400	0.60114100
N	-1.04685800	0.19459000	-1.52675500
C	-1.90167500	-0.95282600	-1.85234300
H	-2.72874000	-0.59867500	-2.47926400
H	-1.29912700	-1.61255700	-2.48513500
C	-2.45457900	-1.74807600	-0.67799900
C	-1.78086300	-1.84004900	0.54418400
C	-3.65225000	-2.45380400	-0.85458800
C	-2.29962300	-2.63353000	1.56966400
H	-0.86250900	-1.28980700	0.71995500
C	-4.16537300	-3.25033000	0.16924900
H	-4.18667000	-2.38169200	-1.79985200
C	-3.48794700	-3.34204900	1.38688200
H	-1.76463900	-2.69215300	2.51290900
H	-5.09469600	-3.79220000	0.01787900

H	-3.88673000	-3.95822700	2.18766800
C	0.28207700	0.13263000	-1.79577900
C	1.17763100	1.14733600	-1.56170600
C	0.68025600	2.53578500	-1.22348800
H	0.77840200	3.18437200	-2.10843500
H	1.29247600	2.99073100	-0.43807100
H	0.63239500	-0.81500400	-2.19238100

32

IMP Eelec= -673.48291789 a. u.

C	1.60620700	2.58788500	-0.27713200
C	0.81474200	1.48138800	-0.57674000
C	1.27528000	0.17561200	-0.32549400
C	2.55209400	-0.00465700	0.25886200
C	3.32037400	1.12478600	0.54733300
C	2.86989400	2.41853200	0.28478500
H	1.22337900	3.58388600	-0.48097300
H	-0.17537600	1.64000200	-0.98548200
H	2.44783500	-3.51205500	0.34366900
H	4.30237200	0.97842700	0.99253900
H	3.49213100	3.27602900	0.52183200
N	0.48475700	-0.94169600	-0.64808700
C	-0.78804300	-0.79381700	-1.33426300
H	-0.67236400	-0.11280600	-2.18749400
H	-1.03124900	-1.77115200	-1.76643400
C	-1.95832900	-0.33128000	-0.47253100
C	-1.98610600	-0.55545800	0.90772800
C	-3.05716100	0.28946800	-1.07988600
C	-3.09377700	-0.16995900	1.66499400
H	-1.13268200	-1.02353100	1.38866400
C	-4.16713200	0.67109200	-0.32559200
H	-3.04379100	0.47668700	-2.15182900
C	-4.18828600	0.44184200	1.05166000
H	-3.09966200	-0.34617100	2.73706000
H	-5.01083900	1.15316700	-0.81160400
H	-5.04878200	0.74268200	1.64232600
C	0.97372600	-2.22308700	-0.38441000
H	3.33008200	-1.44707600	1.66260600
H	0.30066300	-3.02287800	-0.67564200
C	2.16023300	-2.47908500	0.17894400
C	3.10684000	-1.38422000	0.58486300
H	4.08165200	-1.51760700	0.08864800

31

17	Eelec= -2600.02689863 a. u.		
Zn	1.05083800	0.21121500	-0.05214100
O	2.59680200	-0.62235000	-1.23081900
C	3.33703600	-0.51087400	-0.20656100
O	2.84596800	-0.06990100	0.88831300
C	4.80063200	-0.86883700	-0.27834000
H	5.16263900	-1.20607100	0.69437100
H	4.97249200	-1.62895700	-1.04197200
H	5.36584900	0.02726600	-0.55714500
O	-0.08592500	1.56101900	1.12173100
C	-0.18160300	2.26185300	0.06721400
O	0.35034500	1.85138200	-1.01824700
C	-0.94515900	3.56224800	0.08849400
H	-0.67222400	4.14017100	0.97466800
H	-0.75809600	4.13997900	-0.81674900
H	-2.01526700	3.33992800	0.15715300
C	-1.60410000	-1.26420700	-0.45265800
C	-2.18368400	-0.93431100	0.79879200
C	-3.48716300	-0.44065800	0.91466300
C	-4.21592400	-0.29572000	-0.25911900
C	-3.66360200	-0.63109300	-1.51356200
C	-2.36572300	-1.11058000	-1.62328200
H	-3.91190900	-0.18266800	1.87992900
H	-5.23275800	0.08206500	-0.21038700
H	-4.26661400	-0.50608300	-2.40765300
H	-1.94240400	-1.35648000	-2.59227600
C	-0.24970000	-1.69661500	-0.18356500
H	0.43328100	-2.17053200	-0.87616600
H	0.76760800	-1.93243600	1.79571100
N	-1.24280800	-1.20984500	1.77837300
C	-0.08781500	-1.65212600	1.19714400
H	-1.30478900	-0.88938800	2.73297800

31			
TS15	Eelec= -2599.99164469 a. u.		
Zn	-1.17078200	-0.15549600	0.01412900
O	-0.37841000	2.68967800	0.54719200
C	-1.52420200	2.63192300	-0.01795400
O	-2.09894200	1.55412700	-0.35755100
C	-2.21917700	3.93736100	-0.31570300
H	-3.27979000	3.85549700	-0.06798200
H	-1.75481500	4.75814700	0.23101700
H	-2.14692600	4.13589000	-1.39039900
O	-2.39839500	-1.56559500	0.87161700

C	-2.38956300	-2.16292400	-0.25315900
O	-1.73086700	-1.66409100	-1.22619500
C	-3.17231300	-3.43538300	-0.45095300
H	-4.11610900	-3.19292200	-0.95114100
H	-2.62074800	-4.12000600	-1.09840200
H	-3.39536600	-3.90450400	0.50783200
C	1.90145500	0.09142900	-0.10429100
C	2.90657500	-0.44732300	0.73772200
C	4.19997800	-0.73734900	0.29653200
C	4.48766100	-0.47150000	-1.03818800
C	3.51151400	0.06723700	-1.89927400
C	2.22799600	0.34994000	-1.44535700
H	4.95083700	-1.15173400	0.96343100
H	5.48126800	-0.68258300	-1.42222200
H	3.76950900	0.26291400	-2.93590700
H	1.48508800	0.76456100	-2.12188100
C	0.68388800	0.27700600	0.68475800
H	0.09820900	1.57068800	0.64180900
H	0.43887300	-0.20048300	2.85733500
N	2.33493600	-0.59588000	1.99569200
C	1.03833000	-0.17032500	1.95603000
H	2.80892800	-0.95290300	2.81129800

31

18 Eelec= -2599.99878989 a. u.

Zn	-1.10004100	-0.21603000	0.28485600
O	-0.34711400	2.80427000	-0.39189800
C	-1.62871700	2.55790100	-0.55783500
O	-2.16338500	1.46948500	-0.30378500
C	-2.40832400	3.72186600	-1.09952600
H	-3.47092700	3.48430600	-1.11234400
H	-2.21952700	4.61121200	-0.49250700
H	-2.06449000	3.94124600	-2.11531100
O	-2.46717600	-1.42276800	1.20139400
C	-2.53283600	-2.09304400	0.11849600
O	-1.85202000	-1.72239600	-0.89291300
C	-3.43011900	-3.30037100	0.02323600
H	-4.33442800	-3.02480500	-0.52984700
H	-2.93126700	-4.09440900	-0.53669900
H	-3.71591900	-3.65020500	1.01554700
C	1.91960300	-0.27153500	-0.06204100
C	3.09878100	0.13828700	0.61703500
C	4.38258600	-0.19644500	0.17354800
C	4.47700300	-0.96835400	-0.97942000

C	3.32380500	-1.39735000	-1.66809700
C	2.05305200	-1.05750000	-1.21970400
H	5.27171200	0.12866600	0.70708200
H	5.45744300	-1.24954100	-1.35316800
H	3.43499300	-2.00654300	-2.56048000
H	1.16663100	-1.40470200	-1.74494100
C	0.76413900	0.24481800	0.65691700
H	0.11970700	1.99007600	-0.03085500
H	0.81341900	1.46069700	2.53071100
N	2.69063100	0.87378300	1.71427700
C	1.31023300	0.92885900	1.72852300
H	3.30178800	1.30690900	2.38801400

63

TS16 Eelec= -3273.47275579 a. u.

Zn	2.07757000	-0.62031000	0.96168300
O	2.53381000	-0.73816700	2.96655000
C	1.34360400	-0.39765800	3.24575100
O	0.50192200	-0.18730000	2.31045400
C	0.91090000	-0.25847400	4.68637300
H	1.77047500	-0.29111900	5.35606800
H	0.36013900	0.67607200	4.82211100
H	0.22960600	-1.07894400	4.93503500
C	2.36196900	2.09627800	-0.38595500
C	2.94762200	2.67792500	-1.54866500
C	2.87146500	4.04698900	-1.82707600
C	2.18880700	4.85116400	-0.91914300
C	1.59718500	4.30460600	0.23810000
C	1.68014400	2.94265700	0.50896600
H	3.32846800	4.47158500	-2.71739800
H	2.11248300	5.91879500	-1.10517600
H	1.07576700	4.96167800	0.92867500
H	1.23381800	2.52311600	1.40757400
C	2.61362800	0.66720800	-0.39732900
H	3.72634800	-0.46151100	-1.96340700
N	3.53549600	1.64612500	-2.24976000
C	3.33412100	0.46009200	-1.55223500
H	4.06992000	1.74598200	-3.09763500
C	-3.66638300	-2.72808200	0.84066500
C	-2.94962600	-1.54478600	0.66919300
C	-2.16867100	-1.35825100	-0.47684500
C	-2.09821200	-2.36292200	-1.46255500
C	-2.82011300	-3.54033200	-1.26197200
C	-3.60396900	-3.73153000	-0.12382800

H	-4.26869700	-2.85984500	1.73408700
H	-3.00482200	-0.77653600	1.42814700
H	-2.76252000	-4.31955500	-2.01763500
H	-4.15732900	-4.65634000	0.00757800
N	-1.40400800	-0.15686700	-0.64846100
C	-1.56934400	0.97680700	0.28574500
H	-1.35419900	0.63095700	1.30000600
H	-0.77666800	1.68984100	0.04168000
C	-2.92154900	1.65887100	0.19509700
C	-3.56460400	1.86396300	-1.03148200
C	-3.51530800	2.15756600	1.36092100
C	-4.77824700	2.54913600	-1.08968200
H	-3.11779000	1.48217600	-1.94527800
C	-4.72526300	2.85099500	1.30392900
H	-3.02404300	2.00449800	2.31899600
C	-5.36169500	3.04644900	0.07751200
H	-5.26755500	2.69701300	-2.04821000
H	-5.17212500	3.23197700	2.21775400
H	-6.30610700	3.58074500	0.03084900
C	-0.44233300	-0.11178000	-1.57372900
H	0.17841500	0.77782400	-1.55488400
C	-1.28232500	-2.14999700	-2.72223100
O	1.62154100	-2.89550100	-1.71972000
C	1.99175700	-3.23795500	-0.54598800
O	1.89158300	-2.53880000	0.49586200
C	2.58930500	-4.62465700	-0.40646700
H	3.56342800	-4.55347900	0.08491300
H	1.94375000	-5.22277000	0.24440500
H	2.68802200	-5.11337700	-1.37579300
C	-0.15289900	-1.16222000	-2.45710300
H	0.42099700	-0.84393300	-3.32864400
H	0.82551700	-1.91173700	-1.87936600
H	-0.87423700	-3.10667100	-3.06402000
H	-1.93922300	-1.78618400	-3.52834900

63

19 Eelec= -3273.49028314 a. u.

Zn	2.75586700	-0.99772700	0.37370800
O	3.34454000	-1.33621900	2.32104900
C	2.17198700	-1.11294800	2.74490500
O	1.22589500	-0.84866200	1.92865000
C	1.88296800	-1.14275500	4.22816100
H	1.58213400	-0.14293200	4.55714400
H	1.04463200	-1.81627400	4.42813600

H	2.76083800	-1.46235400	4.78982500
C	2.32206400	1.94844000	-0.31495000
C	2.75853600	2.91775200	-1.26662200
C	2.27607500	4.23119800	-1.28392800
C	1.33524800	4.58519400	-0.32128800
C	0.89247000	3.65273100	0.63943000
C	1.37767300	2.34768600	0.65113900
H	2.62362500	4.95332700	-2.01863500
H	0.94443000	5.59888100	-0.30445900
H	0.17613700	3.96778700	1.39403800
H	1.05444400	1.63944700	1.41009700
C	2.99753600	0.69000900	-0.58047300
H	4.49132400	0.31630000	-2.19024600
N	3.67044200	2.28452300	-2.08250200
C	3.80532300	0.96512000	-1.66025700
H	4.19658700	2.72235500	-2.82133100
C	-4.97702200	-1.23574900	-1.92741600
C	-3.91667800	-1.28412900	-1.02261800
C	-2.73173900	-0.60462000	-1.31144500
C	-2.59292600	0.12943000	-2.50385500
C	-3.66705200	0.16376400	-3.39275400
C	-4.85616700	-0.51112900	-3.11202700
H	-5.89550900	-1.76762800	-1.70057300
H	-4.02415900	-1.84826500	-0.10571700
H	0.83565200	0.46650000	-2.28030200
H	-3.56470700	0.72524300	-4.31742000
H	-5.68116400	-0.47309100	-3.81666000
N	-1.62127300	-0.62020400	-0.39281800
C	-1.84074900	-0.96766100	1.03628100
H	-2.24119900	-1.98417100	1.07504100
H	-0.85073500	-0.99273200	1.50192600
C	-2.74999200	0.00921200	1.75269400
C	-2.50613700	1.38826000	1.69518500
C	-3.81082800	-0.46006000	2.53486900
C	-3.31776300	2.27736200	2.39877800
H	-1.67743500	1.76972700	1.10410100
C	-4.61795700	0.42879000	3.24745600
H	-4.00415600	-1.52885300	2.59385000
C	-4.37552700	1.80066400	3.17699300
H	-3.11999400	3.34395600	2.34407300
H	-5.43679100	0.04881800	3.85150100
H	-5.00474000	2.49492300	3.72620200
C	-0.39912700	-0.41323000	-0.81515600
H	-1.27451400	1.81348900	-2.26225400

H	0.37199900	-0.36683300	-0.06290900
C	-0.13549100	-0.02942400	-2.23227800
C	-1.28398200	0.83538500	-2.76344800
H	-1.15482300	1.02585700	-3.83235500
O	2.54502600	-2.76959800	-0.39603700
C	1.46063200	-3.22294800	-0.90831000
O	0.38686700	-2.59777900	-1.06711000
C	1.52855900	-4.67616800	-1.36227700
H	2.33406100	-4.79271500	-2.09369400
H	1.77718900	-5.31318700	-0.50808600
H	0.58115900	-4.99407700	-1.79906600
H	-0.06269700	-0.96492100	-2.79938000

63

TS17 Eelec= -3273.47553883 a. u.

Zn	-1.62003200	0.66530400	0.91969400
O	-0.39297700	-0.23013200	2.39808500
C	-1.45053800	-0.38134400	3.09685200
O	-2.57384100	0.00431600	2.65589000
C	-1.36903900	-1.05624100	4.44771700
H	-0.35448000	-1.01016300	4.84659000
H	-2.07381600	-0.59303000	5.14112400
H	-1.65554400	-2.10816900	4.33813300
C	-2.01080200	-1.96487900	-0.61692000
C	-2.94092900	-2.32279400	-1.62753700
C	-3.35919600	-3.63441900	-1.85315500
C	-2.82628100	-4.62327500	-1.02807000
C	-1.91437700	-4.30101100	-0.00699100
C	-1.50740800	-2.98511900	0.20573400
H	-4.07655500	-3.87909600	-2.63175100
H	-3.12924200	-5.65646700	-1.16992300
H	-1.53297800	-5.09162900	0.63279900
H	-0.83552500	-2.73691400	1.02273500
C	-1.78161800	-0.51802600	-0.66982000
H	-2.82414300	0.92608400	-2.00333000
N	-3.29932000	-1.14064600	-2.26913200
C	-2.63813800	-0.09340300	-1.68836200
H	-4.01032600	-1.05907800	-2.98059300
C	3.18277900	2.98911100	0.54055100
C	2.72091400	1.67817000	0.44634600
C	1.78761300	1.32940000	-0.53908100
C	1.30926700	2.30349200	-1.43917700
C	1.79247300	3.60793000	-1.32392900
C	2.72156600	3.96041700	-0.34554700

H	3.90483500	3.24326600	1.31006900
H	3.10037600	0.93616100	1.13485100
H	-0.59961000	0.15404200	-3.35756800
H	1.42343700	4.35925000	-2.01724300
H	3.08066700	4.98271800	-0.27790000
N	1.31180600	-0.02063500	-0.63529800
C	1.74171600	-1.02453700	0.35924600
H	1.53799700	-0.64196200	1.36150100
H	1.07350900	-1.87875300	0.22943900
C	3.18262700	-1.48085400	0.20847600
C	3.80800000	-1.58294700	-1.03940600
C	3.88761200	-1.87799400	1.35202800
C	5.11210000	-2.06882000	-1.14197600
H	3.27964100	-1.27161700	-1.93606300
C	5.18891000	-2.37148600	1.25043000
H	3.41254000	-1.80065100	2.32710400
C	5.80606600	-2.46671000	0.00208800
H	5.58604700	-2.13610000	-2.11709100
H	5.72168300	-2.67448000	2.14719400
H	6.82100400	-2.84460200	-0.07851000
C	0.40251400	-0.37887100	-1.54897300
H	0.42855400	2.53257900	-3.38495300
H	0.24112600	-1.44388100	-1.63670100
C	0.27436200	0.46318800	-2.78451400
C	0.25782300	1.95784500	-2.46874900
H	-0.72583700	2.25228200	-2.08249900
O	-2.44990900	2.92417600	-0.94670100
C	-1.98778000	3.32236600	0.13451300
O	-1.49404900	2.56852400	1.06676600
C	-1.95073000	4.81044300	0.45666200
H	-2.40980900	5.39004800	-0.34532600
H	-2.47233500	4.99873200	1.39964400
H	-0.91232900	5.12760800	0.59677300
H	1.16382400	0.22080600	-3.39124300

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D-R1 Eelec= -673.40162957 a. u.

C	1.15890700	2.58563100	-1.05213700
C	0.81907500	1.23989200	-1.20214500
C	1.06349500	0.32680600	-0.16715600
C	1.65572800	0.78652800	1.01651700
C	2.00776200	2.12799900	1.15775600
C	1.75834100	3.03436100	0.12495400
H	0.95588900	3.28296000	-1.86034000

H	0.35780600	0.90827500	-2.12682300
H	1.82899600	0.07800500	1.81858700
H	2.46523500	2.46841400	2.08255300
H	2.02177200	4.08184600	0.23964100
N	0.73512800	-1.07342700	-0.26801700
C	-0.50719900	-1.38671100	-0.98521400
H	-0.47807500	-1.10480000	-2.05319200
H	-0.60040300	-2.48095200	-0.97176400
C	-1.73874500	-0.78586700	-0.33696100
C	-1.93113000	-0.87956400	1.04794200
C	-2.72807500	-0.17699400	-1.11570000
C	-3.08932200	-0.37566700	1.63763700
H	-1.15852100	-1.34055600	1.65574900
C	-3.89202900	0.32406800	-0.52829500
H	-2.58738300	-0.09342500	-2.19098500
C	-4.07521600	0.22642900	0.85098500
H	-3.22430300	-0.45251100	2.71305300
H	-4.64990500	0.79564900	-1.14769600
H	-4.97725700	0.61925100	1.31160000
C	1.85045800	-1.90775500	-0.75904400
H(Iso=2)	1.47222900	-2.93406100	-0.84779000
H	2.16975700	-1.60496200	-1.77389300
C	3.02559300	-1.92856000	0.11405600
C	4.01740800	-1.99045900	0.79935300
H	4.88796300	-2.02997200	1.41213400

16

D-R2 Eelec= -363.82233437 a. u.

C	0.25002800	0.75163800	0.00000000
C	0.24798600	-0.67175500	-0.00003300
C	-0.93552000	-1.41917000	-0.00000500
C	-2.13587100	-0.71888300	0.00003500
C	-2.15918500	0.69211700	0.00001000
C	-0.98264700	1.42952600	-0.00001900
H	-0.91785200	-2.50572500	-0.00002100
H	-3.07338700	-1.26741300	0.00006700
H	-3.11628000	1.20577600	0.00001400
H	-1.01084500	2.51583100	-0.00003700
C	1.62636400	1.16711700	0.00005400
H(Iso=2)	1.99894100	2.18160900	-0.00000300
H	3.46491000	-0.08511000	0.00001500
N	1.56656000	-1.08146800	-0.00021500
C	2.39025100	0.02995800	0.00005600
H	1.88015300	-2.03797100	0.00088700

47

D-TS10	Eelec= -2909.58318858 a. u.		
Zn	-2.00432800	-1.14168200	-0.41151000
O	-2.33400600	0.53245000	-1.31302900
C	-1.71666500	1.40465600	-1.99109400
O	-0.51360100	1.33055800	-2.39933100
C	-2.46492700	2.67318000	-2.33186800
H	-3.53416000	2.47551800	-2.41711400
H	-2.31076700	3.38228900	-1.51072800
H	-2.07359300	3.11822900	-3.24746500
O	-3.72713400	-2.16019800	-0.00916200
C	-3.58802600	-1.81841600	1.21195200
O	-2.58429800	-1.11290100	1.55683200
C	-4.62111000	-2.22812200	2.22898200
H	-5.50353100	-1.59034100	2.11063100
H	-4.93470500	-3.25886200	2.05020200
H	-4.23502300	-2.11280100	3.24200500
C	4.80300900	-2.40764600	-0.20099800
C	3.71843700	-1.72489900	-0.74848200
C	3.30658000	-0.48489400	-0.21950200
C	4.01643200	0.02867600	0.88633600
C	5.10343100	-0.66223800	1.41724400
C	5.51142600	-1.88454700	0.88123100
H	5.09880500	-3.35838500	-0.63674000
H	3.19888600	-2.15332900	-1.59782900
H	3.69651600	0.95204900	1.35591900
H	5.62580100	-0.24113200	2.27214300
H	6.35569800	-2.42088800	1.30266100
N	2.22017200	0.21751900	-0.76283300
C	2.09193900	1.65907300	-0.58429000
H	3.08026600	2.06829600	-0.34824300
H	1.80572600	2.10264600	-1.54579800
C	1.08045300	2.10911100	0.46545100
C	0.43651700	1.20375800	1.31394600
C	0.77033200	3.47247800	0.57487300
C	-0.50988500	1.64492200	2.24473700
H	0.67783500	0.14769900	1.24376900
C	-0.16252400	3.91792100	1.51064500
H	1.26099400	4.18927700	-0.08078200
C	-0.81056500	3.00298400	2.34615900
H	-1.01881400	0.91991900	2.87221500
H	-0.38872200	4.97831800	1.58463500
H	-1.54587500	3.34795600	3.06737000

C	1.33178400	-0.40292500	-1.71830600
H(Iso=2)	0.29239300	0.43072800	-2.00229400
H	1.72097300	-0.51325800	-2.74132600
C	0.55905000	-1.46518100	-1.28252500
C	-0.36236200	-2.23252600	-0.89043900
H	-0.36773800	-3.28755700	-0.65489700

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D-TS15	Eelec= -2599.99164469 a. u.		
Zn	-1.17078200	-0.15549600	0.01412900
O	-0.37841000	2.68967800	0.54719200
C	-1.52420200	2.63192300	-0.01795400
O	-2.09894200	1.55412700	-0.35755100
C	-2.21917700	3.93736100	-0.31570300
H	-3.27979000	3.85549700	-0.06798200
H	-1.75481500	4.75814700	0.23101700
H	-2.14692600	4.13589000	-1.39039900
O	-2.39839500	-1.56559500	0.87161700
C	-2.38956300	-2.16292400	-0.25315900
O	-1.73086700	-1.66409100	-1.22619500
C	-3.17231300	-3.43538300	-0.45095300
H	-4.11610900	-3.19292200	-0.95114100
H	-2.62074800	-4.12000600	-1.09840200
H	-3.39536600	-3.90450400	0.50783200
C	1.90145500	0.09142900	-0.10429100
C	2.90657500	-0.44732300	0.73772200
C	4.19997800	-0.73734900	0.29653200
C	4.48766100	-0.47150000	-1.03818800
C	3.51151400	0.06723700	-1.89927400
C	2.22799600	0.34994000	-1.44535700
H	4.95083700	-1.15173400	0.96343100
H	5.48126800	-0.68258300	-1.42222200
H	3.76950900	0.26291400	-2.93590700
H	1.48508800	0.76456100	-2.12188100
C	0.68388800	0.27700600	0.68475800
H(Iso=2)	0.09820900	1.57068800	0.64180900
H	0.43887300	-0.20048300	2.85733500
N	2.33493600	-0.59588000	1.99569200
C	1.03833000	-0.17032500	1.95603000
H	2.80892800	-0.95290300	2.81129800

47

S-TS1	Eelec= -2909.60549084 a. u.		
Zn	2.67416000	-0.20584600	0.09219000

O	3.99815700	-0.85162500	-1.28181300
C	3.51997200	-2.04015000	-1.24528000
O	2.53558100	-2.31376300	-0.50081100
C	4.17616000	-3.11445900	-2.08094000
H	3.47087000	-3.91917100	-2.29445100
H	4.57671800	-2.69378400	-3.00526400
H	5.01393100	-3.53493900	-1.51395300
O	3.32764200	1.79153500	0.84763200
C	3.47478200	1.16888800	1.93604300
O	3.19822100	-0.08130200	2.01856900
C	4.01279900	1.87093300	3.16155200
H	3.58432200	1.44380700	4.07024600
H	5.09757500	1.72311000	3.20139900
H	3.81599800	2.94276300	3.10690800
C	-1.35885600	3.49394300	-0.89907900
C	-0.98363000	2.15181800	-0.81046300
C	-1.94670900	1.12291200	-0.97038000
C	-3.28404800	1.49554600	-1.19955200
C	-3.63465700	2.84148900	-1.29003300
C	-2.68135000	3.85212400	-1.14730100
H	-0.59940800	4.26028400	-0.76398400
H	1.08855200	1.69449400	-1.43736700
H	-4.05417200	0.74083900	-1.29060800
H	-4.67360600	3.09981300	-1.47441600
H	-2.96626500	4.89657900	-1.21671800
N	-1.53955100	-0.20661600	-0.83890100
C	-2.50483900	-1.28984400	-1.00927800
H	-3.03677800	-1.19629100	-1.96947800
H	-1.92386800	-2.21614800	-1.07768500
C	-3.51426000	-1.43397400	0.12036800
C	-3.15311000	-1.19546100	1.45116900
C	-4.81250600	-1.87541400	-0.16092300
C	-4.07424100	-1.39352400	2.47991000
H	-2.14974800	-0.84646500	1.67586300
C	-5.73415600	-2.07914000	0.86755300
H	-5.10507700	-2.06205800	-1.19217600
C	-5.36692400	-1.83710600	2.19200200
H	-3.78126200	-1.20201200	3.50826000
H	-6.73835400	-2.42060200	0.63292300
H	-6.08304200	-1.99031200	2.99407000
C	-0.14578600	-0.53287700	-1.15567400
H	0.07854600	-1.54892100	-0.81906100
H	0.06999900	-0.53790400	-2.24673500
C	0.82902500	0.39964700	-0.51608700

C	0.41229500	1.76080000	-0.48750300
H	1.01057900	2.43295300	0.13358900
47			
S-1	Eelec= -2909.68283292 a. u.		
Zn	2.02641000	-0.01416100	0.24084400
O	3.95319700	-0.62308000	0.06622100
C	3.56702200	-1.73117500	-0.44124900
O	2.33305900	-1.93089000	-0.65681000
C	4.58185600	-2.80344700	-0.75056500
H	4.24106700	-3.42474600	-1.58041700
H	5.55494000	-2.36134600	-0.96992500
H	4.69060700	-3.44534100	0.13044200
O	1.97452300	1.54659100	1.68938500
C	1.13666400	0.82539400	2.30474400
O	0.79413600	-0.30768000	1.81177100
C	0.52214500	1.27727700	3.60463200
H	-0.54730600	1.45338000	3.45145900
H	0.61755800	0.48521800	4.35201300
H	0.99548500	2.19194500	3.96121200
C	-0.55933800	3.53062700	-0.38297400
C	-0.24038800	2.26272400	-0.88912700
C	-1.26478400	1.29188200	-1.09090300
C	-2.58923700	1.65454100	-0.78686400
C	-2.87960400	2.92934500	-0.30366000
C	-1.87412500	3.87825400	-0.09632400
H	0.24634400	4.24191100	-0.22203500
H	2.40868900	0.55525800	-2.24420900
H	-3.39279000	0.94053000	-0.90801300
H	-3.91352600	3.18106000	-0.08429800
H	-2.11397500	4.86472100	0.28628000
N	-0.90482900	0.01240900	-1.51719600
C	-1.94952700	-0.97374100	-1.79777800
H	-2.66514000	-0.58426100	-2.54081200
H	-1.44683700	-1.82060500	-2.27744000
C	-2.71140200	-1.49719500	-0.58897600
C	-2.12180500	-1.58920500	0.67684600
C	-4.02179400	-1.96024800	-0.76640200
C	-2.83674900	-2.14016900	1.74230500
H	-1.11495300	-1.22003800	0.84147600
C	-4.73190400	-2.51664700	0.29821500
H	-4.49051300	-1.88690200	-1.74588000
C	-4.13916900	-2.60800500	1.55892300
H	-2.36673600	-2.20172700	2.71977100

H	-5.74709100	-2.87164600	0.14360100
H	-4.69004600	-3.03637300	2.39155500
C	0.28539500	-0.11480700	-2.37027300
H	0.59735100	-1.16163700	-2.36443600
H	0.06304900	0.16113100	-3.42154500
C	1.41015800	0.74781100	-1.86125200
C	1.12614100	1.90410700	-1.20603000
H	1.91868700	2.59394600	-0.92801400

47

S-TS2 Eelec= -2909.63360612 a. u.

Zn	1.73785500	-0.23331300	0.03554400
O	1.46646100	-2.15530300	-0.24123700
C	0.90442000	-2.95926200	-1.03472100
O	0.31038900	-2.64050800	-2.11979600
C	0.91140300	-4.42589200	-0.67178000
H	0.64860600	-5.04341600	-1.53060600
H	1.89019000	-4.70508400	-0.27644200
H	0.17582400	-4.58832700	0.12339200
O	3.33431500	-0.01741600	1.34190200
C	2.47260100	0.19705100	2.25242800
O	1.22832500	0.17572200	1.96534400
C	2.90212300	0.47576800	3.67033400
H	2.50395400	1.44445600	3.98580600
H	2.47276700	-0.28109800	4.33332800
H	3.98850600	0.47175600	3.75704100
C	0.91105200	3.40573600	-0.50702400
C	0.65419000	2.11534300	-0.96639500
C	-0.67748300	1.64956400	-1.02724900
C	-1.72578200	2.48554300	-0.64079300
C	-1.44905700	3.77275900	-0.16396200
C	-0.13785600	4.23488700	-0.09497700
H	1.93758400	3.76166800	-0.46890100
H	1.96392800	0.14784900	-3.39027400
H	-2.75030400	2.13492800	-0.66939300
H	-2.26970100	4.40623500	0.15975300
H	0.07461800	5.23211000	0.27837700
N	-0.82875100	0.29425400	-1.45122300
C	-2.16513300	-0.30131200	-1.44998700
H	-2.86716200	0.28908100	-2.06260700
H	-2.06390600	-1.27177300	-1.94879200
C	-2.76702100	-0.52781200	-0.07258700
C	-1.97770400	-0.90344100	1.02047700
C	-4.15287600	-0.42281200	0.09917700

C	-2.56412300	-1.16231800	2.25957800
H	-0.90252700	-0.98094800	0.90866100
C	-4.74216300	-0.69175900	1.33552900
H	-4.77657900	-0.12659200	-0.74181000
C	-3.94724200	-1.06062400	2.42181500
H	-1.93323100	-1.43705600	3.09989200
H	-5.81897800	-0.60407800	1.45103400
H	-4.40131800	-1.26128300	3.38810400
C	-0.01722800	-0.08830000	-2.60096100
H	0.25668600	-1.43573900	-2.36336900
H	-0.52251100	-0.16372500	-3.57173800
C	1.28676700	0.41908200	-2.58195500
C	1.71764400	1.19515000	-1.48162000
H	2.72405700	1.60656600	-1.53087500

47

S-2 Eelec= -2909.64887153 a. u.

Zn	1.96653200	0.15079200	-0.07142300
O	1.99822400	-1.92686900	-0.20803700
C	1.67292700	-2.82961000	-0.98365900
O	0.98147800	-2.64244100	-2.08932300
C	2.02921800	-4.26830400	-0.73539400
H	2.50612000	-4.69188200	-1.62326600
H	2.68924300	-4.34489900	0.12710800
H	1.11292300	-4.83887800	-0.55362700
O	3.65928800	0.51367600	1.04547000
C	2.91315600	0.49684700	2.07843900
O	1.66703500	0.26347600	1.95544100
C	3.49443800	0.77697400	3.44177900
H	3.26238400	1.81078300	3.71952300
H	3.03375300	0.12493400	4.18693100
H	4.57740900	0.64959400	3.43447300
C	0.41180300	3.35384500	-0.56585100
C	0.14921800	2.06478600	-1.03468200
C	-1.17366500	1.57357400	-0.94185300
C	-2.17303900	2.34962100	-0.34815000
C	-1.87385600	3.62303600	0.14708300
C	-0.58434600	4.13230400	0.03083700
H	1.42362100	3.74352200	-0.65381500
H	1.19442000	0.10666400	-3.59864800
H	-3.18110700	1.96661300	-0.24515300
H	-2.65716200	4.20761800	0.62051900
H	-0.34664800	5.12264600	0.40803700
N	-1.43429100	0.27644700	-1.48487300

C	-2.76600800	-0.30165400	-1.36719800
H	-3.53782000	0.39885200	-1.72279500
H	-2.79823800	-1.15940600	-2.04863700
C	-3.12934300	-0.78112700	0.03186700
C	-2.15479600	-1.21806200	0.93537300
C	-4.47618400	-0.83663700	0.41098700
C	-2.52057100	-1.70000500	2.19288700
H	-1.10688400	-1.16586000	0.65774200
C	-4.84493500	-1.32656600	1.66449500
H	-5.24284400	-0.49061200	-0.27945900
C	-3.86596600	-1.75899100	2.56093600
H	-1.74988600	-2.02135500	2.88765700
H	-5.89441100	-1.36075700	1.94359700
H	-4.14900700	-2.13119500	3.54141700
C	-0.64910000	-0.09253800	-2.59324400
H	0.72961500	-1.68112300	-2.20879100
H	-1.14418100	-0.68442100	-3.35828800
C	0.62988000	0.32661400	-2.69602800
C	1.21610000	1.17294100	-1.61625200
H	2.04499600	1.77524800	-2.00037200

47

S-TS3 Eelec= -2909.62506301 a. u.

Zn	1.78456000	-0.64734600	-0.12258900
O	3.59254000	-1.34854900	-0.54898600
C	4.49129400	-0.46647300	-0.41873700
O	4.22963800	0.77158300	-0.20744700
C	5.94085900	-0.86410500	-0.49447100
H	6.36450100	-0.83781800	0.51511000
H	6.03895000	-1.87193100	-0.89742200
H	6.49527500	-0.14552900	-1.10214800
O	1.28485300	-1.17704100	1.82030800
C	0.39571600	-1.92474000	1.31463700
O	0.27243800	-1.97852900	0.03835800
C	-0.52671100	-2.73411900	2.18567200
H	-1.53634900	-2.31736200	2.11145400
H	-0.56839800	-3.76490800	1.82438400
H	-0.19901600	-2.70801700	3.22468700
C	0.93309400	2.58113600	1.35208000
C	0.57013800	1.89989400	0.18846100
C	-0.81181300	1.72719400	-0.08458400
C	-1.75985900	2.21969700	0.82415200
C	-1.36342100	2.89603500	1.97969300
C	-0.01230500	3.08745700	2.24646100

H	1.99242800	2.71457100	1.55948400
H	1.72540600	0.45873400	-2.79654500
H	-2.81602700	2.06202700	0.64503100
H	-2.12058900	3.26465900	2.66549300
H	0.30920400	3.61044100	3.14185800
N	-1.22650200	1.07530700	-1.27284900
C	-2.62984900	1.05717900	-1.66353700
H	-3.05683100	2.06206400	-1.54523100
H	-2.65470800	0.84736700	-2.73883200
C	-3.51407900	0.04366500	-0.94754500
C	-3.01758200	-1.20133600	-0.54293000
C	-4.86957300	0.33320100	-0.74940800
C	-3.87136800	-2.13863000	0.04286300
H	-1.96408200	-1.43439600	-0.66856000
C	-5.72184300	-0.60448200	-0.16372100
H	-5.26255200	1.30088300	-1.05524200
C	-5.22376500	-1.84617200	0.23342500
H	-3.47640300	-3.10404200	0.34735700
H	-6.77048700	-0.36282500	-0.01414200
H	-5.88314200	-2.57845200	0.69067500
C	-0.26656800	0.65504300	-2.18602000
H	3.03772700	0.93108900	-0.28614300
H	-0.66868600	0.20811500	-3.08876600
C	1.06089200	0.76941000	-1.99587200
C	1.65037000	1.37732200	-0.74305900
H	2.30496500	2.21579400	-1.02811900

47

S-TS4 Eelec= -2909.58461282 a. u.

Zn	-2.84923900	-0.15046400	0.24826500
O	-2.43139000	-2.05514300	-0.17167100
C	-1.43315100	-2.76905700	0.10772900
O	-0.38783800	-2.38764900	0.73936800
C	-1.46359200	-4.21693400	-0.33725200
H	-1.60372100	-4.25645600	-1.42132100
H	-0.54800600	-4.73820700	-0.05770000
H	-2.32719900	-4.71106200	0.11739600
O	-4.89164900	-0.06634400	0.50186300
C	-4.96781300	0.40400600	-0.67929300
O	-3.91034100	0.56746800	-1.36853800
C	-6.31731800	0.73638200	-1.26888400
H	-6.77922700	-0.18767600	-1.63323100
H	-6.97293600	1.15404200	-0.50190600
H	-6.21400700	1.42735600	-2.10652700

C	0.70311200	4.11366400	0.04517900
C	0.93920600	2.99859500	0.84720300
C	1.82474600	2.00123300	0.41479800
C	2.48236600	2.13791800	-0.81474200
C	2.24703800	3.26416200	-1.60268200
C	1.35570000	4.25195400	-1.18082200
H	0.01458000	4.88033600	0.38716400
H	0.46284300	2.90641900	1.81646200
H	3.15577400	1.36263400	-1.16077300
H	2.75624900	3.36070800	-2.55693800
H	1.17241700	5.12358800	-1.80152800
N	2.07429100	0.87502600	1.25858100
C	3.45925500	0.39722100	1.42696900
H	4.11219500	1.27375800	1.44639500
H	3.51092200	-0.06253500	2.42146700
C	3.95756700	-0.59184400	0.38228000
C	3.16286400	-1.65202400	-0.07592700
C	5.26892200	-0.47036600	-0.09535100
C	3.67804900	-2.56800400	-0.99412500
H	2.13954000	-1.77142000	0.26740400
C	5.78472000	-1.39145800	-1.00844500
H	5.89178400	0.35179700	0.24981700
C	4.98810500	-2.44354300	-1.46137500
H	3.05015700	-3.38195500	-1.34445300
H	6.80344600	-1.28167000	-1.36891500
H	5.38327700	-3.15952900	-2.17605500
C	1.06874900	0.20633200	1.87457100
H	-0.31440500	-1.17214700	1.13217200
H	1.42378100	-0.50382200	2.62223900
C	-0.25681900	0.12348700	1.49078000
C	-1.42102400	0.73318200	1.27395700
H	-1.55467600	1.71848500	1.73523100

47

S-3 Eelec= -2909.60834525 a. u.

Zn	-2.91491900	-0.24972500	-0.11126300
O	-3.61440400	-1.75623800	-1.24137800
C	-3.58669500	-2.61558400	-0.28885400
O	-3.17824300	-2.31375800	0.86125000
C	-4.09792200	-4.01233300	-0.58401300
H	-3.81649300	-4.31965900	-1.59395000
H	-3.72292500	-4.72390800	0.15358000
H	-5.19231200	-4.00550500	-0.53448700
O	-4.30348700	0.86520400	0.87301700

C	-4.34975300	1.70650400	-0.09012400
O	-3.62753600	1.56210200	-1.11415300
C	-5.31814500	2.86682100	0.01005900
H	-6.31972100	2.51506100	-0.26050700
H	-5.36578200	3.23786200	1.03650500
H	-5.03461900	3.66676000	-0.67581100
C	1.45066200	3.52607100	0.41833600
C	1.57782800	2.33137700	1.12649500
C	1.94231200	1.16916000	0.44270600
C	2.20635100	1.18878600	-0.92811200
C	2.07618600	2.39036900	-1.62549500
C	1.69656100	3.55545000	-0.95614500
H	1.15186900	4.42983400	0.93978500
H	1.37379200	2.29116600	2.19202400
H	2.48994700	0.27510100	-1.43827800
H	2.26542600	2.41188200	-2.69398000
H	1.58815300	4.48506800	-1.50592200
N	2.09260000	-0.05988400	1.19260800
C	3.45824000	-0.33137300	1.72218500
H	3.79130100	0.57602300	2.23363800
H	3.35916700	-1.12204700	2.47108100
C	4.45343000	-0.72523800	0.65052800
C	4.35180800	-1.96876400	0.01097700
C	5.49028100	0.14289000	0.29227600
C	5.26980600	-2.33393100	-0.97218400
H	3.55333700	-2.65564000	0.28135300
C	6.41405800	-0.22375000	-0.68863500
H	5.57592700	1.10916900	0.78248500
C	6.30374500	-1.46111300	-1.32314200
H	5.18260700	-3.29990300	-1.46033100
H	7.21588400	0.45773000	-0.95637000
H	7.02062000	-1.74756200	-2.08678400
C	1.09862800	-0.90306800	1.43955800
H	-0.82080000	-1.73633900	1.48649800
H	1.41107400	-1.74213100	2.06129600
C	-0.26792900	-0.90026400	1.05934800
C	-0.95907300	-0.03883900	0.23950700
H	-0.38000800	0.77046500	-0.20369500

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S-TS5 Eelec= -2909.57496617 a. u.

Zn	-2.53384000	0.12659800	0.48720000
O	-3.52739800	-1.49563700	-0.30445700
C	-3.81265700	-1.88523200	0.87871100

O	-3.41224800	-1.22794900	1.88343400
C	-4.66329400	-3.12096000	1.06408900
H	-4.39412800	-3.88184300	0.32790700
H	-4.56196600	-3.51262000	2.07700700
H	-5.71233900	-2.85504200	0.89498400
O	-3.42126300	1.92201000	0.82006700
C	-3.29904800	2.27438100	-0.40356300
O	-2.74551100	1.51362200	-1.24663600
C	-3.86394300	3.60950000	-0.83714900
H	-3.92476400	4.29979500	0.00577400
H	-3.26143300	4.03446800	-1.64257700
H	-4.87652100	3.45244500	-1.22480200
C	-0.71010000	-1.27340600	-1.84516800
C	-0.04732000	-0.12017300	-1.36768200
C	1.33993700	-0.20376200	-1.03270800
C	2.01731200	-1.41656400	-1.18651700
C	1.32785700	-2.53776900	-1.65645900
C	-0.03814800	-2.48379100	-1.96034400
H	-1.75734600	-1.19361300	-2.11528700
H	-0.52868100	0.83994500	-1.52139900
H	3.06287100	-1.49456600	-0.91314700
H	1.86711900	-3.47460300	-1.76766100
H	-0.55834800	-3.37004700	-2.30733700
N	1.98992300	0.96037600	-0.54764100
C	3.37631000	1.24760200	-0.91185000
H	3.51606200	0.96392700	-1.95982000
H	3.49436600	2.33846000	-0.86772400
C	4.45633600	0.58985900	-0.05918100
C	4.27117200	0.33555800	1.30543300
C	5.68870100	0.27293200	-0.64548100
C	5.30116200	-0.21930800	2.06716400
H	3.31832100	0.56169400	1.77468100
C	6.72027800	-0.27720200	0.11626200
H	5.84266200	0.45857700	-1.70625500
C	6.52854900	-0.52512700	1.47661700
H	5.14189000	-0.41462000	3.12369900
H	7.66920700	-0.51809700	-0.35424600
H	7.32782200	-0.95805200	2.07082200
C	1.35398900	1.71979800	0.42321000
H	-0.35016300	2.08240300	1.58466200
H	1.80365300	2.69099200	0.61049300
C	0.20069900	1.33404300	1.01666200
C	-0.50972700	0.10494000	0.70753900
H	-0.00959600	-0.81847000	1.01094600

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S-4 Eelec= -2909.62241705 a. u.

Zn	2.57588400	0.17754000	-0.41877500
O	3.66363400	-1.43466300	0.29016400
C	3.96442000	-1.74322900	-0.91381100
O	3.53213300	-1.05046900	-1.88058700
C	4.86089400	-2.93437900	-1.16328100
H	4.53184800	-3.78392500	-0.55928500
H	4.87149400	-3.19952000	-2.22086000
H	5.87877700	-2.68529000	-0.84575200
O	3.28942200	2.05674700	-0.69668000
C	3.09191000	2.34891400	0.53190100
O	2.57472000	1.50551100	1.32061600
C	3.52135400	3.70645400	1.03991400
H	3.44409500	4.45490000	0.24910500
H	2.92728000	3.99705500	1.90793900
H	4.57107200	3.64981500	1.34828300
C	0.51884500	-1.72531100	1.53179400
C	0.07386600	-0.43606700	0.92194300
C	-1.40789100	-0.19461300	1.02695300
C	-2.24831200	-1.06689300	1.77273800
C	-1.71240700	-2.18312700	2.35848700
C	-0.32038900	-2.52678000	2.22438000
H	1.56883000	-1.97641500	1.40086200
H	0.55946500	0.39938400	1.46044900
H	-3.31472900	-0.88505100	1.83440500
H	-2.36792500	-2.85619200	2.90404400
H	0.03789800	-3.44898100	2.67121900
N	-1.86387400	0.89573200	0.38980000
C	-3.23135700	1.40261200	0.60793400
H	-3.43378400	1.38206000	1.68186800
H	-3.21207600	2.45737600	0.31553000
C	-4.32973900	0.66771300	-0.14487800
C	-4.10505300	0.05835400	-1.38475300
C	-5.61766200	0.63818600	0.40533700
C	-5.15338300	-0.56840000	-2.06021300
H	-3.11070800	0.06889100	-1.82008600
C	-6.66663800	0.01791000	-0.27423600
H	-5.80234400	1.10338200	1.37123500
C	-6.43620100	-0.58841700	-1.51012200
H	-4.96518200	-1.04222500	-3.01920500
H	-7.65956100	0.00261600	0.16562400
H	-7.24950000	-1.07669200	-2.03868400

C	-1.12045400	1.48888300	-0.64657000
H	0.21189500	1.05595400	-2.23290500
H	-1.54293300	2.39693200	-1.05327300
C	-0.10007900	0.77987600	-1.22793300
C	0.53665300	-0.30786700	-0.56354400
H	0.63714300	-1.23033600	-1.14621800

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S-TS6	Eelec= -2909.61328100 a. u.		
Zn	2.65813800	-0.26104700	-0.57787400
O	3.91669800	-1.12679400	0.87639100
C	4.60590200	-1.56640400	-0.09673100
O	4.26916300	-1.29908000	-1.29786400
C	5.85098800	-2.38038600	0.16323100
H	5.76459900	-2.92205500	1.10672700
H	6.03939400	-3.06854800	-0.66258900
H	6.70564400	-1.69914100	0.23899700
O	2.99208500	1.66838300	-0.64471300
C	2.22680200	2.53567700	-0.10919500
O	1.14851600	2.30536400	0.50582400
C	2.68121500	3.98048500	-0.21693800
H	2.93026200	4.21058900	-1.25629400
H	1.91300700	4.66143700	0.14998600
H	3.59554400	4.11003100	0.37086800
C	0.61450800	-0.65340300	1.98693300
C	0.10443800	-0.18275000	0.71141900
C	-1.31943200	0.18668800	0.67695900
C	-2.05177300	0.25261900	1.89028000
C	-1.45255800	-0.11343400	3.07749300
C	-0.11277300	-0.57339700	3.14316100
H	1.63770800	-1.02276400	1.99715800
H	0.58723500	0.95953300	0.67842800
H	-3.09961400	0.52611000	1.88550200
H	-2.04198200	-0.06971300	3.98993500
H	0.31187900	-0.87516500	4.09459300
N	-1.85615700	0.54972800	-0.50836700
C	-3.16699700	1.19707800	-0.59951900
H	-3.23628300	1.96117400	0.18081900
H	-3.17869200	1.73672000	-1.55264900
C	-4.36586500	0.26198300	-0.52198500
C	-4.29461000	-1.06570300	-0.95966600
C	-5.58553500	0.75379600	-0.03987300
C	-5.42505500	-1.88347600	-0.91773300
H	-3.35359300	-1.46202900	-1.32922200

C	-6.71665000	-0.06242300	-0.00180400
H	-5.65143600	1.78240600	0.30838700
C	-6.63883600	-1.38511800	-0.44114400
H	-5.35542600	-2.91282700	-1.25754600
H	-7.65475700	0.33287300	0.37715400
H	-7.51652400	-2.02388000	-0.40821300
C	-1.17766900	0.24537100	-1.72624000
H	0.33436300	-0.76547500	-2.73124300
H	-1.70593700	0.56686000	-2.61460300
C	-0.03346200	-0.45649000	-1.75530900
C	0.73479800	-0.83897600	-0.55180900
H	0.74728800	-1.93621000	-0.45770300

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1' -2893.59464115 a. u.

Zn	2.50484900	0.07266000	-0.00191900
O	3.96263200	-1.28196600	-0.35615900
C	3.08658500	-2.19133800	-0.54503700
O	1.85157500	-1.89741500	-0.48439700
C	3.52340700	-3.61036800	-0.80513700
H	4.52349400	-3.63223400	-1.23985200
H	3.55133400	-4.14803900	0.14892600
H	2.80695700	-4.11700700	-1.45413100
O	3.31189300	1.72702900	1.01753400
C	2.43415700	1.51186900	1.90915300
O	1.59778300	0.55699900	1.75411600
C	2.39400800	2.35334000	3.15871200
H	3.11226200	1.94550500	3.87830000
H	2.69198700	3.37917500	2.93468900
H	1.40203900	2.32757700	3.61137800
C	-3.05194400	3.02149000	-1.55919700
C	-2.46884300	1.77797000	-1.80207400
C	-1.66433000	1.15752600	-0.83441400
C	-1.45513500	1.81727800	0.38369500
C	-2.03904800	3.06236900	0.62926800
C	-2.83961600	3.66789900	-0.33936800
H	-3.67250000	3.48514000	-2.32114000
H	-2.64665900	1.28823400	-2.75702400
H	-0.82414200	1.35394900	1.13758300
H	-1.86771300	3.55793200	1.58088100
H	-3.29438900	4.63565400	-0.14781000
C	-2.04472300	-1.32431400	-1.38418200
H	-2.66959600	-1.04323900	-2.24007100
H	-1.48363200	-2.21831900	-1.68287000

C	-2.91751800	-1.66301600	-0.19455600
C	-2.40643300	-2.45006600	0.84788400
C	-4.23321200	-1.19446600	-0.09590400
C	-3.19017000	-2.76009900	1.95902300
H	-1.38581700	-2.82121800	0.78476800
C	-5.02127900	-1.50427900	1.01427900
H	-4.64243100	-0.57938800	-0.89304400
C	-4.50209600	-2.28831800	2.04518200
H	-2.77791500	-3.37279200	2.75594300
H	-6.04080900	-1.13313200	1.07216300
H	-5.11473100	-2.53171800	2.90864700
C	0.02327400	-0.13822900	-2.24578700
H	0.42456300	-1.14285000	-2.41430000
H	-0.45181800	0.19439600	-3.17733700
C	1.14715400	0.75520400	-1.97280300
C	2.08724200	1.49611100	-1.75274200
H	2.84378700	2.24154800	-1.63570300
C	-1.01942200	-0.19623700	-1.09132600
H	-0.47312500	-0.48809700	-0.18918100

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R1' Eelec= -657.38792865 a. u.

C	1.92191700	2.37581800	-1.01095400
C	1.56146000	1.03360600	-1.12881300
C	1.11794000	0.30420200	-0.01525000
C	1.04575700	0.96047500	1.21890500
C	1.40456900	2.30404400	1.34258100
C	1.84428200	3.01702600	0.22736100
H	2.26545100	2.92072900	-1.88600100
H	1.63127500	0.55143000	-2.10109200
H	0.70345200	0.41179700	2.09233000
H	1.34025200	2.79181100	2.31127200
H	2.12544300	4.06212400	0.32066000
C	-0.52451500	-1.36443700	-1.04938800
H	-0.31056900	-0.95639000	-2.04419100
H	-0.67411600	-2.44355800	-1.18089300
C	-1.79707200	-0.75240700	-0.50330700
C	-2.56781700	-1.44883500	0.43871900
C	-2.22762600	0.51878900	-0.90541500
C	-3.73353600	-0.89285500	0.96617900
H	-2.25391500	-2.44092900	0.75650500
C	-3.39409500	1.07868800	-0.38163800
H	-1.64167100	1.07516800	-1.63179000
C	-4.15107400	0.37505200	0.55636400

H	-4.31853500	-1.45162900	1.69157000
H	-3.71162700	2.06513900	-0.70815900
H	-5.06055600	0.80900000	0.96206300
C	1.88730700	-2.05061000	-0.64130100
H	1.51904000	-3.07838300	-0.76000900
H	2.19515000	-1.72155200	-1.64246700
C	3.04788600	-2.05888900	0.24756100
C	3.99765700	-2.07428100	0.99329700
H	4.83767100	-2.07907800	1.64809400
C	0.71729800	-1.15873100	-0.13701500
H	0.45123400	-1.51560300	0.86480600

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TS10' Eelec= -2893.55978309 a. u.

Zn	-2.23851800	-1.19726800	-0.45202000
O	-2.50343300	0.64755700	-0.95997200
C	-1.81803200	1.58958800	-1.45938400
O	-0.57100600	1.57120200	-1.69839300
C	-2.53916600	2.87844000	-1.78709000
H	-3.61773400	2.72451700	-1.81714300
H	-2.29756000	3.60822000	-1.00736000
H	-2.17719200	3.27910400	-2.73633500
O	-3.97926100	-2.26055100	-0.36522800
C	-3.91476900	-2.16978400	0.90602100
O	-2.94010000	-1.55374900	1.44654100
C	-5.00542500	-2.76993400	1.75562000
H	-5.88574900	-2.12006600	1.70938000
H	-5.29627300	-3.74492600	1.35844000
H	-4.68441100	-2.85680200	2.79391500
C	5.40381500	-1.77955900	-0.85790400
C	4.32384400	-0.89723800	-0.86322900
C	3.32421400	-0.97543100	0.11836400
C	3.43896000	-1.96374600	1.10396400
C	4.51807300	-2.85047000	1.11228300
C	5.50528800	-2.76094200	0.13096200
H	6.16735400	-1.70123300	-1.62696100
H	4.26045500	-0.14174300	-1.64246700
H	2.67396500	-2.04036500	1.87307500
H	4.58580500	-3.60912000	1.88710100
H	6.34613700	-3.44846500	0.13521200
C	2.61476700	1.45547400	0.25779900
H	3.41909600	1.46614400	1.00440100
H	3.07478500	1.77667200	-0.68387500
C	1.55617500	2.46282600	0.66701800

C	0.80424600	2.28679400	1.83871200
C	1.34272000	3.62342900	-0.08654000
C	-0.13709700	3.23548100	2.23859800
H	0.96057500	1.40413000	2.45390200
C	0.41116800	4.58291000	0.31494600
H	1.91197000	3.77732200	-0.99958100
C	-0.33564000	4.39074300	1.47837100
H	-0.70931600	3.07642200	3.14818800
H	0.26932300	5.47909300	-0.28299700
H	-1.06084100	5.13541400	1.79428000
C	1.23309200	-0.24248600	-1.11054500
H	0.22115600	0.65514200	-1.28501700
H	1.72305300	-0.04666600	-2.07066600
C	0.41153300	-1.34699900	-1.11148600
C	-0.56336300	-2.15118500	-1.05247000
H	-0.58834900	-3.22866800	-1.14169600
C	2.13804300	-0.01577700	0.12376700
H	1.53503500	-0.25458500	1.00657000