

Supplementary Material

Mechanistic details of the dehydrative carbon-heteroatom bond construction *via* the benzoisochalcogenazolone-catalyzed acylative oxidation–reduction–condensation strategy

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Cartesian Coordinates (in Å) of all the reported structures	S2
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Cartesian Coordinates (in Å) of all the reported structures**P(OMe)₃**

P -3.03414500 -0.60582300 -0.16311000
O -3.90786500 -1.64867000 -1.07700500
O -3.31758800 -1.33300300 1.30791300
O -3.93429500 0.77030400 -0.02416800
C -5.16159900 -2.25056900 -0.69686100
H -5.28629600 -3.13823600 -1.31936200
H -5.15393900 -2.53842500 0.35546400
H -5.98800700 -1.56040000 -0.88639100
C -5.24647200 0.82692000 0.56652100
H -5.35129400 1.80614500 1.03802800
H -6.00957400 0.71771900 -0.20927500
H -5.37505900 0.04668800 1.32012000
C -2.68301400 -0.74035900 2.44831900
H -2.76894500 -1.45190900 3.27103500
H -1.62164900 -0.54134300 2.25791100
H -3.17482900 0.19664100 2.73003500

OP(OMe)₃

P -3.52628700 -0.58312000 0.04629200
O -4.73767900 -1.29580000 -0.72089400
O -3.80932400 -1.04538200 1.56187800
O -3.92737200 0.96113200 -0.05848900
C -4.79780300 -2.74039100 -0.74495800
H -5.64789700 -3.00144900 -1.37378100
H -3.88004000 -3.15148500 -1.17231200
H -4.94662400 -3.12584100 0.26605400
C -5.21390600 1.41766100 0.42046600
H -5.20368200 2.50328300 0.33259600
H -6.01273300 0.99846900 -0.19454900
H -5.35504000 1.12885500 1.46429400
C -2.78975200 -0.81739100 2.56068000
H -3.13257400 -1.31424300 3.46746800
H -1.83799300 -1.24182600 2.23522200
H -2.67554600 0.25367500 2.74748600
O -2.15067200 -0.83029000 -0.44784900

RCO-O-P(OMe)₃, plus

P -3.65523100 -0.57899100 0.05088600
O -4.76587900 -1.33679800 -0.73039900

O -3.58861800 -1.20497300 1.47799800
O -3.97945200 0.94283500 0.01316100
C -4.90846700 -2.79886200 -0.73002500
H -5.82156600 -2.99006800 -1.28716600
H -4.04802100 -3.24060100 -1.23151100
H -4.99481800 -3.15032600 0.29689500
C -5.29045000 1.48042800 0.40361600
H -5.19814700 2.55617500 0.28170700
H -6.05243500 1.07493600 -0.26041600
H -5.49076500 1.22407300 1.44349400
C -2.55335500 -0.86263200 2.46075200
H -2.78874000 -1.46069800 3.33688700
H -1.57738600 -1.12840500 2.05666900
H -2.61233100 0.20088100 2.69013400
O -2.19109800 -0.73266000 -0.55415500
C -1.85448100 -0.33700500 -1.89471300
O -2.69561500 0.09420600 -2.62358100
C -0.40317800 -0.57441000 -2.12493700
H -0.14494300 -0.26897200 -3.13726200
H 0.17984700 -0.00923900 -1.39279800
H -0.18189500 -1.63531000 -1.97801000

Structure 1_S

N 0.60415600 1.13276300 -0.22727700
S -0.96546800 0.42346200 -0.53692500
C 1.65236400 0.22245100 -0.07878100
C 1.11762600 -1.13764800 -0.22888100
C -0.25861900 -1.18420200 -0.48076100
O 2.82082000 0.54281300 0.13382400
C 1.86056500 -2.31946800 -0.14864700
C -0.92534400 -2.39978900 -0.65361100
C 1.20950800 -3.53579100 -0.31808700
C -0.17360000 -3.56971100 -0.56775100
H -1.99143900 -2.43514800 -0.84889900
H -0.66996800 -4.52605700 -0.69807300
H 1.76713200 -4.46422700 -0.25807800
H 2.92686600 -2.26321500 0.04403700
C 0.72604400 2.54692800 -0.16870500
C -0.02627800 3.34609900 -1.03834900
C 1.58115800 3.14074800 0.76950900
C 0.07265600 4.73505600 -0.96477600
H -0.67664600 2.88394100 -1.77358100
C 1.68503200 4.52984800 0.81884700

H 2.15784000 2.51704900 1.43861100
C 0.93145700 5.33264600 -0.04087400
H -0.51713800 5.34713100 -1.63964000
H 2.35134200 4.98568800 1.54457900
H 1.01198400 6.41363400 0.01044900

Structure A

N 2.00947700 2.11933600 -0.77976300
S -0.91933900 1.73612200 -0.36216500
C 1.81015200 1.34948400 -1.89548100
C 0.94309100 0.14107200 -1.67433000
C -0.28479900 0.15097400 -0.97954000
O 2.30971700 1.58138700 -2.99512900
C 1.38936600 -1.05495800 -2.25181000
C -1.01789700 -1.03211700 -0.85856500
C 0.66444000 -2.23427600 -2.11791300
C -0.53990700 -2.21801300 -1.41368500
H -1.96652300 -1.02932100 -0.33603100
H -1.12241000 -3.12695700 -1.30272000
H 1.03130000 -3.15359800 -2.56148200
H 2.32256000 -1.03711300 -2.80422100
C 2.68986500 3.34864200 -0.65654300
C 3.29978200 4.00587900 -1.73527800
C 2.72893700 3.92493200 0.62296100
C 3.93641100 5.22852400 -1.51713600
H 3.27258800 3.55687200 -2.71676500
C 3.37017200 5.14377500 0.82330700
H 2.25377800 3.41487800 1.45648100
C 3.97819800 5.80493500 -0.24692300
H 4.40655900 5.73200100 -2.35656500
H 3.39203900 5.57669500 1.81853200
H 4.47812800 6.75544800 -0.09126500
S -2.75231600 1.29341500 0.49155000
N -5.50570000 1.52950400 1.60816600
C -3.88535700 1.05208000 -0.90652000
C -5.80069200 0.51221400 0.73897000
C -5.81247500 1.64409700 2.98015400
C -5.21812900 0.67491200 -0.63754500
C -3.44929100 1.14514800 -2.23053100
O -6.50690300 -0.45477700 1.01978400
C -6.51973900 0.66849900 3.69825300
C -5.36044800 2.80046100 3.63536700
C -6.07048500 0.37538200 -1.70854600
C -4.32321600 0.87361000 -3.28193500

H -2.42463300 1.42356900 -2.44389200
C -6.76202000 0.86488600 5.05859000
H -6.86978100 -0.21749500 3.19017000
C -5.61304500 2.98161900 4.99189800
H -4.80935400 3.55278300 3.07787000
C -5.63763800 0.48191400 -3.02588700
H -7.08321600 0.06101300 -1.48079800
H -3.96519200 0.95769100 -4.30299700
C -6.31590800 2.01349600 5.71363100
H -7.31026800 0.10571700 5.60836800
H -5.25723100 3.88122700 5.48431000
H -6.31507100 0.25733300 -3.84266600
H -6.51303500 2.15416800 6.77144700
H 1.65830500 1.74175700 0.09043200
H -5.03662400 2.33327300 1.21166600

Structure 2

N 1.04493900 1.32506000 -0.23962800
S -0.59443900 0.69499000 -0.27502800
C 2.05576300 0.36955900 -0.17578700
C 1.43808500 -0.96309400 -0.14987900
C 0.03775500 -0.94982600 -0.19776100
O 3.25897500 0.62887500 -0.15325900
C 2.13551200 -2.17283900 -0.08646400
C -0.69310100 -2.14188900 -0.17733000
C 1.41917500 -3.36354600 -0.06625300
C 0.01531300 -3.34005600 -0.10953600
H -1.77507600 -2.14777400 -0.19992700
H -0.53647300 -4.27453300 -0.08970500
H 1.94088300 -4.31319500 -0.01537600
H 3.21992800 -2.15559600 -0.05308000
C 1.24096400 2.73057800 -0.28776800
C 0.39972800 3.52281100 -1.07932600
C 2.25717000 3.32735800 0.47128200
C 0.57091900 4.90643700 -1.10555700
H -0.37655100 3.05842200 -1.67830500
C 2.42922000 4.70957500 0.42071900
H 2.90259800 2.70979800 1.08060400
C 1.58807900 5.50541100 -0.36074000
H -0.08833500 5.51271100 -1.71861600
H 3.21980600 5.16668500 1.00771200
H 1.72373200 6.58178400 -0.38751000
P -3.89815100 -0.31361800 -0.14527100
O -4.61159900 -1.21311200 -1.30938700

O -3.80101900 -1.50883700 1.01061500
O -5.05395400 0.67038200 0.48611300
C -5.59043100 -2.25153300 -1.09264800
H -5.59685300 -2.86613700 -1.99398400
H -5.32304100 -2.86348600 -0.23024700
H -6.58194200 -1.81577900 -0.94609900
C -6.26766500 0.19928200 1.10624500
H -6.55011900 0.93211700 1.86404600
H -7.06206400 0.12706400 0.35852300
H -6.11606700 -0.77347100 1.57937500
C -3.15574600 -1.16305900 2.24535300
H -2.99536400 -2.09260500 2.79271800
H -2.18805400 -0.68018400 2.06803700
H -3.78502100 -0.49404400 2.84046500

Structure 3

O 1.31555700 1.97564200 -0.21292500
S -1.17523100 0.74712100 -0.89512400
C 1.86802300 0.79829900 -0.67924700
C 1.22406300 -0.47991000 -0.30829100
C -0.17619000 -0.61806200 -0.34856600
N 2.96287100 0.82346400 -1.32480500
C 2.02304200 -1.57370400 0.05096700
C -0.75514200 -1.85104200 -0.03137000
C 1.43915600 -2.79712600 0.36773400
C 0.04873200 -2.93461400 0.32206400
H -1.83456100 -1.95498800 -0.06307100
H -0.41238900 -3.88550600 0.57021600
H 2.06335800 -3.63849300 0.64977000
H 3.09953900 -1.44597800 0.07243400
P -0.20811700 2.32208800 0.34554400
O -1.20215700 3.28844500 -0.52694000
O -0.70867900 1.49792000 1.66195100
O 0.52895600 3.56825200 1.17754100
C -1.00015600 4.69038400 -0.81437800
H -1.31285900 4.82876200 -1.85001300
H -1.62727000 5.29312100 -0.15572700
H 0.04603800 4.97067700 -0.69892200
C -0.22170800 4.39534200 2.07547700
H 0.19642600 4.29079900 3.07947600
H -0.12635600 5.43620100 1.75823300
H -1.28317600 4.13107000 2.10821700
C -0.00721000 1.48061300 2.92714200
H -0.57989300 2.04704300 3.66323800

H 0.04866400 0.43255600 3.22471700
H 0.99575700 1.89606700 2.83387500
C 3.60740700 2.01457100 -1.71349200
C 5.00014100 2.07759700 -1.55601300
C 2.93711000 3.08912800 -2.32380800
C 5.70562800 3.20928500 -1.96217700
H 5.51178800 1.23350800 -1.10469100
C 3.65255500 4.20741900 -2.74733700
H 1.86475600 3.03754500 -2.47199000
C 5.03598900 4.27899300 -2.56107100
H 6.78144500 3.24995200 -1.82058600
H 3.12469100 5.02911300 -3.22228300
H 5.58664900 5.15563900 -2.88738600

Structure 4

C -2.09364500 -2.23477000 -0.79589700
C -0.88581900 -2.04439800 -0.04196400
C -0.64151500 -0.89398400 0.75858500
C -1.59855600 0.09232200 0.82358700
C -2.79927100 -0.06227400 0.09175500
C -3.03819200 -1.17899800 -0.68689400
S -2.35763300 -3.64711200 -1.75387600
C 0.08392500 -3.04054200 -0.10778000
H 0.29229800 -0.81186300 1.30401400
H -1.43407400 0.97726900 1.42746700
H -3.55368000 0.71745300 0.14329100
H -3.96837500 -1.27136400 -1.23743300
N 0.93591900 -3.83356400 -0.11972400
C 1.89173500 -4.82391700 -0.20267000
C 3.01478800 -4.76687400 0.63278100
C 1.70472800 -5.86205600 -1.12607800
C 3.96719100 -5.77708800 0.53300500
H 3.12558900 -3.94913800 1.33516800
C 2.66956800 -6.86127900 -1.20498300
H 0.82204800 -5.86951600 -1.75477700
C 3.79790500 -6.82136800 -0.38041200
H 4.84307300 -5.74783700 1.17194600
H 2.53945300 -7.67197600 -1.91364400
H 4.54548000 -7.60433500 -0.45013100

4_dimer_S

C -0.89846200 -3.21295100 -0.68893900
C 0.32690400 -2.53588600 -0.55803400
C 0.37066700 -1.32360500 0.13644000

C -0.77558200 -0.82194800 0.75131500
C -1.98258500 -1.51689900 0.65206700
C -2.04816000 -2.70226100 -0.07946400
S -0.99759200 -4.73218700 -1.62149900
C 1.56834900 -3.08800700 -1.18466200
H 1.30929100 -0.78313000 0.20212100
H -0.72600400 0.11047200 1.30365300
H -2.87796700 -1.12657900 1.12448700
H -2.99045200 -3.22693600 -0.19353200
N 2.31054900 -4.01569400 -0.72381600
C 2.04114100 -4.58582100 0.54376900
C 2.12647600 -3.83749300 1.72621300
C 1.74432000 -5.95466300 0.60807500
C 1.89918900 -4.45254700 2.95739600
H 2.37988100 -2.78447300 1.67530100
C 1.50064800 -6.55578700 1.84201900
H 1.68553700 -6.52603900 -0.31112100
C 1.57838100 -5.81023600 3.02146800
H 1.97058200 -3.86544700 3.86808700
H 1.25473200 -7.61278700 1.88116300
H 1.39692500 -6.28418100 3.98093800
C -0.41852700 -4.16799100 -3.24765100
N 0.05919900 -4.96832400 -4.10969800
C -0.56914200 -2.71667400 -3.56658600
C -1.79574900 -2.24337500 -4.04023100
C 0.49772600 -1.81611300 -3.38998200
C -1.95031800 -0.90009000 -4.38210000
H -2.62385700 -2.93628300 -4.14823400
C 0.33533200 -0.46874800 -3.72445300
S 2.07634500 -2.36761000 -2.75020600
C -0.88215400 -0.01455900 -4.23145500
H -2.90331400 -0.54719600 -4.76204400
H 1.15908200 0.22045500 -3.57382800
H -0.99973000 1.03278400 -4.48939400
C 0.30501600 -6.32411300 -3.79549400
C 1.46410100 -6.66574000 -3.08121000
C -0.55754500 -7.32720600 -4.25275300
C 1.74321400 -8.00593700 -2.81855300
H 2.12087000 -5.87681400 -2.72884800
C -0.27050300 -8.66533100 -3.97736800
H -1.44516800 -7.05059200 -4.81244000
C 0.87783800 -9.01065400 -3.26175800
H 2.63970600 -8.26499900 -2.26297800
H -0.94783400 -9.43891200 -4.32630900

H 1.09935100 -10.05265700 -3.05433900

Structure 5

N 1.32633200 1.67749100 -0.52241000
S -0.37431200 1.22138100 -0.41021900
C 2.16735700 0.65140000 -0.61384800
C 1.52610300 -0.62381400 -0.59918600
C 0.12831700 -0.46201700 -0.47688300
O 3.46124500 0.91127700 -0.69099300
C 2.11008500 -1.90356200 -0.66722200
C -0.70410500 -1.59043400 -0.41570500
C 1.28021200 -3.00784100 -0.61005100
C -0.11552000 -2.84539400 -0.48189000
H -1.77466000 -1.48776600 -0.30159700
H -0.74754400 -3.72606800 -0.43086800
H 1.70267600 -4.00495200 -0.65951500
H 3.18438500 -2.02876800 -0.76092700
C 1.78511800 3.04104200 -0.46411500
C 2.11974400 3.69172100 -1.64932200
C 1.93403100 3.65145000 0.77850400
C 2.60961400 4.99522200 -1.58653300
H 1.99053500 3.18356900 -2.59854300
C 2.42142000 4.95653800 0.82907200
H 1.63106600 3.12707800 1.67535600
C 2.75895600 5.62719500 -0.34933100
H 2.87260900 5.51555200 -2.50156800
H 2.53482300 5.44967700 1.78884800
H 3.13886000 6.64285600 -0.30345900
P -3.25430200 0.26645300 1.54601700
O -3.03316300 0.64827800 -0.04354500
O -3.87697200 -1.25331200 1.27062200
O -4.58493900 1.09780700 2.03643400
C -3.91396200 0.31351700 -1.13644400
H -3.30690900 0.33814200 -2.04250800
H -4.33860500 -0.68203700 -1.00218700
H -4.71183100 1.05564000 -1.21356700
C -5.89852800 0.95102900 1.46148600
H -6.62328100 1.14274400 2.25466100
H -6.03671400 1.68278500 0.66100300
H -6.04598000 -0.05769000 1.06968000
C -4.12580700 -2.06802300 2.42495900
H -4.30280100 -3.08356400 2.06826300
H -3.26505000 -2.07075500 3.10352000
H -5.00904200 -1.71712100 2.96848400

H 3.97789500 0.09310400 -0.75184300
O -1.09349900 3.68389400 1.72676700
C -1.12942800 4.29333200 0.62755600
O -0.97868100 3.79746800 -0.53159500
C -1.31486700 5.82411400 0.67453900
H -1.86407000 6.18790800 -0.19879500
H -1.82199200 6.13912400 1.59059300
H -0.32301700 6.29220100 0.65804100

Structure 6

N 1.48627700 1.20277400 0.17309200
S -0.51660400 -0.32203700 1.81335800
C 1.76607800 0.18505500 -0.69130900
C 1.03801500 -1.11549900 -0.46659700
C 0.07382800 -1.41628800 0.54800900
O 2.57841000 0.30304000 -1.62367700
C 1.39013400 -2.11489200 -1.39796600
C -0.46716200 -2.72792800 0.54025200
C 0.84166500 -3.38668700 -1.37646300
C -0.10256100 -3.69091500 -0.38747600
H -1.19973300 -2.97048600 1.30380800
H -0.55303000 -4.67909200 -0.34147300
H 1.13906900 -4.12829700 -2.11133900
H 2.12300400 -1.84406000 -2.14901900
C 2.00647500 2.50259300 0.19774300
C 2.94023400 3.00640500 -0.72543000
C 1.54403200 3.34513800 1.22768500
C 3.38911800 4.32280600 -0.60577900
H 3.29557500 2.36226300 -1.51536100
C 2.00149800 4.65464500 1.33270000
H 0.82291800 2.95917500 1.94253900
C 2.92981600 5.15589500 0.41531100
H 4.11036600 4.69813700 -1.32654100
H 1.63077500 5.28557700 2.13529200
H 3.28750700 6.17749700 0.49659200
H 0.79072800 0.96849700 0.90372400

Structure 7

N 1.09422600 0.96399300 -0.07919500
S 0.19634400 -1.18074600 2.25424700
C 1.84839900 -0.14301000 -0.33106300
C 1.03621800 -1.40911000 -0.42830500
C 0.22620400 -1.90440400 0.61119500
O 3.06500500 -0.14984700 -0.51811300

C 1.12726700 -2.13263800 -1.62291200
C -0.49104400 -3.09341700 0.42914800
C 0.40094400 -3.30751000 -1.80437400
C -0.41497700 -3.78603500 -0.77821900
H -1.09917900 -3.47595500 1.24143400
H -0.98221200 -4.70151100 -0.90991000
H 0.47434400 -3.84855100 -2.74201900
H 1.76949000 -1.75603900 -2.41204000
C 1.51177500 2.28280800 0.18395600
C 2.84461600 2.70660300 0.07760700
C 0.51863800 3.19527400 0.57806500
C 3.16458800 4.03338500 0.36973200
H 3.60318400 2.00060600 -0.22706800
C 0.85551600 4.51525000 0.86345800
H -0.51114400 2.86016800 0.66168300
C 2.18186900 4.94353100 0.76205900
H 4.19847800 4.35504900 0.28602800
H 0.07801600 5.20921300 1.16772400
H 2.44430300 5.97259100 0.98546600
H 0.09444700 0.80139700 0.00088200
C -1.03615800 0.12082200 2.10198100
O -1.54173100 0.43180300 1.03775600
C -1.32392300 0.83118700 3.39885400
H -0.82842800 1.80767400 3.36149700
H -2.40041200 1.00063600 3.47712400
H -0.96512700 0.28340200 4.27119000

Structure 8

N 1.42373000 1.21339400 0.07494500
S 0.30058200 -0.68424100 2.32057500
C 1.97473500 0.09681400 -0.48749800
C 1.15662300 -1.16355200 -0.36306700
C 0.41886700 -1.58095700 0.76466200
O 3.03366400 0.09479000 -1.11743600
C 1.17344400 -1.99008700 -1.49753700
C -0.31051200 -2.77605300 0.70921400
C 0.43448100 -3.16661700 -1.55324700
C -0.32023800 -3.55492100 -0.44551000
H -0.85833100 -3.10244100 1.58699400
H -0.89771700 -4.47349200 -0.46718500
H 0.45047300 -3.77652600 -2.45026900
H 1.77496400 -1.67500500 -2.34272300
C 1.94061200 2.52193100 0.14177900
C 3.15297800 2.91071700 -0.44851300

C 1.17769900 3.46685600 0.84750600
C 3.58150500 4.23291600 -0.32197500
H 3.73649000 2.18284400 -0.99179900
C 1.61917800 4.78151300 0.96298400
H 0.23923300 3.16447400 1.30409600
C 2.82611700 5.17424100 0.37858600
H 4.52084700 4.52566600 -0.78167100
H 1.01729100 5.49906100 1.51201200
H 3.17093800 6.19933300 0.46797400
H 0.53787200 1.08180300 0.54777100
H 1.57363600 -0.25295100 2.39675400

Structure 1_Se

N 0.88270100 1.33043100 -0.28486400
Se -0.87519100 0.62600500 -0.34094300
C 1.89491600 0.39041600 -0.13515600
C 1.33107800 -0.96993100 -0.05697200
C -0.06163000 -1.07274600 -0.14510200
O 3.09237100 0.67478500 -0.08716400
C 2.10856600 -2.12274200 0.09084400
C -0.70300900 -2.31011000 -0.08722700
C 1.48235500 -3.36275400 0.15137900
C 0.08388200 -3.45110300 0.06290600
H -1.78220000 -2.38843800 -0.15691400
H -0.39688100 -4.42302500 0.11115800
H 2.07281200 -4.26533000 0.26720100
H 3.18714100 -2.02316500 0.15498900
C 1.08027900 2.73109000 -0.39870600
C 0.28922800 3.47261600 -1.28521400
C 2.04460400 3.37837500 0.38662800
C 0.45711900 4.85335600 -1.38183500
H -0.44620400 2.96781300 -1.90369800
C 2.21515700 4.75663900 0.26777900
H 2.65213900 2.80173700 1.07057000
C 1.42330100 5.50084400 -0.61008100
H -0.16406600 5.41885300 -2.06911900
H 2.96540000 5.25188100 0.87644200
H 1.55699300 6.57482700 -0.69001300

Structure A-Se

N 2.18909000 2.10710600 -0.88438300
Se -0.69182200 1.99472000 -0.05850400
C 1.82199700 1.33617200 -1.96015900
C 0.95580100 0.16352300 -1.60385700

C -0.16621500 0.24852300 -0.75669500
O 2.16680300 1.55555700 -3.11910600
C 1.27513200 -1.06342200 -2.19996000
C -0.92274200 -0.89583000 -0.50100300
C 0.52404100 -2.20409400 -1.93632000
C -0.57395100 -2.11566500 -1.07885200
H -1.79347600 -0.83380600 0.14131900
H -1.17269600 -2.99509400 -0.86366100
H 0.78887900 -3.15002400 -2.39650000
H 2.12678000 -1.10225400 -2.87079000
C 2.90360300 3.32368100 -0.86413900
C 3.32032800 3.99218700 -2.02432900
C 3.17586000 3.87742500 0.39648600
C 4.00263100 5.20372900 -1.90484700
H 3.11424600 3.55983100 -2.99199200
C 3.85936300 5.08553500 0.49771900
H 2.84623400 3.35968400 1.29317400
C 4.27729700 5.75756600 -0.65371600
H 4.32323500 5.71633400 -2.80680700
H 4.06296900 5.50169300 1.47938700
H 4.81019500 6.69962600 -0.57534000
Se -2.81458200 1.54789600 0.85352500
N -5.70441500 1.48143300 1.64560300
C -3.90024100 1.26337000 -0.74452600
C -5.85050000 0.47247800 0.72547100
C -6.07833500 1.50626000 3.00593700
C -5.20636700 0.75579900 -0.60015100
C -3.38214300 1.47294600 -2.02323300
O -6.45884600 -0.57437200 0.93635000
C -6.66717700 0.41676400 3.66388900
C -5.81364000 2.68897400 3.71371800
C -5.95188800 0.44254200 -1.74420700
C -4.14827500 1.18324400 -3.15138700
H -2.37424600 1.85336100 -2.14086500
C -6.98226000 0.52816200 5.01889000
H -6.87356000 -0.48955100 3.11459000
C -6.13655200 2.78412400 5.06413100
H -5.35023600 3.52831000 3.20251200
C -5.43584700 0.66112800 -3.01722400
H -6.94561800 0.02819000 -1.61167000
H -3.72819700 1.35780200 -4.13691000
C -6.72343900 1.70286300 5.72640200
H -7.43867700 -0.31863000 5.52259800
H -5.92618500 3.70529600 5.59846400

H -6.02833400 0.42382200 -3.89432600
H -6.97532200 1.77646100 6.77937100
H 2.00562800 1.70919100 0.02769800
H -5.35810300 2.36153200 1.28550400

Structure 2_Se

N 0.91673700 1.34525600 -0.27418200
Se -0.89739700 0.65339000 -0.24981900
C 1.91672700 0.40343500 -0.19035800
C 1.33945800 -0.95540200 -0.12551700
C -0.05856000 -1.06228700 -0.14453100
O 3.12687400 0.65312100 -0.18276100
C 2.13605900 -2.10144400 -0.04918000
C -0.66806700 -2.31861000 -0.08646600
C 1.53590700 -3.35359600 0.01085600
C 0.13809500 -3.45379000 -0.00683900
H -1.74343600 -2.43237400 -0.09494100
H -0.33365900 -4.43016200 0.04158000
H 2.14384800 -4.25000600 0.07181100
H 3.21444500 -1.98181000 -0.03820200
C 1.11854900 2.74399700 -0.32749700
C 0.25941900 3.53460900 -1.10442100
C 2.14520400 3.35608500 0.40860900
C 0.41949000 4.91921300 -1.13885500
H -0.52324100 3.06220000 -1.68919500
C 2.30502100 4.73953700 0.35356100
H 2.80905900 2.74549900 1.00503200
C 1.44458100 5.52886100 -0.41366500
H -0.25506300 5.51855300 -1.74242300
H 3.10364900 5.20350000 0.92457700
H 1.57211100 6.60618900 -0.44554100
P -3.62060800 -0.56548700 -0.02800900
O -4.41601000 -1.22104200 -1.28456100
O -3.88356600 -1.76452200 1.07827200
O -4.51809600 0.67254200 0.54748300
C -5.61715700 -2.02229400 -1.19585300
H -5.69494400 -2.56391100 -2.13891100
H -5.54998500 -2.72709000 -0.36646100
H -6.49189900 -1.38001100 -1.07155700
C -5.87278300 0.52604900 1.02766500
H -6.03432700 1.30693000 1.77177200
H -6.57379800 0.65983400 0.20011700
H -6.02119900 -0.45352800 1.48736500
C -3.26810500 -1.60038300 2.36921400

H -3.38363300 -2.54778800 2.89571300
H -2.20233800 -1.36898200 2.26908400
H -3.75988200 -0.80359700 2.93436700

Structure 3_Se

O 1.51077500 1.83370200 0.06028400
Se -1.01712100 0.77514400 -1.15013200
C 1.97154800 0.70074800 -0.59187100
C 1.32362600 -0.58452600 -0.24242700
C -0.06482400 -0.71526700 -0.41493100
N 2.97167100 0.77123000 -1.36870600
C 2.08049400 -1.66435600 0.22173200
C -0.68452900 -1.92907600 -0.11393700
C 1.45521100 -2.87429700 0.52215400
C 0.07468400 -3.00440500 0.35270000
H -1.75617800 -2.03246900 -0.24646700
H -0.41522400 -3.94426100 0.58755100
H 2.04241100 -3.71105100 0.88578900
H 3.15235800 -1.54742300 0.34118200
P -0.03939700 2.33470100 0.36618800
O -0.75475800 3.40908800 -0.64782100
O -0.84527700 1.54780300 1.55016800
O 0.66627700 3.48104600 1.34930800
C -0.36223800 4.78853600 -0.84305000
H -0.49613900 4.98381700 -1.90767500
H -1.01383100 5.44305000 -0.26241700
H 0.67867000 4.94574400 -0.56354800
C -0.13640400 4.37063100 2.13578400
H 0.08981200 4.20612400 3.19189000
H 0.12139800 5.39909600 1.87360400
H -1.20930100 4.22323700 1.97903400
C -0.38500700 1.44392500 2.91925300
H -1.01261500 2.06700400 3.55844900
H -0.49957600 0.39450800 3.19424300
H 0.65857000 1.74261000 3.01406200
C 3.50955300 2.01622100 -1.76491400
C 4.89257200 2.21431800 -1.66711300
C 2.70506000 3.01920600 -2.33138000
C 5.45864500 3.41642900 -2.09247400
H 5.50837300 1.42586400 -1.24644700
C 3.28054300 4.20953800 -2.76992300
H 1.63816000 2.85112000 -2.43332700
C 4.65739200 4.41809600 -2.64507200
H 6.53009900 3.56579100 -1.99926500

H 2.65007100 4.97730800 -3.20838500
H 5.10169100 5.34868900 -2.98371100

Structure_4

C -2.02065900 -2.19646800 -0.85048900
C -0.86489100 -2.02165800 -0.02660100
C -0.68648300 -0.90249200 0.83057800
C -1.66595200 0.06481100 0.87829700
C -2.81996500 -0.08017900 0.07586200
C -2.99132200 -1.17138600 -0.75857300
Se -2.20034500 -3.69094500 -1.96044500
C 0.12168100 -3.00615500 -0.08009100
H 0.21242000 -0.82487400 1.43227900
H -1.55227300 0.92756700 1.52458600
H -3.59134400 0.68337600 0.11469800
H -3.88670600 -1.25853100 -1.36452500
N 0.99615400 -3.77458300 -0.05691500
C 1.92313300 -4.79005400 -0.16335300
C 3.10545700 -4.73167200 0.58419900
C 1.64025900 -5.85636200 -1.02896500
C 4.02168100 -5.77198400 0.45543900
H 3.28878000 -3.89093500 1.24284600
C 2.57168000 -6.88334600 -1.14036200
H 0.71100700 -5.85770000 -1.58745800
C 3.75876500 -6.84390900 -0.40204200
H 4.94301600 -5.74400200 1.02690800
H 2.36963400 -7.71617300 -1.80521100
H 4.47921600 -7.64955400 -0.49532600

Structure 4_dimer_Se

C -0.86080700 -3.14250200 -0.61234700
C 0.39629400 -2.51986300 -0.54136300
C 0.50756600 -1.26774500 0.07252800
C -0.60197400 -0.67347100 0.67037300
C -1.84201000 -1.31463200 0.63227900
C -1.97342500 -2.53958100 -0.02116900
Se -1.05811900 -4.81715400 -1.52881200
C 1.60424100 -3.15396100 -1.14877000
H 1.47124300 -0.76891100 0.08614000
H -0.49924000 0.28916800 1.16017800
H -2.71073300 -0.85272500 1.08991000
H -2.94225800 -3.02173600 -0.09046700
N 2.29852500 -4.11228700 -0.68118600
C 1.99647900 -4.66978100 0.58468600

C 2.04747500 -3.91512800 1.76496700
C 1.69713700 -6.03825400 0.64692800
C 1.78498500 -4.52437200 2.99208900
H 2.30132200 -2.86220100 1.71650800
C 1.41687400 -6.63327600 1.87578400
H 1.66388600 -6.61255200 -0.27171700
C 1.46128300 -5.88156800 3.05320900
H 1.83119100 -3.93333900 3.90186500
H 1.16922100 -7.68991900 1.91336200
H 1.25218500 -6.35072000 4.00943400
C -0.44479300 -4.19352000 -3.29140400
N 0.03900900 -4.97973700 -4.15833300
C -0.62039500 -2.74190500 -3.57515700
C -1.88106500 -2.26962600 -3.95397300
C 0.44677000 -1.83524700 -3.45116100
C -2.06942800 -0.92240500 -4.25846000
H -2.71011400 -2.96728400 -4.01354200
C 0.25123800 -0.48428200 -3.74643000
Se 2.17896800 -2.42521500 -2.85294600
C -1.00048600 -0.02996400 -4.16187800
H -3.04903300 -0.57093500 -4.56519300
H 1.07550000 0.21122100 -3.63358000
H -1.14303100 1.02148300 -4.38910100
C 0.32288000 -6.32901000 -3.85677200
C 1.46111900 -6.63742700 -3.09455000
C -0.48130400 -7.35525300 -4.36539500
C 1.77782200 -7.97022500 -2.83827100
H 2.07138800 -5.82987600 -2.70321400
C -0.15862700 -8.68579000 -4.09279900
H -1.35313300 -7.10241300 -4.95998600
C 0.96940100 -8.99898500 -3.33146500
H 2.65857800 -8.20515300 -2.24783900
H -0.79142800 -9.47854300 -4.48011500
H 1.21952800 -10.03516600 -3.12731600

Structure 6_Se

Se -3.22112000 2.97983700 0.32233300
N -5.50641300 1.45281700 1.76259200
C -4.11721400 1.79588600 -0.89277400
C -5.92458800 0.70817700 0.70039800
C -5.99327500 1.46081300 3.07593900
C -5.20707800 0.91773200 -0.61145300
C -3.62838400 1.80201800 -2.22136800
O -6.85545900 -0.10974700 0.78480000

C -7.03810500 0.64584900 3.54661400
C -5.37278100 2.35774600 3.96757900
C -5.72652000 0.11717400 -1.65110200
C -4.15708300 1.00538200 -3.22584400
H -2.80054900 2.46618400 -2.44800400
C -7.43967900 0.73986100 4.88036000
H -7.51443500 -0.04191100 2.86457500
C -5.78510700 2.43866400 5.29358800
H -4.56574700 2.98769300 3.60463200
C -5.22458700 0.14548200 -2.94190500
H -6.55279400 -0.53636600 -1.39742400
H -3.73842500 1.05409900 -4.22763500
C -6.82416900 1.62909200 5.76237300
H -8.24834300 0.10409200 5.23023600
H -5.29236500 3.13783100 5.96295500
H -5.65287200 -0.48670600 -3.71357100
H -7.14691900 1.69187900 6.79684300
H -4.71897600 2.09662800 1.56771900

Structure 7_Se

N 1.11168500 0.98414300 -0.07592500
Se 0.40257700 -1.17723500 2.38856300
C 1.86318900 -0.10393100 -0.40507600
C 1.06987700 -1.38322000 -0.47148600
C 0.34648300 -1.91944400 0.60751500
O 3.06255200 -0.08440200 -0.68335100
C 1.09209200 -2.07610200 -1.68827500
C -0.35683400 -3.11852300 0.44609900
C 0.37971700 -3.26203700 -1.84869700
C -0.35206700 -3.78204300 -0.78006300
H -0.90019800 -3.53345700 1.28756100
H -0.90906300 -4.70629500 -0.89383400
H 0.39782400 -3.77888800 -2.80260700
H 1.67018500 -1.66701000 -2.51021900
C 1.52590400 2.30891500 0.15873400
C 2.84780600 2.74713100 -0.01271300
C 0.54283800 3.21452500 0.59197100
C 3.16633800 4.07964100 0.25313200
H 3.59916300 2.04744900 -0.34786400
C 0.87803700 4.54042800 0.85042500
H -0.47799600 2.87012600 0.72735100
C 2.19306000 4.98270500 0.68348500
H 4.19168900 4.41140600 0.11863200
H 0.10780800 5.22846400 1.18532100

H 2.45398800 6.01651200 0.88591900
H 0.12338200 0.80300800 0.07998900
C -1.02732200 0.14227800 2.22649200
O -1.48361000 0.47277200 1.14974400
C -1.49332700 0.69612200 3.54554300
H -1.79716900 1.73660000 3.41170700
H -2.36453500 0.11765500 3.87277200
H -0.72453300 0.61933100 4.31702400

Structure 8_Se

Se -4.19969700 3.51715100 0.20188500
N -5.43262400 1.19554800 1.77300600
C -4.40419400 1.98488700 -0.95510000
C -6.11171500 0.87561200 0.62622400
C -5.91986200 1.32174100 3.09046000
C -5.28650900 0.93706900 -0.62757200
C -3.70471500 1.93531600 -2.16812300
O -7.29322200 0.53340900 0.59652800
C -7.26327800 1.12057200 3.44046900
C -4.98948900 1.68224200 4.07820000
C -5.46820100 -0.11603100 -1.53576500
C -3.87749000 0.86754200 -3.04529700
H -3.02695400 2.73864000 -2.43490100
C -7.65382800 1.28441600 4.77031600
H -7.97487000 0.83852400 2.67903500
C -5.39551600 1.83911400 5.40011100
H -3.95017700 1.84193800 3.80451300
C -4.76559000 -0.16444600 -2.73398300
H -6.17313400 -0.89804400 -1.27507700
H -3.32117200 0.85017800 -3.97714900
C -6.73226800 1.64164700 5.75546200
H -8.69540300 1.12690200 5.03404600
H -4.66407100 2.11793800 6.15223300
H -4.90890600 -0.99366200 -3.41843500
H -7.04938500 1.76386900 6.78607700
H -4.43254700 1.31732400 1.67891300
H -3.32495300 4.23129100 -0.73457400

Structure 1_Te

N 0.79146600 1.36594800 -0.33340300
Te -1.17662600 0.66805300 -0.34625400
C 1.78003700 0.40886200 -0.19613500
C 1.23587100 -0.96753300 -0.08332600

C -0.15043500 -1.16065800 -0.12279200
O 2.98578400 0.67105200 -0.17846000
C 2.08514700 -2.07150500 0.05719400
C -0.70196400 -2.43822400 -0.02479300
C 1.54643500 -3.34939200 0.15888000
C 0.15689100 -3.52890100 0.11795700
H -1.77540400 -2.59142900 -0.05744000
H -0.26138100 -4.52751900 0.19734900
H 2.19993400 -4.20836000 0.26949600
H 3.15605800 -1.89844200 0.08326300
C 1.05847300 2.75762700 -0.42650000
C 0.32895400 3.54176200 -1.32931000
C 2.01618400 3.36431200 0.39968400
C 0.54919600 4.91685800 -1.40404000
H -0.40096800 3.07267000 -1.98264400
C 2.23996700 4.73682900 0.30662800
H 2.57763800 2.75893000 1.09839000
C 1.50861700 5.52034600 -0.58975200
H -0.02629700 5.51179100 -2.10622900
H 2.98389700 5.19750000 0.94949700
H 1.68338900 6.58974700 -0.65036800

Structure A_Te

N 2.19558800 2.00669500 -1.17502900
Te 0.08679600 2.20028700 1.41234900
C 1.01332100 1.67715600 -1.78206400
C 0.34090800 0.47989000 -1.17404300
C -0.04800600 0.43876400 0.17527000
O 0.52784600 2.27790300 -2.74036000
C 0.04597300 -0.59960200 -2.01611900
C -0.69157800 -0.70071500 0.67007500
C -0.60232600 -1.72604700 -1.51973200
C -0.96451800 -1.77779800 -0.17131700
H -1.01213900 -0.73448400 1.70533000
H -1.47005500 -2.65249700 0.22554200
H -0.82620300 -2.55816200 -2.17903500
H 0.32651500 -0.53912400 -3.06253400
C 3.03581800 3.11524400 -1.40646100
C 2.74475900 4.11812900 -2.34276700
C 4.20328800 3.20149900 -0.63229700
C 3.62614900 5.19017900 -2.48977200
H 1.84730400 4.04604400 -2.93875600
C 5.07247000 4.27646500 -0.79286200
H 4.42323500 2.42553000 0.09580400

C 4.78916200 5.27926100 -1.72370700
H 3.39514000 5.96337300 -3.21636800
H 5.97155700 4.32948200 -0.18690400
H 5.46638600 6.11790300 -1.84887800
Te -2.73153400 2.15501000 1.96801900
N -5.72729200 1.39842100 1.61469200
C -3.30911800 1.72919400 -0.07419000
C -5.31615300 0.39894600 0.75803400
C -6.50866100 1.28686100 2.78512000
C -4.40824200 0.88688000 -0.32733100
C -2.51406000 2.14944700 -1.14228500
O -5.64633600 -0.77915000 0.86050500
C -6.79717200 0.05952000 3.39883400
C -6.96985800 2.48026400 3.36087400
C -4.66046800 0.44511700 -1.63237700
C -2.78251600 1.71603300 -2.44029100
H -1.65319400 2.78439800 -0.97076100
C -7.54624900 0.04508200 4.57606700
H -6.44593400 -0.85813000 2.95109800
C -7.71650500 2.44848000 4.53517800
H -6.73787300 3.43017600 2.88718800
C -3.85298700 0.85612600 -2.68904300
H -5.49823700 -0.22393200 -1.79941200
H -2.12155100 2.03075800 -3.24026000
C -8.01029300 1.22921200 5.15073900
H -7.76730900 -0.90860200 5.04580500
H -8.06706800 3.37980700 4.96881700
H -4.05444200 0.50538100 -3.69586000
H -8.59246600 1.20380900 6.06617900
H 2.53204200 1.34604700 -0.48691900
H -5.61768500 2.34156500 1.26349500

Structure 2_Te

N 0.88642500 1.46395100 -0.34030200
Te -1.18157500 0.87535300 -0.27357700
C 1.81396400 0.46251000 -0.25513100
C 1.18668900 -0.88737800 -0.19100200
C -0.21022400 -1.01093800 -0.18968000
O 3.04287300 0.62426100 -0.24678100
C 1.98824600 -2.03346800 -0.13595200
C -0.80218300 -2.27514800 -0.14385200
C 1.40338300 -3.29367400 -0.08043500
C 0.00870600 -3.40961600 -0.08519500
H -1.87726100 -2.40034000 -0.15347600

H -0.45547700 -4.39018700 -0.04564100
H 2.02341800 -4.18310200 -0.03615200
H 3.06537400 -1.90319700 -0.13877200
C 1.22607700 2.83582100 -0.35279900
C 0.47229800 3.72002900 -1.14035800
C 2.26700300 3.34880900 0.44015700
C 0.74594500 5.08763500 -1.13147700
H -0.31816700 3.33058100 -1.77482200
C 2.54098000 4.71509800 0.43293300
H 2.85302500 2.67230200 1.04710700
C 1.78368000 5.59327000 -0.34719500
H 0.14978900 5.75472500 -1.74674000
H 3.34862600 5.09689200 1.05071400
H 2.00034700 6.65683700 -0.34294200
P -3.75533100 -0.57249900 0.05004700
O -4.41263000 -1.37563600 -1.19086500
O -3.91588900 -1.71483200 1.21623400
O -4.77615200 0.60669400 0.50555700
C -5.47373000 -2.35698500 -1.08557800
H -5.48978900 -2.88665600 -2.03776100
H -5.26983300 -3.05345500 -0.27207300
H -6.43380300 -1.86225600 -0.92489000
C -6.13813100 0.35752700 0.92759100
H -6.42619700 1.19023500 1.56920700
H -6.79269600 0.32359900 0.05377100
H -6.20500600 -0.57811200 1.48653000
C -3.27155800 -1.46260000 2.48170900
H -3.46444600 -2.33425400 3.10635400
H -2.19279600 -1.34105800 2.34544900
H -3.68649500 -0.57005100 2.95742600

Structure 3_Te

O 1.50105100 1.81202000 0.09634600
Te -1.14193000 0.74535800 -1.42230000
C 1.94502800 0.68928700 -0.58810900
C 1.31925800 -0.60814700 -0.22394700
C -0.04845900 -0.82069500 -0.47084200
N 2.92508800 0.76918500 -1.38828300
C 2.10080800 -1.61988900 0.34548500
C -0.61790400 -2.05239300 -0.13748200
C 1.52249700 -2.84416700 0.67831300
C 0.16414700 -3.05832300 0.43563600
H -1.67224200 -2.22820500 -0.32411600
H -0.29110500 -4.00935900 0.69477100

H 2.12934400 -3.62642100 1.12247900
H 3.15612300 -1.43846400 0.52082600
P -0.03413200 2.39314400 0.32941300
O -0.62985300 3.51720000 -0.71881300
O -0.92210200 1.59870400 1.45384700
O 0.66238000 3.48412600 1.37138800
C -0.20656300 4.90213700 -0.81105300
H -0.29417900 5.16057700 -1.86687900
H -0.87115800 5.53316200 -0.21956300
H 0.82460400 5.02115200 -0.48210600
C -0.14564000 4.36001400 2.16901500
H 0.04501400 4.14757100 3.22350900
H 0.14263100 5.39150400 1.95588100
H -1.21582100 4.24207900 1.97458500
C -0.48274700 1.39706400 2.82165000
H -1.09119900 2.01040900 3.48809200
H -0.64440300 0.33957400 3.03480200
H 0.57140600 1.64498100 2.94334000
C 3.45798200 2.01575900 -1.78653100
C 4.84642600 2.19509500 -1.73947300
C 2.64500600 3.03814500 -2.30362800
C 5.41132700 3.39738900 -2.16519300
H 5.46749400 1.39137400 -1.35722500
C 3.21916700 4.22851100 -2.74453200
H 1.57292800 2.88695400 -2.36598900
C 4.60216300 4.41817300 -2.66941900
H 6.48737300 3.53203600 -2.11086400
H 2.58246300 5.01150500 -3.14546400
H 5.04497700 5.34906600 -3.00918300

Structure 4_Te

C -2.12444300 -2.24208200 -0.72998000
C -0.89771600 -2.04260500 -0.03420100
C -0.61342200 -0.87004500 0.71453200
C -1.56397500 0.12815900 0.77606500
C -2.78524600 -0.03923600 0.09444200
C -3.05542500 -1.18894700 -0.63688000
Te -2.49895700 -4.02019100 -1.82316400
C 0.07824100 -3.04537200 -0.09060900
H 0.33894600 -0.77509200 1.22440400
H -1.37008200 1.03195900 1.34234700
H -3.53256600 0.74726900 0.14189800
H -4.00626200 -1.28714900 -1.14960000
N 0.96404700 -3.79921100 -0.06935200

C 1.91062800 -4.79762800 -0.17239600
C 3.00555800 -4.80259800 0.70036000
C 1.73463300 -5.78102300 -1.15604200
C 3.94443600 -5.82282100 0.57675800
H 3.10573300 -4.02480500 1.44819800
C 2.68432900 -6.79240100 -1.25624900
H 0.87011300 -5.73688600 -1.80884900
C 3.78627400 -6.81448800 -0.39553600
H 4.80024100 -5.84315800 1.24252600
H 2.56464700 -7.56316800 -2.00983800
H 4.52320800 -7.60569000 -0.48349900

Structure 4_dimer_Te

C -0.83732100 -3.05079000 -0.51623200
C 0.45304000 -2.49175900 -0.49023600
C 0.63245400 -1.20106900 0.02720800
C -0.43821000 -0.49901200 0.57369100
C -1.71309200 -1.06846700 0.57672100
C -1.91142400 -2.33200300 0.02054900
Te -1.19225000 -4.95336100 -1.41442400
C 1.63793600 -3.20200100 -1.05937900
H 1.62270700 -0.75707700 0.00283200
H -0.27921600 0.49151200 0.98730400
H -2.55565800 -0.52273300 0.98933100
H -2.90968400 -2.75507300 -0.01197500
N 2.28635300 -4.18270700 -0.57364100
C 1.97230200 -4.73967100 0.68781400
C 1.87715200 -3.97335900 1.85850300
C 1.81583600 -6.13205700 0.75617400
C 1.60957800 -4.59646900 3.07741900
H 2.02424500 -2.90081900 1.81187300
C 1.52619200 -6.74323200 1.97425900
H 1.90009600 -6.71377300 -0.15508100
C 1.42342700 -5.97931400 3.14033000
H 1.54454400 -3.99650400 3.98019400
H 1.38888700 -7.81963900 2.01411500
H 1.20947300 -6.45866900 4.09043300
C -0.47995300 -4.22484000 -3.36705200
N 0.04687400 -4.98835000 -4.22518000
C -0.68442900 -2.77281400 -3.62256400
C -1.97905500 -2.32017800 -3.90817700
C 0.37188300 -1.84636300 -3.54350300
C -2.21884100 -0.97248800 -4.16509400
H -2.79437100 -3.03624300 -3.92929900

C 0.11841600 -0.49154900 -3.78415600
Te 2.34092400 -2.44754800 -2.96202200
C -1.16733200 -0.05647400 -4.10707500
H -3.22429400 -0.63844600 -4.39967900
H 0.92570400 0.22839700 -3.70376700
H -1.34878000 0.99763200 -4.29136700
C 0.35357400 -6.33444400 -3.94709600
C 1.45866600 -6.63740200 -3.13431800
C -0.40605100 -7.36482900 -4.51385300
C 1.78904400 -7.96914300 -2.89136500
H 2.03177000 -5.82875400 -2.69285200
C -0.07198500 -8.69440500 -4.25106400
H -1.25248000 -7.11509200 -5.14525600
C 1.02496300 -9.00187400 -3.44320200
H 2.64502500 -8.20053200 -2.26414800
H -0.67085500 -9.49066200 -4.68249300
H 1.28492300 -10.03731600 -3.24766700

Structure 6_Te

N 1.45264600 1.21271900 0.14194800
Te -0.08071500 -0.49435200 2.56046600
C 1.86609600 0.13708600 -0.58722100
C 1.10916100 -1.15745100 -0.39843200
C 0.31261000 -1.56305700 0.70677400
O 2.78258800 0.20815700 -1.41818300
C 1.26241000 -2.03174400 -1.49587500
C -0.29109500 -2.83722300 0.62952100
C 0.65027700 -3.27436000 -1.54708300
C -0.13682100 -3.67933600 -0.46564700
H -0.89881600 -3.17031000 1.46442100
H -0.62808200 -4.64861500 -0.47266900
H 0.78333200 -3.91671000 -2.41212100
H 1.88692400 -1.69313700 -2.31429000
C 1.97711300 2.51460200 0.16669900
C 3.02931700 2.96201100 -0.65039500
C 1.38553300 3.41191900 1.07557400
C 3.46884600 4.28276300 -0.54515500
H 3.48249200 2.27469800 -1.34833900
C 1.83755600 4.72437800 1.16923800
H 0.57084500 3.06659200 1.70552000
C 2.88438000 5.17160900 0.35808600
H 4.28241000 4.61651800 -1.18308400
H 1.36805000 5.39993200 1.87818900
H 3.23611400 6.19600300 0.42899300

H 0.75326400 1.02062800 0.86474200

Structure 7_Te

N 1.17095300 0.95157700 -0.04935700
Te 0.37232900 -1.21468900 2.55799000
C 1.91895200 -0.13917900 -0.38044100
C 1.11558100 -1.40810300 -0.49874500
C 0.35982700 -1.96533000 0.54855900
O 3.12695900 -0.12676500 -0.62020800
C 1.16709800 -2.06396700 -1.73618500
C -0.34666700 -3.15559900 0.32649600
C 0.45074800 -3.23811800 -1.95233200
C -0.31308600 -3.78237400 -0.91929400
H -0.92105300 -3.59766000 1.13299100
H -0.87449400 -4.69797000 -1.07583400
H 0.49130500 -3.72669700 -2.92046400
H 1.77073600 -1.63429200 -2.52896100
C 1.59788300 2.26404700 0.22961100
C 2.93773700 2.67386000 0.14922500
C 0.61085100 3.18688800 0.61516600
C 3.26928200 3.99438200 0.45565200
H 3.69271900 1.96207300 -0.14998300
C 0.95951900 4.50048400 0.91557500
H -0.42404400 2.86617000 0.68035500
C 2.29195700 4.91415400 0.83869300
H 4.30851700 4.30322900 0.39117900
H 0.18534400 5.20154200 1.21229400
H 2.56308200 5.93847300 1.07346300
H 0.17469400 0.78438200 0.06744800
C -1.19489100 0.27862000 2.19315600
O -1.50857100 0.59260000 1.06472600
C -1.82901000 0.84725900 3.43292100

H -2.31875800 1.79302300 3.19111100

H -2.57690300 0.13496900 3.79838600

H -1.08905700 0.98963100 4.22467200

Structure 8_Te

N 1.44728400 1.17164600 -0.02640400
Te 0.91141200 -0.75533900 2.72885900
C 2.03503700 0.06299800 -0.56662100
C 1.24166100 -1.20732900 -0.40891900
C 0.69687200 -1.68765000 0.79578800
O 3.09782900 0.07330600 -1.18844500
C 1.08319300 -1.96451400 -1.58070800
C -0.02658900 -2.88772100 0.79015800
C 0.34690600 -3.14400600 -1.58309800
C -0.21940100 -3.60083000 -0.39208300
H -0.42901900 -3.28151700 1.71796500
H -0.79078200 -4.52353100 -0.37392200
H 0.22039300 -3.70426700 -2.50358100
H 1.54127900 -1.59811800 -2.49327300
C 1.95937100 2.47730000 0.09933200
C 3.18166800 2.88535300 -0.45593600
C 1.18677500 3.39410300 0.83022700
C 3.61146400 4.19981600 -0.26914000
H 3.77144500 2.17752800 -1.01901200
C 1.62922600 4.70218100 1.00484500
H 0.24195400 3.07489200 1.26139300
C 2.84634800 5.11431700 0.45635500
H 4.55871300 4.50837500 -0.70142900
H 1.02043300 5.39892600 1.57272200
H 3.19188200 6.13403000 0.59239700
H 0.55366800 1.02119300 0.42337600
H 2.44134300 -0.20232100 2.42838200