

Supplementary information for

Study on the Formation of Secondary Organic Aerosol by Ozonolysis of Citral in the Atmosphere

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Table S1. The T1 diagnostic values of the key transition states involved in the reactions of CIs at CCSD/6-311+G(d,p) level.

Species	T1 Diagnostic
TS1-H ₂ O	0.021
TS1-NO(1)	0.038
TS1-NO(2)	0.032
TS2-NO ₂ (2)	0.029
TS1-SO ₂	0.023
TS2-SO ₂	0.021

Table S2. Cartesian coordinates for all the optimized structures of reactants, transition states and products

Neral			
C	-2.04337100	-0.00997600	0.08200300
C	-3.34296100	-0.20356400	0.82175400
H	-3.21029000	-0.92117700	1.63985200
H	-3.72291700	0.73230900	1.23481000
H	-4.10213100	-0.62432400	0.15193400
C	-1.43317400	1.18839500	0.14053500
C	-1.59323600	-1.26961200	-0.63302800
H	-1.94766000	-2.10430400	-0.01318500
H	-2.16790300	-1.34907600	-1.56637800
C	-0.10140600	-1.51568900	-0.92895300
H	-0.01210900	-2.57502000	-1.20510000
H	0.21943800	-0.95567200	-1.80979200
C	0.77414300	-1.22885600	0.26011500
H	0.37441800	-1.57652400	1.21505000
C	1.94677400	-0.58168300	0.28309100
C	2.64582500	-0.01840900	-0.92640800
H	2.67118500	1.07729800	-0.86722800
H	3.68522400	-0.36427100	-0.95268000
H	2.17879900	-0.30335300	-1.87091700
C	2.66025500	-0.31967000	1.58319300
H	3.67300200	-0.73883300	1.56582500

H	2.76163700	0.76074600	1.74316000
H	2.12263500	-0.74509600	2.43393200
C	-0.19122400	1.59639800	-0.53527100
H	0.17548900	0.96452100	-1.36049200
O	0.40534600	2.61560200	-0.24683900
H	-1.87133000	1.97396100	0.75373700
O ₃			
O	0.00000000	0.00000000	0.42403200
O	0.00000000	1.06278900	-0.21201600
O	0.00000000	-1.06278900	-0.21201600
PRC1			
C	1.97265500	0.97546200	0.15360300
C	1.53503900	2.13255300	1.00589700
H	0.49501900	2.01009100	1.32745300
H	2.17268500	2.25896000	1.88304800
H	1.56401100	3.05519400	0.41358300
C	3.09035400	0.28579400	0.45281100
C	1.08186800	0.65770800	-1.03274100
H	0.40398000	1.50344900	-1.19110000
H	1.68247500	0.56335000	-1.94353100
C	0.25086900	-0.63127800	-0.86037000
H	-0.35024900	-0.77433700	-1.76576900
H	0.93925300	-1.48639900	-0.81074900
C	-0.62693100	-0.63221300	0.36207600
H	-0.25692100	-0.07650500	1.22285000
C	-1.79114600	-1.29203200	0.51399100
C	-2.38203000	-2.22790000	-0.50846500
H	-2.25908700	-3.26310700	-0.16754600
H	-3.45687900	-2.05063500	-0.61710900
H	-1.91832800	-2.14295000	-1.49259500
C	-2.57061100	-1.18760600	1.79483900
H	-3.55846500	-0.75541800	1.59505300
H	-2.73218300	-2.17874000	2.23467900
H	-2.06243700	-0.55702500	2.52796500
O	-2.36667200	1.52617400	-0.88113100
O	-3.23182200	0.63481700	-0.81097600
O	-1.84233800	1.88916000	0.18876500
C	3.63237100	-0.81210300	-0.35875100
H	3.11132500	-1.03930100	-1.31031400
O	4.61540900	-1.45178900	-0.04400700
H	3.67456000	0.53616100	1.33552900

PRC2

C	3.27163300	-0.39451400	-0.25733100
H	3.27942700	0.04248200	-1.26176700
H	3.70155700	0.32714500	0.43887200
H	3.91478100	-1.28229400	-0.28705600
C	1.28295400	-1.83309100	-0.78998700
H	1.65754500	-1.58153700	-1.79176300
H	1.76029800	-2.79261100	-0.54516800
C	-0.23757300	-2.04102200	-0.90828200
H	-0.38531500	-2.72629100	-1.75400600
H	-0.63486200	-2.56404500	-0.03660300
C	-0.97791800	-0.75991600	-1.18177700
H	-0.52492600	-0.13723300	-1.95685800
C	-2.10200600	-0.30842500	-0.60636800
C	-2.87866100	-1.02948800	0.46488800
H	-2.81314600	-0.48136700	1.41349900
H	-3.93777300	-1.07463500	0.18851000
H	-2.53798100	-2.05262700	0.63405700
C	-2.68683100	1.02568000	-0.99211700
H	-3.73550400	0.91791200	-1.29121800
H	-2.66654700	1.70887000	-0.13336200
H	-2.14067900	1.48773200	-1.81807200
C	0.00877600	-0.50190800	1.83355400
H	-0.49834400	-1.43202000	1.53439400
O	-0.49482600	0.21461000	2.67618400
C	1.87048900	-0.78728700	0.13812400
C	1.31717400	-0.21050400	1.22533300
H	1.87445400	0.56376400	1.74941700
O	1.35917700	1.82742600	-1.14506600
O	0.20049200	2.38816300	0.54356700
O	0.24500700	2.08475200	-0.65457300

TS1

C	2.44439600	-0.87971500	0.03307700
C	3.31003700	-2.00940800	-0.46872800
H	2.77330000	-2.58536000	-1.23131700
H	4.24514600	-1.64742300	-0.89847800
H	3.54408800	-2.70369800	0.34635400
C	2.83251600	0.38612900	-0.22410000
C	1.23323700	-1.39551300	0.77984000
H	0.83951500	-2.23633300	0.19186100
H	1.60512100	-1.84447900	1.71105100
C	0.06009200	-0.47327600	1.09938200
H	-0.70942000	-1.07807900	1.60664600

H	0.34382500	0.29038900	1.83413600
C	-0.55383400	0.14565100	-0.12325200
H	-0.05698000	-0.01334300	-1.07789100
C	-1.61582000	1.01143900	-0.07611300
C	-2.13097700	1.56274200	1.22923100
H	-1.55000300	2.45336900	1.50345800
H	-3.17746100	1.86322300	1.13828700
H	-2.05240800	0.84167800	2.04564800
C	-2.11862100	1.66787000	-1.32683100
H	-1.85666700	2.73289800	-1.32515300
H	-1.69570900	1.20293000	-2.21983600
H	-3.20927400	1.59361600	-1.38074000
O	-2.54220800	-1.68276900	0.05817500
O	-3.26085200	-0.65045100	-0.08836700
O	-1.64379700	-1.79324500	-0.82694000
C	2.20975000	1.66973000	0.14569900
H	1.30635700	1.67098800	0.77454700
O	2.68137700	2.72801700	-0.22229800
H	3.74975800	0.53332600	-0.79237200

TS2

C	3.17341400	-0.68417100	0.68600000
H	3.15630800	-1.77050700	0.80715500
H	3.71249800	-0.44575700	-0.23258200
H	3.72115600	-0.26030000	1.53612300
C	0.90584100	-0.65116900	1.78211000
H	0.99868600	-1.74397800	1.78067100
H	1.41063100	-0.31870500	2.70114400
C	-0.57895100	-0.28795700	1.88649000
H	-0.92685300	-0.69351300	2.84632200
H	-0.70499300	0.79631700	1.96453500
C	-1.40484400	-0.87947800	0.77564300
H	-1.07346900	-1.86247000	0.43845900
C	-2.47986900	-0.35116800	0.17526700
C	-3.09051200	0.98057200	0.52553900
H	-3.10754500	1.63984300	-0.35103100
H	-4.13297700	0.84100400	0.83502700
H	-2.57210500	1.49869400	1.33448500
C	-3.17574000	-1.08396700	-0.94180600
H	-4.22848900	-1.26437500	-0.69502400
H	-3.16169600	-0.48468900	-1.86014100
H	-2.69926500	-2.04469700	-1.15124300
C	0.38518500	1.88777500	-0.18095300
H	-0.60625200	1.42379500	-0.06219800

O	0.49381000	3.07438400	-0.40827700
C	1.77189700	-0.12713900	0.65289400
C	1.56979600	0.99934900	-0.12361800
H	2.43800400	1.42337300	-0.62329700
O	1.18338300	-1.65527900	-0.91333500
O	1.04405900	0.07569000	-2.10973300
O	0.44363000	-0.93853400	-1.65538000

TS3

C	2.13649500	-1.05331200	-0.02009400
C	1.91742400	-2.33235000	-0.77580000
H	2.41271100	-2.32369700	-1.74871800
H	2.30661400	-3.17467700	-0.19114200
H	0.84581800	-2.51923500	-0.91361800
C	2.94611900	-0.09085300	-0.50335400
C	1.35524700	-0.92639700	1.27398100
H	1.01650000	-1.92185100	1.57851800
H	1.98822800	-0.54035300	2.07910000
C	0.11235200	-0.02111300	1.14197900
H	-0.46528300	-0.08549700	2.06740900
H	0.43177500	1.01776100	0.99354900
C	-0.75455000	-0.47914100	-0.03155100
H	-0.28584000	-0.31054100	-1.01899700
C	-2.11218400	0.85702700	-0.17925000
C	-2.63367900	1.05189800	1.22118500
H	-1.98842500	1.73877800	1.77139900
H	-3.63130000	1.49986500	1.13764800
H	-2.72563300	0.10470200	1.75113200
C	-1.58182300	2.05194600	-0.91968700
H	-1.40086300	1.80500700	-1.96754700
H	-2.29524200	2.88035600	-0.86197300
H	-0.64402400	2.38549000	-0.46798400
O	-3.28165800	-0.98236600	-0.35717700
O	-2.86422800	0.08620600	-0.97746100
O	-1.42290200	-1.55850600	0.11675600
C	3.22197900	1.18022800	0.17711300
H	2.79576400	1.31104200	1.19252500
O	3.88729200	2.07030600	-0.31313500
H	3.44688600	-0.21988000	-1.46030800

TS4

C	-2.08670000	-0.96932000	0.06614000
C	-1.89974400	-2.26622100	0.80125600
H	-2.14360200	-3.10361200	0.13692100

H	-0.85338900	-2.40235900	1.09694000
H	-2.53326800	-2.32724500	1.68816600
C	-3.00069900	-0.07071200	0.47984600
C	-1.17739600	-0.75320900	-1.12963500
H	-0.71856600	-1.70607000	-1.41226500
H	-1.74835000	-0.41009500	-1.99781100
C	-0.05107800	0.27140900	-0.87192000
H	0.58386400	0.33749400	-1.75796900
H	-0.48006100	1.25588200	-0.66645000
C	0.78890100	-0.12900200	0.31631900
H	0.40086300	0.08076600	1.31507800
C	2.46026500	0.74672200	0.14795700
C	2.02860600	2.19485800	-0.12392200
H	1.29757400	2.55472500	0.60604100
H	2.92445200	2.81765200	-0.03901200
H	1.63606100	2.30238200	-1.13497300
C	3.13396200	0.53602600	1.50236700
H	3.29281100	-0.52910600	1.67984400
H	4.11178400	1.02766200	1.48117300
H	2.55315300	0.96682800	2.32388600
O	1.86648600	-1.58988800	-0.87048900
O	2.95627700	0.10159600	-0.84468000
O	1.32565500	-1.35273500	0.29723500
C	-3.28994400	1.20054800	-0.19895200
H	-2.76693100	1.39331600	-1.15739200
O	-4.07242800	2.02087000	0.23480600
H	-3.60135900	-0.26356800	1.36609300

TS5

C	-1.44206700	2.41384500	-0.68820600
H	-0.65435100	3.10839800	-0.99699100
H	-2.05188500	2.18128600	-1.56387800
H	-2.05420500	2.90624600	0.07385800
C	-0.13222200	1.29652600	1.23986600
H	0.37858200	2.26948100	1.21956800
H	-0.90785500	1.39399500	2.00917200
C	0.88727400	0.20090000	1.58003300
H	1.02070500	0.18514900	2.66917500
H	0.50324200	-0.78056000	1.29366300
C	2.22081500	0.44086500	0.92568100
H	2.76548400	1.30996500	1.30037400
C	2.79105100	-0.27557100	-0.05141000
C	2.18219400	-1.48477800	-0.70784800
H	2.87732700	-2.33121000	-0.65683400

H	1.22681400	-1.78555900	-0.27810800
H	2.00271500	-1.27123500	-1.76784700
C	4.13893000	0.11518200	-0.60103200
H	4.86137000	-0.69914900	-0.47032800
H	4.07111700	0.30932500	-1.67798500
H	4.53505900	1.00903000	-0.11266100
C	-1.95034200	-1.02922500	1.20002600
H	-1.90837900	-0.64932000	2.23839500
O	-1.76647900	-2.18815800	0.94002800
C	-0.76953700	1.14869600	-0.15917200
C	-2.34044700	0.01310800	0.18699900
H	-3.14342000	0.68265000	0.49844200
O	-0.15863000	0.42450700	-1.01410300
O	-2.49884400	-0.35164400	-1.07920600
O	-1.45557500	-0.99417700	-1.51267300

TS6

C	1.69810800	-2.24830600	-0.23609600
H	0.95358400	-2.96234500	-0.60825500
H	2.41935700	-2.05049400	-1.02754400
H	2.19663200	-2.68278500	0.63329200
C	0.25443000	-1.04054200	1.52252800
H	-0.12198400	-2.06506300	1.65329800
H	1.01823200	-0.90542800	2.29867500
C	-0.90468300	-0.04680400	1.71345600
H	-1.13179100	-0.02536100	2.78601000
H	-0.59343400	0.96268300	1.43981000
C	-2.14396600	-0.45308600	0.96150600
H	-2.62533500	-1.36307400	1.32534400
C	-2.70047000	0.17124900	-0.08491400
C	-2.16093500	1.41769500	-0.73349400
H	-1.26983700	1.82215700	-0.25220900
H	-1.89644100	1.20292600	-1.77603900
H	-2.93271800	2.19605000	-0.75238000
C	-3.94952800	-0.37402000	-0.72786700
H	-4.75593400	0.36778100	-0.69445600
H	-3.76813400	-0.59793500	-1.78559400
H	-4.29750400	-1.28504700	-0.23487100
C	1.89512100	1.45457900	0.91062500
H	2.15348400	1.40077900	1.99161000
O	1.23833700	2.36166300	0.46845600
C	0.96241900	-1.00067000	0.18432200
C	2.40232400	0.30686400	0.06800800
H	3.14035600	-0.34561800	0.56423600

O	0.26422500	-0.36627900	-0.76163500
O	2.50043000	0.48622800	-1.19094300
O	0.92132600	-0.33048500	-1.89454900

IM1

C	2.49749200	-0.67482300	0.05163900
C	3.51371200	-1.65569500	-0.47832600
H	3.04832500	-2.30886600	-1.22535400
H	4.36806700	-1.15462500	-0.93549100
H	3.87554200	-2.30401900	0.32772700
C	2.67319000	0.63550000	-0.21896900
C	1.40922600	-1.37277700	0.84285100
H	1.19633100	-2.31121300	0.31432000
H	1.86303000	-1.68011600	1.79528500
C	0.06778000	-0.69360900	1.12461500
H	-0.56156400	-1.40926300	1.66548900
H	0.18718800	0.16788500	1.78476200
C	-0.66358500	-0.31932700	-0.16006100
H	0.00459400	0.18352700	-0.86725600
C	-1.99376700	0.49951700	-0.00761000
C	-2.42926700	0.74989800	1.43062600
H	-1.72714500	1.40757000	1.95178800
H	-3.40719400	1.23764100	1.42029200
H	-2.51677300	-0.18842700	1.98328600
C	-1.97238800	1.77748600	-0.83221000
H	-1.70325200	1.55336300	-1.86741300
H	-2.95623900	2.25409400	-0.81875600
H	-1.24369800	2.48246900	-0.42010500
O	-2.41899000	-1.65645600	-0.38235000
O	-2.94350500	-0.37510300	-0.64317800
O	-1.08377700	-1.50424900	-0.84145200
C	1.85547800	1.79466800	0.17017100
H	0.99233100	1.63874400	0.83960100
O	2.10856900	2.91841200	-0.21639200
H	3.53486000	0.92538900	-0.81756900

IM2

C	3.08301100	0.95979000	-0.08670600
H	3.29083900	1.74107300	0.64901800
H	3.68807600	0.08359800	0.15041600
H	3.36274800	1.32780300	-1.07775600
C	0.78020400	1.89667000	-0.30864300
H	1.02367200	2.53498500	0.54988800
H	1.22955600	2.38696000	-1.17934500

C	-0.74710400	1.88206200	-0.48684000
H	-1.05767200	2.93528500	-0.44443500
H	-1.00703500	1.54686400	-1.49384300
C	-1.48469700	1.09184300	0.55841200
H	-1.09318800	1.18290800	1.57098900
C	-2.53129600	0.27935000	0.36653200
C	-3.19503400	0.02205900	-0.96074400
H	-3.02654200	-1.01941600	-1.26215900
H	-4.27808200	0.16175100	-0.87011000
H	-2.84588500	0.67951500	-1.75957900
C	-3.10497000	-0.51862900	1.50593000
H	-4.17634000	-0.32107300	1.62763000
H	-2.99336800	-1.58976500	1.29720300
H	-2.59844300	-0.29950000	2.44848100
C	-0.07378600	-1.03605700	-1.27146600
H	-0.52651700	-0.37515600	-2.03848100
O	-0.65379100	-2.00555900	-0.86315400
C	1.59023500	0.61804200	-0.05689500
C	1.35614500	-0.68466900	-0.87242700
H	1.96765400	-0.67318300	-1.78606300
O	1.22304300	0.11036700	1.22721400
O	1.87130800	-1.67975400	-0.01815700
O	1.93497400	-1.09573200	1.31600100

IM3

C	-0.33230100	0.88704000	0.26777600
C	0.36754800	2.17868200	-0.04999400
H	-0.18424500	2.77220700	-0.78121300
H	0.48453800	2.76994000	0.86582500
H	1.37911200	1.99596700	-0.43200300
C	-1.54621600	0.61409600	-0.24586700
C	0.43266800	-0.06290300	1.17012600
H	1.19610400	0.50217500	1.71515100
H	-0.22580700	-0.51164000	1.91861000
C	1.13648000	-1.20065600	0.39256500
H	1.73620400	-1.79957700	1.08293700
H	0.38268700	-1.83694500	-0.08484300
C	2.05141700	-0.63708700	-0.66768400
H	1.57280000	-0.33811400	-1.62372500
O	3.23701800	-0.47393500	-0.50427900
C	-2.31219500	-0.61070000	0.02838500
H	-1.86808500	-1.33877400	0.73659700
O	-3.38980100	-0.84450400	-0.47789700
H	-2.03544000	1.32144000	-0.91177700

IM4

C	-0.51832300	0.90364100	0.24901800
C	0.29182400	2.10515500	-0.14410600
H	0.38076400	2.77485700	0.72031800
H	1.31696800	1.81990500	-0.40639800
H	-0.16799800	2.65633800	-0.96627300
C	-1.74497400	0.68635500	-0.26387900
C	0.16802600	-0.03599300	1.22336800
H	1.00744500	0.48301900	1.68736300
H	-0.51268200	-0.36312200	2.01380700
C	0.71664300	-1.31042200	0.52788900
H	1.47571200	-1.75813500	1.18343300
H	-0.08873100	-2.02840500	0.35497900
C	1.37791100	-1.05227400	-0.77317100
H	1.01519900	-1.42293400	-1.72948500
O	2.97760700	0.11574400	0.26845100
O	2.44237600	-0.39838100	-0.87152600
C	-2.60931200	-0.44505100	0.09620000
H	-2.24658300	-1.12301800	0.89576900
O	-3.68297000	-0.65763300	-0.42857000
H	-2.16696700	1.37519600	-0.99226600

IM5

C	2.81960700	-0.75223700	1.01533200
H	2.33709900	-0.68753900	1.99705800
H	3.13659900	-1.77896200	0.83218800
H	3.68516800	-0.08246300	1.03582600
C	1.49439100	1.16632600	-0.09320700
H	1.56672600	1.59179700	0.91550600
H	2.29030200	1.64254800	-0.68403300
C	0.11864300	1.43647500	-0.70976100
H	0.03443800	2.50861200	-0.92219400
H	0.05229100	0.90977700	-1.66419800
C	-0.98764500	1.02835200	0.22500800
H	-1.08425100	1.65178800	1.11674500
C	-1.83284700	-0.00409900	0.10310400
C	-1.84616400	-0.97865700	-1.04395200
H	-2.81175600	-0.93664400	-1.56258100
H	-1.04477000	-0.81020000	-1.76199700
H	-1.73105600	-1.99986400	-0.66247600
C	-2.87977400	-0.26824700	1.15528800
H	-3.88392600	-0.24241900	0.71531600
H	-2.74940200	-1.26722900	1.58782800

H	-2.83861500	0.46676100	1.96306000
C	1.83128900	-0.31588100	-0.04099900
O	1.34201900	-1.10476900	-0.82136600
IM6			
C	2.83929400	-0.08211500	0.95736200
H	2.51169700	-0.75070200	1.76215100
H	3.56362700	-0.66659700	0.37980200
H	3.27988900	0.83239400	1.35316000
C	1.15894900	1.58492700	-0.18210500
H	1.16757700	2.13443000	0.76827100
H	1.89949400	2.08472000	-0.82360600
C	-0.23996000	1.62196700	-0.81440800
H	-0.44550200	2.66021600	-1.09817200
H	-0.23795500	1.03287500	-1.73437700
C	-1.29313900	1.14209200	0.14840700
H	-1.47951500	1.80940200	0.99211200
C	-1.98153800	-0.00656600	0.10257800
C	-1.84472200	-1.05798800	-0.96647000
H	-1.30060100	-0.71415600	-1.84643300
H	-1.30324400	-1.92588800	-0.57095300
H	-2.83581500	-1.39971300	-1.28431700
C	-2.96679200	-0.35290300	1.18895000
H	-3.97199000	-0.48058800	0.77109100
H	-2.69456900	-1.30540200	1.65853300
H	-3.00892500	0.41668800	1.96361300
C	1.67439200	0.20786200	0.09557800
O	1.07171100	-0.74107100	-0.46139000
O	1.52540400	-2.01784600	-0.22238900
OHCCHO			
C	0.76989500	0.47688600	-0.00003600
H	1.25305600	1.47468800	0.00009000
O	1.40350400	-0.54200000	0.00001200
C	-0.76989100	0.47688600	-0.00001600
H	-1.25306700	1.47468100	0.00006600
O	-1.40350500	-0.54200000	0.00000700
OHCCHOO			
C	1.26227400	0.21295300	0.00000000
H	2.15829200	0.86237100	0.00000000
O	1.34459000	-0.98982800	0.00000000
C	0.00000000	0.98782400	0.00000000
H	0.00842200	2.07347400	0.00000000

O	-1.17230500	0.50710200	0.00000000
O	-1.38982900	-0.78483700	0.00000000

CH₃COCH₃

C	0.00005300	0.18413900	0.00000000
C	-0.00002200	-0.61249300	1.28747300
H	0.00052400	0.06295700	2.14260000
H	-0.88105100	-1.26130400	1.32598200
H	0.88059000	-1.26191400	1.32542600
C	-0.00002200	-0.61249300	-1.28747300
H	0.88059000	-1.26191400	-1.32542600
H	-0.88105100	-1.26130400	-1.32598200
H	0.00052400	0.06295700	-2.14260000
O	-0.00002200	1.39570100	0.00000000

CH₃COOCH₃

C	0.37381400	0.02156100	-0.00005200
C	0.04920900	1.46260000	-0.00007700
H	0.95057400	2.07459100	-0.00060200
H	-0.58537400	1.67488500	-0.86819800
H	-0.58383300	1.67522400	0.86915000
C	1.75917200	-0.52459000	0.00002100
H	1.74184500	-1.61450100	0.00068800
H	2.29777900	-0.16385800	-0.88233900
H	2.29792200	-0.16269300	0.88186100
O	-1.84226500	-0.33493700	0.00004600
O	-0.55924500	-0.82019700	-0.00003600

TS7

C	-0.71663100	0.95241100	0.25123900
C	-0.09262800	2.28346300	-0.05438500
H	-0.03991100	2.88014300	0.86431000
H	0.93436300	2.16146200	-0.41121500
H	-0.67014000	2.83767900	-0.79620800
C	-1.87770800	0.58473800	-0.32351700
C	0.03337900	0.07619400	1.24321700
H	0.83712500	0.66015500	1.70089300
H	-0.63207300	-0.23807000	2.05279800
C	0.64222900	-1.18458800	0.61447900
H	1.11701800	-1.80289700	1.39494700
H	-0.10672100	-1.83093700	0.14318800
C	1.72973300	-0.94140100	-0.36355600
H	2.07249600	-1.73133500	-1.03182400
O	3.62998400	-0.39843200	-0.40035200

O	2.28261100	0.19671400	-0.45225000
C	-2.60749900	-0.65610300	-0.02453600
H	-2.21349300	-1.29057100	0.79639700
O	-3.61324700	-0.99420200	-0.61227100
H	-2.35870400	1.23343900	-1.05194400
DO			
C	-0.74965000	0.95440300	0.21078500
C	-0.13071800	2.25664300	-0.21254800
H	-0.12070000	2.95200100	0.63508100
H	0.91656600	2.11618900	-0.50794700
H	-0.67351100	2.71985200	-1.03837600
C	-1.90154000	0.52275600	-0.33577200
C	0.03164400	0.17890600	1.25504000
H	0.71555000	0.86624300	1.76426000
H	-0.63127400	-0.23151000	2.02119100
C	0.86061100	-0.97219000	0.65252700
H	1.50503700	-1.41246300	1.41873800
H	0.19730500	-1.75237200	0.26179000
C	1.74237800	-0.49278300	-0.46389900
H	1.25867600	-0.20739000	-1.40183600
O	2.98877600	-1.07953900	-0.61022800
O	2.82895900	0.29743400	-0.10883500
C	-2.58195200	-0.72724400	0.03550200
H	-2.12625100	-1.32822000	0.84796400
O	-3.60068300	-1.11192200	-0.49917700
H	-2.40245700	1.10694200	-1.10475900
TS1-NO(1)			
C	1.14362200	0.93451000	0.02456800
C	0.30088100	1.88055200	0.82857700
H	-0.03487200	2.69895600	0.17917600
H	-0.60954100	1.37968700	1.17791200
H	0.84968500	2.30488200	1.67128800
C	2.45748200	0.77078600	0.27649100
C	0.38621200	0.16597400	-1.04535100
H	-0.59037100	0.63036100	-1.18522600
H	0.91917500	0.17943400	-2.00028000
C	0.15165400	-1.31611200	-0.65554800
H	-0.70230100	-1.69937100	-1.22481200
H	1.04014500	-1.91498900	-0.87295800
C	-0.17474100	-1.49826400	0.79319100
H	0.52931500	-2.02899400	1.44929500
O	-2.22426600	-0.31387900	0.30212600

O	-1.20091900	-1.10125700	1.33289800
C	3.34479900	-0.10866100	-0.49570100
H	2.91038100	-0.59887600	-1.39099900
O	4.50755500	-0.30695500	-0.20887500
H	2.93601800	1.31315500	1.08896200
N	-3.53160300	0.56096400	-0.73603000
O	-4.60560300	0.32662900	-0.43833800

TS1-NO(2)

C	-1.49829800	0.97380000	0.15603000
C	-1.18306800	2.36232800	-0.32443000
H	-1.22040600	3.06032400	0.52019400
H	-0.16456500	2.42167400	-0.72560800
H	-1.88674900	2.69968100	-1.08739400
C	-2.59022000	0.32028300	-0.28273200
C	-0.50282400	0.37842200	1.13599700
H	0.13086200	1.17366800	1.54180900
H	-1.01298000	-0.08660400	1.98405700
C	0.42016900	-0.69380800	0.50633600
H	1.13289600	-1.04023900	1.25449200
H	-0.16239100	-1.54420200	0.14299300
C	1.14179300	-0.10447500	-0.66125800
H	0.70148600	-0.12357900	-1.65792600
O	2.76353000	0.67691500	0.57650200
O	2.00444000	0.84635000	-0.54325000
C	-3.00281200	-1.01902100	0.16734400
H	-2.40160200	-1.49338100	0.96910300
O	-3.96248200	-1.60196800	-0.29052600
H	-3.25390600	0.78083600	-1.01129000
N	3.37422900	-1.04499100	0.21597000
O	2.67067600	-1.40109800	-0.69596900

TS2-NO(2)

C	-1.47439400	1.00621600	0.10909000
C	-1.08021300	2.33664700	-0.46796800
H	-1.20932900	3.11705600	0.29140700
H	-0.01818400	2.34951400	-0.74111000
H	-1.67970300	2.59781200	-1.34192500
C	-2.52882400	0.32650000	-0.37985000
C	-0.59511100	0.49968500	1.23828800
H	-0.00411500	1.33599300	1.62476200
H	-1.20100100	0.12786200	2.06950700
C	0.36852400	-0.61615000	0.79871200
H	1.04677600	-0.86787900	1.62053000

H	-0.18298300	-1.52342800	0.52928100
C	1.20046200	-0.21005500	-0.40193100
H	0.61530900	-0.04772600	-1.31338000
O	3.22739800	0.13209400	0.43767900
O	1.99661600	0.90421200	-0.20845900
C	-3.01405300	-0.95713000	0.14906400
H	-2.50075000	-1.36259600	1.04418400
O	-3.94115000	-1.56654500	-0.34182300
H	-3.10218200	0.72347300	-1.21494900
N	3.36772600	-0.89358000	-0.31407100
O	2.14260300	-1.28342400	-0.71767700

TS3-NO(2)

C	-1.61854800	0.98104800	0.12950100
C	-1.38425200	2.35584500	-0.42936900
H	-1.56785000	3.10404400	0.35093200
H	-0.33846300	2.48153900	-0.73370500
H	-2.03663100	2.56911700	-1.27804200
C	-2.60512100	0.19690000	-0.34577700
C	-0.65988600	0.55241400	1.22645400
H	-0.15035400	1.43822000	1.61807800
H	-1.19672900	0.09435400	2.06193200
C	0.41100200	-0.43846600	0.73103600
H	1.11709100	-0.64175400	1.54280500
H	-0.04750100	-1.38156000	0.41742200
C	1.17196100	0.15880900	-0.43781500
H	0.65882400	0.08934700	-1.41492000
O	3.55746100	-0.17137700	0.55338200
O	1.87477700	1.20765100	-0.27372700
C	-2.92566600	-1.14179100	0.17116700
H	-2.34328100	-1.49790800	1.04461300
O	-3.78944400	-1.84901100	-0.30412600
H	-3.24215300	0.54056800	-1.15789100
N	3.35864000	-1.04289000	-0.23029800
O	2.26965800	-1.12280100	-0.86431800

IM1-NO(2)

C	-1.44736200	1.00481200	0.11750900
C	-1.03952200	2.33503800	-0.45125400
H	-1.15357900	3.11092500	0.31511200
H	0.02005000	2.33907800	-0.73339400
H	-1.64207300	2.61081900	-1.31858900
C	-2.51658900	0.34642200	-0.36802400
C	-0.56601200	0.47382400	1.23406200

H	0.03928500	1.29763000	1.62540800
H	-1.17046300	0.10223800	2.06638000
C	0.37739500	-0.65237800	0.77666400
H	1.06283300	-0.92014500	1.58714700
H	-0.18938900	-1.55050700	0.50871400
C	1.19556400	-0.25903800	-0.43739800
H	0.59859000	-0.06206400	-1.33201200
O	3.13899000	0.24224400	0.42312100
O	2.01404200	0.86307700	-0.23680500
C	-3.01804200	-0.93452400	0.15275900
H	-2.50459600	-1.35704700	1.03990100
O	-3.95847200	-1.52378600	-0.33690500
H	-3.09096300	0.76072400	-1.19392400
N	3.33984100	-0.94665300	-0.20180300
O	2.14779300	-1.28028700	-0.76166600

IM2-NO(2)

C	-1.60220700	0.97330800	0.14761400
C	-1.45671000	2.36763300	-0.39283400
H	-1.70202800	3.09103700	0.39413400
H	-0.41845400	2.57026100	-0.67951300
H	-2.11278200	2.54647700	-1.24662300
C	-2.53248400	0.13320300	-0.34500400
C	-0.62745800	0.59323000	1.24818100
H	-0.15614600	1.50264500	1.63257900
H	-1.15242500	0.12839000	2.08828300
C	0.47056700	-0.37368700	0.78079000
H	1.17993900	-0.54968800	1.59222200
H	0.04213700	-1.33533600	0.48149400
C	1.23039300	0.16699800	-0.44243200
H	0.50163100	0.30792700	-1.26841600
O	3.43897100	-0.47141000	0.65842200
O	1.80140300	1.36248400	-0.26725500
C	-2.78735300	-1.22277100	0.16630600
H	-2.21003900	-1.54439800	1.05619300
O	-3.59968800	-1.97595200	-0.32779500
H	-3.17962000	0.44356100	-1.16256400
N	3.28514200	-1.09616300	-0.32922000
O	2.11472700	-0.82952400	-1.00824500

TS1-H₂O

C	-1.21752600	1.00812300	0.12395400
C	-0.82540400	2.36083600	-0.39995200
H	-0.85026400	3.08966200	0.41887000

H	0.20492600	2.35551600	-0.77324900
H	-1.49538200	2.70174400	-1.19140700
C	-2.32952200	0.39116200	-0.31939200
C	-0.27631200	0.40723800	1.15378300
H	0.41412000	1.17768900	1.51101900
H	-0.83035300	0.03969200	2.02241000
C	0.57782700	-0.76332700	0.61445600
H	1.26919900	-1.08527500	1.39060400
H	-0.04481500	-1.60949900	0.31339800
C	1.32656700	-0.28966400	-0.59382000
H	0.86558600	-0.40554500	-1.57746200
O	2.99232800	0.50989000	0.60935700
O	2.18176400	0.65799300	-0.56201800
C	-2.82166600	-0.90324500	0.17521700
H	-2.27453900	-1.36316400	1.02264800
O	-3.79134600	-1.46438100	-0.29080400
H	-2.94914200	0.85388000	-1.08452700
O	2.70683600	-1.73251200	-0.44018300
H	3.23597800	-1.81287200	-1.24403500
H	3.13424000	-0.97648700	0.13543100

HAHP

C	-1.07504900	1.01882800	0.05446300
C	-0.55765300	2.27901300	-0.57881500
H	-0.50690800	3.07238800	0.17667800
H	0.46577200	2.13714300	-0.94190900
H	-1.19609500	2.61649400	-1.39775000
C	-2.24610700	0.48252300	-0.34118300
C	-0.19317500	0.41166100	1.13056300
H	0.54892000	1.15279800	1.44390300
H	-0.78632600	0.16056300	2.01503700
C	0.55103100	-0.85111200	0.67223000
H	1.18758300	-1.21936200	1.48101500
H	-0.15264600	-1.64875000	0.41386900
C	1.42275600	-0.61619800	-0.54707300
H	0.82107300	-0.37133200	-1.43398800
O	2.98014700	0.45221500	0.77932000
O	2.24699700	0.53272900	-0.43665600
C	-2.85921300	-0.71471400	0.24934800
H	-2.34160300	-1.17405800	1.11520200
O	-3.89530600	-1.19974500	-0.15850200
H	-2.82209600	0.94496000	-1.13993500
O	2.20095500	-1.76211200	-0.74497800
H	2.57580000	-1.74485800	-1.63376200

H	3.68864900	-0.17068000	0.55096200
PRC-SO ₂			
C	-1.95570700	0.88840100	0.37957600
C	-1.61895300	2.33338700	0.14885900
H	-1.55356400	2.84456300	1.11720100
H	-0.63227000	2.44108100	-0.31409300
H	-2.37229900	2.83527100	-0.46074100
C	-3.12635500	0.36877300	-0.03770300
C	-0.88320200	0.08042000	1.09119100
H	-0.14154000	0.75792000	1.51560200
H	-1.30602300	-0.50608100	1.91144900
C	-0.15067500	-0.92256200	0.16120300
H	0.77008100	-1.25221500	0.65162700
H	-0.77291900	-1.79956400	-0.03218400
C	0.19229100	-0.34598900	-1.16397800
H	-0.20765100	-0.73687100	-2.09919500
O	1.50967400	1.21050700	-0.24142200
O	0.88427000	0.68252100	-1.35460800
C	-3.56138400	-1.01396400	0.21040000
H	-2.91314200	-1.63992500	0.85699000
O	-4.58723400	-1.47854800	-0.24065400
H	-3.84014500	0.98444600	-0.58070300
S	3.23699100	-0.16592000	0.12624400
O	2.90448100	-0.45449200	1.51596700
O	2.76400000	-1.16057400	-0.84467600
TS1-SO ₂			
C	-2.15630400	0.87743700	0.34058700
C	-2.03080200	2.35616700	0.10284200
H	-2.06776500	2.88436000	1.06292800
H	-1.06253500	2.60572000	-0.34642900
H	-2.83012300	2.73606300	-0.53572900
C	-3.21331700	0.18646600	-0.12591600
C	-1.01465900	0.24544000	1.11915300
H	-0.40070400	1.03155900	1.56782300
H	-1.38693900	-0.38005800	1.93521400
C	-0.07790800	-0.64786700	0.26051900
H	0.77018700	-0.95699600	0.87001000
H	-0.60019900	-1.53525700	-0.10341900
C	0.36319100	0.12959400	-0.92890800
H	-0.11636800	0.01691900	-1.90096900
O	1.87408200	1.25349300	0.24374800
O	1.07824500	1.17358500	-0.88420300

C	-3.44736500	-1.24745800	0.11149800
H	-2.74326200	-1.77100000	0.78928900
O	-4.37109000	-1.85585100	-0.38529900
H	-3.98513900	0.68558400	-0.70781100
S	3.22351300	-0.35882500	-0.05079300
O	3.07596100	-0.98476000	1.25854500
O	2.38150500	-0.95826400	-1.11989900

TS2-SO₂

C	1.82289500	0.89731200	-0.25978700
C	1.18246300	2.22787900	0.00940700
H	0.79459900	2.65522500	-0.92232100
H	0.33017100	2.10679500	0.68447100
H	1.89252500	2.92966300	0.45074200
C	3.08364600	0.64972200	0.14629600
C	0.98875700	-0.12862000	-1.01162200
H	0.12538400	0.36891600	-1.46247700
H	1.57684600	-0.53439600	-1.83999600
C	0.50509200	-1.31469200	-0.15793800
H	0.27791400	-2.17721100	-0.79180100
H	1.29394600	-1.62763400	0.53689900
C	-0.71036100	-1.04168200	0.69501400
H	-1.03839800	-1.88332000	1.32723200
O	-1.80441900	1.08008200	-0.10450500
O	-0.87883100	0.10379500	1.27868700
C	3.81677800	-0.59853500	-0.10196000
H	3.31612500	-1.36606000	-0.72746500
O	4.93134400	-0.81387700	0.32870700
H	3.64147300	1.40512700	0.69476000
S	-2.86838400	0.05743000	-0.38962500
O	-4.04984800	-0.01205100	0.44665700
O	-2.00475400	-1.22598600	-0.40360900

IM1-SO₂

C	-2.15261600	0.91375100	0.23989500
C	-1.98963500	2.35016100	-0.17104200
H	-2.14847800	2.99943200	0.69831400
H	-0.96835700	2.54930200	-0.51630100
H	-2.69653900	2.63487400	-0.95256700
C	-3.14536800	0.15933200	-0.26860600
C	-1.12466800	0.39588500	1.23056000
H	-0.61336500	1.24949200	1.68680400
H	-1.60908600	-0.15280400	2.04328000
C	-0.06641800	-0.52033700	0.59228000

H	0.69594600	-0.78340300	1.33098200
H	-0.51777300	-1.45324500	0.23786200
C	0.59998700	0.12727000	-0.60616700
H	-0.09175100	0.33578500	-1.42738400
O	2.37429900	0.98385600	0.42976600
O	1.22935000	1.35839100	-0.32057100
C	-3.41087200	-1.23703300	0.10933800
H	-2.77591100	-1.67531000	0.90527500
O	-4.28722900	-1.90452100	-0.39897100
H	-3.83527200	0.57404900	-1.00042500
S	3.06356300	-0.42212500	-0.30384200
O	3.18568500	-1.34319900	0.81220700
O	1.65803400	-0.67682000	-1.13516900

PRC3

C	0.02102500	-0.92135500	1.00253200
C	0.83981900	-0.57164500	2.21074100
H	0.26367400	-0.01222800	2.95104600
H	1.20645500	-1.49553400	2.67455300
H	1.72239900	0.00182800	1.91226600
C	-1.30107300	-0.63104700	0.95844900
C	0.73855300	-1.64479400	-0.11306900
H	1.70041100	-2.00998500	0.25944700
H	0.13194200	-2.49540800	-0.43318600
C	0.98269700	-0.75480100	-1.33677900
H	1.24815500	-1.36782500	-2.20923900
H	0.07224000	-0.21660200	-1.62474800
C	2.09064300	0.24464700	-1.15117600
H	2.22337500	0.96767000	-1.98251900
O	2.82283100	0.28900500	-0.18929100
C	-2.23211100	-1.00913200	-0.11677700
H	-3.29419900	-0.76787800	0.08922300
O	-1.93231800	-1.55144200	-1.16413200
H	-1.75682900	-0.12260100	1.80696800
O	0.31925200	2.00482100	0.21283100
O	-0.87102800	2.35698100	0.21490000
O	-1.63310400	1.80654900	-0.59522500

TS8

C	0.19151900	0.00292300	1.04582300
C	-0.37396000	-0.92956000	2.08464100
H	0.17742800	-1.87215500	2.12862200
H	-0.30524800	-0.44392000	3.06637500
H	-1.42808600	-1.12797000	1.87881800

C	1.54257300	-0.08129900	0.72340000
C	-0.62435300	1.24445400	0.74865100
H	-1.46673800	1.26991400	1.44620800
H	0.00977000	2.11562600	0.93385600
C	-1.17119400	1.35484500	-0.67495500
H	-1.47392400	2.39161300	-0.87686400
H	-0.41023600	1.11144500	-1.42264600
C	-2.38342600	0.48985500	-0.89877300
H	-2.74343400	0.42529800	-1.94556300
O	-2.96781100	-0.09757000	-0.01793300
C	2.32782800	0.98170000	0.06180500
H	3.42502300	0.84836900	0.12096300
O	1.85740400	1.93437700	-0.52294600
H	2.13251200	-0.86854700	1.18744300
O	-0.46419000	-1.38461200	-0.61994800
O	0.63135900	-2.00485500	-0.81824000
O	1.57186500	-1.22573600	-1.15352900
TS9			
C	0.06315000	-0.49874400	0.55747700
C	0.32755800	-1.60028500	1.54955500
H	1.18563400	-2.20727300	1.26537200
H	0.48018200	-1.16457400	2.53913400
H	-0.56813000	-2.23256200	1.57402500
C	1.86880500	0.06938900	0.14501200
C	-0.82447300	0.63803900	1.00584300
H	-1.53614200	0.22722000	1.73069800
H	-0.19778800	1.36500600	1.53347300
C	-1.59855500	1.32214100	-0.11481900
H	-2.02075800	2.26954000	0.24378300
H	-0.96645700	1.58839100	-0.97030500
C	-2.74577800	0.47519200	-0.61594900
H	-3.30942500	0.88333000	-1.47762100
O	-3.06372100	-0.57724700	-0.11726500
C	1.67871900	1.44211600	-0.43643500
H	1.62947500	1.46640000	-1.54419400
O	1.57645400	2.43778900	0.24202000
H	2.20387400	0.04784900	1.19333200
O	-0.15660400	-0.87386900	-0.71231200
O	0.68347600	-1.80968700	-1.08234200
O	2.27076700	-0.84328800	-0.65907700
TS10			
C	-0.00411000	-0.39771200	0.67139300

C	-0.61950000	-1.37545600	1.67205900
H	-1.01374800	-0.83333500	2.53356600
H	-1.40976200	-1.97746700	1.21361400
H	0.17570500	-2.04246600	2.01678800
C	-1.58999300	0.52288800	0.10936000
C	0.60543400	-1.04543500	-0.58578900
H	1.21324500	-1.88887700	-0.23673400
H	-0.16341400	-1.46785200	-1.24012700
C	1.51489400	-0.07141400	-1.32338100
H	1.78810700	-0.47085100	-2.30947000
H	1.03639400	0.89810400	-1.49417300
C	2.81181200	0.15015000	-0.57149900
H	3.32561400	1.11366800	-0.75593400
O	3.30228900	-0.67517600	0.16013100
C	-2.31042600	-0.23329800	-0.95077400
H	-2.09594700	0.07379800	-1.99199100
O	-3.04647500	-1.15130000	-0.68312800
H	-2.04684300	0.61549200	1.09304100
O	0.64461100	0.60133200	1.15965000
O	-0.31799300	2.19417800	0.60054200
O	-0.98968500	1.61614800	-0.35679400

IM8

C	0.26160800	-0.46550800	0.66599300
C	0.62703100	-1.24482100	1.91961700
H	1.23691800	-2.11431600	1.66099100
H	1.19388500	-0.60645500	2.60492300
H	-0.28182500	-1.58549800	2.42051500
C	1.56866100	-0.08663000	-0.14289200
C	-0.68458800	0.69760700	0.96026400
H	-1.47269100	0.33638900	1.62762500
H	-0.11867900	1.46263200	1.49816500
C	-1.33684600	1.27167800	-0.29605700
H	-1.57871000	2.33484600	-0.16287300
H	-0.68572800	1.21895200	-1.17796100
C	-2.63318600	0.57641600	-0.65828400
H	-3.01658100	0.78260700	-1.67743700
O	-3.25320600	-0.13213200	0.09497900
C	1.74658100	1.37529500	-0.49717700
H	1.68400100	1.62554600	-1.57427900
O	1.95842200	2.21184600	0.34488600
H	2.44753000	-0.41286900	0.42834800
O	-0.40168800	-1.31029800	-0.28352800
O	0.65886600	-1.93015600	-0.97352500

O	1.44964500	-0.81251800	-1.35241200
IM9			
C	0.79573500	0.45469300	-0.07409400
C	1.92014300	0.99311100	0.71532400
H	1.73321700	2.01941700	1.02930100
H	2.07234900	0.33196100	1.57657500
H	2.83726100	0.90643600	0.12242700
C	-0.44316800	1.22881500	-0.40279800
H	-0.74458400	1.76752800	0.50166500
H	-0.17170600	1.98790600	-1.14835300
C	-1.58503900	0.35736800	-0.90716700
H	-2.42443600	0.97688600	-1.24673300
H	-1.28471600	-0.25514900	-1.76455900
C	-2.10222800	-0.55997300	0.17786200
H	-2.89127100	-1.27562400	-0.12358700
O	-1.70586900	-0.52352600	1.31713500
O	0.86569000	-0.71019400	-0.53598400
O	2.01033200	-1.42921100	-0.28133800
CH ₃ COCH ₂ CH ₂ CHO			
C	1.08903500	-0.20872400	0.15701100
C	2.19179300	0.64496700	-0.41388600
H	2.63346900	0.17311500	-1.29727400
H	1.75045700	1.59547300	-0.73400800
H	2.95420300	0.83028300	0.34253800
C	0.08311600	-0.78462900	-0.83245300
H	0.01438200	-0.13020700	-1.70675300
H	0.48186000	-1.74742500	-1.17597600
C	-1.27822400	-0.97212000	-0.18309100
H	-1.98037700	-1.50145400	-0.83929600
H	-1.19340300	-1.56597000	0.73508800
C	-1.89222200	0.35436700	0.18828900
H	-2.88237100	0.31495300	0.68413900
O	-1.36220600	1.41802700	-0.03136200
O	0.99480500	-0.43951900	1.34340300