Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

For

A DFT-Weaving of Single Component Bifunctional Organocatalysts for Carbon dioxide/Propylene Oxide Coupling Reaction

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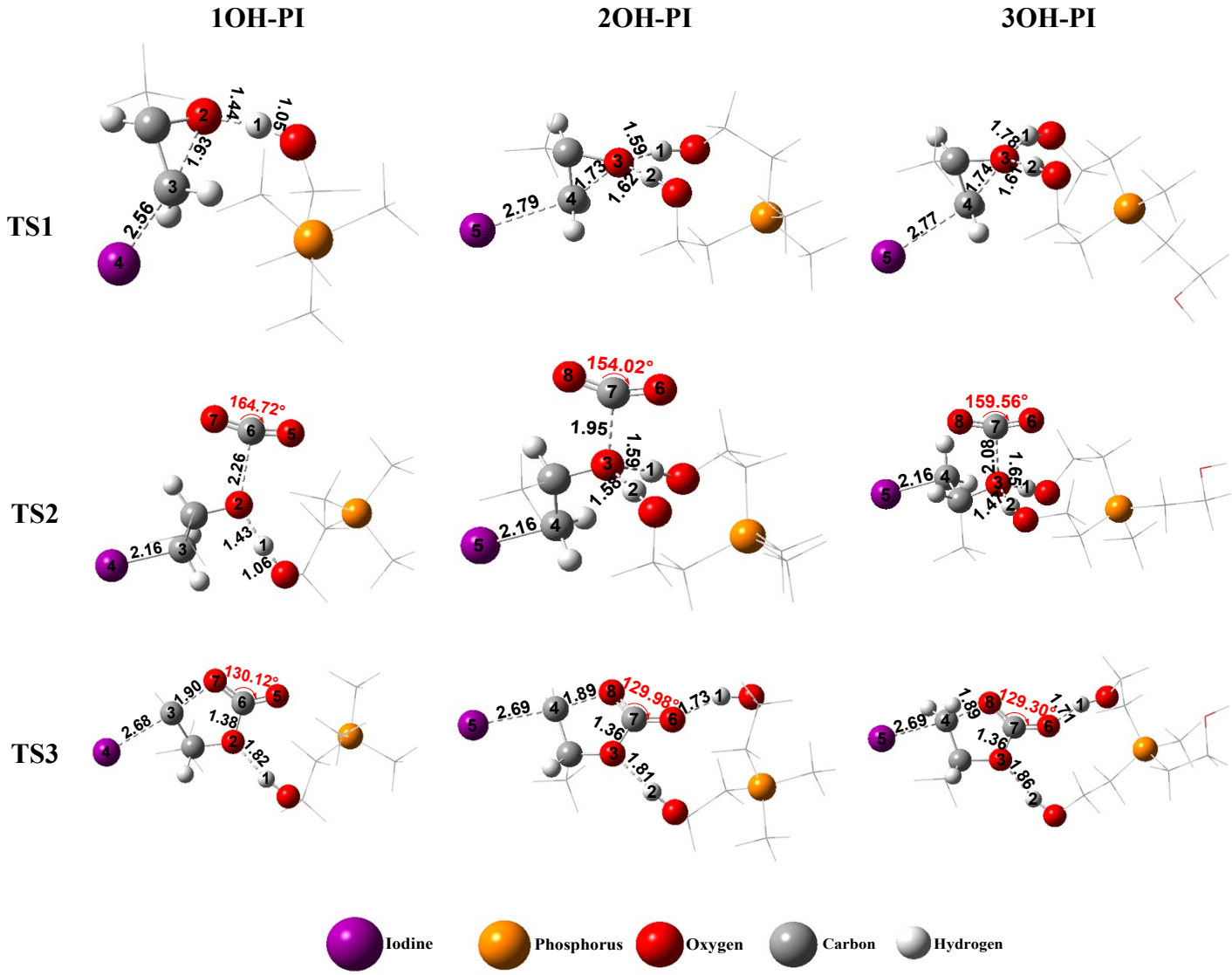
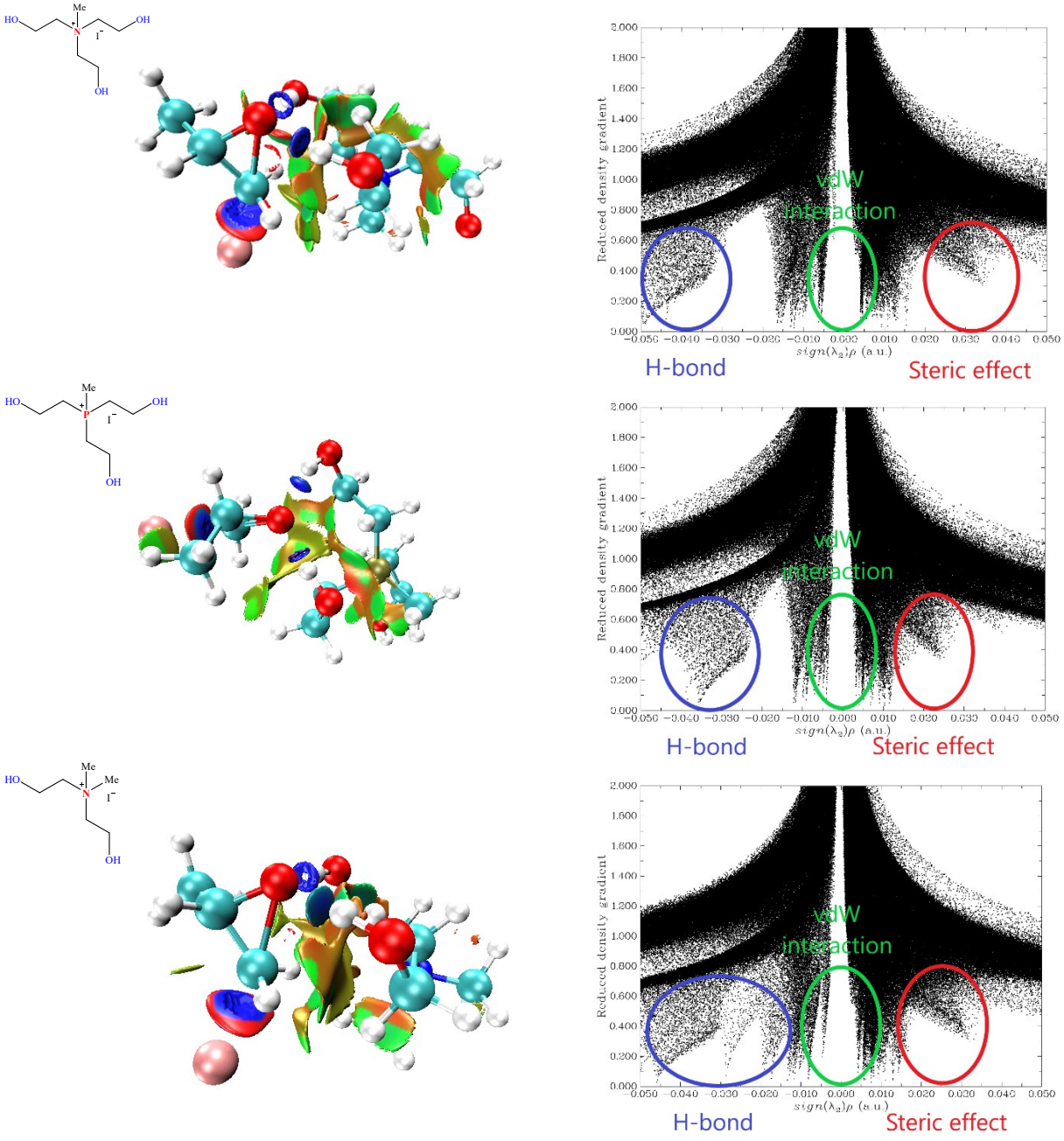


Fig. S1. The optimized structures of the transition stats of **1OH-PI**, **2OH-PI**, and **3OH-PI** catalysts. Dotted lines indicate hydrogen-bonding interactions, the bond formed, and bond breaking. Distances are shown in Å. Nonessential atoms were selected as low-layer.



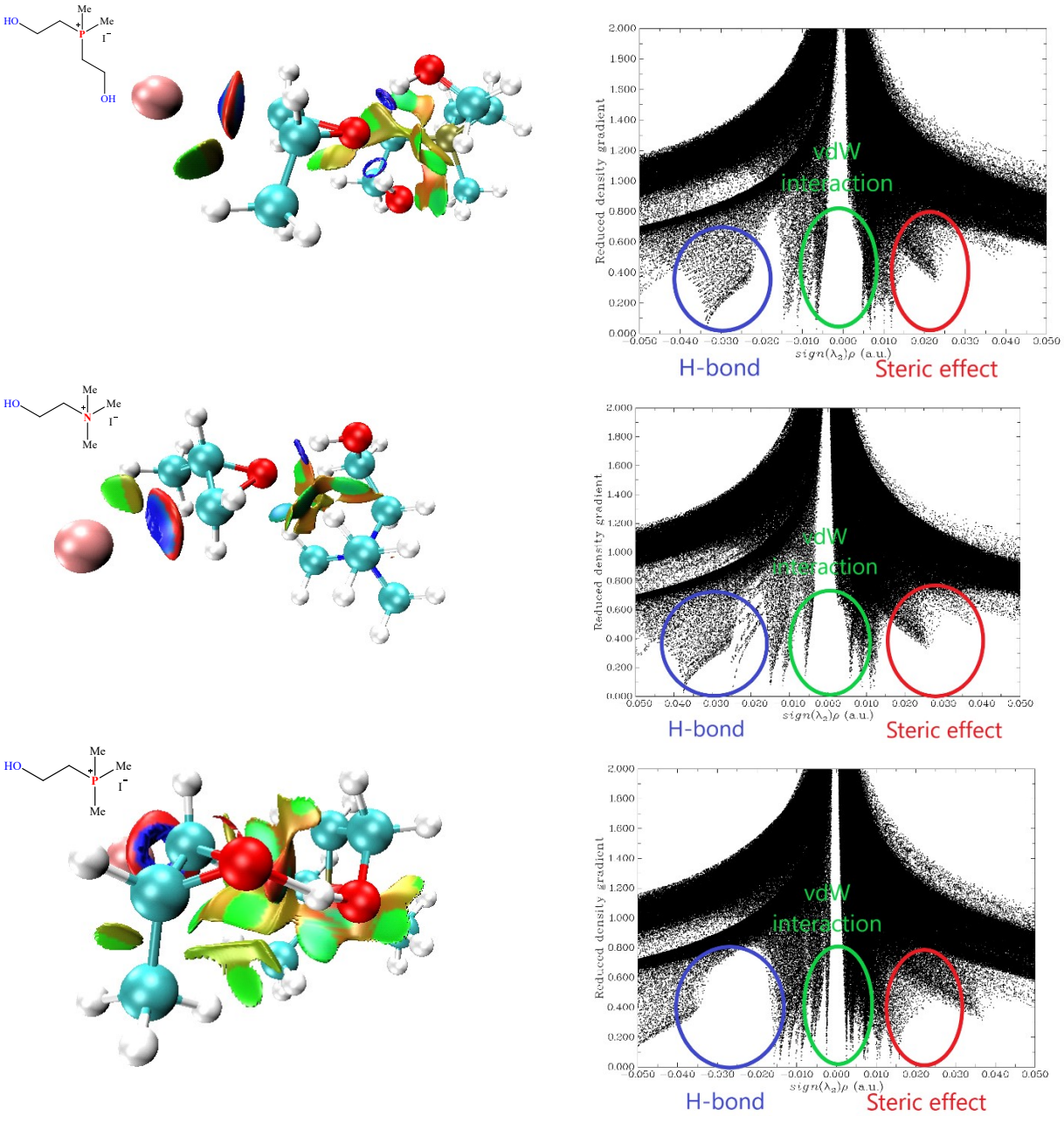


Fig. S2. 2D NCI plots for TS1 at right and the corresponding 3D plots are displayed at left.

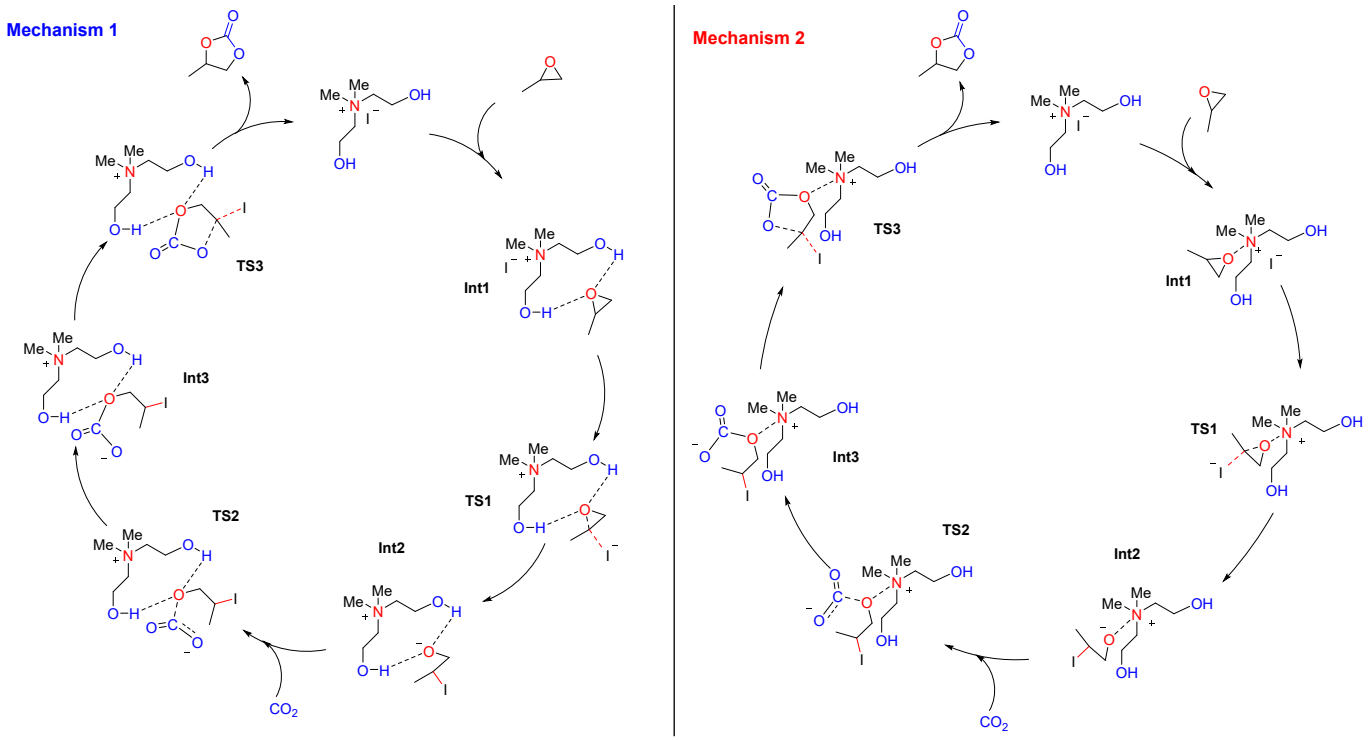


Fig. S3. Other suggested mechanisms for CO_2 fixation with propylene oxide.

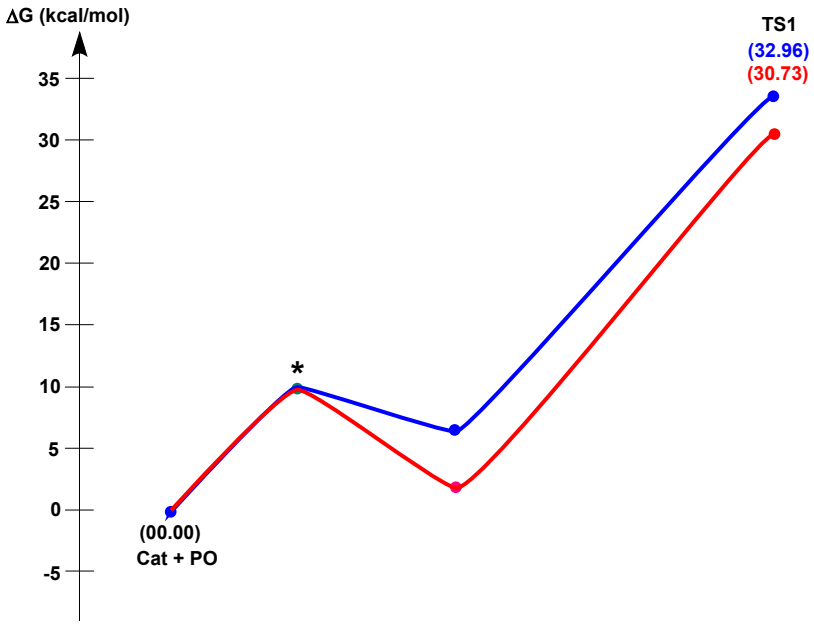


Fig. S4. The free energy profile of ring-opening step for other suggested mechanisms. (—) represent mechanism 1 and (—) represent mechanism 2.

The cartesian coordinates of the optimized geometry of the transition states:

[HTEA]I-TS1

N	-2.06488700	-0.33068800	0.42036900
C	-1.72950900	-1.52798700	1.26557900
C	-3.25505000	0.39840400	0.97364500
C	-3.32878400	1.85707200	0.51831900
O	-3.20765700	2.02153100	-0.86180900
C	-0.27822500	-1.95935100	1.17232600
O	0.49220700	-0.96740800	1.78109400
C	-2.18153600	-0.71799700	-1.03354800
H	-2.25179400	2.16470300	-1.01725600
H	-2.42485800	-2.32436200	0.97224600
H	-1.91748000	-1.24986700	2.31006700
H	-4.14643100	-0.18666600	0.71799200
H	-3.15020100	0.38162300	2.06634700
H	-2.54864400	2.42758900	1.04771400
H	-4.30643800	2.24268100	0.84990300
H	-0.19722300	-2.92909500	1.69558100
H	0.03372500	-2.14111700	0.12644900
H	-1.51073200	-1.57485200	-1.17724400
H	-1.80126700	0.12168200	-1.62189200
C	-3.57675100	-1.07271700	-1.48755200
H	-4.20861300	-0.17046300	-1.45506600
H	-3.49442000	-1.38411600	-2.54335200
O	-4.07251300	-2.10970400	-0.67116300
H	-4.95633800	-2.35351300	-0.96577500
H	-1.28220400	0.40351600	0.39648100
H	1.41303000	-0.98858700	1.45087300
I	3.29845800	-0.33459800	-0.34229000
O	-0.61499300	1.71632800	-0.42524000
C	0.70949500	2.05309300	-0.10016300
C	0.89626000	0.76693500	-0.77808000
H	1.08215500	2.90451600	-0.69186200
H	0.97516500	0.74740600	-1.86334000
H	0.59249400	-0.12632800	-0.25737600
C	1.02024200	2.20977300	1.36642000
H	2.10615600	2.29005400	1.51423800
H	0.54003000	3.12302400	1.74780500
H	0.65658700	1.34136400	1.93150100

E= -1009.376348 Hartree $\bar{\upsilon}$ = -515.60 cm^{-1}

[HTEA]I-TS2

N	-2.34457800	0.75324200	-0.71663600
C	-1.89798600	2.09379100	-1.20110000
C	-2.77496800	-0.09495700	-1.86067300
C	-2.93606600	-1.59245700	-1.59155000

O	-3.98497800	-1.94642200	-0.73886900
C	-0.54525200	2.55782500	-0.67389200
O	-0.45599300	2.74087800	0.70223200
C	-3.47794500	0.90780100	0.23522200
H	-3.61719400	-2.07817400	0.14781900
H	-2.66867000	2.83965000	-0.94992300
H	-1.83335000	2.06568400	-2.29893300
H	-3.72075000	0.30782900	-2.26566400
H	-2.00880800	0.00364700	-2.64381900
H	-1.97317400	-2.00731700	-1.24912500
H	-3.13352300	-2.04365600	-2.57797500
H	0.23289700	1.86764100	-1.04541700
H	-0.33624600	3.52984800	-1.14675500
H	-3.86580400	-0.08950400	0.45170600
H	-4.28565600	1.46504700	-0.27303100
C	-3.10774300	1.61929600	1.52590400
H	-2.84595000	2.67124200	1.34225400
H	-3.99784100	1.61053500	2.17891900
O	-1.99314300	1.04121300	2.15500400
H	-2.12391900	0.07780300	2.18911200
H	-1.29497000	0.01714700	-0.14511700
H	-0.73867000	1.94549500	1.19427100
I	3.77245300	0.00005000	-0.03187400
O	-0.50767600	-0.70153500	0.29111800
C	0.80595100	-0.83823000	-0.24710200
C	1.69690200	0.13108800	0.52620400
H	1.12318500	-1.85792800	0.01474500
H	1.66418800	-0.12776600	1.59026300
H	1.40974400	1.18178000	0.41114700
C	0.79162000	-0.72564900	-1.76469500
H	0.12440400	-1.49447100	-2.17964500
H	0.45518300	0.25908400	-2.11826800
H	1.79727500	-0.90177700	-2.16753200
O	-0.33566200	-2.84841800	1.28697300
C	-1.14180100	-1.99218600	1.19276000
O	-2.26837500	-1.65010300	1.47857600

E= -1198.018506 Hartree $\bar{\upsilon}$ = -539.13 cm^{-1}

[HTEA]I-TS3

N	-2.82609000	0.20987200	-0.99991800
C	-2.75067500	1.60060100	-1.58804000
C	-2.61572500	-0.85227300	-2.04315400
C	-2.11867600	-2.19651800	-1.51468800
O	-2.98505700	-2.83333500	-0.63056000
C	-1.62032100	2.42941100	-0.98674200
O	-1.87543900	2.85349400	0.31132600

C	-4.08830400	-0.02058700	-0.22323000
H	-2.63509900	-2.69238700	0.26742400
H	-3.71116900	2.10101900	-1.40979000
H	-2.61565000	1.49384800	-2.67156400
H	-3.57134900	-0.96042900	-2.57687800
H	-1.86363600	-0.46588800	-2.74382800
H	-1.11518500	-2.05240000	-1.08192000
H	-1.98516400	-2.82542600	-2.41032800
H	-0.67203300	1.86540800	-1.07654200
H	-1.51495300	3.32596000	-1.61479300
H	-4.09752100	-1.08545900	0.03262500
H	-4.93043900	0.18189700	-0.90083400
C	-4.14674400	0.86082800	1.01842200
H	-4.30053200	1.91631800	0.74831100
H	-5.02300100	0.54125600	1.60803100
O	-2.95909000	0.80835600	1.75401300
H	-2.67746500	-0.12283200	1.88539800
H	-2.03783900	0.11932100	-0.32404300
H	-1.92525100	2.09795100	0.92691000
I	4.05890300	0.06717800	-0.41967800
O	-0.38001700	-0.14765700	0.46916300
C	0.99862100	0.30727900	0.49765800
C	1.85310300	-0.89721200	0.87279700
H	1.22633100	0.61283000	-0.52798700
H	1.96505100	-1.72900700	0.18306600
H	2.49519400	-0.87464500	1.74672600
C	1.12979600	1.45913600	1.47069700
H	2.16176000	1.83232600	1.44267300
H	0.44135700	2.27145200	1.20027600
H	0.89667000	1.11645200	2.49007700
O	0.45191800	-1.68808000	1.79670900
C	-0.59158000	-1.21023400	1.30820700
O	-1.77060300	-1.56524100	1.44657200

E= -1198.001233 Hartree $\bar{\upsilon}$ = -520.91 cm^{-1}

[1OH-NI] TS1

N	-3.30585500	-1.00817100	0.22718200
C	-4.25252000	0.10728800	-0.16449100
C	-3.63630100	1.48885400	-0.36657000
O	-2.80958800	1.55985500	-1.47234600
H	-1.87996600	1.60253100	-1.11722100
O	-0.70886200	1.27510200	-0.04367300
C	0.63151400	1.68729800	0.10448500
C	0.72757500	0.26960800	-0.20578500
H	-4.73071800	-0.21955600	-1.09879600

H	-5.01157600	0.14608800	0.63050800
H	-4.50748800	2.15790600	-0.49105300
H	-3.11975800	1.81139300	0.55417900
H	0.71570800	-0.05967600	-1.24082300
I	3.36278100	-0.48374200	-0.13346500
C	-4.12299400	-2.21893400	0.51025200
C	-2.35070100	-1.32312800	-0.88476300
C	-2.52659400	-0.63785400	1.45081300
H	-4.78333000	-2.01412000	1.36088700
H	-4.71821800	-2.46147100	-0.37777000
H	-3.45108200	-3.05125100	0.74912100
H	-1.98175200	-1.52936200	1.78475900
H	-1.81633900	0.16177700	1.18348700
H	-3.23272800	-0.31747600	2.22701000
H	-1.74358200	-2.18178600	-0.57303500
H	-2.93194500	-1.56579400	-1.78146500
H	-1.72019300	-0.44890200	-1.05958900
H	0.59890800	-0.45308100	0.59570900
H	0.97867000	2.35432700	-0.69922000
C	1.02982300	2.16715200	1.47439400
H	0.59066200	3.15388100	1.67965800
H	0.68234100	1.45648000	2.23893900
H	2.12473900	2.23229700	1.53620900

E= -819.587231 Hartree $\bar{\upsilon}$ = -502.77 cm^{-1}

[1OH-NI] TS2

N	-4.05399800	-0.29629600	-0.03834800
C	-3.02665600	-0.37109200	-1.15701500
C	-2.16398400	-1.62895300	-1.14319200
O	-1.57639800	-1.83666800	0.08030300
H	-1.07063100	-0.91651100	0.30786200
O	-0.51382900	0.35189400	0.49647400
C	0.81063800	0.16391600	0.86759100
C	1.58552600	-0.02752900	-0.43925100
H	-3.59697900	-0.28980300	-2.09499900
H	-2.39930700	0.51775200	-1.02225700
H	-2.76737500	-2.50958300	-1.43453600
H	-1.44010200	-1.47611000	-1.97248200
H	1.46148000	0.85261800	-1.07931300
I	3.73699900	-0.23735300	-0.22025800
C	-4.90147800	0.89948700	-0.31036900
C	-4.88976100	-1.52337200	-0.02208600
C	-3.41050900	-0.12545000	1.31733900
H	-4.23781400	1.76652500	-0.40533700
H	-5.45710900	0.73846500	-1.24160400
H	-5.59787000	1.04243600	0.52386200

H	-4.16721900	0.29754200	1.98914800
H	-3.06131700	-1.10169900	1.65789700
H	-2.53288200	0.52539300	1.21551300
H	-5.66780500	-1.40750700	0.74251200
H	-5.34734000	-1.66083800	-1.00979300
H	-4.24271200	-2.37238100	0.22406100
H	1.24927900	-0.93323200	-0.96078200
O	0.28312200	2.87139100	0.16309900
C	-0.80478100	2.52578800	-0.03125200
O	-1.94204900	2.48646400	-0.31454900
H	1.21253400	1.07457100	1.35449500
C	0.96783200	-1.00878000	1.83505900
H	0.65016400	-1.94627200	1.35323200
H	2.00348700	-1.11919500	2.18481400
H	0.31881600	-0.83711400	2.70623300

E= -1008.227416 Hartree $\bar{\upsilon}$ = -155.54 cm^{-1}

[1OH-NI] TS3

N	4.52884200	-0.04739700	-0.09647200
C	3.46164600	-0.61387200	0.81949500
C	2.82926900	-1.93167300	0.39259300
O	2.08352500	-1.84463200	-0.77559800
H	1.37925800	-1.18286500	-0.63039600
O	0.36111100	0.15219000	0.05920700
C	-1.00844800	-0.07007400	0.45069400
C	-1.84757200	1.07987800	-0.09031800
H	3.94256100	-0.71978600	1.80278400
H	2.68843700	0.16294500	0.86876300
H	3.58742300	-2.72002000	0.25371300
H	2.22085900	-2.24770100	1.26143400
H	-1.95213900	1.22512700	-1.16147600
I	-4.12859000	-0.31446900	-0.21710000
C	4.84869500	1.32525800	0.40479500
C	5.74718500	-0.89475500	-0.05983200
C	4.05458900	0.08064100	-1.51627300
H	3.93277100	1.92524600	0.32580200
H	5.17946200	1.24861200	1.44738100
H	5.64993500	1.74381000	-0.21573100
H	4.85268100	0.57999600	-2.07933500
H	3.84202800	-0.91431000	-1.91415700
H	3.14190200	0.68816900	-1.49929300
H	6.51363300	-0.43851500	-0.69720600
H	6.10894000	-0.95926300	0.97338600
H	5.50302300	-1.89331500	-0.43741000
H	-2.40014000	1.73579700	0.57229200
O	-0.33926500	2.24007000	0.00522900

C	0.66739400	1.50056600	-0.06404700
O	1.85162800	1.78235500	-0.21650900
C	-1.09674700	-0.18318900	1.95958800
H	-2.13211100	-0.40976700	2.24561600
H	-0.44075000	-0.98634000	2.32205900
H	-0.79316400	0.76774500	2.42253600
H	-1.30330700	-1.00346000	-0.03795200

E= -1008.215627 Hartree $\bar{\upsilon}$ = -498.66 cm^{-1}

[2OH-NI] TS1

N	-2.56348900	-1.03466200	0.33740000
C	-2.49518200	-0.02503500	-0.78826700
C	-3.74945700	-1.91156100	0.13152400
C	-2.74300100	-0.28450800	1.64204800
C	-1.65539400	0.72713700	2.03619300
O	-1.80450000	1.96628400	1.43684900
C	-1.79206900	-0.42409200	-2.08598300
O	-1.60973800	0.74337500	-2.81781800
C	-1.35453300	-1.91672800	0.41648200
H	-1.20145100	2.12832000	0.65520400
H	-1.12663500	1.39228100	-2.25913700
O	-0.34970600	2.26926100	-0.78347100
C	0.78039400	0.83345600	-0.63898900
C	1.02727900	2.26979600	-0.50294300
C	1.43697800	2.81461200	0.84278000
H	-3.52686200	0.29286000	-0.98897200
H	-1.96287600	0.84326800	-0.40347400
H	-3.77085300	-2.67771100	0.91559700
H	-3.66866700	-2.38536600	-0.85368200
H	-4.65605500	-1.29855200	0.17886400
H	-2.84576100	-1.05995800	2.41457000
H	-3.69137100	0.26378600	1.55293100
H	-1.79299200	0.84692800	3.12466300
H	-0.64687400	0.28499400	1.92230700
H	-0.83952300	-0.93890800	-1.86467800
H	-2.40222000	-1.11358900	-2.69139400
H	-0.42096000	-1.34327600	0.43998600
H	-1.43648200	-2.51467800	1.33202600
H	-1.34029300	-2.57798800	-0.45610100
H	0.74416200	0.40901900	-1.63849500
H	0.22784000	0.37703500	0.16617200
H	1.63106700	2.69311900	-1.32101500
H	1.26650900	3.89965700	0.87622100
H	2.49965900	2.60605900	1.02676600
H	0.84609100	2.34858100	1.64509100
I	2.63095200	-0.89741600	0.09175900

E= -934.118028 Hartree $\bar{\upsilon}$ = -486.20 cm^{-1}

[2OH-NI] TS2

N	3.76243800	-0.47031900	0.44921100
C	2.71730300	-1.50396100	0.05998500
C	5.10340900	-1.11007600	0.41897000
C	3.48532000	-0.00471000	1.86288700
C	2.28748600	0.93344800	2.04311400
O	1.06021200	0.34263900	1.81202600
C	2.56944100	-1.77650600	-1.43215300
O	2.06792300	-0.71330600	-2.15645100
C	3.77895300	0.71025600	-0.47204000
H	0.76108600	0.47020800	0.84727000
H	1.33961000	-0.25314400	-1.62670500
O	0.31426900	0.45314300	-0.63112800
C	-1.77675000	0.23154300	0.44827100
C	-0.95745800	-0.11206700	-0.79787900
C	-0.85210500	-1.61478800	-1.04413200
H	2.99830000	-2.42089700	0.59764400
H	1.76628800	-1.14498500	0.46314400
H	5.86741100	-0.34744300	0.60997900
H	5.26122600	-1.55403500	-0.57016900
H	5.14617700	-1.88640800	1.19181200
H	4.40191400	0.50234600	2.19938900
H	3.34095400	-0.91641700	2.46028100
H	2.35289000	1.24156500	3.10209100
H	2.43292800	1.84937500	1.44475700
H	3.53284500	-2.08955400	-1.87655100
H	1.91747100	-2.67372600	-1.47644700
H	2.77297700	1.13023400	-0.55941500
H	4.46678700	1.44982300	-0.04137300
H	4.11412200	0.38287300	-1.45975000
H	-1.80597100	1.31646400	0.59303000
H	-1.37459000	-0.25452300	1.34590500
H	-1.45916000	0.35815100	-1.66458100
H	-0.23191900	-1.79746000	-1.93339100
H	-1.83810200	-2.06990000	-1.20853400
H	-0.38747900	-2.10998300	-0.17406700
I	-3.85359700	-0.35978900	0.32055300
O	1.37953700	2.73716500	-0.53271400
C	0.30590700	2.47360300	-0.94161500
O	-0.75209400	2.65761600	-1.40054800

E= -1122.771530 Hartree $\bar{\upsilon}$ = -205.04 cm^{-1}

[2OH-NI] TS3

N	4.01410700	-0.72027800	-0.40994600

C	3.19073400	-0.68361300	0.86712000
C	4.71635600	-2.02601000	-0.53264100
C	5.05719900	0.37444700	-0.36257800
C	4.53863100	1.80924300	-0.32363200
O	3.96571100	2.14858900	0.89466100
C	2.34520100	-1.92093900	1.12454900
O	1.51266500	-2.25809500	0.05708900
C	3.14952200	-0.52413700	-1.62406800
H	3.00985000	2.26754400	0.73905900
H	0.93266800	-1.49322800	-0.11768600
O	0.02242100	0.12491700	-0.19060400
C	-2.16257800	1.09236000	0.10380300
C	-1.34011300	-0.18703300	0.18650700
C	-1.34067800	-0.80156000	1.57218500
H	3.89617300	-0.51608600	1.69209600
H	2.55694600	0.20308400	0.77525800
H	5.35444500	-1.99695200	-1.42361200
H	3.96653700	-2.81756300	-0.63749200
H	5.32920900	-2.18850500	0.36266600
H	5.68071600	0.23102200	-1.25678000
H	5.66947000	0.18278200	0.52988900
H	5.43369000	2.43096100	-0.50382000
H	3.85209200	1.99354400	-1.16600200
H	2.97029400	-2.79833100	1.34791600
H	1.77919000	-1.70186300	2.04928600
H	2.47448200	0.31981000	-1.43517800
H	3.81089100	-0.32327400	-2.47653600
H	2.57226600	-1.43721200	-1.78402700
H	-2.36361400	1.55325300	-0.85853600
H	-2.64093200	1.51148300	0.98178000
H	-1.69417300	-0.89807300	-0.56591100
H	-0.71242400	-1.70381100	1.58385100
H	-2.36616100	-1.08062200	1.84625800
H	-0.95476600	-0.07469300	2.30344900
I	-4.50663900	-0.17879100	-0.25458200
O	1.52399300	1.76246300	-0.13828700
C	0.34550300	1.44410900	0.03531800
O	-0.62509000	2.14630300	0.38928900

E= -1122.755387 Hartree $\bar{\upsilon}$ = -503.29 cm^{-1}

[3OH-NI] TS1

N	-2.07311000	-0.42678500	0.49674100
C	-1.26129500	0.09861300	1.67757900
C	-1.87764100	-1.91856700	0.51987300
C	-1.56971500	0.03879300	-0.84700300
C	-1.70836300	1.53112700	-1.18554500

O	-0.94481000	1.79896000	-2.30978600
C	-1.17625000	1.61710000	1.96938400
O	0.02139400	2.22295600	1.66235000
C	-3.51722100	-0.07038000	0.70644900
H	-0.10259100	2.18801800	-1.96002900
H	0.24186400	2.43302800	0.70272100
H	-1.72137700	-0.40615500	2.53809100
H	-0.24689000	-0.31445200	1.56211800
H	-2.46013600	-2.36225800	-0.29040200
H	-2.22281800	-2.29681300	1.48962500
H	-0.80250900	-2.11484000	0.39635000
H	-2.09388100	-0.56311000	-1.60191700
H	-0.52013000	-0.26431400	-0.87607600
H	-2.76793800	1.77208200	-1.38931100
H	-1.39313800	2.16008300	-0.34374000
H	-2.05717000	2.14337900	1.55454600
H	-1.28647100	1.69033700	3.06271000
H	-3.55967700	1.01121300	0.88728700
H	-3.82814200	-0.57749500	1.63275400
C	-4.47194800	-0.40098600	-0.43526800
H	-5.44464800	0.03989000	-0.15632000
H	-4.15577300	0.11058200	-1.35399700
O	-4.57965200	-1.76280400	-0.73984200
H	-5.15282600	-2.19769000	-0.09880000
I	2.39947000	-1.60755500	-0.06232000
O	1.03392900	2.58616800	-0.73719000
C	1.51956700	0.77145900	-0.61438000
C	2.30907200	2.01534900	-0.60617000
C	3.06832900	2.37701700	0.64849400
H	1.15621400	0.43017400	-1.57927100
H	0.92923700	0.62765700	0.27637800
H	2.92582200	2.14706600	-1.51033300
H	2.44205400	2.20167200	1.53364500
H	3.34542900	3.44017700	0.61788100
H	3.98123800	1.77026400	0.72713100

E= -1048.640850 Hartree $\bar{\upsilon}$ = -455.55 cm^{-1}

[3OH-NI] TS2

N	2.84006200	-1.29788300	0.13949300
C	1.47538100	-1.81252700	-0.29518300
C	3.87046200	-2.30629100	-0.24016700
C	2.82871100	-1.16989100	1.64729500
C	2.03135300	0.00521700	2.22822200
O	0.66422000	-0.06592800	2.02668700
C	1.11805000	-1.66745500	-1.77007700
O	0.91421300	-0.36879100	-2.19913000

C	3.13836400	0.03176700	-0.51570500
H	0.39963900	0.44956100	1.19218100
H	0.52599200	0.19436400	-1.46069400
H	1.46102700	-2.87268500	-0.00505100
H	0.74125300	-1.28089900	0.31628000
H	4.86301900	-1.90533700	-0.01581500
H	3.78591000	-2.49871700	-1.31595100
H	3.67518100	-3.22859900	0.31971100
H	3.87882100	-1.10145100	1.96358700
H	2.41611200	-2.11751400	2.02206600
H	2.24529000	-0.04147100	3.31098400
H	2.44635600	0.96143600	1.86914400
H	1.88540200	-2.14027600	-2.41117300
H	0.21319200	-2.30003900	-1.88537200
H	2.26623500	0.67136800	-0.34657200
H	3.19014600	-0.15720600	-1.59496900
C	4.38695700	0.75250100	-0.03493400
H	4.30389500	1.77551000	-0.43668900
H	4.39634400	0.86403900	1.05706400
O	5.60194300	0.13485300	-0.39226600
H	5.78746800	0.32153400	-1.31912600
I	-4.03946000	-0.56939900	0.21118500
O	-0.02004700	1.04224900	-0.18691400
C	-1.89163200	-0.36473400	0.05924300
C	-1.42011900	1.04414100	-0.31226900
C	-1.83919400	1.45727500	-1.71780900
H	-1.50964600	-0.65615600	1.04461000
H	-1.58459800	-1.09585500	-0.70121900
H	-1.85694700	1.75636600	0.41227400
H	-1.41786300	0.75647800	-2.45545500
H	-1.44980400	2.46249600	-1.92502800
H	-2.93237900	1.47772500	-1.82560900
O	-0.25071400	3.57045700	0.07752300
C	0.70211400	2.89688800	0.13790800
O	1.85016600	2.65807100	0.28690100

E= -1237.302480 Hartree $\bar{\upsilon}$ = -208.32 cm^{-1}

[3OH-NI] TS3

N	-3.68456300	-0.49928300	-0.34780500
C	-2.75359200	-0.05695500	-1.46707700
C	-4.43935600	-1.71004500	-0.78690000
C	-4.68696500	0.59989200	-0.07897100
C	-4.11426700	1.93474300	0.39235900
O	-3.47275000	2.63881100	-0.62066000
C	-1.92456900	-1.16038900	-2.10580400
O	-1.15846700	-1.89092900	-1.19569200

C	-2.87582400	-0.80832400	0.90359800
H	-2.52774300	2.67402600	-0.38536800
H	-0.58508600	-1.26005300	-0.72248300
H	-3.38387500	0.43417200	-2.22055100
H	-2.10248200	0.70214100	-1.02503200
H	-5.18855200	-1.94690900	-0.02753300
H	-3.73111700	-2.53923300	-0.89391100
H	-4.91297500	-1.49030500	-1.75197800
H	-5.39266600	0.19389300	0.65805300
H	-5.22729500	0.75709000	-1.02300100
H	-4.98907100	2.50581000	0.75153100
H	-3.44830800	1.79130000	1.25809500
H	-2.55407300	-1.87419400	-2.65691700
H	-1.30101600	-0.65022100	-2.86400300
H	-2.10778000	-0.02416700	0.97870200
H	-2.37177900	-1.75925300	0.70040700
C	-3.67297100	-0.86707100	2.19755100
H	-2.94357900	-1.09665600	2.99233800
H	-4.09375900	0.11526200	2.44750800
O	-4.74669500	-1.77536800	2.18717700
H	-4.41251600	-2.66819600	2.32987500
I	4.82661300	-0.37672400	0.33191300
O	0.33733200	0.19322800	0.00237800
C	2.56364500	1.07413900	0.24783600
C	1.72062500	-0.04363900	-0.35179800
C	1.83920800	-0.12752300	-1.86065100
H	2.67741100	1.15754800	1.32439600
H	3.13747900	1.74558900	-0.38071800
H	1.98284400	-0.99408700	0.12260300
H	1.54758700	0.83301900	-2.31240000
H	1.18982300	-0.92678200	-2.24577600
H	2.87854500	-0.35383900	-2.13135100
O	1.08779500	2.25039900	0.22252300
C	0.06970000	1.52630700	0.22716600
O	-1.11125800	1.82993200	0.40638800

E= -1237.286505 Hartree $\bar{\upsilon}$ = -503.03 cm^{-1}

[1OH-PI] TS1

C	1.85454800	-0.10759000	-1.36909300
C	2.10023100	1.42304700	-1.34682000
O	1.86211300	1.95529700	-0.08921700
H	0.94357700	2.47605800	-0.14395400
H	2.46168200	-0.61744100	-2.13475300
H	0.80379600	-0.38911100	-1.54492600
H	3.14964600	1.60043900	-1.64902400
H	1.45717500	1.88772900	-2.11387800
I	-2.17953900	-1.06185800	-0.13024200

C	3.99816100	-0.29867000	0.60943600
C	1.25921600	-0.46241900	1.61871300
C	2.27777300	-2.63902500	0.00574500
H	4.68165300	-0.55095100	-0.21232300
H	3.94654400	0.79288000	0.73478400
H	4.34433800	-0.76994400	1.53870800
H	2.59243200	-3.13763300	0.93219200
H	1.23727800	-2.91884700	-0.22002100
H	2.93049300	-2.94720400	-0.82128700
H	1.60252900	-1.05610400	2.47774200
H	1.33905600	0.61210800	1.81600100
H	0.21731200	-0.73212000	1.37398300
P	2.32195000	-0.84398100	0.21886400
C	-1.46531000	2.41597300	0.13280200
C	-1.06855100	1.19418200	-0.59716700
O	-0.36357300	2.98599200	-0.48181100
H	-1.26298400	1.15837900	-1.66693500
H	-0.14442300	0.77562600	-0.22835600
H	-2.41986600	2.84059400	-0.22608200
C	-1.44057900	2.36175300	1.64591600
H	-0.50150600	1.90433800	1.99189500
H	-1.49026800	3.38195000	2.05145100
H	-2.28343100	1.77361800	2.03564100

E= -1106.231392 Hartree $\bar{\upsilon}$ = -459.96 cm^{-1}

[1OH-PI] TS2

C	2.47065600	-0.74485600	-1.33386800
C	1.53886600	-1.88654500	-0.89987200
O	1.20270200	-1.70735800	0.43198400
H	0.78251300	-0.73332300	0.46083500
H	1.89322100	0.18295600	-1.43798000
H	3.03528200	-0.94264200	-2.25880400
H	0.66228600	-1.89255700	-1.57651900
H	2.04580400	-2.85967200	-1.03056700
I	-3.89025800	-0.30888900	-0.20224700
C	3.04382400	0.25129000	1.53804700
C	4.45053300	-2.02705000	0.38254800
C	4.94587600	0.66733700	-0.65942600
H	2.92586100	-0.57407900	2.25007100
H	3.75209300	1.00203000	1.91189900
H	2.04909000	0.68663900	1.34738400
H	4.46685800	1.62785300	-0.89015700
H	5.73012900	0.81657200	0.09467600
H	5.38736900	0.24219100	-1.57025000
H	3.66232000	-2.66969400	0.79978800
H	4.86969600	-2.48621000	-0.52270600

H	5.24441100	-1.88281700	1.12740100
P	3.67162200	-0.44089100	-0.00768900
C	-1.01402700	0.62550400	0.63979700
C	-1.72506100	-0.31749700	-0.33840100
O	0.32703700	0.61286400	0.28971800
H	-1.50524600	-0.01882300	-1.36910900
H	-1.41999200	-1.35935200	-0.17159400
H	-1.44182100	1.63830700	0.49901100
C	-1.21454000	0.20926500	2.09654800
H	-0.64979600	0.89452500	2.74522400
H	-2.27107800	0.23262400	2.39912300
H	-0.82503700	-0.81061400	2.24869400
C	1.11338800	2.62881400	-0.35546900
O	0.13019500	3.23213700	-0.26325900
O	2.22235100	2.29398200	-0.53861900

E= -1294.87011 Hartree $\bar{\upsilon}$ = -124.75 cm^{-1}

[1OH-PI] TS3

C	-3.14814900	-0.84237300	0.99487000
C	-2.57887000	-2.11945500	0.36348600
O	-1.96773900	-1.87003000	-0.86091100
H	-1.21960800	-1.26393200	-0.69825600
H	-2.33399900	-0.14833500	1.23748600
H	-3.71653300	-1.06481300	1.91246600
H	-1.88831600	-2.57025600	1.09884300
H	-3.38049600	-2.85654900	0.19293000
I	4.37736700	-0.22160400	-0.23081400
C	-3.79738700	0.25730300	-1.81178400
C	-5.84484000	-0.83947700	-0.08595100
C	-4.59586900	1.70239900	0.63373200
H	-3.56817000	-0.73254700	-2.22244000
H	-4.63314700	0.73078900	-2.34587600
H	-2.90114400	0.88822500	-1.84171200
H	-3.65015300	2.26035300	0.58966300
H	-5.37430200	2.21474000	0.05254400
H	-4.92805900	1.58701300	1.67406400
H	-6.22559900	-0.93825200	0.93941800
H	-6.58796400	-0.31208800	-0.69905400
H	-5.68197900	-1.84034800	-0.50911600
P	-4.27913800	0.08039700	-0.08543700
C	1.24781000	-0.18004800	0.43791200
C	2.01811400	1.03878500	-0.05296000
O	-0.13528800	-0.01513800	0.06394100
H	2.11759400	1.23212900	-1.11702200
H	2.53621600	1.69429300	0.63727000
H	1.58974300	-1.07201600	-0.09481500

C	1.34844000	-0.35698800	1.93971700
H	0.74055700	-1.21217700	2.26518400
H	2.39612300	-0.53588700	2.21400900
H	0.99241700	0.55291800	2.44610600
C	-0.51249200	1.31380600	-0.00151600
O	0.45161100	2.10670400	0.08687700
O	-1.71322100	1.53872700	-0.13016200

E= -1294.856347 Hartree $\bar{\upsilon}$ = -499.85 cm^{-1}

[2OH-PI] TS1

C	4.00031300	0.88892400	-1.09639200
C	4.85070300	-1.87941300	-0.92296700
C	2.19478100	-1.27968100	0.17621600
C	1.62497500	-0.82034500	1.52659700
O	1.74129500	0.55828600	1.66964900
C	2.75209900	1.77324900	-1.16026600
C	4.64874600	-0.31303100	1.53318200
H	0.99472300	0.94839100	1.12588900
H	4.88296300	1.43705300	-0.73178200
H	4.21272000	0.54016400	-2.11861200
H	4.36825000	-2.11721000	-1.88120400
H	4.90570600	-2.78853200	-0.30935900
H	5.86503800	-1.50311100	-1.11313900
H	2.25362100	-2.37593400	0.09539200
H	1.58618900	-0.88818900	-0.65281600
H	0.57910300	-1.16475200	1.58987400
H	2.16986500	-1.31229900	2.34919200
H	4.03782200	0.43090900	2.06302600
H	4.67651800	-1.24619200	2.11174400
H	5.67211300	0.05491800	1.38231100
I	-4.15465000	-0.56117300	-0.20902000
P	3.87280700	-0.61469600	-0.07130500
C	-1.45628600	0.16656400	-0.22209900
C	-1.41953400	1.57373400	0.12921500
O	-0.06498800	1.17462200	-0.04015500
H	-1.36845500	-0.57934000	0.56284800
H	-1.44880200	-0.14060700	-1.26384600
H	-1.76629100	2.25964000	-0.65572100
C	-1.80809700	1.99661200	1.51839800
H	-1.42299300	3.00122800	1.74285800
H	-2.90375600	1.99377900	1.59984500
H	-1.40206200	1.28704900	2.25460900
H	2.43439900	2.05819800	-0.14398100
O	1.75971100	1.08357800	-1.84591600
H	0.91689500	1.19609600	-1.33290900

H	3.04644200	2.69979500	-1.68650000

E= -1220.761421 Hartree $\bar{\upsilon}$ = -510.20 cm^{-1}

[2OH-PI] TS2

C	3.31552300	0.54238100	-0.77653700
C	3.68163800	-2.30600700	-1.29439700
C	1.69922800	-1.61784400	0.72376900
C	1.43577400	-0.88483500	2.04644000
O	1.72379700	0.46659600	1.94121200
C	2.48123900	0.59676800	-2.06329100
C	4.52268200	-1.12917200	1.29034400
H	1.06568900	0.85928900	1.27799300
H	2.92599800	1.25488600	-0.03565600
H	4.37742600	0.77582000	-0.95901500
H	2.85971600	-2.29372000	-2.02503200
H	3.77560200	-3.30994300	-0.86041600
H	4.61970800	-2.02787700	-1.79343900
H	1.74775000	-2.71132500	0.85236800
H	0.93765700	-1.38460900	-0.03177800
H	0.38797100	-1.08357200	2.34469400
H	2.06876500	-1.31858100	2.83919300
H	5.51490300	-0.91388900	0.87300000
H	4.24441000	-0.34769400	2.01262900
H	4.53281100	-2.10882400	1.78677200
I	-3.72988200	-0.82139700	-0.22908500
P	3.27224600	-1.09557600	-0.01427200
C	-1.60948200	-0.40739000	-0.12260600
C	-1.28055100	1.02596200	0.30037500
O	0.09115400	1.21683000	0.08832300
H	-1.21345300	-1.14385400	0.58903600
H	-1.22646500	-0.61280100	-1.12951300
H	-1.84990800	1.71319100	-0.35136200
C	-1.64952100	1.32169600	1.74816000
H	-1.07611200	0.67142800	2.42875900
H	-1.39491800	2.36566500	1.97328700
H	-2.72205700	1.17433900	1.93585900
H	2.39871400	1.65799200	-2.35243600
O	1.24323000	-0.01371200	-1.88362400
H	0.73466800	0.50826700	-1.18320400
H	3.01042300	0.07195600	-2.87703300
C	0.53140000	3.08805300	-0.20821300
O	1.70672900	3.03293300	-0.32877700
O	-0.50076700	3.64658600	-0.17005600

E= -1409.413597 Hartree $\bar{\upsilon}$ = -175.62 cm^{-1}

[2OH-PI] TS3

C	-3.21390800	-0.88012100	1.16269900
C	-4.87302000	-1.96304700	-1.01286100
C	-3.78283000	0.76429900	-1.31932500
C	-3.91988100	2.19444200	-0.77354100
O	-3.56747600	2.27824500	0.57418600
C	-2.16850000	-1.88409400	0.64602500
C	-5.89282100	0.21920200	0.65882200
H	-2.59871600	2.12797600	0.62518100
H	-2.75667900	0.07174600	1.45931500
H	-3.77970500	-1.28745400	2.01507000
H	-3.97312600	-2.34230500	-1.51566700
H	-5.65660200	-1.74019800	-1.74910300
H	-5.24485500	-2.71087000	-0.29897900
H	-4.33466500	0.62962700	-2.26258000
H	-2.73014100	0.49439700	-1.47414500
H	-3.31623400	2.86444900	-1.40889000
H	-4.96729200	2.52452200	-0.86252900
H	-6.32629000	-0.52632500	1.33840400
H	-5.58930600	1.11530000	1.21752200
H	-6.63288400	0.48979000	-0.10670000
I	4.98150700	-0.03900700	-0.25594000
P	-4.41153800	-0.45365100	-0.13054800
C	2.51231600	0.85918100	0.33518000
C	1.82142200	-0.46940300	0.05045100
O	0.44632700	-0.18928000	-0.28571400
H	2.94193400	1.07385100	1.30692800
H	2.66907700	1.57671800	-0.46467200
H	2.25407600	-0.92552400	-0.84404100
C	1.86706000	-1.41376700	1.23467300
H	1.32485100	-2.34086200	1.00277000
H	2.91230000	-1.65889100	1.46312400
H	1.40903100	-0.93305100	2.11310000
H	-1.27726700	-1.82621100	1.29183800
O	-1.84803800	-1.66701200	-0.69794700
H	-1.02532700	-1.14288700	-0.73472100
H	-2.57281500	-2.90538400	0.74202500
C	-0.01481400	0.96346400	0.29155900
O	-1.22597100	1.16966300	0.18859800
O	0.87187100	1.64622700	0.84933500

E= -1409.396998 Hartree $\bar{\upsilon}$ = -501.56 cm^{-1}

[3OH-PI] TS1

C	2.40939800	1.52935100	-0.96372800
C	3.82521600	-1.01283200	-1.25809600
C	1.64987600	-0.79548100	0.74466500
C	1.26329000	-0.12280300	2.07230200

O	1.26330800	1.26516200	1.97153900
C	1.43322400	1.17129500	-2.10874800
O	0.56569700	2.21721800	-2.35650300
C	4.83565400	-1.95726800	-0.62137900
O	4.22393100	-2.55385700	0.49555000
C	4.22429600	0.60868000	1.18460000
H	1.87497100	2.14063900	-0.22307700
H	3.27513800	2.10387400	-1.32761400
H	4.31254400	-0.38751200	-2.02087900
H	3.01946400	-1.57590300	-1.75502600
H	1.96998200	-1.83808500	0.87438200
H	0.81202700	-0.76641200	0.03168800
H	0.28759100	-0.53137500	2.39406600
H	1.99417900	-0.40974700	2.84559200
H	2.00296000	0.96257800	-3.02806300
H	0.88673400	0.24043100	-1.85401800
H	5.73658600	-1.38801100	-0.32689400
H	5.14682500	-2.70426600	-1.37043000
H	4.79389200	-3.24311900	0.85427900
H	3.70334000	1.28675300	1.87498900
H	4.58188300	-0.28338900	1.71553700
H	5.06257000	1.12764200	0.70092800
I	-3.99322700	-0.94436400	-0.21424200
P	3.01469600	0.09584100	-0.05129900
C	-1.60157400	0.44907200	-0.22339000
C	-1.84568000	1.75364900	0.36444700
O	-0.45279500	1.72484000	0.07813900
H	-1.27540400	-0.36283700	0.42101500
H	-1.59182400	0.32922800	-1.30401700
H	-2.40129200	2.45461700	-0.27475500
C	-2.22270900	1.84796900	1.81743400
H	-2.03943800	2.86133600	2.20095800
H	-3.28579300	1.59517700	1.93093200
H	-1.63206800	1.13461200	2.41167900
H	0.53484600	1.52681500	1.33432000
H	0.02382600	2.28391600	-1.53969900

E= -1335.295628 Hartree $\bar{\upsilon}$ = -506.99 cm^{-1}

[3OH-PI] TS2

C	2.25475200	0.42550600	1.59479700
C	4.93084600	0.27732800	0.44042500
C	2.60921200	-0.28814700	-1.30242200
C	1.42263400	-1.24785000	-1.51040400
O	0.63487600	-1.32515800	-0.37125300
C	2.11524000	1.94184200	1.30331000
O	0.87801100	2.40471900	1.70522500

C	6.02603400	-0.66509100	-0.03661100
O	5.63258300	-1.19843800	-1.27709600
C	3.37366900	-2.20245200	0.82834600
H	1.25717700	-0.03070900	1.53410000
H	2.67122800	0.22609700	2.59435700
H	5.12682100	0.59380000	1.47563700
H	4.89546800	1.18473300	-0.18269200
H	3.44711100	-0.47154900	-1.98920500
H	2.27365000	0.75501500	-1.40883200
H	0.86234500	-0.90359100	-2.39935200
H	1.80922000	-2.25479500	-1.74578800
H	2.89905600	2.49077800	1.85043400
H	2.28378700	2.13233300	0.22455700
H	6.17470900	-1.46449700	0.71279600
H	6.97285100	-0.10385000	-0.11197000
H	6.34182500	-1.74140400	-1.63802100
H	2.34956600	-2.59969500	0.79635000
H	4.00928600	-2.71149400	0.09187600
H	3.79354900	-2.31058600	1.83729700
I	-4.53252400	-0.71777100	-0.00509600
P	3.25482700	-0.45754900	0.38155900
C	-2.46951800	-0.26573900	-0.48135600
C	-1.76533100	0.61428800	0.55256700
O	-0.48504300	0.87815700	0.05317500
H	-1.96159800	-1.23291900	-0.58435000
H	-2.51235100	0.25164400	-1.44541400
H	-2.33608800	1.55962300	0.63398000
C	-1.66048800	-0.03569000	1.93026400
H	-1.06220900	0.61389200	2.58614100
H	-2.64392600	-0.19647400	2.39254500
H	-1.15151200	-1.01008300	1.84115400
H	0.15879900	-0.40881200	-0.22707900
H	0.23359900	1.91740700	1.12034500
C	-0.41152200	2.31685000	-1.44429100
O	0.73045200	2.24100200	-1.71311900
O	-1.52140200	2.67411500	-1.47942200

E= -1523.937616 Hartree $\bar{\upsilon}$ = -196.80 cm^{-1}

[3OH-PI] TS3

C	2.86373800	1.03354300	1.19627500
C	4.76631100	1.51357200	-0.96729800
C	3.28233700	-1.05287300	-0.91992500
C	3.24495500	-2.39994700	-0.18070800
O	2.86016100	-2.25078900	1.15132800
C	1.83362300	1.89328000	0.44126700
O	0.84610200	2.33268600	1.30910000

C	6.13057300	1.14361900	-1.53192000
O	6.04327800	-0.15710400	-2.06084500
C	5.39649300	-0.49572300	1.09424500
H	2.33349100	0.23173700	1.72689700
H	3.42114500	1.64618600	1.92224700
H	4.83379700	2.44523600	-0.38605400
H	4.03721100	1.68018100	-1.77567900
H	3.85371300	-1.10553200	-1.85616200
H	2.25822800	-0.70295700	-1.11739900
H	2.58043600	-3.08131900	-0.73870900
H	4.25125300	-2.84841700	-0.19190300
H	2.33881400	2.77369500	0.00658000
H	1.40675000	1.30334300	-0.38850300
H	6.88787500	1.19791600	-0.72836600
H	6.41141100	1.88316700	-2.30034000
H	6.86761600	-0.38597700	-2.50427400
H	4.94525200	-1.25235400	1.75031900
H	6.11898900	-0.96131600	0.41114600
H	5.88394000	0.28715700	1.69047600
I	-5.41704600	0.11950300	-0.71049500
P	4.05826300	0.22030000	0.11666200
C	-3.01631800	-0.86341300	0.00062200
C	-2.52364500	0.42417400	0.64959700
O	-1.08170600	0.42872900	0.57868200
H	-3.59492300	-1.58973000	0.55974900
H	-2.86735900	-1.03476100	-1.06124900
H	-2.84481600	1.28479500	0.05673800
C	-2.96440900	0.54712700	2.09383500
H	-2.54282900	1.45443800	2.54644000
H	-4.06018300	0.60164200	2.13138100
H	-2.62583300	-0.33065100	2.66428300
H	1.91998200	-1.96141700	1.13915900
H	0.10309900	1.70925400	1.23688900
C	-0.55350900	-0.82856100	0.56050100
O	0.67782400	-0.90706500	0.62525700
O	-1.40171600	-1.74286400	0.45818800

E= -1523.922240 Hartree $\bar{\upsilon}$ = -500.78 cm^{-1}

[2OH-AsI] TS1

C	2.34274900	0.74767700	1.07216700
C	3.96446100	-1.72789700	0.05428600
C	2.22053900	-0.18825400	-1.97295400
C	1.11181300	0.82743700	-2.29921200
O	1.33012300	2.03274800	-1.65284900
C	1.50274900	0.60506600	2.35945200
O	1.01331900	1.83387600	2.76268300

C	0.92416100	-2.03365500	0.23522200
H	0.65890100	2.23175100	-0.93427300
H	0.49740000	2.21142800	2.01371700
O	-0.23324000	2.43389300	0.40955300
C	-1.17422000	0.87289100	0.47766400
C	-1.60116300	2.23290200	0.15230200
C	-2.07565900	2.54884100	-1.24333400
H	3.39892000	0.97457500	1.27676300
H	1.93937300	1.57103500	0.46980400
H	3.97596700	-2.57881700	-0.63871300
H	4.05618500	-2.09365000	1.08522400
H	4.80413900	-1.05797100	-0.17077900
H	2.12782200	-1.10430100	-2.57663800
H	3.19606600	0.27337700	-2.18872800
H	1.14616300	0.97262900	-3.39343800
H	0.12154300	0.38068800	-2.09054400
H	0.69648700	-0.13628700	2.19312500
H	2.12959200	0.20173800	3.16971300
H	-0.09360700	-1.62872100	0.10370700
H	1.06175400	-2.87315700	-0.45959700
H	1.03241900	-2.39413600	1.26650100
H	-1.09616000	0.59901800	1.52631400
H	-0.59113600	0.34644200	-0.26679400
H	-2.25055500	2.68263700	0.91950900
H	-2.04063700	3.63357100	-1.41446900
H	-3.10468500	2.18957800	-1.37942100
H	-1.43669400	2.05970100	-1.99276500
I	-2.95635300	-1.04026200	0.04910000
As	2.31161400	-0.75883200	-0.12997500

E= -3115.278109 Hartree $\bar{\upsilon}$ = -496.11 cm^{-1}

[2OH-BiI] TS1

C	-2.56393200	1.42363900	-0.56200900
C	-3.37418600	-1.83667000	0.46092400
C	-0.42544200	-0.72523600	1.95616200
C	-0.20966200	0.63642900	2.65405100
O	-0.84953300	1.70699700	2.02549600
C	-2.25794600	1.69150900	-2.02727300
O	-0.90256000	1.59365600	-2.31713900
C	-0.53796300	-1.52893400	-1.58287100
H	-0.28399900	2.08189400	1.29968800
H	-0.39360200	2.09593400	-1.62861700
O	0.42995700	2.42616300	-0.20153900
C	1.44812800	0.93735800	-0.32948800
C	1.83619400	2.34618000	-0.27562200
C	2.58827100	2.85262300	0.92690500

H	-3.63514900	1.30612600	-0.34792500
H	-2.12150800	2.15950000	0.11778100
H	-3.01046600	-2.83865700	0.71947300
H	-3.99267800	-1.88521000	-0.44371300
H	-3.95751100	-1.42246800	1.29236400
H	0.50571000	-1.21831400	1.63226200
H	-1.01575800	-1.43369800	2.55314600
H	-0.60619700	0.56297900	3.67726200
H	0.87742800	0.80444600	2.74729000
H	-2.79664800	0.97475400	-2.67007900
H	-2.67075400	2.69276800	-2.26494200
H	0.49081900	-1.71601400	-1.23864500
H	-1.06545300	-2.46319600	-1.80586400
H	-0.54964100	-0.82713600	-2.42484300
H	1.11403500	0.52655800	-1.27811700
H	1.17884100	0.47409500	0.60779300
H	2.23787100	2.73996400	-1.22161800
H	2.53190700	3.94857300	0.97617700
H	3.64094300	2.54375400	0.87090000
H	2.15227800	2.44070000	1.84914300
I	3.34584100	-0.93999000	-0.23264500
Bi	-1.61932200	-0.50992500	0.07147100

E= -1093.837035 Hartree $\bar{\upsilon}$ = -495.11 cm^{-1}

[2OH-SbI] TS1

C	-1.41285900	-1.32449300	-0.74533900
C	-3.97350600	1.25469800	-0.78183100
C	-2.28588100	0.30555400	2.22070700
C	-1.01623300	1.06736000	1.83972000
O	-1.26021300	1.58061300	0.55158900
C	-1.38766700	-1.04215500	-2.25160200
O	-1.41591500	0.31990500	-2.54154100
C	-4.44912000	-1.77868500	0.62175000
H	-0.40908000	1.52333700	-0.03195800
H	-0.56249500	0.70643200	-2.24815200
O	0.65058400	1.10205000	-1.00275300
C	1.94815000	0.11155900	-0.47913800
C	2.00215400	1.49119200	-0.95273000
C	2.34299000	2.58684000	0.01872800
H	-0.47483300	-0.99890400	-0.27475600
H	-1.56310700	-2.39399100	-0.53576600
H	-5.05410100	1.07169700	-0.79248700
H	-3.54235800	1.28266500	-1.79019300
H	-3.73615000	2.19041000	-0.26279000
H	-2.12150100	-0.56272700	2.87283400
H	-3.05601900	0.94568600	2.67463300

H	-0.79676300	1.87199600	2.55977300
H	-0.14952900	0.38253700	1.83563700
H	-0.49514900	-1.53933800	-2.67357200
H	-2.26432900	-1.50631600	-2.73215300
H	-5.28027100	-1.35676000	1.20226500
H	-4.83730300	-2.14279300	-0.33908800
H	-4.01515800	-2.62139800	1.17556800
H	1.99304000	-0.72165000	-1.17440300
H	1.75697200	-0.06746400	0.57540300
H	2.44665100	1.63068900	-1.94730100
H	1.95961900	3.55511600	-0.33269700
H	3.43455500	2.63949200	0.12779100
H	1.91391000	2.36627700	1.00803100
I	4.55825500	-0.60903300	0.26571800
Sb	-2.96348900	-0.27505900	0.27490900

E= -1119.550206 Hartree $\bar{\upsilon}$ = -515.63 cm^{-1}

PO

O	0.80852200	-0.76827500	-0.26411400
C	1.04805700	0.60227600	-0.04712900
C	-0.14879100	-0.06015900	0.48903900
C	-1.50154200	0.11107000	-0.14375000
H	1.88553800	0.83932000	0.61754100
H	0.94732100	1.24613700	-0.92834700
H	-0.14706600	-0.31054100	1.55779200
H	-2.07024800	0.90835600	0.35517100
H	-2.08042800	-0.82054700	-0.07150000
H	-1.38963900	0.36435700	-1.20670700

CO_2

C	0.00000000	0.00000000	-0.00257500
O	0.00000000	1.17961900	0.00096600
O	0.00000000	-1.17961900	0.00096600