

“Supporting Information for”

Proton Supplier Role of Binuclear Gold Complexes in Promoting Hydrofunctionalization of unactivated Alkenes

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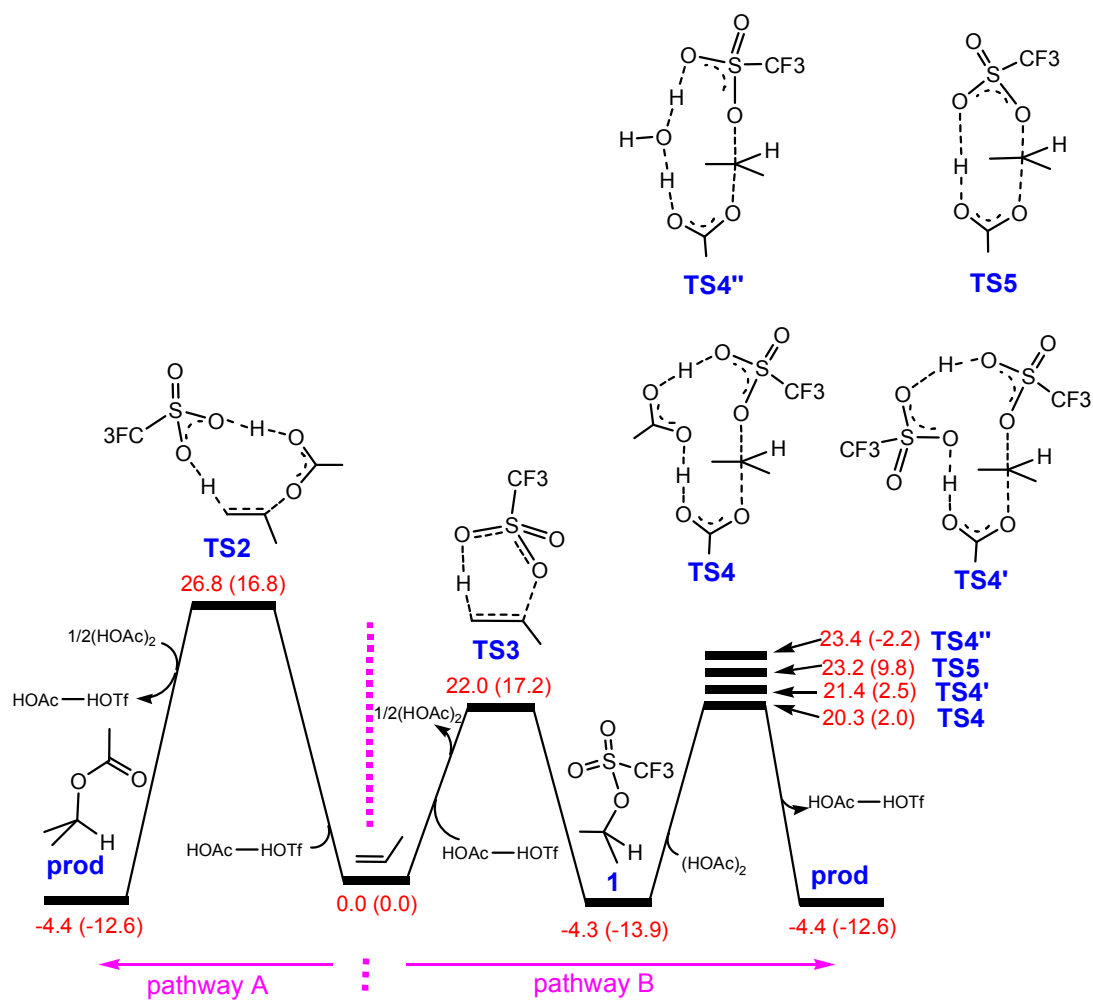


Fig. S1 Energy profile for HOF-catalyzed hydroacetoxylation of propene calculated at M06-D3-CPCM/BS2//B3LYP-CPCM/BS1 level of theory. Free energies (potential energies) are given in kcal/mol.

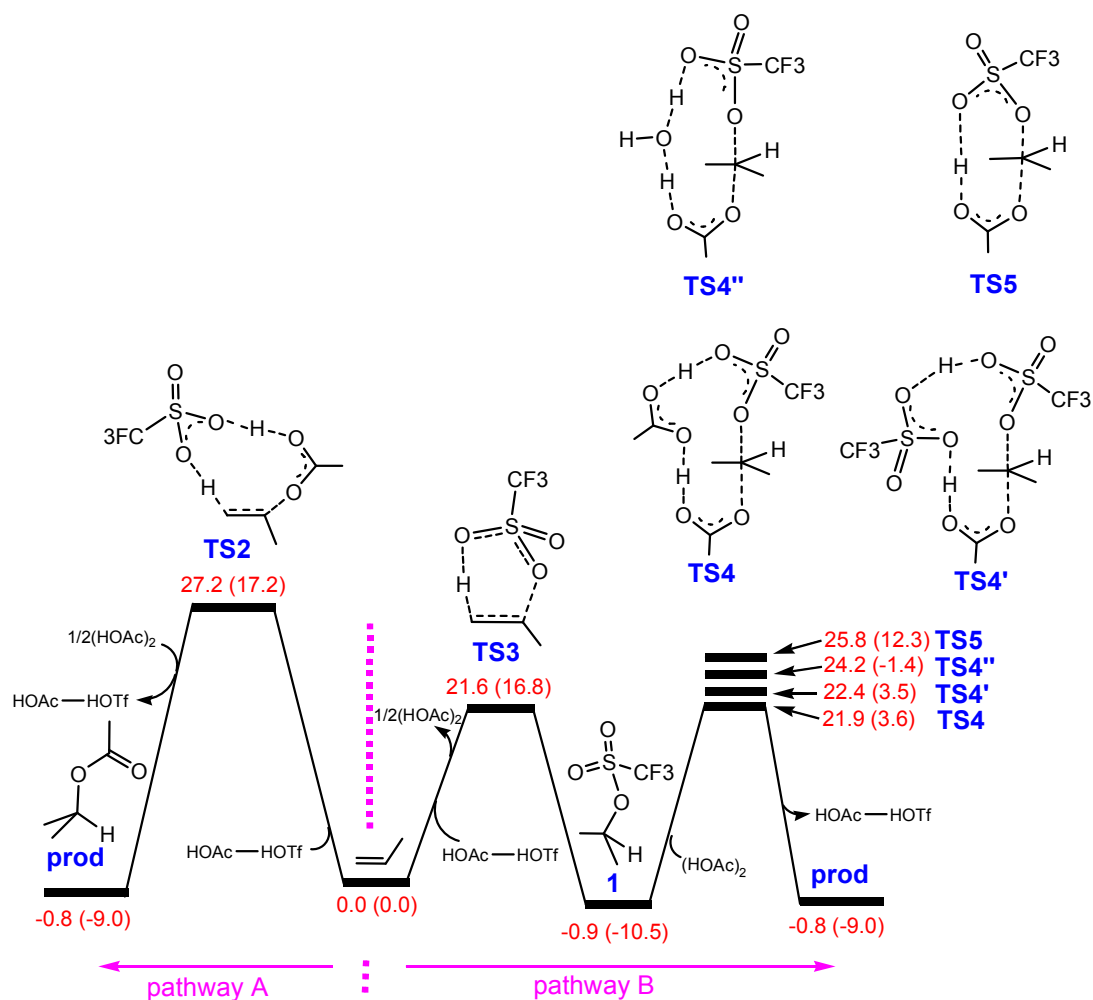


Fig. S2 Energy profile for HOTf-catalyzed hydroacetoxylation of propene calculated at B3LYP-D3-CPCM/BS2//B3LYP-CPCM/BS1 level of theory. Free energies (potential energies) are given in kcal/mol.

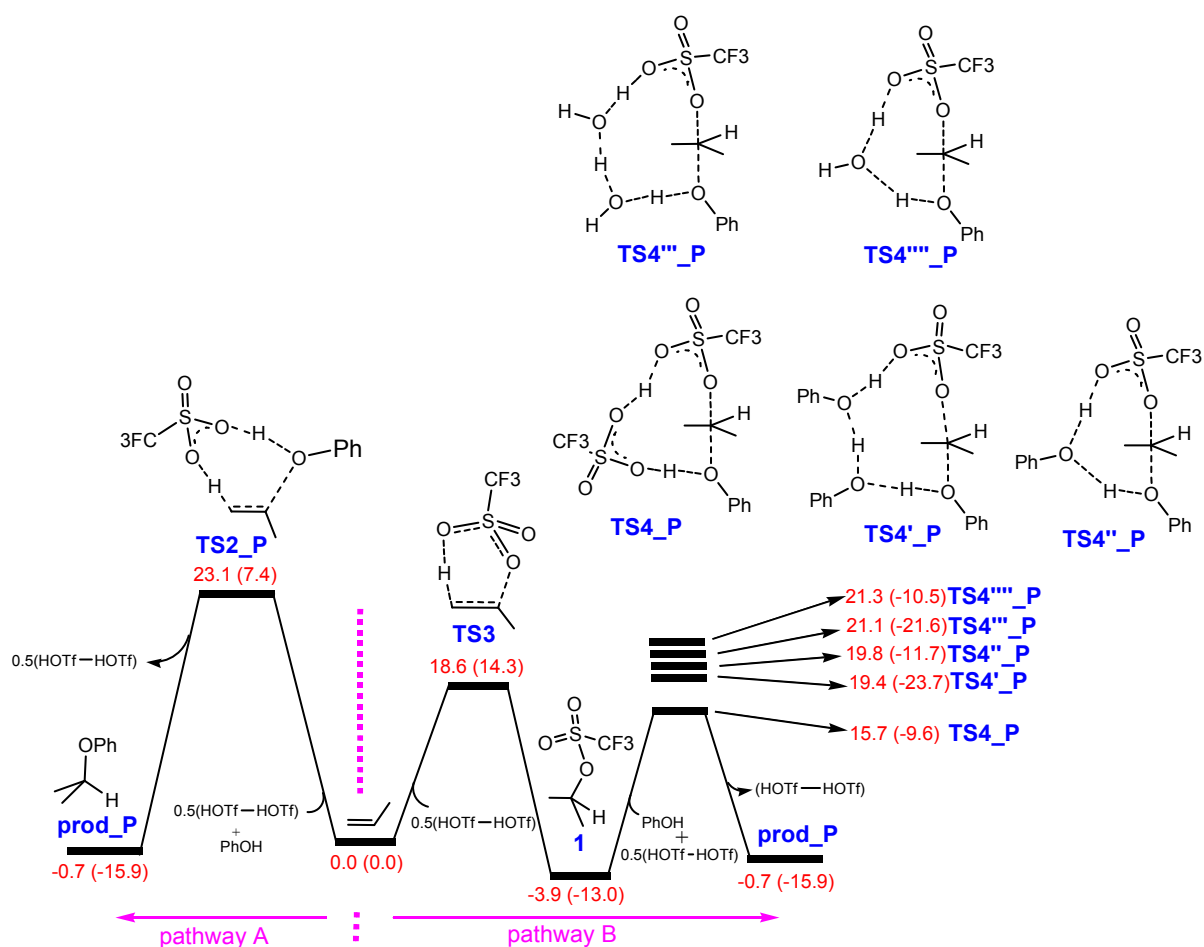


Fig. S3 Energy profile for HOTf-catalyzed hydroaryloxylation of propene calculated at B3LYP-D3-CPCM/BS2//B3LYP-CPCM/BS1 level of theory. Free energies (potential energies) are given in kcal/mol.

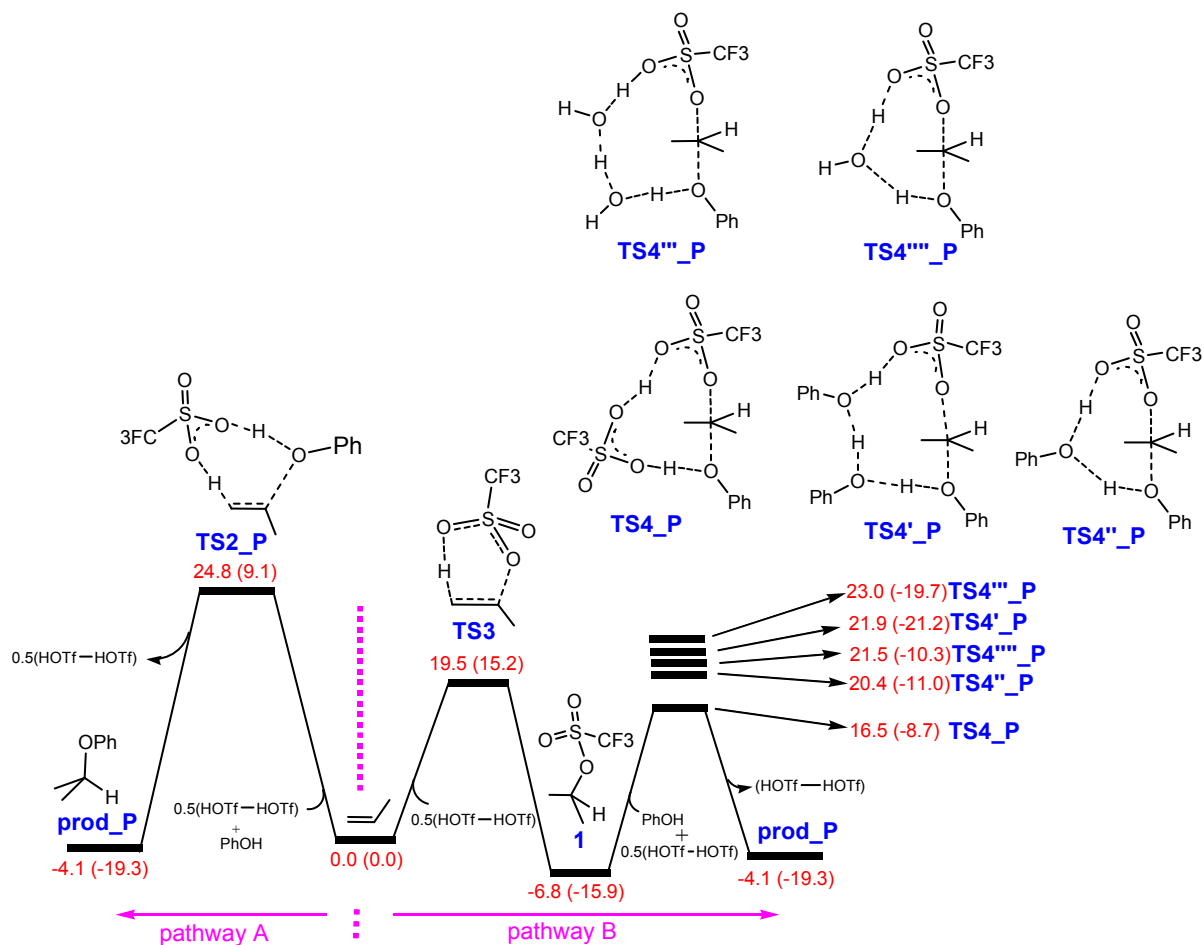
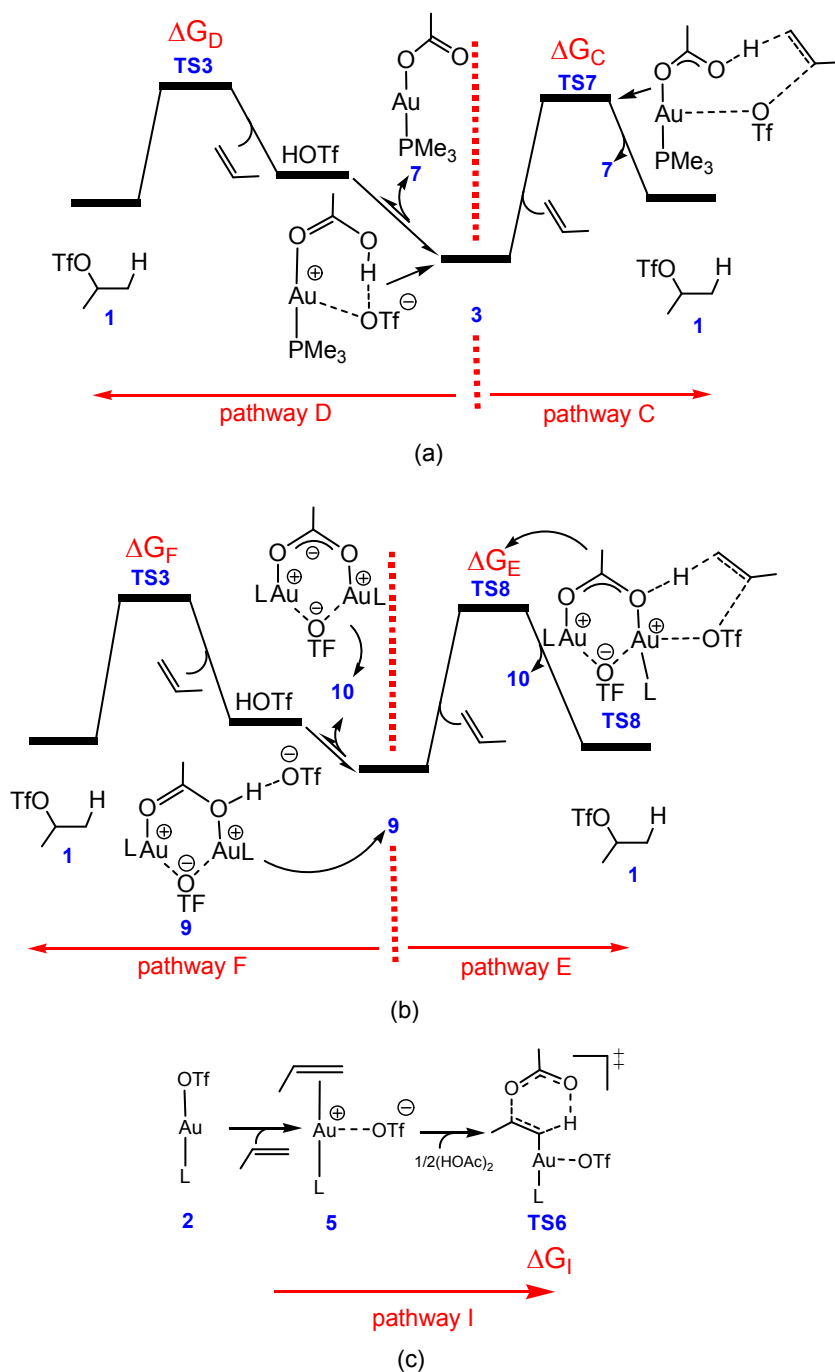


Fig. S4 Energy profile for HOFt-catalyzed hydroaryloxylation of propene calculated at M06-D3-CPCM/BS2//B3LYP-CPCM/BS1 level of theory. Free energies (potential energies) are given in kcal/mol.

Table S1. Free energy changes calculated for **TS3** (ΔG_D and ΔG_F), **TS7** (ΔG_C), **TS8** (ΔG_E) and **TS6** (ΔG_I) calculated at different levels of theory for pathways C-F and I where L = PMe_3 and PPh_3 . Free energies are given in kcal/mol. It follows that regardless of the method and the nature of the phosphine ligands (PMe_3 or PPh_3) used in the calculations, pathways E and F (binuclear mechanism) are the most favorable.



L	method	ΔG_C	ΔG_D	ΔG_E	ΔG_F	ΔG_I
PMe ₃	B3LYP-D3 -CPCM/BS2//B3LYP -CPCM/BS1	37.5	39.2	27.9	29.2	51.1
PMe ₃	M06-D3-CPCM/BS2//B3LYP-CPCM/BS1	37.2	38.2	31.6	31.6	45.8
PMe ₃	B97D-CPCM/BS2//B3LYP-CPCM/BS1	35.6	36.7	24.2	24.8	48.2
PMe ₃	B3LYP-D3-CPCM/BS2//B3LYP-D3-CPCM/BS1	37.4	38.7	28.5	29.2	51.3
PMe ₃	B3LYP-D3 -CPCM/BS2//B3LYP -CPCM/BS3*	36.9	38.1	26.1	28.5	49.2
PPh ₃	B3LYP-D3 -CPCM/BS2//B3LYP -CPCM/BS1	38.2	38.5	24.5	26.8	49.6
PPh ₃	M06-D3-CPCM/BS2//B3LYP-CPCM/BS1	37.9	38.0	26.5	27.4	44.5

* BS3 utilizes def2-SVP with its ECP for gold and 6-31G(d) for the other atoms

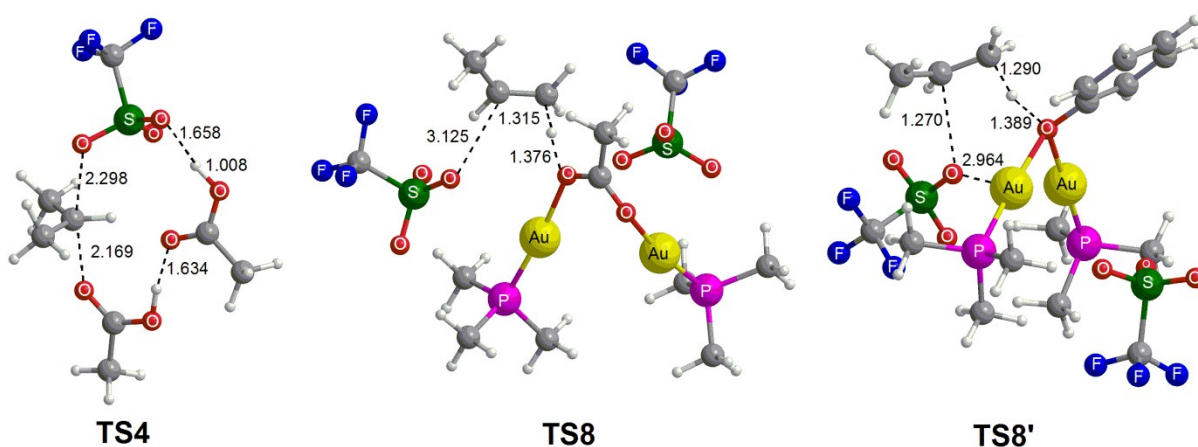


Fig. S5 Optimized structures for TS4, TS8, TS8' along with some structural parameters (bond lengths in Å).

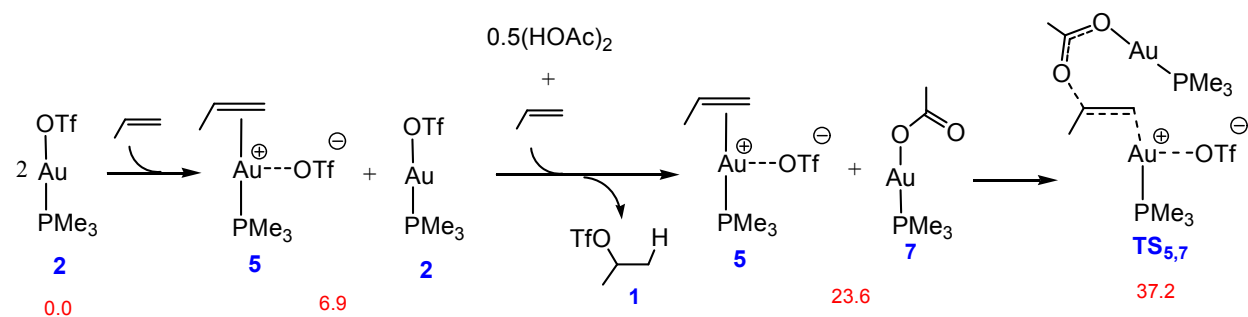


Fig. S6 Calculated mechanism for C-O bond formation via transition structure **TS_{5,7}** in which LAuOAc (**7**) reacts with the alkene complex **5**. Free energies are given in kcal/mol.

Table S2. Cartesian coordinates and total energies for all of the calculated structures in water

1

E (B3LYP-CPCM/BS1) = -1079.939306au

H(B3LYP-CPCM/BS1) = -1079.802629au

G(B3LYP-CPCM/BS1) = -1079.854963au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1080.352247au

H	-3.49371100	-0.85743800	-0.79101600
O	-0.91622800	-0.15254200	-0.68011800
S	0.38049500	-0.88515700	-0.08606300
O	0.13846900	-1.39217200	1.25986600
O	0.92464300	-1.71935300	-1.14381600
C	1.51328800	0.58777000	0.09190200
F	2.64825600	0.19300700	0.66344300
F	1.76735300	1.11260500	-1.10297100
F	0.91970100	1.50545200	0.86461500
C	-3.10829700	-0.71208700	0.22345800
C	-2.00118100	0.32811700	0.23273400
H	-3.93149100	-0.37463500	0.86282700
H	-2.74562100	-1.66984300	0.60709600
H	-1.56889700	0.41878200	1.23111700
C	-2.40470100	1.69020800	-0.30553100
H	-3.20285800	2.10479300	0.31933800
H	-1.55683100	2.38079400	-0.28875900
H	-2.77601800	1.60895900	-1.33219700

TS1

E (B3LYP-CPCM/BS1) = -2290.841988au

H(B3LYP-CPCM/BS1) = -2290.370177au

G(B3LYP-CPCM/BS1) = -2290.480484au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2291.982022au

C	5.16764600	-1.12453200	-0.17013100
C	4.27318200	-1.19610400	-1.23396500
C	4.42589400	-2.10133600	-2.27881400
C	5.51917900	-2.96917700	-2.25091100
C	6.43731200	-2.91558600	-1.19847300
C	6.26090900	-1.99404300	-0.16377000
O	3.15645200	-0.32817100	-1.28809300
O	2.47918000	0.86520500	0.76399000
C	2.46156600	2.21874900	1.10536100
C	3.40297000	2.67728100	2.02824000
C	3.44144800	4.03705200	2.34717400
C	2.53652100	4.92310000	1.75759100
C	1.59611500	4.44728300	0.83924100
C	1.55619800	3.09361600	0.49957400
C	1.22391000	0.06151700	1.07470700
C	0.96698300	-0.99138600	0.01066500
Au	-1.07809200	-1.71901100	0.33311900
P	-3.32846700	-2.25438900	0.62146200
C	1.42843100	-0.49985000	2.47639800

O	-2.22235700	1.44572700	0.39892900
S	-2.01535100	1.57493500	-1.06706200
O	-0.60925200	1.38620100	-1.51369200
O	-3.03421300	0.90257800	-1.90555100
C	-2.30808200	3.38526800	-1.37851300
F	-2.14767700	3.68139600	-2.67684500
F	-3.55095100	3.73738900	-1.01510100
F	-1.43929300	4.13339500	-0.66910400
H	0.83851400	2.71842200	-0.22427300
H	0.88773500	5.12785200	0.37600300
H	2.56391600	5.97878100	2.01237700
H	4.17520000	4.39971800	3.06189800
H	4.09238600	1.97229700	2.48325000
H	0.59277300	-0.63390100	-0.95960500
H	1.45962700	-1.96529700	0.10461800
H	0.41854500	0.79579600	1.05565400
H	2.22700100	-1.25079600	2.48253700
H	0.50753800	-0.97381000	2.83079600
C	-3.70680100	-3.93401400	1.27270900
C	-4.12840500	-1.08622100	1.79130300
C	-4.29054800	-2.10519000	-0.93486400
H	3.16231100	0.37601400	-0.53757100
H	2.15556100	-0.78974900	-0.87450400
H	3.70940200	-2.11482700	-3.09378200
H	5.65482700	-3.68211800	-3.05859000
H	7.28864000	-3.58935600	-1.18589300
H	6.97149900	-1.94920600	0.65610000
H	5.01012300	-0.41099200	0.63249000
H	-5.35812400	-2.26080200	-0.74449100
H	-4.12238700	-1.10631900	-1.35021100
H	-3.93869000	-2.85025900	-1.65487200
H	-4.78749000	-4.07088000	1.38697300
H	-3.31926400	-4.69036500	0.58382600
H	-3.22208600	-4.06774600	2.24421500
H	-5.21084100	-1.24947000	1.82699800
H	-3.70730800	-1.22541100	2.79163600
H	-3.90791200	-0.06806300	1.45737800
H	1.69662900	0.29874000	3.17533800

2

E (B3LYP-CPCM/BS1) = -1558.053701au

H(B3LYP-CPCM/BS1) = -1557.891227au

G(B3LYP-CPCM/BS1) = -1557.960786au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1558.843932au

Au	0.72834800	-0.26581300	-0.27522200
P	2.87461300	0.29000800	0.19578500
C	3.09169300	2.08344200	0.51974000
H	2.45585800	2.37973900	1.35864300
H	4.13715500	2.30550800	0.75865100
H	2.79077000	2.65338300	-0.36361700
C	4.05543500	-0.11508700	-1.14932000

H	5.07303900	0.17172000	-0.86416400
H	4.02354400	-1.18943000	-1.35094900
H	3.76840100	0.41907900	-2.05933000
C	3.51870000	-0.55539000	1.69164600
H	3.49300000	-1.63791400	1.53953400
H	4.54724300	-0.23956700	1.89581600
H	2.88465900	-0.30935200	2.54790900
O	-1.26325400	-0.78176800	-0.77328100
S	-2.35592000	-0.75093800	0.30940900
O	-3.39907000	-1.74304000	0.04400700
O	-1.80866600	-0.64014600	1.66956400
C	-3.12993700	0.90361400	-0.03898100
F	-4.11523500	1.13696900	0.83411100
F	-2.20960900	1.87397000	0.08104900
F	-3.62905600	0.93696100	-1.27828800

TS2

E (B3LYP-CPCM/BS1) = -1308.979166au

H(B3LYP-CPCM/BS1) = -1308.779635au

G(B3LYP-CPCM/BS1) = -1308.849572au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1309.517086au

C	-2.19849700	0.73143400	-0.16643700
F	-2.79214300	1.18596000	0.94189900
F	-1.33748700	1.65979200	-0.60606300
S	-1.29636000	-0.85053800	0.20840100
O	-0.26279400	-0.46266100	1.21319900
F	-3.12677000	0.52254300	-1.10399800
O	-2.31835600	-1.78789500	0.68247600
O	-0.68936400	-1.18615900	-1.13226700
C	1.62395200	-2.64726800	-1.01966800
C	2.61820900	-1.91807200	-0.35349300
H	0.72163500	-1.84584300	-1.01994300
H	1.78403300	-2.83806600	-2.08177400
H	1.16592100	-3.46696500	-0.46055300
H	3.30148900	-1.31084100	-0.93972600
O	2.35950300	0.73878400	-0.68596600
C	2.11326200	1.75033100	-0.04010500
O	1.23042500	1.79833500	0.95420600
C	2.77184500	3.08517800	-0.28890600
H	3.15645400	3.49891900	0.64832900
H	3.57963200	2.97470800	-1.01301800
H	2.02778300	3.79018100	-0.67590900
H	0.74704300	0.92929500	1.02355600
C	2.79699400	-1.90979600	1.10603200
H	3.63575700	-2.59820700	1.31400300
H	3.10417400	-0.92460300	1.46474300
H	1.91553100	-2.26870900	1.64160700

TS2_P

E (B3LYP-CPCM/BS1) = -1387.358608au

H(B3LYP-CPCM/BS1) = -1387.114783au

G(B3LYP-CPCM/BS1) = -1387.188015au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1387.922442au

C	-3.46627800	-0.58473300	0.37914800
F	-3.67514500	-1.90130600	0.48572200
F	-3.51612600	-0.03740200	1.59837000
S	-1.80584100	-0.27806700	-0.39753200
O	-0.85321500	-0.92300300	0.55187500
F	-4.43263800	-0.05125200	-0.37588600
O	-1.87048800	-0.86571100	-1.74099500
O	-1.72514000	1.22767800	-0.36279900
C	0.34504500	2.72317300	-1.41530700
C	1.39357700	2.70834600	-0.47599700
O	1.49957400	0.38298200	0.93022800
C	2.54629100	-0.38777500	0.50066500
H	-0.42336000	1.95722700	-0.92050900
H	-0.26927700	3.62816400	-1.42550500
H	0.56428400	2.30110000	-2.39673700
H	2.24273900	2.05118100	-0.64599500
H	0.64346800	-0.10875800	0.82411700
C	2.35675900	-1.61990500	-0.14228700
C	3.46684300	-2.34854400	-0.57036900
C	4.76299100	-1.86356500	-0.37261400
C	4.94314300	-0.63578300	0.26921700
C	3.84322100	0.10254800	0.70844600
H	1.34962300	-1.99409500	-0.29798600
H	3.31320900	-3.30379700	-1.06535700
H	5.62098400	-2.43712400	-0.71070900
H	5.94531000	-0.25031400	0.43770600
H	3.97704400	1.04530000	1.23199300
C	1.42544300	3.52481000	0.74456400
H	1.60439700	2.87079700	1.60677000
H	2.30595000	4.18524300	0.68204300
H	0.52622000	4.12679600	0.88756400

3

E (B3LYP-CPCM/BS1) = -1787.153322au

H(B3LYP-CPCM/BS1) = -1786.921818au

G(B3LYP-CPCM/BS1) = -1787.003144au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1788.063134au

Au	-1.07785400	0.80012000	-0.05639500
P	-2.38602600	-1.06002700	-0.00902600
C	-4.16843000	-0.71567800	-0.28666100
H	-4.30479900	-0.24413900	-1.26381400
H	-4.74376200	-1.64689900	-0.24929000
H	-4.53410900	-0.03312500	0.48560200
C	-2.27969200	-1.93774800	1.59496000
H	-2.93481500	-2.81554800	1.58769900
H	-1.24177500	-2.25051000	1.74022400
H	-2.57674900	-1.26640600	2.40529400

C	-1.90121800	-2.28935600	-1.27858900
H	-0.86587900	-2.58437300	-1.09025900
H	-2.55256800	-3.16785500	-1.21939500
H	-1.97744300	-1.84380700	-2.27412900
O	2.07116300	2.18382700	0.77314900
C	1.20442800	2.96077500	0.19164000
O	3.18155500	-1.90350900	1.47330800
S	1.91035900	-1.55545300	0.82661900
O	0.89282200	-2.62147100	0.71482300
O	1.31857400	-0.24381000	1.28592500
C	2.37305700	-1.18809600	-0.93758200
F	1.27508500	-0.92571900	-1.67606800
F	3.17632600	-0.11385500	-0.99677500
F	3.00538700	-2.22990200	-1.48584100
O	0.05446700	2.63425200	-0.16775900
C	1.69972900	4.36052800	-0.04667100
H	0.89950800	4.98532700	-0.44264400
H	2.08354700	4.77961500	0.88821800
H	2.53216000	4.32923200	-0.75800900
H	1.76471400	1.22510200	0.92519300

3'

E (B3LYP-CPCM/BS1) = -1865.525058au

H(B3LYP-CPCM/BS1) = -1865.249515au

G(B3LYP-CPCM/BS1) = -1865.335054au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1866.460883au

Au	-1.34405700	0.27687200	-0.29846400
P	-3.04186900	-1.01086100	0.47387600
C	-4.70853300	-0.59421200	-0.16942700
H	-4.70827200	-0.66550400	-1.26052600
H	-5.45587100	-1.28183600	0.24026000
H	-4.96353800	0.43060900	0.11453600
C	-3.18899900	-0.96066900	2.30189400
H	-3.97750000	-1.64303000	2.63673900
H	-2.23598600	-1.25778500	2.74801900
H	-3.42652600	0.05650800	2.62523400
C	-2.73857100	-2.76669100	0.04447900
H	-1.73627700	-3.04085200	0.38523300
H	-3.48832400	-3.41413100	0.51115900
H	-2.77791900	-2.88595100	-1.04197200
O	0.38029600	1.37567500	-1.05820800
H	1.10144100	0.65816200	-1.15994200
O	0.72559500	-1.76531600	0.36176100
S	1.87533200	-1.81907200	-0.57507300
O	2.00966300	-3.03913100	-1.38127800
O	2.06970300	-0.54270700	-1.35232300
C	3.35854800	-1.81298000	0.54320100
F	4.48945200	-1.86225100	-0.16964200
F	3.37498600	-0.69215800	1.28891100
F	3.32284500	-2.86638600	1.36950900
C	0.86185300	2.51911800	-0.41980900

C	2.09820300	2.50654000	0.22713400
C	0.08027200	3.67316400	-0.47008500
C	2.55378600	3.68174700	0.82950500
H	2.68422100	1.59430400	0.26500400
C	0.54691600	4.83666200	0.14319400
H	-0.87304000	3.65240900	-0.99034500
C	1.78472000	4.84707800	0.79234600
H	3.51616700	3.67887500	1.33361100
H	-0.05783800	5.73848100	0.10588800
H	2.14572600	5.75538800	1.26562000

TS3

E (B3LYP-CPCM/BS1) = -1079.885669au

H(B3LYP-CPCM/BS1) = -1079.756316au

G(B3LYP-CPCM/BS1) = -1079.809045au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1080.308721au

H	-2.02732300	-1.24838500	-1.01961900
C	-2.57505100	-0.67490800	-0.27563800
C	-2.35388300	-0.96023300	1.07467400
H	-1.35759900	-0.24441600	1.26447100
H	-1.94047300	-1.94285600	1.30869700
H	-3.07998200	-0.57087800	1.79053600
O	-0.12230500	0.51118100	1.50599000
S	0.47120300	0.86343800	0.15214000
O	-0.56445700	0.81719800	-0.90984600
O	1.37298400	2.01192800	0.17693100
C	1.53261300	-0.61711800	-0.20579100
F	2.11230500	-0.49286700	-1.40274300
F	2.47793400	-0.75917300	0.72544400
F	0.76345900	-1.72255000	-0.21267800
C	-3.51789800	0.33963000	-0.78304200
H	-3.04929100	0.94042000	-1.56782100
H	-4.35440200	-0.20228300	-1.25458100
H	-3.91791400	0.97800600	0.00804800

4

E (B3LYP-CPCM/BS1) = -825.535130au

H(B3LYP-CPCM/BS1) = -825.341232au

G(B3LYP-CPCM/BS1) = -825.398039au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -826.070420au

Au	0.07942900	-0.21355500	-0.00034000
P	-2.16721900	0.15245500	0.00064200
C	-2.74155400	0.96317900	1.54036200
H	-2.23331500	1.92392600	1.65908300
H	-3.82330700	1.12700700	1.49697500
H	-2.50407400	0.33019100	2.39963000
C	-3.13610500	-1.39418300	-0.16128200
H	-4.20720100	-1.16688900	-0.15939800
H	-2.87253900	-1.89555000	-1.09646500
H	-2.90471300	-2.06143700	0.67334900

C	-2.69807800	1.23804200	-1.37702900
H	-2.42820600	0.77885700	-2.33187100
H	-3.78211500	1.38754000	-1.33906500
H	-2.19464600	2.20525200	-1.29631800
O	2.20269800	-0.65481900	0.00016200
C	3.11990100	0.17265200	-0.00026100
C	4.56317900	-0.23785700	0.00235200
H	5.06797700	0.16667300	-0.88220000
H	5.06367400	0.16484600	0.89023200
O	2.81658300	1.46377600	-0.00271000
H	4.63981900	-1.32444100	0.00156100
H	3.61375000	2.02536200	-0.00273400

TS4

E (B3LYP-CPCM/BS1) = -1538.095929au

H(B3LYP-CPCM/BS1) = -1537.823272au

G(B3LYP-CPCM/BS1) = -1537.908746au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1538.747620au

H	-0.30158800	-3.30874400	0.33350700
O	-1.24230600	-0.86470200	0.86295600
S	-1.81131000	0.12112200	-0.11447900
O	-1.87619200	1.51454500	0.41518900
O	-1.29536100	-0.01782100	-1.48627100
C	-3.60147000	-0.36801900	-0.19628200
F	-4.25725400	0.43829300	-1.03808700
F	-3.70681600	-1.62862800	-0.63693300
F	-4.16610800	-0.28572500	1.01342400
C	0.47445600	-2.79684000	-0.24391000
C	0.90980700	-1.58010000	0.48939900
H	1.32618200	-3.48023200	-0.32908700
H	0.09357900	-2.55268400	-1.23603800
H	0.92078400	-0.62772000	-0.01303000
C	1.22672700	-1.63646600	1.94096400
H	1.84991000	-2.50826000	2.16219000
H	1.71387000	-0.72280900	2.28547000
H	0.28245900	-1.75469100	2.48305000
C	3.91597700	-0.98609100	-0.36493200
O	3.85570900	0.32706900	-0.31243600
O	2.97928100	-1.76020300	-0.13314700
C	5.27919100	-1.50001700	-0.75017000
H	5.28964600	-2.58965600	-0.73264600
H	5.53246100	-1.14114500	-1.75331300
H	6.03105500	-1.10406300	-0.06022200
H	2.94321300	0.69378900	-0.08893800
C	1.34693400	2.68105700	0.15758900
O	0.15420700	3.22552600	0.23510000
O	1.52654400	1.45781300	0.19411200
C	2.45778600	3.68864700	0.01699000
H	3.42992700	3.19463400	0.01440400
H	2.32546500	4.24589100	-0.91639900
H	2.40752100	4.41081500	0.83771000

H -0.56342600 2.52061900 0.29745100

TS4_P

E (B3LYP-CPCM/BS1) = -2349.388330au

H(B3LYP-CPCM/BS1) = -2349.092835au

G(B3LYP-CPCM/BS1) = -2349.187671au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2350.320044au

H	-0.47155700	-3.86046700	1.59056700
O	-2.51341600	-1.29371200	1.22204200
S	-2.90647500	-0.21690700	0.26667300
O	-3.99120400	0.66712100	0.69455400
O	-1.69966900	0.48041200	-0.31827200
C	-3.54225100	-1.14991500	-1.20877700
F	-3.85442800	-0.30514400	-2.19336700
F	-2.60286900	-2.00281500	-1.65094200
F	-4.62889500	-1.84695200	-0.86681100
C	-0.21916500	-3.07984900	0.86883400
C	-0.18446800	-1.73788800	1.48186700
H	0.77442000	-3.30289800	0.44960200
H	-0.91859600	-3.08693600	0.02916300
H	-0.22318400	-0.87865600	0.82715200
C	-0.22199800	-1.54428100	2.94663700
H	0.44813700	-2.25282200	3.44421800
H	0.01139300	-0.51930500	3.23827500
H	-1.24375300	-1.77884500	3.27282600
O	2.02805500	-1.24135200	1.40369800
H	1.90369300	-0.27251900	1.30146000
C	2.81988700	-1.73664900	0.38625200
C	3.37191600	-3.00876300	0.56764400
C	3.05133100	-1.01212700	-0.78781700
C	4.16932000	-3.55649100	-0.43920700
H	3.19172400	-3.53982900	1.49718300
C	3.85947400	-1.56901100	-1.77877800
H	2.60726300	-0.03091400	-0.92300000
C	4.41772500	-2.84010900	-1.61195700
H	4.60298300	-4.54234400	-0.29882800
H	4.04822700	-1.00604900	-2.68824200
H	5.04247500	-3.26707300	-2.39052000
O	-0.87338900	2.73374700	0.48665600
O	1.07766500	1.35919900	1.25116300
H	-1.25018100	1.80398100	0.18666300
S	0.65554500	2.70592900	0.83659900
O	0.98856900	3.85835800	1.65259200
C	1.42250400	2.96120200	-0.84179300
F	1.07585400	4.14487900	-1.33124100
F	1.00484700	1.99131000	-1.66244100
F	2.74919000	2.89021500	-0.72028400

TS4'

E (B3LYP-CPCM/BS1) = -2271.008686au

H(B3LYP-CPCM/BS1) = -2270.757394au

G(B3LYP-CPCM/BS1) = -2270.850957au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2271.913462au

H	1.69454900	3.86400500	0.29035800
O	2.00258100	1.25621400	0.81693200
S	2.09959900	-0.02571400	0.05022000
O	1.93605200	-1.24192600	0.91662100
O	1.34159800	-0.05016300	-1.20928400
C	3.89544800	-0.11956800	-0.41796400
F	4.12486400	-1.24537300	-1.09799500
F	4.20442200	0.92780400	-1.19056000
F	4.66350700	-0.09900800	0.67378000
C	0.81173300	3.54126200	-0.27011600
C	0.09611500	2.49052300	0.49641400
H	0.15122900	4.40990900	-0.36947500
H	1.10713400	3.19237400	-1.26017800
H	-0.17617700	1.57280900	0.00157300
C	-0.17635200	2.65571100	1.94634800
H	-0.56832300	3.65811600	2.14487800
H	-0.85964200	1.89418900	2.32334900
H	0.77869400	2.56582100	2.47595500
C	-2.96835700	2.65225900	-0.44118300
O	-3.25170400	1.36981000	-0.29447500
O	-1.89281300	3.18000800	-0.14471500
C	-4.11191000	3.43910800	-1.02205600
H	-3.83735800	4.48995200	-1.11002500
H	-4.36815800	3.03520900	-2.00704300
H	-4.99431400	3.33151300	-0.38337900
H	-2.51193300	0.85142000	0.10947800
O	-0.22518100	-2.49103900	1.26888700
O	-1.37914200	-0.31970900	0.83269100
H	0.63080400	-1.91528600	1.07008200
S	-1.57811000	-1.78150700	0.93197300
O	-2.64166200	-2.31188000	1.76558000
C	-1.89304000	-2.36112900	-0.81302500
F	-2.16417800	-3.66239400	-0.80861600
F	-0.82456400	-2.12184200	-1.56474600
F	-2.94071500	-1.68296600	-1.28842400

TS4'_P

E (B3LYP-CPCM/BS1) = -2002.329493au

H(B3LYP-CPCM/BS1) = -2001.854604au

G(B3LYP-CPCM/BS1) = -2001.963557au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2003.177757au

H	1.69690500	-3.64863000	-0.40419700
O	2.29178700	-1.32034700	-1.88731200
S	2.84463200	-0.06384500	-1.28676500
O	3.27021800	0.96021200	-2.24576200
O	2.01730800	0.41500800	-0.13424000
C	4.39705500	-0.63602200	-0.44283100

F	4.97658100	0.38677500	0.19497300
F	4.11197800	-1.59464600	0.45320800
F	5.25550700	-1.13157800	-1.34024800
C	1.00494000	-2.94609500	0.07171100
C	0.30503800	-2.15869500	-0.96631100
H	0.27143000	-3.55169200	0.62362300
H	1.54072400	-2.30837500	0.77447100
H	0.22512300	-1.09043300	-0.84271500
C	-0.16090100	-2.77885600	-2.22845200
H	-0.48036400	-3.81287500	-2.06966500
H	-0.95789400	-2.19997900	-2.69843000
H	0.69926900	-2.79245600	-2.90976100
O	-1.75034300	-2.05597100	-0.10878800
H	-1.88567200	-1.06935700	-0.17393700
O	-2.06966700	0.58707500	-0.45578500
H	-1.32335100	1.21603500	-0.26123600
C	-2.05076800	-2.50617200	1.15875000
C	-2.20786300	-3.88526100	1.33581400
C	-2.18631000	-1.62530500	2.23841200
C	-2.50128400	-4.38341900	2.60674000
H	-2.12168400	-4.54526200	0.47798900
C	-2.49183300	-2.13786500	3.49903200
H	-2.06588400	-0.55677500	2.08664300
C	-2.64509100	-3.51451600	3.69064100
H	-2.62552000	-5.45371200	2.74455100
H	-2.60580600	-1.45519500	4.33623700
H	-2.87771800	-3.90520100	4.67665800
C	-2.81554900	1.00960700	-1.53665900
C	-2.47830400	2.16224400	-2.25374700
C	-3.92927600	0.24571500	-1.89859700
C	-3.27136500	2.54801400	-3.33650600
H	-1.60458700	2.74024600	-1.96789400
C	-4.70934500	0.64300000	-2.98491000
H	-4.17508800	-0.64574000	-1.32891500
C	-4.38734700	1.79476500	-3.70820700
H	-3.00801200	3.44369300	-3.89252000
H	-5.57472300	0.04792800	-3.26395600
H	-4.99861900	2.10066200	-4.55203600
O	0.02982800	2.20257300	0.07654100
H	0.84494300	1.65513800	-0.07051900
C	0.11743800	2.90655000	1.25744500
C	1.27362100	2.87745000	2.04473300
C	-0.98916600	3.66763500	1.64724900
C	1.31243300	3.61807200	3.22787900
H	2.12415100	2.27948900	1.73121100
C	-0.93507600	4.40088600	2.83264400
H	-1.87585100	3.67984800	1.02011700
C	0.21357000	4.38143900	3.62906900
H	2.21170500	3.59472600	3.83766700
H	-1.79648100	4.99177700	3.13247000
H	0.25154300	4.95529500	4.55036700

TS4''

E (B3LYP-CPCM/BS1) = -1385.425470au

H(B3LYP-CPCM/BS1) = -1385.194345au

G(B3LYP-CPCM/BS1) = -1385.268194au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1386.013854au

H	-0.14604800	2.69451200	1.16219900
O	1.05860800	0.31219100	1.23904900
S	1.82842200	-0.64835500	0.37366900
O	2.78730900	-1.48375600	1.10278900
O	0.96140200	-1.34417400	-0.62144800
C	2.85619100	0.47003100	-0.69553000
F	3.60018500	-0.25167700	-1.53875700
F	2.06345400	1.28440200	-1.41303200
F	3.66202100	1.22034700	0.06341700
C	-0.74746000	2.22177600	0.37975600
C	-1.08279500	0.83049400	0.78718000
H	-1.67656100	2.79355600	0.28501400
H	-0.20327200	2.24869100	-0.56433400
H	-0.92015800	0.02088000	0.09804500
C	-1.54946500	0.54240800	2.17141100
H	-2.32440200	1.25718300	2.46425900
H	-1.92611300	-0.47695800	2.26907500
H	-0.69984500	0.67272900	2.84937800
C	-3.84893200	0.06972200	-0.53545700
O	-3.62951800	-1.21606000	-0.66892100
O	-3.06712500	0.89544700	-0.04196600
C	-5.19782000	0.49612000	-1.05631600
H	-5.26362300	0.26654800	-2.12494500
H	-5.98383500	-0.07314800	-0.55001500
H	-5.34493200	1.56399400	-0.89575400
H	-2.72986300	-1.54974000	-0.34104500
O	-1.44167000	-2.43760100	0.03329100
H	-1.36289600	-2.77943100	0.93703000
H	-0.53449500	-2.13447200	-0.22088800

TS4''_P

E (B3LYP-CPCM/BS1) = -1694.849193au

H(B3LYP-CPCM/BS1) = -1694.487901au

G(B3LYP-CPCM/BS1) = -1694.577551au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1695.555789au

H	-0.39925900	-2.89585300	1.33939600
O	-2.12544200	-0.81255800	1.42490900
S	-2.62555800	-0.34641600	0.09152800
O	-3.74881200	0.59541100	0.13443700
O	-1.51602400	0.01196200	-0.84780900
C	-3.29509500	-1.90280900	-0.66927200
F	-3.71024000	-1.67326800	-1.91860500
F	-2.33530400	-2.84387500	-0.70096400
F	-4.32138300	-2.36561400	0.05238600
C	0.43767600	-2.36954500	1.81109200

C	0.24594400	-0.91969600	1.61929400
H	0.52757300	-2.65424100	2.86180200
H	1.34215400	-2.68710100	1.27068000
H	-0.00913000	-0.58745800	0.62832700
C	0.25790400	0.02822300	2.75374600
H	1.13839300	-0.14830200	3.38081100
H	0.21724200	1.07046200	2.43481700
H	-0.62609500	-0.18866900	3.36689800
O	2.24106900	-0.19251300	0.86104000
H	1.82741500	0.49060300	0.26758800
O	0.75026500	1.50549500	-0.68217100
H	-0.13267200	1.07205800	-0.80248900
C	3.05242300	-1.03384400	0.12922000
C	3.87541900	-1.91517200	0.83893100
C	3.05289500	-1.02032000	-1.27063100
C	4.70850700	-2.78737500	0.13615000
H	3.86798100	-1.89334500	1.92438000
C	3.89838900	-1.89184800	-1.95717700
H	2.40644400	-0.33096100	-1.80600100
C	4.72467200	-2.77892700	-1.26065000
H	5.35089900	-3.46980800	0.68533400
H	3.90628900	-1.87823100	-3.04329700
H	5.37685000	-3.45677800	-1.80302200
C	0.59895900	2.85890500	-0.45570700
C	-0.66648500	3.45194800	-0.39731000
C	1.75548600	3.62564500	-0.28841200
C	-0.76362200	4.82636200	-0.16970900
H	-1.55894500	2.84565600	-0.52484600
C	1.64097500	4.99713800	-0.05988500
H	2.72786500	3.14471900	-0.34361200
C	0.38363100	5.60479700	0.00011200
H	-1.74693200	5.28638700	-0.12446400
H	2.54112000	5.59205800	0.06913000
H	0.29956900	6.67300700	0.17678000

TS4'''_P

E (B3LYP-CPCM/BS1) = -1540.234311au

H(B3LYP-CPCM/BS1) = -1539.931511au

G(B3LYP-CPCM/BS1) = -1540.015052au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1540.903003au

H	0.62588700	-0.66341200	3.11301800
O	-2.02481900	0.21846800	1.32516900
S	-2.72463100	0.22060200	-0.00229700
O	-4.10376000	0.71850400	0.02394500
O	-1.85538100	0.73589100	-1.10332300
C	-2.85509100	-1.58756700	-0.40509500
F	-3.35639200	-1.76323900	-1.63142800
F	-1.63608200	-2.15646300	-0.35479800
F	-3.64623300	-2.20400000	0.47957800
C	0.57505500	-0.76877100	2.02678000
C	0.27826500	0.51177200	1.34694500

H	1.52756000	-1.17064000	1.65610100
H	-0.19301200	-1.49733500	1.75344300
H	0.08151600	0.48349100	0.28449800
C	0.14558700	1.78651200	2.09601900
H	1.06082500	1.96456900	2.67120500
H	-0.06337000	2.63336100	1.44045100
H	-0.67465000	1.67655300	2.81362700
O	2.32988000	1.07190200	0.64672400
H	2.08661200	1.75757500	-0.06413800
O	1.70800600	2.84145100	-1.17373200
H	0.72798500	3.04622300	-1.16805100
C	3.17099500	0.11837400	0.12314600
C	3.94280800	-0.63434000	1.01743400
C	3.25363000	-0.11382500	-1.25675300
C	4.79543900	-1.62540100	0.52680600
H	3.88349300	-0.41887900	2.07993500
C	4.11860200	-1.09922500	-1.73178000
H	2.65620600	0.48296100	-1.93880900
C	4.88715500	-1.86192000	-0.84644900
H	5.39469300	-2.20634900	1.22229500
H	4.18775000	-1.27448300	-2.80182700
H	5.55383200	-2.63080300	-1.22543700
O	-0.91282700	3.30222200	-0.96377400
H	-1.33907900	2.41360500	-1.04327700
H	-1.32526000	3.84529700	-1.65356100
H	2.14798400	3.68079700	-0.96527600

TS4''''_P

E (B3LYP-CPCM/BS1) = -1463.801988au

H(B3LYP-CPCM/BS1) = -1463.526592au

G(B3LYP-CPCM/BS1) = -1463.602787au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1464.418257au

H	0.10829400	-0.31696400	-2.13783300
O	2.03623000	1.09364600	-0.84765600
S	2.61805500	0.39427300	0.34499600
O	3.88444000	0.94765600	0.83505800
O	1.59519500	0.07854200	1.38631500
C	3.03615500	-1.28410200	-0.33011100
F	3.48512800	-2.08489600	0.64162200
F	1.94135100	-1.84601300	-0.87549600
F	3.97554100	-1.18238700	-1.27669100
C	-0.63974300	0.47458700	-2.03186500
C	-0.31920000	1.28403000	-0.83932600
H	-0.70115200	1.07172900	-2.94475100
H	-1.60524000	-0.02924100	-1.87185900
H	-0.02483500	0.75780700	0.05154700
C	-0.26131300	2.76244100	-0.89031100
H	-1.15399900	3.15780100	-1.38607900
H	-0.14641500	3.20894700	0.09847900
H	0.60496300	3.03638200	-1.50476700
O	-2.22753200	1.32136400	0.32937400

H	-1.74247800	1.27154200	1.21055200
O	-0.71137400	1.12530300	2.50506700
H	0.16773500	0.77731100	2.22362000
C	-3.13950800	0.29769400	0.21735200
C	-4.02833300	0.33637000	-0.86381800
C	-3.18456000	-0.75402800	1.14198900
C	-4.96903700	-0.68380200	-1.01562200
H	-3.98593400	1.17117200	-1.55685300
C	-4.13694200	-1.76018800	0.98097900
H	-2.48979600	-0.76945000	1.97637500
C	-5.02844200	-1.73347800	-0.09602400
H	-5.66078200	-0.65135800	-1.85262300
H	-4.17828300	-2.57192200	1.70182200
H	-5.76387600	-2.52343100	-0.21519800
H	-0.52540800	1.95173900	2.97799900

5

E (B3LYP-CPCM/BS1) = -1675.962651au

H(B3LYP-CPCM/BS1) = -1675.712610au

G(B3LYP-CPCM/BS1) = -1675.792027au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1676.816609au

Au	-1.10774200	-0.35909400	-0.03652800
P	-1.30305900	1.96580700	0.15001800
C	-3.01774600	2.55659000	0.45392200
H	-3.39570000	2.12504500	1.38507000
H	-3.03621600	3.64922500	0.52763500
H	-3.66628500	2.23947700	-0.36769400
C	-0.73047400	2.83181000	-1.36020200
H	-0.83196700	3.91535400	-1.23591600
H	0.32094900	2.57264800	-1.51298100
H	-1.31854700	2.50648300	-2.22289900
C	-0.28751400	2.64502700	1.51690900
H	0.75341200	2.37062700	1.32731400
H	-0.38307000	3.73553500	1.55361800
H	-0.61242100	2.21800300	2.46981500
O	3.77132000	0.00899700	-1.54473200
S	2.51521600	0.29065700	-0.83036600
O	2.28773200	1.70498000	-0.43998000
O	1.30962900	-0.38944100	-1.38944100
C	2.73264000	-0.56115600	0.81030200
F	1.71161800	-0.26044000	1.64696100
F	2.74753800	-1.90020800	0.66186300
F	3.87221000	-0.19040100	1.40489400
C	-0.66278700	-2.60022800	-0.33951300
H	-0.62875600	-2.70216700	-1.42216000
H	0.28893800	-2.65302000	0.18166900
C	-1.85498600	-2.64174000	0.33753000
H	-1.82578800	-2.68019600	1.42641300
C	-3.20071400	-2.85209100	-0.29769800
H	-3.53603400	-3.87580700	-0.08234900
H	-3.95246400	-2.17415400	0.11900200

H -3.16423600 -2.72237900 -1.38297100

TS5

E (B3LYP-CPCM/BS1) = -1308.988224au

H(B3LYP-CPCM/BS1) = -1308.784348au

G(B3LYP-CPCM/BS1) = -1308.853311au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1309.524727au

H	0.88082300	2.82158500	1.28956500
O	-1.04883400	1.47602700	0.29019800
S	-1.50080100	0.13821100	0.81492300
O	-0.35617600	-0.77967600	1.10289400
O	-2.54904700	0.19306200	1.83420900
C	-2.27543000	-0.63664800	-0.68439300
F	-2.67810300	-1.88173000	-0.41599200
F	-3.32381100	0.08193000	-1.09608300
F	-1.36835900	-0.68228200	-1.67794500
C	1.57360800	2.01135500	1.04057800
C	1.13773100	1.40038600	-0.24397100
H	2.56880400	2.45244400	0.92052900
H	1.57996700	1.28877800	1.85750500
H	0.77583000	0.39771100	-0.28677200
C	1.13182300	2.19894500	-1.49524600
H	2.16967800	2.36820500	-1.80657300
H	0.59222800	1.69345800	-2.29731300
H	0.68733300	3.18174100	-1.30735400
C	3.15363900	-0.84566800	-0.03857700
O	2.26196300	-1.54443800	0.64473200
O	2.97806000	0.28149400	-0.51585900
C	4.46233300	-1.57381900	-0.18751100
H	5.16514900	-0.96855500	-0.75955700
H	4.87362300	-1.79130400	0.80359800
H	4.29349200	-2.53153300	-0.69005400
H	1.36838900	-1.12422900	0.75317400

6

E (B3LYP-CPCM/BS1) = -714.362688au

H(B3LYP-CPCM/BS1) = -714.149983au

G(B3LYP-CPCM/BS1) = -714.207312au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -714.841016au

Au	-0.39571500	-0.19765600	0.01384200
P	1.91642100	0.16553500	-0.00804500
C	2.37287200	1.78326400	-0.74152900
H	1.91527900	2.59074500	-0.16362200
H	3.46091700	1.90552100	-0.73716700
H	2.00681000	1.83565800	-1.77052900
C	2.80299300	-1.10788200	-0.98615000
H	3.87929100	-0.90688200	-0.97613700
H	2.61567000	-2.09658600	-0.55819700
H	2.44210200	-1.09692800	-2.01834900
C	2.66279200	0.13243200	1.66681200

H	2.47236900	-0.83715500	2.13515200
H	3.74337100	0.29637400	1.59911300
H	2.21587600	0.91576500	2.28509400
C	-2.54213200	-1.02188100	-0.25372000
H	-2.66554400	-1.06279100	-1.33425500
H	-2.44457700	-1.97031400	0.26940900
C	-2.78848100	0.13681600	0.43887700
H	-2.79818500	0.08904600	1.52789800
C	-3.22005500	1.43598200	-0.17292600
H	-4.27601800	1.60244700	0.07978500
H	-2.66004600	2.28048400	0.24232400
H	-3.12011200	1.43405600	-1.26158100

TS6

E (B3LYP-CPCM/BS1) = -1904.999318au

H(B3LYP-CPCM/BS1) = -1904.684488au

G(B3LYP-CPCM/BS1) = -1904.774395au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1905.964959au

Au	-0.34647700	-1.35402000	0.00319800
P	-2.66930300	-1.37874200	0.00931600
C	-3.37229400	-3.03387100	0.40066300
H	-3.04152900	-3.34853700	1.39465300
H	-4.46690500	-3.00000200	0.37837600
H	-3.01934700	-3.76546500	-0.33201100
C	-3.38516300	-0.90907100	-1.61205300
H	-4.47842900	-0.97019400	-1.57674400
H	-3.07803700	0.11892300	-1.82548200
H	-3.00709800	-1.57576000	-2.39223000
C	-3.43141600	-0.22907400	1.21848300
H	-3.12152400	0.78657300	0.96165300
H	-4.52317300	-0.30583800	1.17328100
H	-3.09011100	-0.47096500	2.22893100
O	-0.52629200	3.81481400	-1.64097300
S	-0.81042800	2.52399300	-0.98954600
O	-2.24096800	2.12935300	-0.92853400
O	0.11661800	1.41452200	-1.34892200
C	-0.39572400	2.83481800	0.79725200
F	-0.72425400	1.76667400	1.56371600
F	0.92432800	3.05044900	0.95527400
F	-1.05452100	3.89725100	1.27656500
C	1.91298600	-1.42768600	-0.06893800
H	1.84613400	-2.25241800	0.64919900
H	1.74723200	-1.61341400	-1.13548000
C	2.36165500	-0.06040400	0.39099600
C	2.28710500	0.17472200	1.88997500
H	2.77515400	-0.63424600	2.44533500
H	2.76011200	1.12457700	2.15210500
H	1.23722600	0.22316100	2.19074700
H	1.86914700	0.73409600	-0.16658600
O	3.83689800	0.26718800	0.03486900
C	4.69703200	-0.63006400	-0.32277200

C	6.06129300	-0.12592700	-0.68069500
H	6.07904600	0.09546700	-1.75464400
H	6.28787000	0.79145600	-0.13480200
H	6.80524900	-0.89794500	-0.47561200
O	4.42395000	-1.85993500	-0.40590900
H	3.19258400	-1.89220400	-0.26201800

7

E (B3LYP-CPCM/BS1) = -825.114633au

H(B3LYP-CPCM/BS1) = -824.933783au

G(B3LYP-CPCM/BS1) = -824.990172au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -825.651361au

Au	0.14933800	-0.25193200	-0.00026000
P	-2.09031500	0.16481900	-0.00018800
C	-2.96234500	-0.37990800	1.52348900
H	-2.51469900	0.11130100	2.39214600
H	-4.02676000	-0.12721400	1.47104300
H	-2.85121900	-1.46148600	1.64152000
C	-3.01396300	-0.62448500	-1.37947200
H	-4.07823800	-0.37133000	-1.32724500
H	-2.60506800	-0.27991200	-2.33359300
H	-2.89606200	-1.71037400	-1.32392600
C	-2.47178000	1.95697100	-0.14228300
H	-2.04967100	2.34556600	-1.07334300
H	-3.55374500	2.12634400	-0.13315600
H	-2.01197000	2.49199000	0.69345500
O	2.17959400	-0.69320600	0.00204900
C	2.95906100	0.35878500	0.00003900
C	4.44204000	0.00580800	0.00142100
H	5.05017800	0.91239600	0.00292200
H	4.68198400	-0.59947500	0.88228400
O	2.57171900	1.52906700	-0.00297700
H	4.68374400	-0.59735500	-0.88046100

7'

E (B3LYP-CPCM/BS1) = -903.487446au

H(B3LYP-CPCM/BS1) = -903.261907au

G(B3LYP-CPCM/BS1) = -903.324881au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -904.051071au

Au	0.47020400	-0.34064300	0.00059000
P	2.64536600	0.34522100	-0.00007600
C	3.03364200	1.58324700	-1.30174600
H	2.40438900	2.46696300	-1.16256300
H	4.08783100	1.87648700	-1.25609700
H	2.81759400	1.15635500	-2.28524000
C	3.84895800	-1.01769900	-0.27475900
H	4.87580100	-0.63679800	-0.26633400
H	3.73426800	-1.76885000	0.51197500
H	3.64612100	-1.49243000	-1.23898800
C	3.18041500	1.13403900	1.57170800

H	3.05159800	0.42666000	2.39583600
H	4.23060700	1.43937000	1.51490100
H	2.55731500	2.01107200	1.76846000
O	-1.41966300	-1.09961900	0.00127800
C	-2.54252700	-0.37516600	0.00050500
C	-3.77967100	-1.06105100	-0.00069900
C	-2.58146400	1.03721000	0.00106000
C	-4.98683300	-0.36578600	-0.00134000
H	-3.76258300	-2.14784300	-0.00105100
C	-3.79599700	1.72386700	0.00026300
H	-1.64133600	1.58657500	0.00196100
C	-5.01090100	1.03331900	-0.00088400
H	-5.92074300	-0.92417700	-0.00228200
H	-3.78947800	2.81209300	0.00051400
H	-5.95440100	1.57205600	-0.00145300

TS7

E (B3LYP-CPCM/BS1) = -1905.019029au

H(B3LYP-CPCM/BS1) = -1904.704747au

G(B3LYP-CPCM/BS1) = -1904.796553au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1905.984047au

Au	1.64611800	-0.77396400	-0.10862600
P	2.62407600	1.20367200	0.44156700
C	2.40209900	2.49270900	-0.84358100
H	1.32968200	2.65763000	-0.99065400
H	2.87729200	3.42787000	-0.52722700
H	2.84918500	2.15769800	-1.78382400
C	4.43050300	1.12439100	0.76831700
H	4.81189600	2.11132000	1.05107600
H	4.62528700	0.41444000	1.57718600
H	4.94994200	0.77999900	-0.13046800
C	1.87000500	1.90767800	1.95867400
H	2.06033600	1.24088900	2.80469700
H	2.28547300	2.89815900	2.17299500
H	0.78980800	1.98033600	1.80172700
O	0.62947700	-2.53724900	-0.71215800
C	-0.50080600	-2.70654100	-0.13285200
O	-3.37611000	2.29343200	-0.09505100
S	-1.97153200	1.85541900	-0.25663600
O	-1.01160700	2.86804000	-0.73769000
O	-1.47308500	1.02573800	0.88580300
C	-2.07146200	0.62929800	-1.65264400
F	-0.85363900	0.17905600	-1.99853800
F	-2.81830700	-0.43635000	-1.28809000
F	-2.63499400	1.18289600	-2.73262000
C	-3.40077500	-1.54625200	1.68209500
C	-3.43680300	-0.17660600	2.01338100
H	-3.41620200	-2.22985400	2.53615500
H	-2.28021300	-1.72502000	1.27366200
H	-3.82083200	0.54251900	1.29321200
C	-3.07293200	0.35208400	3.34041500

H	-2.52969500	1.29487100	3.24460300
H	-4.02205500	0.58060500	3.85544200
H	-2.51769600	-0.36657000	3.94846200
O	-0.83236700	-2.08258100	0.91008800
C	-1.45722000	-3.68637100	-0.78326400
H	-2.18589800	-3.11178700	-1.36782200
H	-0.93070600	-4.36519700	-1.45608500
H	-2.00258900	-4.25325000	-0.02399600
H	-4.03661000	-1.84509300	0.84703000

TS7'

E (B3LYP-CPCM/BS1) = -1983.395259au

H(B3LYP-CPCM/BS1) = -1983.037634au

G(B3LYP-CPCM/BS1) = -1983.133613au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1984.390142au

Au	-0.14062400	-1.27756300	0.44375700
P	1.69902800	-2.52534700	-0.04741500
C	2.35836500	-2.18070200	-1.72441900
H	2.61311200	-1.11932300	-1.77906200
H	3.25049000	-2.78673000	-1.91550100
H	1.59511000	-2.40798000	-2.47392300
C	1.41367100	-4.34071700	0.00403500
H	2.33396100	-4.87949700	-0.24573500
H	1.08491600	-4.63173500	1.00581300
H	0.63117700	-4.61007600	-0.71104000
C	3.10282900	-2.21472100	1.09132600
H	2.80183200	-2.43291700	2.11980900
H	3.95803200	-2.84341200	0.82042100
H	3.37833700	-1.15966500	1.00869000
O	2.61287100	3.26827400	0.30271900
S	2.11056000	1.91905600	-0.01882600
O	3.12499300	0.87557200	-0.28324800
O	0.98791000	1.46110600	0.86135100
C	1.26754000	2.13803300	-1.66249200
F	0.77759300	0.96451100	-2.11346700
F	0.23736800	2.99843300	-1.55204000
F	2.11790500	2.61326100	-2.57901900
C	-1.80642900	2.32631500	1.94599500
C	-0.61827300	3.06157500	1.80378700
H	-2.12534900	2.13084000	2.97245900
H	-1.62047800	1.20287100	1.48166700
H	-0.41322500	3.52641300	0.84396000
C	0.30354600	3.38793100	2.91159900
H	1.32996700	3.49996900	2.55890900
H	-0.02238900	4.36600100	3.30678400
H	0.23955400	2.66475700	3.72949300
O	-1.85907900	-0.14824500	0.93987000
H	-2.61510600	2.62461700	1.27037300
C	-2.92184800	-0.10412600	0.08695200
C	-4.21598500	-0.29273300	0.60174400
C	-2.76380900	0.17751800	-1.28207300

C	-5.32573900	-0.22277400	-0.24158700
H	-4.33025200	-0.50327600	1.66155500
C	-3.87969900	0.24108900	-2.11748400
H	-1.76461100	0.34873100	-1.67330900
C	-5.16509700	0.04106200	-1.60488800
H	-6.32038400	-0.37817800	0.16899500
H	-3.74308200	0.45364300	-3.17494000
H	-6.03050100	0.09169700	-2.25961200

8

E (B3LYP-CPCM/BS1) = -1787.145941au

H(B3LYP-CPCM/BS1) = -1786.915151au

G(B3LYP-CPCM/BS1) = -1786.997596au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1788.052267au

Au	-2.14247600	0.53339500	0.03175400
P	-3.85700700	-0.95720200	0.10677800
C	-5.37745900	-0.37226400	-0.73747800
H	-5.15468000	-0.16145100	-1.78708100
H	-6.16152900	-1.13436500	-0.67808500
H	-5.72798900	0.54835400	-0.26274500
C	-4.36952900	-1.37436100	1.81850000
H	-5.18862700	-2.10102100	1.80407000
H	-3.51839800	-1.79640400	2.36003900
H	-4.69705800	-0.46737800	2.33410700
C	-3.42990200	-2.55545500	-0.68568600
H	-2.56057900	-2.98912200	-0.18372500
H	-4.27385000	-3.25022000	-0.62082500
H	-3.17647200	-2.38668800	-1.73591900
O	0.78979700	0.42877500	-0.77827600
H	1.79925200	0.21444500	-0.98734900
C	0.57874300	1.62831000	-0.34182300
O	2.96014700	-1.66998600	0.59002800
S	3.86744100	-1.09401500	-0.41704700
O	4.72749400	-2.01118500	-1.17417000
O	3.19600700	-0.04646900	-1.28671700
C	5.04611500	-0.04797700	0.56423300
F	5.89461700	0.60272700	-0.24102300
F	4.36968400	0.86619800	1.29068100
F	5.75270900	-0.80853500	1.40934400
O	-0.57483500	1.97307800	0.01719000
C	1.71073300	2.61595100	-0.27514800
H	1.36727400	3.55361200	0.16066000
H	2.53292500	2.19904300	0.31298000
H	2.09722000	2.79279900	-1.28462300

TS8

E (B3LYP-CPCM/BS1) = -3463.080661au

H(B3LYP-CPCM/BS1) = -3462.603097au

G(B3LYP-CPCM/BS1) = -3462.743820au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -3464.8647658au

Au	-2.39888900	-0.97283000	-1.13512000
P	-4.05648600	-1.76546400	0.21059600
C	-4.39777100	-3.55793900	-0.00538300
H	-3.50193900	-4.13700300	0.23572600
H	-5.21648000	-3.86753500	0.65292300
H	-4.67447100	-3.75777700	-1.04446200
C	-5.64188800	-0.90692600	-0.11682200
H	-6.42661900	-1.30162100	0.53759000
H	-5.49005400	0.15738600	0.08249600
H	-5.93242200	-1.04753700	-1.16167100
C	-3.73074000	-1.52334600	1.99574100
H	-3.57371600	-0.45556200	2.16797600
H	-4.58528500	-1.87689200	2.58269900
H	-2.83474800	-2.07606000	2.28815300
O	0.47435100	0.84680900	-1.22879300
C	-0.27107100	0.86287800	-2.29151000
Au	0.82124400	-0.88150400	0.05964700
P	1.39773600	-2.62872200	1.40523500
C	2.43470800	-3.86371500	0.53838300
H	3.33943500	-3.35719500	0.19103400
H	2.69814900	-4.67787100	1.22228900
H	1.88772000	-4.26815400	-0.31813900
C	2.34891000	-2.09200400	2.87624600
H	2.65934800	-2.96506500	3.46040100
H	3.22423500	-1.52643100	2.54726600
H	1.72116100	-1.44300400	3.49382800
C	-0.03935200	-3.56114300	2.06797900
H	0.30634300	-4.41136600	2.66563000
H	-0.64121200	-2.90095800	2.69842600
H	-0.65607600	-3.92616300	1.24207300
O	-3.93515500	1.67639200	1.03526600
S	-2.58118500	2.22757800	0.77855100
O	-1.50396900	1.63203900	1.60937700
O	-2.23904300	2.40879100	-0.65537900
C	-2.69338300	3.97422600	1.40571700
F	-1.52353600	4.61516000	1.21741700
F	-3.65104300	4.65355700	0.75780700
F	-2.97329000	3.99310400	2.71703700
C	-0.13815200	2.04105700	-3.21749400
H	-0.51615200	1.78268800	-4.20751300
H	-0.75799900	2.84529200	-2.80387300
O	-1.07850500	-0.05328100	-2.56971100
H	0.89666000	2.38467300	-3.28161200
H	0.95759200	2.01412200	-0.68448800
O	3.71804600	0.36422800	-1.07983800
S	4.49970800	-0.10628700	0.09375300
O	4.10756800	0.53563300	1.37688600
O	4.71486300	-1.56899500	0.17066200
C	6.20098300	0.57097300	-0.22840700
F	7.03348200	0.26827400	0.77736400
F	6.70567500	0.06916300	-1.36411000
F	6.15464500	1.91307400	-0.34560300

C	1.10022700	3.09631400	0.04816600
C	2.47459800	3.00088500	0.04631300
H	0.61624100	3.87229200	-0.54484700
H	0.52866900	2.72569100	0.90084300
H	2.95188800	2.30083100	0.73533700
C	3.37653700	3.69755700	-0.89629000
H	4.08492300	4.29913400	-0.30762200
H	3.98494400	2.95552800	-1.42583600
H	2.84842100	4.34626100	-1.59935900

TS8'

E (B3LYP-CPCM/BS1) = -3541.456813au

H(B3LYP-CPCM/BS1) = -3540.934946au

G(B3LYP-CPCM/BS1) = -3541.078225au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -3543.262930au

Au	-0.04083300	0.91768300	1.53127700
P	-0.68099200	-0.26812000	3.36606200
C	-2.26174100	0.31834000	4.08200900
H	-3.02350300	0.27305100	3.29947400
H	-2.54955200	-0.31632100	4.92721500
H	-2.15249100	1.35138400	4.42475600
C	0.55738100	-0.23078300	4.71818000
H	0.20992500	-0.83657800	5.56215100
H	1.49756800	-0.63565700	4.33424700
H	0.71391200	0.79899300	5.05197200
C	-0.92182300	-2.03852300	2.96721800
H	0.02408800	-2.44024800	2.59432500
H	-1.22637600	-2.58434800	3.86714700
H	-1.69542400	-2.12942000	2.20132200
O	0.51591400	2.01922100	-0.33827500
H	1.84643100	2.40504300	-0.23246500
C	-0.23653800	3.14459200	-0.69090700
C	-0.45246400	3.44250400	-2.03962500
C	-0.71903300	3.99698400	0.30630000
C	-1.17436700	4.58649300	-2.38628500
H	-0.06897500	2.77449500	-2.80611300
C	-1.43868600	5.13878600	-0.05132000
H	-0.54223400	3.75655200	1.35096200
C	-1.66960400	5.43773100	-1.39596600
H	-1.35059000	4.80741100	-3.43516900
H	-1.82191500	5.79198700	0.72739700
H	-2.23501000	6.32345400	-1.66955400
O	2.53514600	-0.15264200	0.33950700
S	3.29775800	-1.06609900	1.24536100
O	4.59385700	-0.50889800	1.68704300
O	2.48268900	-1.73224700	2.28264100
C	3.76101000	-2.44796500	0.08903900
F	4.52879000	-3.35587300	0.69808100
F	2.65724900	-3.06920300	-0.37482500
F	4.43324500	-1.96821800	-0.97713700
C	2.93197700	3.10011900	-0.17163500

C	3.88860100	2.10166900	-0.27956900
H	2.77128000	3.74578400	-1.03841900
H	2.80651800	3.57712900	0.80155000
H	4.26162900	1.61962700	0.62146100
C	4.44502100	1.60718800	-1.55679100
H	5.51571300	1.86472500	-1.57733400
H	4.39365800	0.51429100	-1.58754000
H	3.95870300	2.04331900	-2.43304600
Au	0.32103200	0.18858500	-1.60129000
P	0.00589200	-1.70632800	-2.82172800
C	1.51882400	-2.27372800	-3.69643200
H	2.31151800	-2.45373600	-2.96547200
H	1.31304900	-3.19988800	-4.24376200
H	1.85190000	-1.50535300	-4.39987700
C	-1.29600300	-1.52314200	-4.09658900
H	-1.01420400	-0.74094800	-4.80719900
H	-1.43681300	-2.46853000	-4.63165300
H	-2.22061700	-1.23736700	-3.58827000
C	-0.51093400	-3.11862000	-1.77621500
H	-0.66447300	-4.00595600	-2.40033200
H	0.26443000	-3.32543100	-1.03472500
H	-1.44061000	-2.85676600	-1.26730400
O	-5.07668200	0.19450000	-0.61544700
S	-3.83703500	-0.52077800	-0.26459200
O	-2.85897100	-0.68560800	-1.37487000
O	-3.22392900	-0.14422100	1.03624400
C	-4.39322000	-2.26681900	0.04353600
F	-3.33812300	-3.04552100	0.38510100
F	-5.28311600	-2.32468800	1.04434400
F	-4.95281000	-2.79971400	-1.05295000

9

E (B3LYP-CPCM/BS1) = -3345.206689au

H(B3LYP-CPCM/BS1) = -3344.811061au

G(B3LYP-CPCM/BS1) = -3344.941796au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -3346.922370au

Au	2.08413400	-1.80998800	0.02062900
P	4.26090900	-1.17715500	-0.22157400
C	5.30540500	-2.50542400	-0.94493600
H	4.93016700	-2.76814600	-1.93805000
H	6.34418600	-2.16807200	-1.02708400
H	5.26280700	-3.39395800	-0.30873800
C	5.03635200	-0.76344500	1.38786900
H	6.09361800	-0.51826400	1.23883000
H	4.51952200	0.09444600	1.83016500
H	4.95359500	-1.61894900	2.06422800
C	4.53227800	0.28987700	-1.28403500
H	3.95283000	1.12668900	-0.88280100
H	5.59713000	0.54583000	-1.30152600
H	4.19477900	0.07377000	-2.30169200
O	-1.35528300	-1.13949600	0.57173400

C	-0.90525400	-2.32151600	0.79470900
Au	-0.62198200	0.34736000	-0.81314200
P	-0.25487700	1.93642900	-2.39934400
C	1.39933400	1.85962900	-3.18424100
H	1.55095500	0.87309200	-3.63128600
H	1.48763600	2.62887900	-3.95886900
H	2.14835300	2.02588000	-2.40732300
C	-1.46331200	1.79838700	-3.77716700
H	-1.29212700	2.58590900	-4.51885000
H	-1.36342200	0.82015800	-4.25618100
H	-2.47754400	1.88712000	-3.37755700
C	-0.41798000	3.65613000	-1.78538800
H	-0.26010500	4.36085800	-2.60901300
H	-1.41650100	3.80580400	-1.36584000
H	0.32755600	3.82211800	-1.00534600
O	3.18082100	2.04072200	2.30577400
S	1.96553800	1.89457100	1.47602900
O	2.13019300	2.31316100	0.05600400
O	1.22518400	0.61803400	1.66367600
C	0.78168000	3.15944200	2.15193000
F	-0.40725200	3.06702300	1.52196700
F	0.57703400	2.97117500	3.46118200
F	1.25301300	4.40206200	1.96583900
C	-1.79779700	-3.24777200	1.59160200
H	-1.42887500	-4.27236900	1.53848600
H	-1.79482800	-2.92210700	2.63858400
O	0.20900600	-2.75658900	0.41014500
H	-2.82724900	-3.19597600	1.22956700
H	-2.73194500	-0.63306600	1.10957900
O	-3.60003600	-0.27071000	1.52255300
S	-4.67370400	0.17176500	0.44136000
O	-5.54785800	1.16500200	1.04253800
O	-4.05646100	0.38592300	-0.86577200
C	-5.66296800	-1.40055400	0.29617400
F	-6.61184100	-1.22967100	-0.62272000
F	-4.85534600	-2.40015900	-0.08560300
F	-6.21908500	-1.70591800	1.46516900

9'

E (B3LYP-CPCM/BS1) = -3423.583798au

H(B3LYP-CPCM/BS1) = -3423.144617au

G(B3LYP-CPCM/BS1) = -3423.276163au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -3425.327122au

Au	0.57361200	1.36817500	-0.28976800
P	0.25936900	3.41542100	0.65030800
C	1.72011900	4.51003700	0.43785100
H	1.89578800	4.68492000	-0.62755000
H	1.55430400	5.46917400	0.93984800
H	2.60339600	4.02430300	0.86150600
C	-0.03379000	3.32589100	2.45620500
H	-0.17023400	4.33287100	2.86526800

H	-0.93237100	2.72746900	2.62303900
H	0.82044400	2.84668400	2.94277400
C	-1.15872000	4.33636000	-0.05476900
H	-2.06564300	3.74772500	0.10051600
H	-1.25587500	5.30948000	0.43868000
H	-1.00231100	4.48671100	-1.12682700
O	0.97756800	-0.59751000	-1.15249300
H	2.35119000	-0.93226300	-0.63862700
C	0.83215800	-0.69279000	-2.54502100
C	-0.40551100	-0.42541100	-3.13945400
C	1.93618100	-1.05232400	-3.32274200
C	-0.52972100	-0.52196100	-4.52680200
H	-1.24983900	-0.14728400	-2.51487900
C	1.79452400	-1.14425600	-4.71058400
H	2.89297700	-1.25783100	-2.85318100
C	0.56564400	-0.88041800	-5.31815700
H	-1.49142000	-0.31440200	-4.98827100
H	2.65395400	-1.42413700	-5.31377400
H	0.46170700	-0.95324500	-6.39684600
O	2.46831200	-0.52298600	1.91557000
S	3.66670900	-0.88176500	1.15760300
O	4.61026100	-1.86845100	1.65950400
O	3.31214100	-1.22722300	-0.34387100
C	4.63288200	0.69693100	0.91759200
F	5.76735100	0.44379000	0.27028600
F	3.90986800	1.57621800	0.21086300
F	4.90464800	1.21837900	2.11441200
Au	-0.29788700	-1.91327900	0.03055000
P	-1.55417300	-3.33357900	1.28953700
C	-3.19383100	-3.68184500	0.55136900
H	-3.06774700	-4.09429600	-0.45358600
H	-3.74024200	-4.39779700	1.17495300
H	-3.74490000	-2.73882700	0.49706200
C	-0.74606600	-4.96649100	1.52468800
H	-1.37718100	-5.61472500	2.14201800
H	-0.58448600	-5.43917600	0.55170200
H	0.22253500	-4.83159500	2.01413700
C	-1.88810800	-2.68877500	2.97129100
H	-2.45686400	-3.42601300	3.54821400
H	-0.94403800	-2.47569800	3.48019200
H	-2.46961100	-1.76815600	2.87258300
O	-2.60635600	0.36946800	-0.76748400
S	-3.27796700	0.67109700	0.52197700
O	-3.80750400	-0.51305200	1.24245700
O	-2.57347100	1.65713800	1.37856600
C	-4.80428200	1.59115100	-0.00580700
F	-5.55218600	1.92436400	1.05594400
F	-4.46429600	2.72317200	-0.65168500
F	-5.54984800	0.84483100	-0.83356200

TS9

E (B3LYP-CPCM/BS1) = -3463.086544au

H(B3LYP-CPCM/BS1) = -3462.603409au

G(B3LYP-CPCM/BS1) = -3462.743724au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -3464.862341au

Au	-0.04078700	-1.44697200	-0.45436800
P	1.27808000	-3.21921600	-1.05438800
C	0.40163300	-4.31698300	-2.23980600
H	0.14765900	-3.75860700	-3.14508400
H	1.04146700	-5.16512100	-2.50579900
H	-0.52067500	-4.69008400	-1.78575900
C	1.72341300	-4.27753000	0.37080600
H	2.27465100	-5.15633000	0.01861800
H	2.35211400	-3.69699500	1.05292000
H	0.81474900	-4.60000800	0.88697700
C	2.84957300	-2.76784800	-1.87611200
H	3.44075600	-2.13335300	-1.20978200
H	3.41184300	-3.67579200	-2.11967800
H	2.63181100	-2.21937800	-2.79687800
O	-0.31061500	1.55130000	1.05516700
C	-1.39414000	0.93304800	0.97346000
Au	1.33692300	1.71268300	-0.31889200
P	3.01260700	2.34982000	-1.72640900
C	2.49689000	3.71363300	-2.84631500
H	2.15177500	4.56455800	-2.25230300
H	3.33534900	4.02831600	-3.47691600
H	1.67342000	3.37560600	-3.48183200
C	4.45920100	2.99557600	-0.80363800
H	5.25177800	3.29118700	-1.49940500
H	4.15488600	3.86264700	-0.21026600
H	4.82276600	2.21204800	-0.13513800
C	3.67217500	1.04507100	-2.83032700
H	4.46712800	1.45773500	-3.46076100
H	4.07011200	0.24292000	-2.20564000
H	2.87075300	0.65766200	-3.46579800
O	3.78423900	-2.12184500	1.70296400
S	3.74463500	-0.67159900	1.40899700
O	4.28133300	-0.29996900	0.07107600
O	2.47748200	0.01043200	1.77875800
C	4.99525800	0.06065200	2.57276900
F	5.09934600	1.38819300	2.36802400
F	4.63806000	-0.14111200	3.84738700
F	6.20191100	-0.48837400	2.37453400
C	-2.52409500	1.35386400	1.88213800
H	-3.28415700	1.90516900	1.31553300
H	-3.01342900	0.48120600	2.32294800
O	-1.59831300	-0.05163100	0.14688300
H	-2.13424900	2.00073200	2.66862300
H	-4.11112800	-0.75923400	-2.55416500
O	-5.85242000	-0.31454400	-0.88174100
S	-6.45732800	0.91041500	-0.24586900
O	-5.43582600	1.91300000	0.14134600

O	-7.66196100	1.40926600	-0.91990500
C	-7.05879300	0.25580600	1.38496400
F	-7.61531700	1.23359900	2.10916800
F	-7.96239900	-0.71581500	1.20781200
F	-6.02580000	-0.25369300	2.08974100
C	-3.20374100	-0.49982900	-1.99636700
C	-3.56243400	-0.52748600	-0.55471700
H	-2.43909000	-1.24723600	-2.23261500
H	-2.87527000	0.49127300	-2.31413900
H	-3.85174300	0.39736900	-0.08618000
C	-3.72372900	-1.82187400	0.16051700
H	-2.79115800	-2.39590500	0.11901900
H	-4.03625700	-1.68641600	1.19604000
H	-4.48863700	-2.40514000	-0.36371700

10

E (B3LYP-CPCM/BS1) = -2383.190453au

H(B3LYP-CPCM/BS1) = -2382.843388au

G(B3LYP-CPCM/BS1) = -2382.94892au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2384.535360au

Au	-2.14501100	0.25008300	0.12930900
P	-2.72684400	-1.39340900	-1.34472100
C	-4.21532700	-0.92467000	-2.31906300
H	-4.00275100	-0.02903600	-2.90972900
H	-4.50234600	-1.74131300	-2.99025600
H	-5.04481200	-0.70631500	-1.64045500
C	-3.17090300	-2.95373500	-0.49295700
H	-3.51348600	-3.69504400	-1.22328300
H	-2.28163600	-3.32426300	0.02564100
H	-3.96597700	-2.76224900	0.23328700
C	-1.46911000	-1.85686100	-2.59323200
H	-0.55320600	-2.16571000	-2.08264200
H	-1.84826000	-2.67714100	-3.21223400
H	-1.25198700	-0.99398100	-3.22892900
O	0.10417800	2.44664900	1.75832800
C	-1.09283800	2.37043800	2.16306000
Au	1.08801700	1.68521700	0.05087400
P	2.49866700	1.19260500	-1.67382100
C	3.18709900	2.72662100	-2.42240400
H	3.69812500	3.31297800	-1.65350100
H	3.89610100	2.47961300	-3.22001100
H	2.37380900	3.32953500	-2.83661200
C	3.96048800	0.22952100	-1.12761800
H	4.61919100	0.02479000	-1.97859800
H	4.50956900	0.79946600	-0.37246900
H	3.61256100	-0.70860700	-0.69013800
C	1.79255100	0.26304800	-3.08552500
H	2.55230000	0.13944500	-3.86478800
H	1.46890200	-0.71378000	-2.72204900
H	0.93774400	0.80790300	-3.49606300
O	-0.08810900	-3.43225600	0.52227400

S	0.92789700	-2.35792900	0.60787700
O	1.42543700	-1.88031400	-0.71233400
O	0.64052700	-1.28481000	1.58905500
C	2.41920500	-3.21313200	1.31536700
F	3.45380300	-2.35345700	1.40153800
F	2.16518500	-3.68695200	2.54292400
F	2.79533600	-4.23740900	0.53410800
C	-1.42526700	3.10933400	3.44575500
H	-2.42003500	3.55632400	3.37799600
H	-1.43915500	2.38547900	4.26908100
O	-2.04874100	1.73278100	1.62567100
H	-0.67645300	3.87276400	3.66202200

10'

E (B3LYP-CPCM/BS1) = -2461.564206au

H(B3LYP-CPCM/BS1) = -2461.173604au

G(B3LYP-CPCM/BS1) = -2461.284029au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2462.935499au

Au	1.35176800	-1.44519100	0.16016100
P	0.75370300	-3.61189700	0.52539800
C	2.14839600	-4.63075600	1.15552500
H	2.52296300	-4.20386000	2.09014500
H	1.81531300	-5.65868400	1.33443200
H	2.96089500	-4.63733500	0.42338800
C	0.15535200	-4.46883100	-0.97884200
H	-0.08636500	-5.51120800	-0.74400800
H	-0.74023700	-3.94910900	-1.33016000
H	0.92764100	-4.43876300	-1.75277600
C	-0.58045400	-3.77893300	1.77016200
H	-1.43042800	-3.16870700	1.45521200
H	-0.88179400	-4.82820200	1.85952200
H	-0.22058200	-3.41886400	2.73841900
O	1.85198400	0.59359900	-0.13197700
C	3.11103400	1.03482600	-0.42682700
C	3.55669000	2.28223800	0.03687100
C	3.97559700	0.24581400	-1.20191900
C	4.84267200	2.72788600	-0.27272500
H	2.88975300	2.89054800	0.64285600
C	5.26084700	0.69917400	-1.50205600
H	3.62707400	-0.71535600	-1.57133800
C	5.70429600	1.94167900	-1.04183300
H	5.17163800	3.69623000	0.09590800
H	5.91585800	0.07574700	-2.10542900
H	6.70461400	2.29175100	-1.27925500
Au	0.17497200	1.85960100	0.18357600
P	-1.69580400	3.11535200	0.48662100
C	-2.78501600	2.45041000	1.80249400
H	-2.25636000	2.48014500	2.75978100
H	-3.70097900	3.04707400	1.87295700
H	-3.02741100	1.41058200	1.56675200
C	-1.35604200	4.85925500	0.95790600

H	-2.29495600	5.40943600	1.08094100
H	-0.79692800	4.88482800	1.89754800
H	-0.75516200	5.33948300	0.18028800
C	-2.72923000	3.20420600	-1.02401700
H	-3.64256700	3.77596100	-0.82751800
H	-2.16205400	3.68610300	-1.82570300
H	-2.97866100	2.18524000	-1.32934000
O	-2.44928100	-2.51179600	-0.94598500
S	-2.62401300	-1.09882600	-0.53521300
O	-2.36427100	-0.83545900	0.90437700
O	-2.05650700	-0.09331200	-1.46783900
C	-4.45682000	-0.82310000	-0.68464100
F	-4.76622200	0.44596200	-0.34034200
F	-4.87464300	-1.02467300	-1.94234900
F	-5.13661500	-1.64789800	0.12558700

HOAc

E (B3LYP-CPCM/BS1) = -229.081342au

H(B3LYP-CPCM/BS1) = -229.013919au

G(B3LYP-CPCM/BS1) = -229.046873au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -229.196236au

O	-0.77921000	-1.04455400	-0.00000400
C	-0.09216500	0.12363400	-0.00002900
O	-0.64458800	1.20327500	0.00000500
C	1.39704100	-0.11079000	-0.00000700
H	1.91885000	0.84637200	-0.00078800
H	1.68464700	-0.69118600	0.88283700
H	1.68453900	-0.69265400	-0.88190700
H	-1.72691300	-0.80936900	0.00006200

(HOAc)₂

E (B3LYP-CPCM/BS1) = -458.191143au

H(B3LYP-CPCM/BS1) = -458.054059au

G(B3LYP-CPCM/BS1) = -458.102017au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -458.417902au

O	-1.26059600	1.08699800	-0.00002100
O	-1.42469100	-1.16251900	0.00003700
C	1.93698700	-0.05791200	-0.00001100
O	1.42470000	1.16252300	0.00003000
O	1.26060100	-1.08700500	-0.00002900
C	3.44317600	-0.06921300	-0.00000800
H	3.80907200	-1.09605700	-0.00028300
H	3.81660700	0.46148900	-0.88191500
H	3.81656800	0.46096900	0.88223300
H	0.42124700	1.11472300	0.00000900
H	-0.42123300	-1.11471100	0.00002000
C	-1.93699100	0.05790900	0.00000300
C	-3.44318900	0.06921400	-0.00001200
H	-3.80907200	1.09606400	0.00000000
H	-3.81659200	-0.46121100	-0.88209700

H -3.81660700 -0.46122500 0.88205900

HOAc-HOTf

E (B3LYP-CPCM/BS1) = -1191.103968au

H(B3LYP-CPCM/BS1) = -1190.987931au

G(B3LYP-CPCM/BS1) = -1191.045388au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1191.583481au

O	1.94178200	-1.89463200	0.15922200
S	0.96525300	-0.83419100	-0.00078400
O	0.06275700	-0.82142900	-1.16473600
O	0.14049100	-0.65533200	1.33062100
C	1.89706900	0.77808100	-0.06327300
F	1.02531200	1.78708200	-0.06399600
F	2.69664400	0.87472300	0.99445700
F	2.61941400	0.80830700	-1.18108200
C	-3.01557400	0.13243500	0.03956300
O	-2.63112300	-0.21031700	-1.17845400
O	-2.27421100	0.12766500	1.02637200
C	-4.46111300	0.53280300	0.11656500
H	-4.70969800	0.83918200	1.13232300
H	-4.65611100	1.35085600	-0.58393800
H	-5.09004100	-0.31198000	-0.18341400
H	-1.67123300	-0.45639100	-1.18753500
H	-0.82915600	-0.33317400	1.14936500

HOTf

E (B3LYP-CPCM/BS1) = -961.993914au

H(B3LYP-CPCM/BS1) = -961.946748au

G(B3LYP-CPCM/BS1) = -961.988873au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -962.358701au

H	-1.47578700	1.89240000	-0.24043700
O	-1.25864900	0.07790000	1.44904000
S	-0.85101300	-0.14514600	0.06900700
O	-1.21594100	-1.32736700	-0.68666000
O	-1.25723200	1.14398300	-0.83209900
C	1.00841600	0.01065700	-0.00115500
F	1.41632800	-0.07463100	-1.26257000
F	1.36787000	1.18584900	0.51353100
F	1.53759000	-0.97678900	0.71581800

HOTf-HOTf

E (B3LYP-CPCM/BS1) = -1924.010343au

H(B3LYP-CPCM/BS1) = -1923.914239au

G(B3LYP-CPCM/BS1) = -1923.980767au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1924.740995au

O	2.99543800	-2.03297700	-0.06022200
S	2.07801000	-0.91438100	-0.03272400
O	1.04120600	-0.77299300	-1.06906100
O	1.42190900	-0.81558100	1.41487900

C	3.07792000	0.66204800	-0.07191100
F	2.25362900	1.69508800	0.09372900
F	3.97991800	0.63747100	0.90058300
F	3.67955900	0.74583400	-1.25350900
O	-1.18681000	0.73832400	-1.24065100
O	-1.04872400	0.25684900	1.22461600
H	-0.36993400	0.16050900	-1.20413000
H	0.50875300	-0.40901500	1.36806900
S	-1.92773200	0.78395600	0.16863300
C	-3.24930000	-0.50964800	-0.08614800
F	-2.66719100	-1.66546400	-0.39495100
F	-3.93365900	-0.63265200	1.04640500
F	-4.05537000	-0.12736500	-1.06896000
O	-2.57639100	2.06946700	0.31796200

Propene

E (B3LYP-CPCM/BS1) = -117.905896au

H(B3LYP-CPCM/BS1) = -117.820865au

G(B3LYP-CPCM/BS1) = -117.850889au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -117.960996au

C	1.28391000	-0.22038400	-0.00000500
C	0.13350300	0.45578100	-0.00003800
H	1.30660800	-1.30884600	-0.00007900
H	2.24610900	0.28536600	0.00019300
H	0.16315600	1.54653900	-0.00003900
C	-1.23552100	-0.16344300	0.00002300
H	-1.81242800	0.15103200	0.88030600
H	-1.81268300	0.15161200	-0.87989000
H	-1.18211400	-1.25743200	-0.00037400

prod

E (B3LYP-CPCM/BS1) = -347.022565au

H(B3LYP-CPCM/BS1) = -346.866169au

G(B3LYP-CPCM/BS1) = -346.909893au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -347.184318au

H	2.29323000	1.53719500	-0.65749300
O	-0.11641100	0.52376300	-0.23074700
C	2.12726400	1.09540900	0.33146500
C	1.13454100	-0.05607100	0.25075500
H	3.08847300	0.73394900	0.71235100
H	1.76206900	1.87816700	1.00396900
H	0.94038200	-0.46807800	1.24474000
C	1.57086300	-1.17146400	-0.69403000
H	2.51904100	-1.60224800	-0.35333000
H	0.82314400	-1.96919600	-0.72157600
H	1.71346100	-0.78343900	-1.70893200
C	-1.26656500	-0.08123700	0.13254800
C	-2.46015200	0.64349100	-0.44643200
H	-3.37815100	0.14362400	-0.13533500
H	-2.47038300	1.68455000	-0.10738900

H	-2.39733900	0.65642900	-1.53959800
O	-1.32479200	-1.07272700	0.83284100

prod_P

E (B3LYP-CPCM/BS1) = -425.401422au

H(B3LYP-CPCM/BS1) = -425.200891au

G(B3LYP-CPCM/BS1) = -425.246379au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -425.589193au

H	2.61465900	-0.40153500	1.84557100
O	0.95693600	0.72620000	0.02255000
C	2.32148600	-1.04446000	1.00813500
C	2.03755300	-0.19414800	-0.23078800
H	3.13886400	-1.74618200	0.80789900
H	1.44268900	-1.62178000	1.31071300
H	1.76420400	-0.83735700	-1.07725500
C	3.22788300	0.67053500	-0.63207900
H	4.09571900	0.04095700	-0.85514900
H	2.99131900	1.26544500	-1.51975200
H	3.49538000	1.35367700	0.18166500
C	-0.34241400	0.30708000	-0.01677100
C	-1.29713200	1.29020400	0.29336300
C	-0.76964100	-0.98634600	-0.34947600
C	-2.65425700	0.98528000	0.26616000
H	-0.94775500	2.28618400	0.54863000
C	-2.13816300	-1.27744200	-0.37353900
H	-0.05822000	-1.76850300	-0.58714100
C	-3.08721300	-0.30313300	-0.06855000
H	-3.37864800	1.75897900	0.50729200
H	-2.45553300	-2.28421300	-0.63319700
H	-4.14677300	-0.54069700	-0.08839900

PhOH

E (B3LYP-CPCM/BS1) = -307.462564au

H(B3LYP-CPCM/BS1) = -307.351324au

G(B3LYP-CPCM/BS1) = -307.386737au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -307.602826au

C	-1.85860400	0.02910000	0.00000700
C	-1.13080000	1.22060300	0.00000100
C	0.26564400	1.20037800	-0.00001900
C	0.94198000	-0.02507900	-0.00008800
C	0.21968700	-1.22475800	-0.00003200
C	-1.17379900	-1.19057600	0.00002300
H	-2.94438100	0.04928300	0.00004400
H	-1.64780100	2.17657800	0.00003200
H	0.82898100	2.13154000	0.00005700
H	0.76225000	-2.16524200	-0.00003600
H	-1.72823700	-2.12536500	0.00006300
O	2.30760300	-0.11329000	0.00006700
H	2.68371300	0.78151900	-0.00005400

2PhOH

E (B3LYP-CPCM/BS1) = -614.935790au

H(B3LYP-CPCM/BS1) = -614.710722au

G(B3LYP-CPCM/BS1) = -614.767973au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -615.216473au

C	-3.36524800	1.08139000	0.56859000
C	-2.21843400	0.27541600	0.55190100
C	-2.18695100	-0.87300900	-0.25209100
C	-3.29871800	-1.20652000	-1.02834800
C	-4.44433600	-0.40782600	-1.01511700
C	-4.46759300	0.73709500	-0.21196100
O	-1.16795600	0.65586500	1.33448300
O	1.11945200	-0.98916600	0.99666400
C	2.23106400	-0.43673400	0.39377300
C	2.10267800	0.85665400	-0.11949200
C	3.19848300	1.45244000	-0.74258700
C	4.41393700	0.77000200	-0.85438200
C	4.52708300	-0.52072500	-0.33451600
C	3.43777600	-1.13171400	0.29150700
H	-3.37321800	1.96737300	1.19663300
H	-5.35205300	1.36883500	-0.19126500
H	-5.30603500	-0.67218000	-1.62114300
H	-3.26379300	-2.09882400	-1.64848900
H	-1.29386200	-1.49221400	-0.26982200
H	-0.44183600	0.00391100	1.26112400
H	1.33102900	-1.86388800	1.36040400
H	3.52585100	-2.13820500	0.69489500
H	5.46587900	-1.06191800	-0.41346200
H	5.26339000	1.24033100	-1.34047300
H	3.09961100	2.45818200	-1.14147100
H	1.15463000	1.37619100	-0.01977600

7 where L = PPh3

E (B3LYP-CPCM/BS1) = -1400.300144au

H(B3LYP-CPCM/BS1) = -1399.949309au

G(B3LYP-CPCM/BS1) = -1400.031423au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -1401.077524au

Au	1.46850300	-0.48499200	-0.01474200
P	-0.76468700	0.00656200	-0.00205700
O	3.49404300	-0.94974400	-0.04738600
C	4.27942600	0.09593700	0.02002000
C	5.76029700	-0.26486900	-0.00067900
H	6.37322000	0.63656300	0.05835500
H	5.99614000	-0.92556100	0.84055600
O	3.89966500	1.26662100	0.09399300
H	5.99936100	-0.81253500	-0.91868000
C	-1.12585100	1.47844800	-1.03583100
C	-2.33586500	1.61881500	-1.73296500
C	-0.16055700	2.49648100	-1.11486300
C	-2.57844400	2.76590800	-2.49120500

H	-3.08503500	0.83420300	-1.69257700
C	-0.41062300	3.64188600	-1.87114100
H	0.78761700	2.38968500	-0.59468000
C	-1.61840400	3.77790600	-2.56015300
H	-3.51594000	2.86475200	-3.03110500
H	0.34296800	4.42192700	-1.92818700
H	-1.80795300	4.66714400	-3.15479200
C	-1.83231100	-1.34326200	-0.63794000
C	-3.11993600	-1.57304500	-0.12936900
C	-1.34443100	-2.15762300	-1.67299900
C	-3.90869900	-2.59824300	-0.65547600
H	-3.50524900	-0.96050300	0.67971900
C	-2.13788400	-3.17777300	-2.19787400
H	-0.34242400	-1.99640500	-2.06175300
C	-3.42029700	-3.40000200	-1.68926000
H	-4.90277600	-2.77142400	-0.25306700
H	-1.75082000	-3.80327000	-2.99705700
H	-4.03446500	-4.19975900	-2.09346300
C	-1.38726900	0.39505500	1.68006300
C	-2.34625200	1.39360300	1.90719900
C	-0.88787100	-0.34162500	2.76684200
C	-2.80292800	1.64485300	3.20289100
H	-2.73092600	1.98030600	1.07898600
C	-1.35099200	-0.09031700	4.05822300
H	-0.13203400	-1.10496300	2.60203800
C	-2.30813300	0.90391600	4.27793800
H	-3.54182600	2.42339500	3.37024600
H	-0.95708900	-0.66384300	4.89228800
H	-2.66171000	1.10495000	5.28529300

10 where L = PPh₃

E (B3LYP-CPCM/BS1) = -3533.553199au

H(B3LYP-CPCM/BS1) = -3532.866392au

G(B3LYP-CPCM/BS1) = -3533.020481au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -3535.391957au

Au	1.64370000	-0.13057200	-1.36905200
P	2.81035600	1.08402500	0.17708200
O	-1.21225400	-1.60803900	-2.98334100
C	-0.03339600	-1.90001200	-3.35342900
Au	-1.92033800	-0.44019800	-1.38988000
P	-3.10056500	0.66337900	0.22802900
O	2.41529000	-3.08627500	0.23358600
S	0.97209200	-3.40782700	0.13942100
O	0.07141400	-2.22192000	0.23913300
O	0.59694500	-4.38698900	-0.90137700
C	0.61715100	-4.28793900	1.74011700
F	-0.69472600	-4.59157900	1.83109900
F	1.31647200	-5.42732100	1.83585500
F	0.92953600	-3.51091700	2.79169000
C	0.10077000	-3.05994800	-4.31735800
H	0.95803700	-2.91616900	-4.97834400

H	0.27808300	-3.95711700	-3.71189500
O	1.04346100	-1.33876500	-2.99645000
H	-0.81493800	-3.19935800	-4.89485300
C	-3.50163900	-0.41863200	1.65149100
C	-4.62980200	-0.17703100	2.45366000
C	-2.65927000	-1.50431600	1.94484900
C	-4.89982700	-1.00188400	3.54635900
H	-5.30159300	0.64456300	2.22341200
C	-2.93852700	-2.32585100	3.04009900
H	-1.79570200	-1.72409700	1.32192200
C	-4.05412300	-2.07471800	3.84156100
H	-5.77519900	-0.81070300	4.16069000
H	-2.28468000	-3.16709600	3.24755300
H	-4.27174300	-2.71949100	4.68858200
C	-4.71358400	1.25987400	-0.41964500
C	-5.26260500	2.48876300	-0.02453400
C	-5.42364200	0.44391800	-1.31618100
C	-6.50691500	2.89126300	-0.51580200
H	-4.72201500	3.13489400	0.65975800
C	-6.66737000	0.84854800	-1.80012400
H	-5.00043500	-0.50352000	-1.63985200
C	-7.21041100	2.07312500	-1.40131800
H	-6.92228800	3.84634100	-0.20690200
H	-7.20736900	0.21098900	-2.49417500
H	-8.17620300	2.39013900	-1.78460100
C	-2.25477300	2.14742400	0.89139500
C	-2.36524000	2.52894100	2.23674500
C	-1.50056200	2.93753100	0.00824700
C	-1.73770500	3.69222000	2.68795400
H	-2.93272800	1.92041900	2.93336200
C	-0.87897100	4.10009300	0.46302200
H	-1.39508900	2.63748800	-1.03096000
C	-0.99759500	4.47846600	1.80327600
H	-1.82489000	3.97842500	3.73222600
H	-0.28986600	4.69983000	-0.22389900
H	-0.50532700	5.37963200	2.15760400
C	2.33620200	0.79293900	1.92098700
C	1.05888000	0.29652200	2.21625800
C	3.24247700	1.04330800	2.96616100
C	0.68508300	0.07359000	3.54297000
H	0.37749500	0.04563900	1.41127500
C	2.86053000	0.82514800	4.28959100
H	4.24828100	1.39074900	2.74846500
C	1.58076500	0.34282400	4.57900200
H	-0.30083300	-0.32696300	3.75978900
H	3.56630400	1.01893400	5.09236200
H	1.28995500	0.16237100	5.61022500
C	4.58375300	0.61464900	0.08280500
C	5.61160900	1.56525800	0.01359100
C	4.89709900	-0.75681000	0.09223700
C	6.94451700	1.14886300	-0.04225000
H	5.37989000	2.62548300	0.00095700

C	6.23077200	-1.16119800	0.04100900
H	4.10446000	-1.50097600	0.13710500
C	7.25496800	-0.21172400	-0.02786600
H	7.73661800	1.89038900	-0.09854400
H	6.46808200	-2.22119100	0.04829800
H	8.29191700	-0.53295600	-0.07388500
C	2.74171400	2.89474300	-0.12312700
C	2.88786700	3.83017400	0.91247300
C	2.57044000	3.35088600	-1.44041400
C	2.87209100	5.19801900	0.63169300
H	3.00588800	3.49686600	1.93824800
C	2.55752000	4.71858600	-1.71762400
H	2.44226600	2.63346600	-2.24665300
C	2.70838400	5.64450400	-0.68168000
H	2.98615300	5.91334100	1.44138700
H	2.42558900	5.05892600	-2.74072400
H	2.69581400	6.70932500	-0.89709900

Ts6 where L = PPh3

E (B3LYP-D3-CPCM/BS1) = -2480.185018au

H(B3LYP-D3-CPCM/BS1) = -2479.700218au

G(B3LYP-D3-CPCM/BS1) = -2479.814897au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -2481.393293au

Au	0.01788400	1.01779800	0.28612300
P	-2.08875100	0.06440900	0.03271400
O	3.96090200	-2.99808300	1.16170500
S	3.32644300	-1.76834600	0.65665100
O	2.25505100	-1.20049600	1.52389800
O	4.24376600	-0.74975700	0.08580900
C	2.37423900	-2.34552900	-0.83317200
F	1.79358600	-1.30205300	-1.47507600
F	3.17175800	-2.96853000	-1.71074900
F	1.39261100	-3.19340100	-0.47771800
C	2.06699400	1.86132700	0.59557800
H	1.66182200	2.76468100	1.06132500
H	2.12659600	0.89911500	1.13671200
C	2.68931200	1.97568500	-0.78526800
C	2.20238000	3.15807000	-1.60674800
H	2.30873300	4.09419500	-1.04733600
H	2.76626200	3.24002900	-2.54047100
H	1.14304300	3.02054400	-1.84667300
H	2.59263300	1.03920800	-1.33125900
O	4.20453000	2.11522000	-0.79021900
C	4.93155600	2.07133700	0.28989800
C	6.39343600	1.85487800	0.06355700
H	6.54669300	0.76974400	0.02303100
H	6.70958400	2.28798200	-0.88746100
H	6.96889000	2.26608700	0.89436400
O	4.46220800	2.19125400	1.44749100
H	3.20140400	2.05536100	1.26356700
C	-2.36648600	-1.28250100	1.24344900

C	-3.64250900	-1.54374100	1.76838100
C	-1.27493900	-2.07438500	1.63969800
C	-3.82492500	-2.59100300	2.67305600
H	-4.48999700	-0.93011700	1.47842100
C	-1.46772200	-3.12144500	2.54211400
H	-0.27666800	-1.87899300	1.25824600
C	-2.73914400	-3.38042900	3.05952500
H	-4.81414900	-2.78548300	3.07774800
H	-0.61832900	-3.72634600	2.84535800
H	-2.88270400	-4.19192700	3.76745000
C	-3.44926800	1.27051900	0.27707400
C	-4.61660500	1.24294200	-0.50027700
C	-3.31367200	2.24065200	1.28409200
C	-5.63402200	2.17201900	-0.26983000
H	-4.73231100	0.50326600	-1.28623500
C	-4.33459000	3.16234900	1.51384000
H	-2.40884200	2.27551700	1.88539000
C	-5.49529500	3.13052800	0.73566100
H	-6.53290900	2.14582800	-0.87918900
H	-4.22022200	3.90896100	2.29444200
H	-6.28670400	3.85387600	0.91039500
C	-2.33407100	-0.65913600	-1.63345400
C	-3.05597000	-1.84676700	-1.82526800
C	-1.78780500	0.00374700	-2.74480300
C	-3.23282800	-2.35811100	-3.11273700
H	-3.47279300	-2.37669600	-0.97465200
C	-1.97133400	-0.50859500	-4.02878600
H	-1.21385100	0.91594400	-2.60390500
C	-2.69273900	-1.69111800	-4.21401200
H	-3.78834400	-3.28110600	-3.25172500
H	-1.54263900	0.00937900	-4.88181000
H	-2.82708600	-2.09466300	-5.21356400

Ts7 where L = PPh3

E (B3LYP-CPCM/BS1) = -2480.202897au

H(B3LYP-CPCM/BS1) = -2479.718721au

G(B3LYP-CPCM/BS1) = -2479.836006au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -2481.408172au

Au	0.49410500	-1.17608100	-0.74551400
P	2.13714400	0.14482400	0.13245200
O	-0.96082700	-2.42063000	-1.63139100
C	-2.03694700	-2.61596800	-0.96431500
O	-5.28134900	1.64935600	0.28355700
S	-3.80276100	1.72869100	0.23114900
O	-3.22035800	3.08365900	0.25979100
O	-3.11975500	0.73739700	1.11916900
C	-3.39435100	1.10105100	-1.46962800
F	-2.06342600	1.04273800	-1.65629500
F	-3.89333100	-0.13965800	-1.64387800
F	-3.91578100	1.89494800	-2.41362600
C	-4.65025300	-2.17144700	1.39531900

C	-4.78797500	-0.94098500	2.06328100
H	-4.47518400	-3.03954400	2.03727700
H	-3.57412800	-2.08387400	0.83291100
H	-5.31762700	-0.12741300	1.57132900
C	-4.32618800	-0.70273900	3.44401200
H	-3.85105200	0.27810100	3.52378500
H	-5.22781600	-0.67349800	4.07900000
H	-3.66652800	-1.49084000	3.81595800
O	-2.19926400	-2.19114400	0.20956100
C	-3.13343400	-3.38394000	-1.67642300
H	-3.63227100	-4.06981600	-0.98632700
H	-3.87707100	-2.66794600	-2.04342200
H	-2.73238200	-3.93631900	-2.52749700
H	-5.34988300	-2.34306800	0.57499900
C	2.44790300	-0.24088500	1.89783400
C	2.36748100	-1.57670300	2.32407400
C	2.77796700	0.76037300	2.82342500
C	2.62483000	-1.90579600	3.65469700
H	2.09626300	-2.35565500	1.61637700
C	3.03055200	0.42583900	4.15561800
H	2.82970800	1.79826200	2.51000200
C	2.95589400	-0.90482200	4.57204200
H	2.55817400	-2.94134500	3.97567900
H	3.28054500	1.20763600	4.86711400
H	3.14868600	-1.16110700	5.61000900
C	1.73364200	1.92689300	0.04462500
C	2.72402800	2.89659100	-0.18002000
C	0.39797100	2.32430300	0.22024900
C	2.37737900	4.24811900	-0.22290800
H	3.75806900	2.60140400	-0.32928000
C	0.05737600	3.67687200	0.17615300
H	-0.38041900	1.58538300	0.38569700
C	1.04724100	4.63758700	-0.04602800
H	3.14685800	4.99417600	-0.40111000
H	-0.98389700	3.95726500	0.29966500
H	0.78105900	5.69022300	-0.08845500
C	3.74036500	-0.07511500	-0.73089900
C	4.96239000	-0.05478600	-0.04205100
C	3.73670300	-0.25053500	-2.12464000
C	6.16261000	-0.20378900	-0.74064100
H	4.98050800	0.07060200	1.03591000
C	4.93821500	-0.39350100	-2.81795500
H	2.79398100	-0.28002500	-2.66465100
C	6.15260700	-0.37210500	-2.12663500
H	7.10408700	-0.19111600	-0.19887000
H	4.92463600	-0.52949600	-3.89548500
H	7.08766200	-0.49142500	-2.66662400

Ts8 where L = PPh3

E (B3LYP-CPCM/BS1) = -4613.446412au

H(B3LYP-CPCM/BS1) = -4612.628692au

G(B3LYP-CPCM/BS1) = -4612.815850au

E(B3LYP-D3-CPCM/BS2//B3LYP/BS1) = -4615.725639au

Au	1.72824400	-0.58653400	-1.39218600
P	3.71435500	0.41026900	-0.84625900
O	-1.44071500	-1.92243400	-0.67618300
C	-0.79061600	-2.36877800	-1.70418900
Au	-1.46505600	0.10748100	0.08453600
P	-1.72249200	2.14493500	1.08693400
O	2.64755700	-2.49058200	1.50876400
S	1.24498100	-2.94648800	1.65415600
O	0.30325000	-1.91574100	2.16468800
O	0.73274700	-3.76414500	0.52732400
C	1.32003800	-4.16721400	3.05410000
F	0.10314700	-4.70036400	3.27700000
F	2.16814400	-5.16748600	2.77146600
F	1.72897700	-3.57522000	4.18742200
C	-1.22658200	-3.69228300	-2.26817900
H	-0.67952200	-3.90882700	-3.18611800
H	-1.00485900	-4.46785500	-1.52654000
O	0.14601600	-1.73985800	-2.24989600
H	-2.30485600	-3.66977800	-2.45456100
H	-2.11711100	-2.81854300	0.18553500
O	-4.48066400	-2.67050200	-2.26467500
S	-4.59339200	-1.24172900	-1.87434800
O	-4.72366100	-1.02278400	-0.40551800
O	-3.66474700	-0.31971600	-2.56200100
C	-6.26754000	-0.75162200	-2.51871700
F	-6.51957100	0.54275600	-2.24705800
F	-6.33365400	-0.91924700	-3.84692700
F	-7.23174100	-1.49246100	-1.94924700
C	-2.45326600	-3.49575300	1.23227600
C	-3.76577900	-3.67255900	0.84176900
H	-1.76080600	-4.33575300	1.21389800
H	-2.21094700	-2.70904200	1.94820000
H	-4.45458000	-2.83868100	0.96994200
C	-4.29642600	-4.84663500	0.12287800
H	-5.18544400	-5.21254400	0.65651900
H	-4.64907600	-4.50696400	-0.86154500
H	-3.56832200	-5.65407000	0.01733400
C	-1.73537500	1.96110900	2.91197000
C	-2.44946800	2.85200500	3.72949700
C	-1.00405300	0.91371300	3.49921400
C	-2.41829400	2.70687700	5.11764300
H	-3.03635700	3.65093300	3.28695400
C	-0.97734500	0.77783600	4.88878100
H	-0.47144400	0.19143000	2.88563300
C	-1.68079800	1.67264600	5.69865900
H	-2.97647700	3.39849500	5.74228900
H	-0.41413000	-0.03814100	5.33231300
H	-1.66305900	1.55859200	6.77895900
C	-3.27996300	2.98844500	0.62074900

C	-3.37465400	4.39042800	0.62077900
C	-4.40117100	2.21417400	0.28297800
C	-4.58457400	5.00787500	0.30105400
H	-2.50886200	5.00017300	0.86042000
C	-5.60612700	2.84147200	-0.03914800
H	-4.34069200	1.12959100	0.24645300
C	-5.70080400	4.23446900	-0.02776400
H	-4.65077200	6.09224400	0.30102100
H	-6.45959900	2.23328000	-0.32047000
H	-6.63884600	4.71824200	-0.28577800
C	-0.37949200	3.32370300	0.67816900
C	0.14349800	4.21257200	1.62893600
C	0.10369300	3.35704300	-0.64054400
C	1.13216400	5.12835800	1.26090800
H	-0.21517400	4.19171400	2.65321200
C	1.08717300	4.27681200	-1.00340100
H	-0.28520400	2.66043900	-1.37862400
C	1.60246800	5.16286100	-0.05272600
H	1.53437200	5.81132700	2.00375200
H	1.46028100	4.29212100	-2.02281800
H	2.37432200	5.87260800	-0.33603800
C	3.91268600	0.87149800	0.91062700
C	2.78565600	1.23168900	1.66278000
C	5.18185900	0.88380100	1.51106000
C	2.92795800	1.61162500	2.99734400
H	1.79957100	1.20142200	1.21017800
C	5.31810200	1.26620500	2.84622500
H	6.05845800	0.58472200	0.94461400
C	4.19275500	1.62978200	3.58949400
H	2.04789800	1.87599100	3.57593300
H	6.30195300	1.26954500	3.30653100
H	4.30060500	1.91717600	4.63163400
C	5.09610000	-0.73363900	-1.23302100
C	6.15988400	-0.35923500	-2.06637500
C	5.06498400	-2.02312400	-0.67157600
C	7.18639800	-1.26774600	-2.33736300
H	6.19315700	0.63301500	-2.50407600
C	6.09748300	-2.91962900	-0.94577100
H	4.24572600	-2.31944400	-0.02032400
C	7.15636000	-2.54640400	-1.77911200
H	8.00673600	-0.97242000	-2.98547600
H	6.07065900	-3.91395500	-0.50918600
H	7.95455900	-3.25171900	-1.99333300
C	4.00490900	1.92573300	-1.83972900
C	4.77362900	2.99059600	-1.34599800
C	3.47184000	2.00468200	-3.13680700
C	5.00725900	4.11453100	-2.14089800
H	5.18525700	2.94868800	-0.34277300
C	3.71163200	3.12779400	-3.92950400
H	2.86555800	1.19025900	-3.52457900
C	4.47834300	4.18510600	-3.43168800
H	5.60234400	4.93456700	-1.74911100

H	3.29533300	3.17777600	-4.93148300
H	4.66083400	5.06135700	-4.04738700

7 optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -825.131670au

H(B3LYP-D3-CPCM/BS1) = -824.950931au

G(B3LYP-D3-CPCM/BS1) = -825.007173au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -825.651678au

Au	0.14560900	-0.25302600	-0.00011500
P	-2.08691900	0.16438400	-0.00032000
C	-2.96269700	-0.37642000	1.51958800
H	-2.51228000	0.11373300	2.38727500
H	-4.02518500	-0.11715800	1.46208200
H	-2.85539700	-1.45851500	1.63528200
C	-3.01354000	-0.61799000	-1.37817700
H	-4.07586900	-0.35806700	-1.32184300
H	-2.60177400	-0.27231500	-2.33053700
H	-2.89899300	-1.70410300	-1.32218300
C	-2.46338800	1.95528000	-0.14053800
H	-2.03849300	2.34098400	-1.07138800
H	-3.54532900	2.12406100	-0.13124600
H	-2.00093400	2.48536900	0.69673400
O	2.17638200	-0.68381900	0.00250000
C	2.96447800	0.36260400	0.00007000
C	4.44266400	-0.00905200	0.00096500
H	5.06215700	0.88985300	0.00228300
H	4.67232100	-0.61802700	0.88193600
O	2.59135200	1.53716200	-0.00309200
H	4.67348800	-0.61583300	-0.88126200

10 optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -2383.263037au

H(B3LYP-D3-CPCM/BS1) = -2382.916183au

G(B3LYP-D3-CPCM/BS1) = -2383.018037au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -2384.536488au

Au	-1.93779300	-0.68611000	-0.01287600
P	-3.11116000	0.99825400	0.96228800
C	-4.67820600	0.40440400	1.71601400
H	-4.45359700	-0.29962300	2.52222700
H	-5.24752200	1.25006000	2.11637900
H	-5.27408800	-0.10983600	0.95690000
C	-3.63123900	2.25660300	-0.26361100
H	-4.24810300	3.01707600	0.22759700
H	-2.74598500	2.72302400	-0.70579800
H	-4.20954400	1.76917500	-1.05364900
C	-2.29003600	1.94855300	2.29314300
H	-1.37793300	2.39034200	1.88610500
H	-2.96624900	2.73197900	2.65159100
H	-2.03597200	1.28028600	3.12044300
O	0.93003300	-2.18119700	-1.64527100

C	-0.25064000	-2.59697400	-1.83872000
Au	1.56617300	-1.14487300	0.07494400
P	2.34716700	-0.16802000	1.96846000
C	3.50897200	-1.23466000	2.91056100
H	4.38560400	-1.45081300	2.29323300
H	3.82660800	-0.73461500	3.83178600
H	3.01433300	-2.17807700	3.15820500
C	3.24201600	1.41298400	1.74069800
H	3.62610700	1.76150400	2.70516400
H	4.07119100	1.26860000	1.04383100
H	2.55042400	2.14508600	1.32273900
C	0.98740600	0.20743100	3.13390100
H	1.36986000	0.70501500	4.03116200
H	0.28740500	0.85686000	2.60831800
H	0.48016800	-0.72084900	3.41132900
O	-0.60769500	3.30169100	-1.38331900
S	0.18867500	2.10532500	-1.03269400
O	0.31739800	1.86822100	0.43300700
O	-0.08380900	0.89180500	-1.83882000
C	1.92711000	2.55489600	-1.53073000
F	2.75661600	1.50239300	-1.36848700
F	1.97666100	2.93190900	-2.81349000
F	2.39115400	3.56223300	-0.76848200
C	-0.48721500	-3.43694200	-3.07738700
H	-1.10910900	-4.30074600	-2.82704900
H	-1.03942000	-2.83043700	-3.80440400
O	-1.26206600	-2.38936200	-1.09876400
H	0.45513300	-3.76094000	-3.52127800

TS3 optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -1079.903296au

H(B3LYP-D3-CPCM/BS1) = -1079.773864au

G(B3LYP-D3-CPCM/BS1) = -1079.825456au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -1080.308453au

H	-1.90049300	-1.22452800	-0.97943900
C	-2.47814600	-0.66180400	-0.25076800
C	-2.26314900	-0.91844200	1.10442900
H	-1.29575800	-0.15500500	1.28755600
H	-1.80381300	-1.87427500	1.36056700
H	-3.00842600	-0.54338200	1.80788500
O	-0.08724600	0.62809300	1.50416700
S	0.50441000	0.90373200	0.13059400
O	-0.54999400	0.89508000	-0.91300000
O	1.48779600	1.98276000	0.10822500
C	1.44139000	-0.66650500	-0.19885200
F	2.00792300	-0.62666600	-1.40720000
F	2.38492200	-0.86171800	0.72379900
F	0.57944400	-1.70547600	-0.16153900
C	-3.44812700	0.31633200	-0.77931700
H	-2.99588900	0.91041900	-1.57808300
H	-4.27445700	-0.25658100	-1.23125800

H -3.85857400 0.96342800 -0.00036000

TS6 optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -1905.052585au

H(B3LYP-D3-CPCM/BS1) = -1904.737625au

G(B3LYP-D3-CPCM/BS1) = -1904.825127au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -1905.965164au

Au	-0.39575700	-1.26205300	-0.02588000
P	-2.70744800	-1.22868600	0.03096400
C	-3.43571700	-2.84994800	0.50096000
H	-3.08652300	-3.13277300	1.49812000
H	-4.52935500	-2.78974900	0.50157500
H	-3.11401500	-3.61371300	-0.21289100
C	-3.46137500	-0.82037200	-1.58744800
H	-4.55396200	-0.83791000	-1.50989800
H	-3.12042100	0.17923500	-1.86688500
H	-3.13436200	-1.54721000	-2.33642300
C	-3.41904000	-0.02875000	1.21788500
H	-3.09414400	0.96934700	0.91956600
H	-4.51241300	-0.09146900	1.19929800
H	-3.05448900	-0.24781000	2.22523600
O	-0.42244100	3.73565300	-1.57464900
S	-0.71149400	2.41203400	-0.99559800
O	-2.14371300	2.02360600	-0.94485000
O	0.20835600	1.32067300	-1.42029200
C	-0.29332600	2.63534900	0.80774600
F	-0.64492900	1.54433500	1.53297500
F	1.03133400	2.81857800	0.97704600
F	-0.93414900	3.68942400	1.32654400
C	1.85292200	-1.40461500	-0.11197400
H	1.77314700	-2.26249300	0.56526400
H	1.70836800	-1.53729800	-1.18877200
C	2.34447400	-0.07644300	0.41202900
C	2.27749800	0.08162900	1.91999500
H	2.75569700	-0.76492900	2.42532400
H	2.76666700	1.00874400	2.22838800
H	1.22955200	0.12970100	2.22492100
H	1.87735500	0.75557100	-0.10800900
O	3.82807300	0.22663700	0.07098300
C	4.66321500	-0.68576100	-0.30444500
C	6.04260800	-0.21218700	-0.64325400
H	6.76084100	-1.01554400	-0.46977000
H	6.06469100	0.05120600	-1.70753300
H	6.29644100	0.67559500	-0.06139300
O	4.35543000	-1.90514300	-0.42081800
H	3.12386300	-1.90440700	-0.29754000

TS7 optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -1905.073946au

H(B3LYP-D3-CPCM/BS1) = -1904.759812au

G(B3LYP-D3-CPCM/BS1) = -1904.847653au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -1905.986205au

Au	-1.39643700	0.83798400	-0.16926100
P	-2.79895900	-0.82760400	0.45688800
C	-3.11028600	-2.06832900	-0.85385200
H	-2.14671500	-2.48143600	-1.15869400
H	-3.75873700	-2.86550700	-0.47469100
H	-3.58719700	-1.58321700	-1.71008200
C	-4.46236500	-0.25986600	0.98965000
H	-5.07472000	-1.11293200	1.30096900
H	-4.35630100	0.43731100	1.82554000
H	-4.95333900	0.25849800	0.16117400
C	-2.13742200	-1.77560900	1.87746700
H	-1.99212400	-1.10164300	2.72619600
H	-2.82917400	-2.57801600	2.15472100
H	-1.17396400	-2.19268100	1.57847300
O	-0.04584800	2.32077600	-0.84677000
C	0.99734300	2.51335600	-0.13668600
O	2.47387100	-2.69835900	0.23185200
S	1.38726500	-1.75817700	-0.11296200
O	0.09205200	-2.35259900	-0.50179500
O	1.27001900	-0.60063900	0.82908700
C	2.00021200	-0.93710300	-1.66579600
F	1.10308500	-0.06122500	-2.14088400
F	3.14105000	-0.25653000	-1.39738900
F	2.26518900	-1.83897400	-2.61670300
C	3.42574600	1.33455800	1.97256200
C	3.39626900	-0.06649600	1.88391900
H	3.41425500	1.75004100	2.98329800
H	2.32980400	1.69623300	1.54424600
H	3.74414800	-0.54183200	0.97228800
C	3.07306400	-0.96014400	3.01496400
H	2.67268900	-1.91172300	2.66538300
H	4.02743600	-1.16098500	3.53139400
H	2.40239900	-0.48315100	3.73538500
O	1.05631500	2.25517200	1.09858200
C	2.21393200	3.04350400	-0.86848600
H	2.79215300	2.18123800	-1.22031700
H	1.91601600	3.62926700	-1.74001800
H	2.84269200	3.64040000	-0.20377900
H	4.10323700	1.83682800	1.27894300

TS8 optimized by B3LYP-D3 functional

E(B3LYP-D3-CPCM/BS1) = -3463.191916au

H(B3LYP-D3-CPCM/BS1) = -3462.713102au

G(B3LYP-D3-CPCM/BS1) = -3462.847925au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -3464.867238au

Au	-2.41642800	-0.73954300	-1.20594100
P	-3.91343700	-1.51985200	0.30821100
C	-4.22940700	-3.32455700	0.18635100

H	-3.29494700	-3.87254600	0.33446000
H	-4.95559700	-3.63383700	0.94544900
H	-4.61849400	-3.55990300	-0.80826200
C	-5.55448200	-0.72502300	0.15470400
H	-6.22908300	-1.10058200	0.93135800
H	-5.41000900	0.35131500	0.26839200
H	-5.97500900	-0.93760300	-0.83206600
C	-3.38154300	-1.22076500	2.03182400
H	-3.31644100	-0.14161100	2.17687700
H	-4.09912100	-1.66610000	2.72884600
H	-2.39152700	-1.65265100	2.18516500
O	0.49188600	0.82475600	-1.25207200
C	-0.20608100	0.94961800	-2.32640900
Au	0.67634800	-0.88854100	0.06324300
P	1.16849200	-2.75441400	1.25723600
C	2.02430000	-3.99627800	0.21994100
H	2.93920900	-3.53669900	-0.16071700
H	2.26488700	-4.88241200	0.81698700
H	1.37825000	-4.27824900	-0.61629300
C	2.26630800	-2.44991300	2.68646900
H	2.49485800	-3.39538800	3.18951400
H	3.17911000	-1.97702400	2.32115300
H	1.77079400	-1.76789600	3.38285400
C	-0.28417700	-3.64008600	1.94656000
H	0.03659400	-4.58072300	2.40648600
H	-0.76841400	-3.01898300	2.70397400
H	-0.99664300	-3.85180800	1.14513100
O	-3.57997300	1.74833200	0.76067100
S	-2.17327700	2.21367800	0.67657900
O	-1.19061300	1.34062100	1.36999600
O	-1.75500200	2.70149300	-0.65958800
C	-2.16969100	3.75772200	1.71565400
F	-0.94271800	4.31576400	1.72303200
F	-3.03640200	4.65899100	1.23235000
F	-2.50881000	3.47569500	2.98273700
C	0.11078900	2.12102300	-3.21561600
H	-0.28314000	1.95642200	-4.21920700
H	-0.38710700	2.99218500	-2.77527100
O	-1.12630500	0.15902800	-2.65898800
H	1.18741300	2.30432200	-3.24996300
H	1.11405600	1.99494000	-0.63717400
O	3.46376400	0.28148000	-1.14049500
S	4.14722300	-0.30714700	0.04159900
O	3.64476500	0.20993500	1.34281000
O	4.37416100	-1.76821400	-0.00507200
C	5.85457000	0.42551200	-0.06279500
F	6.62115500	0.00966100	0.95357200
F	6.45020700	0.09221000	-1.21550100
F	5.77361700	1.77397600	-0.00515500
C	1.31958800	3.01543300	0.06427200
C	2.69120000	2.90128200	-0.07026100
H	0.78160100	3.78222000	-0.49172400

H	0.84561000	2.67956300	0.98480400
H	3.21511200	2.24282100	0.62051100
C	3.49069900	3.50683400	-1.15189800
H	4.29401300	4.10268500	-0.69544000
H	3.99294700	2.70126900	-1.70034800
H	2.90107500	4.13350300	-1.82505600

Propene optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -117.908550au

H(B3LYP-D3-CPCM/BS1) = -117.823507au

G(B3LYP-D3-CPCM/BS1) = -117.853514au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -117.960991au

C	-1.28373800	0.22058400	0.00000900
C	-0.13367800	-0.45627700	0.00003100
H	-1.30468800	1.30921300	-0.00005800
H	-2.24652800	-0.28428300	0.00000700
H	-0.16262200	-1.54716300	0.00006700
C	1.23531900	0.16361500	-0.00002700
H	1.81179400	-0.15137200	0.88045800
H	1.81199800	-0.15188500	-0.88019900
H	1.18262900	1.25795900	-0.00034900

(HOAc)₂ optimized by B3LYP-D3 functional

E (B3LYP-D3-CPCM/BS1) = -458.201157au

H(B3LYP-D3-CPCM/BS1) = -458.064049au

G(B3LYP-D3-CPCM/BS1) = -458.111872au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -458.417935au

O	-1.25703500	1.08898300	0.00004400
O	-1.42125000	-1.16195200	0.00002100
C	1.93177300	-0.05864500	-0.00002000
O	1.42125300	1.16194600	0.00006600
O	1.25705100	-1.08900200	-0.00002300
C	3.43786800	-0.06842700	-0.00004700
H	3.80462900	-1.09498600	-0.00025500
H	3.80835700	0.46379700	-0.88222500
H	3.80837200	0.46342400	0.88235400
H	0.41743400	1.11733900	0.00011900
H	-0.41742000	-1.11741500	0.00008500
C	-1.93177900	0.05864200	-0.00000500
C	-3.43788100	0.06845900	-0.00005100
H	-3.80464000	1.09501900	-0.00002800
H	-3.80835400	-0.46354200	-0.88237200
H	-3.80841800	-0.46360700	0.88220400

TS_{5,7}

E (B3LYP-D3-CPCM/BS1) = -2501.075808 au

H(B3LYP-D3-CPCM/BS1) = -2500.642757 au

G(B3LYP-D3-CPCM/BS1) = -2500.758703 au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -2502.46837 au

Au	-3.32432700	-0.50406600	0.03296000
P	-3.80161700	1.42081000	1.15522500
C	-5.50930100	1.42439800	1.83710200
H	-5.63209200	0.58121900	2.52280300
H	-5.70224100	2.35943200	2.37386900
H	-6.23110300	1.31977800	1.02201800
C	-3.69004900	2.92946800	0.12049700
H	-3.97599600	3.80549200	0.71333200
H	-2.66601000	3.05866300	-0.24450400
H	-4.36699100	2.83506400	-0.73356800
C	-2.69724300	1.71304900	2.58741700
H	-1.67238100	1.78812700	2.21286700
H	-2.98002400	2.64054200	3.09707500
H	-2.77145400	0.87485800	3.28615600
O	-2.95765700	-2.25818200	-1.11763100
C	-1.86600000	-2.88812900	-0.94653800
C	-1.46698400	-3.86750000	-2.03004800
H	-0.49830600	-3.58197500	-2.45552200
H	-1.35801600	-4.86962400	-1.60335100
O	-1.14538600	-2.72507600	0.09059000
H	-2.21266800	-3.88572000	-2.82527600
Au	2.88071000	-0.68832000	0.65890400
P	4.76622400	0.63985100	0.19056100
C	6.42774600	-0.07770300	0.53319600
H	6.56371400	-0.98945300	-0.05605000
H	7.21868000	0.63638900	0.27933700
H	6.50396800	-0.33578900	1.59366300
C	4.72584800	2.22231900	1.12450200
H	5.58058800	2.85387600	0.85837900
H	3.79288900	2.73349600	0.87042900
H	4.74403100	2.02089000	2.19964800
C	4.82462200	1.16320600	-1.57094100
H	3.88685700	1.67867100	-1.79647200
H	5.66968200	1.83745200	-1.74873900
H	4.91724600	0.28622400	-2.21811700
O	-0.43172100	3.61786700	-0.92250300
S	0.37746000	2.42243300	-0.59864100
O	1.84788400	2.61672400	-0.63046500
O	-0.12441700	1.62586600	0.55134400
C	0.07255900	1.30073400	-2.05133400
F	0.72753600	0.12726400	-1.91461000
F	-1.23957700	1.02203000	-2.17719100
F	0.48781000	1.86962300	-3.19208200
C	0.97757800	-1.58363400	1.07943800
H	0.94246700	-1.97329200	2.10016200
H	0.37209300	-0.68159400	0.95734600
C	0.74149000	-2.57305000	0.06699200
H	0.74578800	-2.21301100	-0.95748900
C	1.19232500	-3.99420200	0.26728500
H	0.76765400	-4.67199300	-0.47553500

H	2.28416300	-4.03370300	0.17184000
H	0.92766900	-4.34598000	1.26879800

PMe₃AuOH

E (B3LYP-D3-CPCM/BS1) = -672.4313894 au

H(B3LYP-D3-CPCM/BS1) = -672.292597 au

G(B3LYP-D3-CPCM/BS1) = -672.340659 au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -672.905225 au

Au	-0.76512600	0.00093900	-0.00041700
P	1.52296100	0.00113800	-0.00008400
C	2.27819600	-0.88822200	-1.42353700
H	1.95799100	-0.41487400	-2.35625300
H	3.37168600	-0.87043000	-1.36293200
H	1.93240300	-1.92604000	-1.42807900
C	2.27687500	-0.78848900	1.48178700
H	3.37045800	-0.76637500	1.42457900
H	1.94917100	-0.25760100	2.38026700
H	1.93815200	-1.82619900	1.55277100
C	2.28073700	1.67658700	-0.05639800
H	1.94846200	2.25603700	0.80984300
H	3.37400700	1.61040700	-0.05067300
H	1.95363200	2.19279600	-0.96354400
O	-2.76475000	-0.11136400	0.00397500
H	-3.09226200	0.80270500	-0.01465300

PMe₃AuOAc...H₂O

E (B3LYP-D3-CPCM/BS1) = -901.5457765 au

H(B3LYP-D3-CPCM/BS1) = -901.336277 au

G(B3LYP-D3-CPCM/BS1) = -901.401305 au

E(B3LYP-D3-CPCM/BS2//B3LYP-D3/BS1) = -902.1365738 au

Au	0.11173800	-0.46999500	0.04545600
P	-2.10847300	0.03484700	-0.06040400
C	-3.26090900	-1.37336200	-0.32198300
H	-3.15333800	-2.09148400	0.49601000
H	-4.29787300	-1.02330100	-0.36313600
H	-3.01185100	-1.87650300	-1.26072000
C	-2.45960500	1.23030700	-1.40662900
H	-3.51205900	1.53349100	-1.39404100
H	-1.81344800	2.09887300	-1.24978100
H	-2.22229800	0.77852800	-2.37398400
C	-2.69722500	0.87370800	1.46358100
H	-2.07903600	1.76226300	1.61680400
H	-3.74728900	1.16885000	1.36545500
H	-2.58398600	0.20849800	2.32413500
O	2.59545000	1.32048600	-0.30708300
C	2.94884400	0.15335800	-0.08089400
O	0.21964800	2.76778600	0.13820100
O	2.15642800	-0.85216700	0.15118100
C	4.42538200	-0.21679900	-0.06712500

H	4.63456300	-0.92091000	-0.88018300
H	5.04484600	0.67339800	-0.18977600
H	4.67897000	-0.72077900	0.87106000
H	0.99930500	2.22166700	-0.11626500
H	0.35214500	2.90215900	1.08938000