

## Supporting Information

# **A Computational Study towards Understanding the Mechanism of Phosphodiester Cleavage by Two Mononuclear Zn(II) Complexes**

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**Figure S1.** Optimized geometries of stationary points in the water-assisted proton transfer mode in the absence of catalyst. Distances are in Å. Certain hydrogen atoms are omitted for clarity.

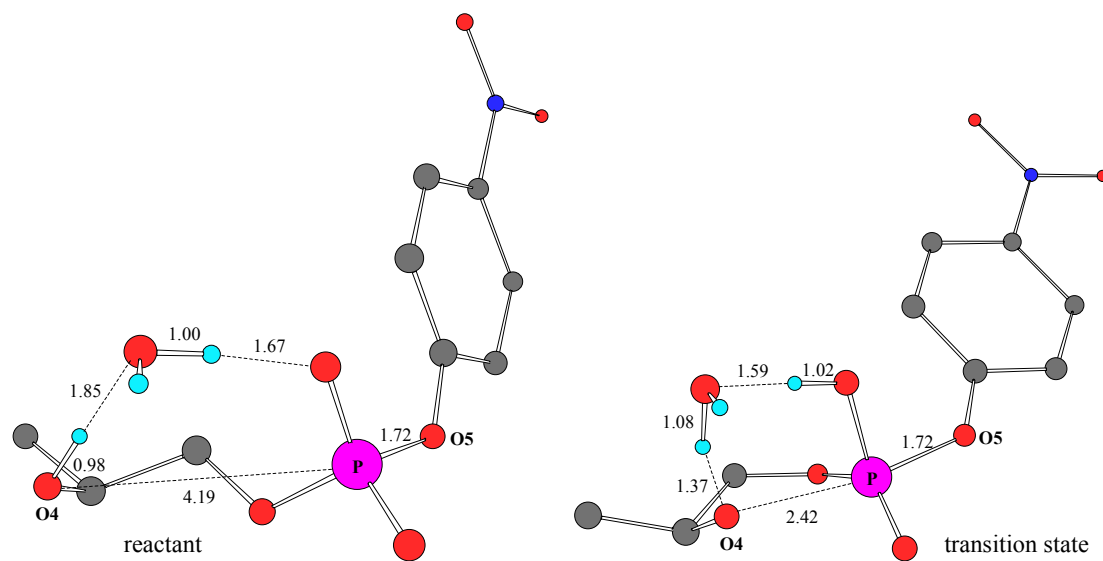
**Figure S2.** Optimized geometries of stationary points in the direct proton transfer mode catalyzed by catalyst **B**. Distances are in Å. Certain hydrogen atoms are omitted for clarity.

**Figure S3.** Optimized geometries of stationary points in the general base mode catalyzed by catalyst **B**. Distances are in Å. Certain hydrogen atoms are omitted for clarity.

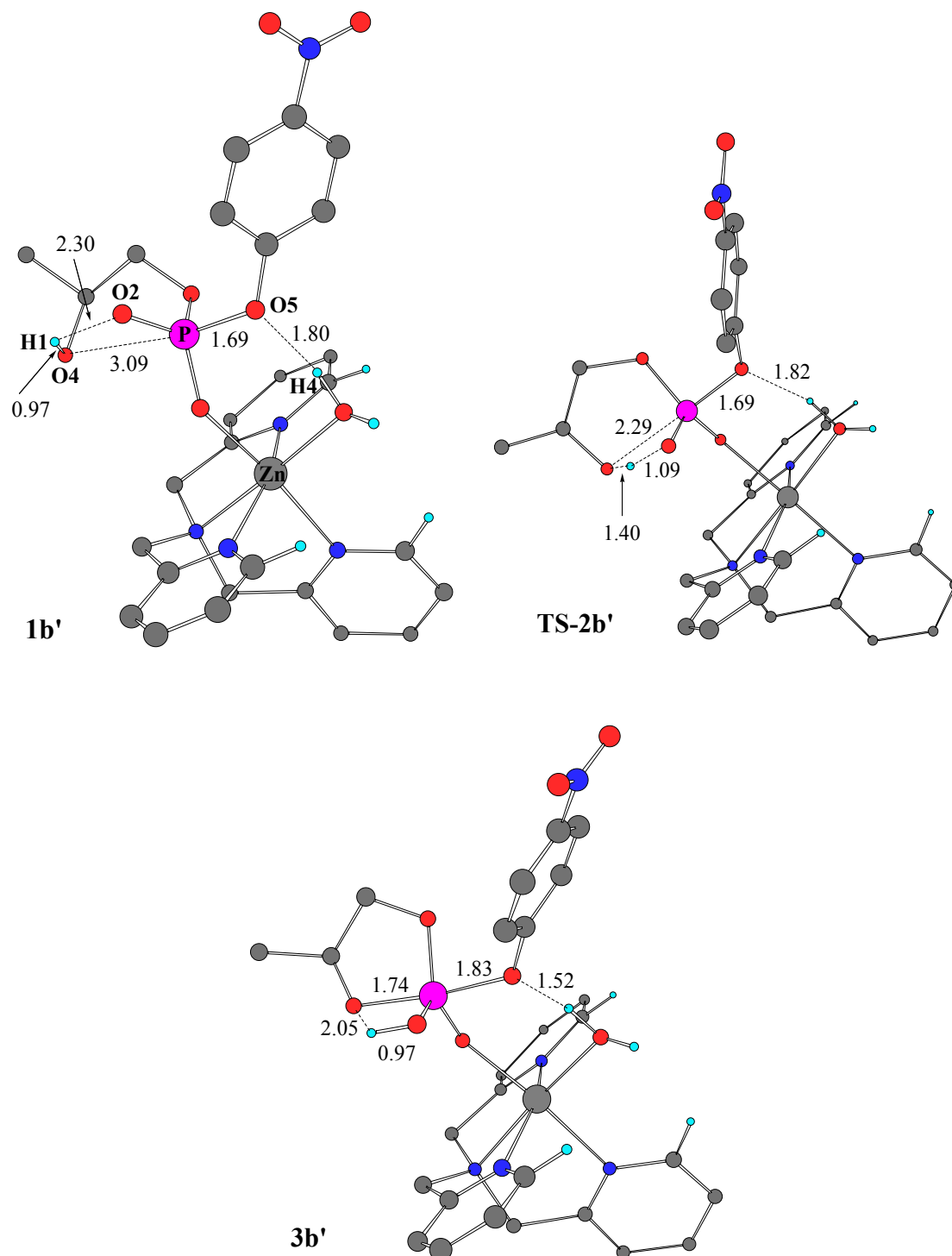
**Figure S4.** Optimized geometries of the reactant and the rate-determining transition state in the general base mode catalyzed by catalyst **B**. The active catalyst is of the Zn-OH form. Distances are in Å. Certain hydrogen atoms are omitted for clarity.

### The coordinates of all species

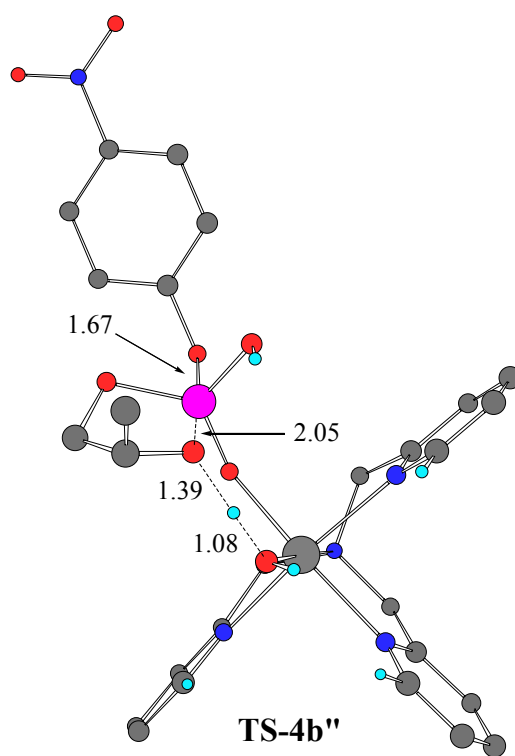
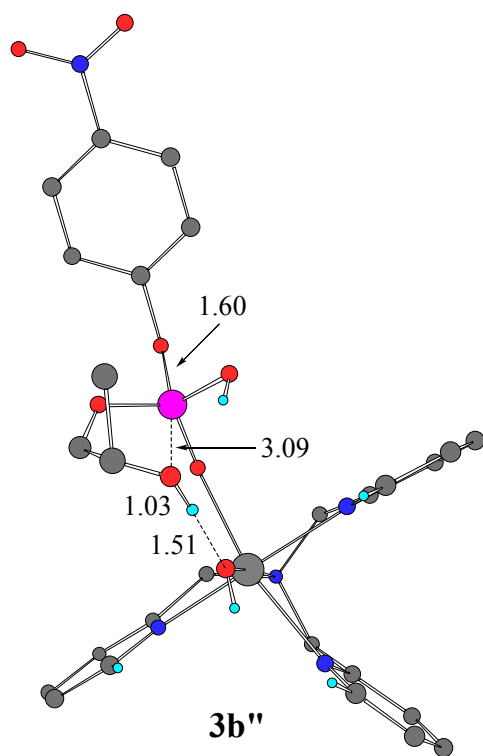
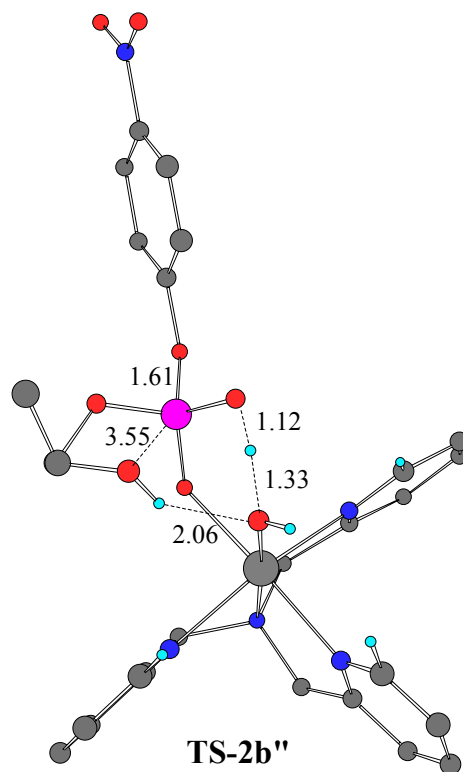
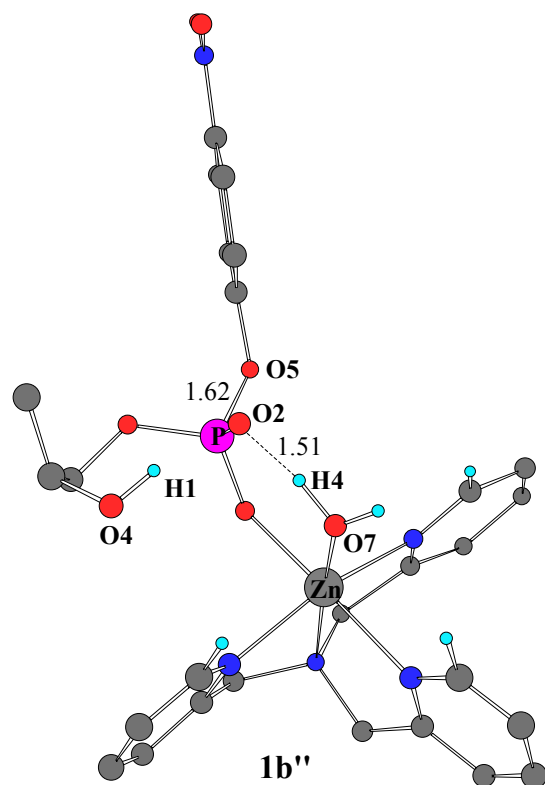
- (1) reaction with catalyst **A**:
- (2) reaction with catalyst **B**:
- (3) species in Gao's mechanism:
- (4) reaction in the water-assisted mode in the absence of catalyst

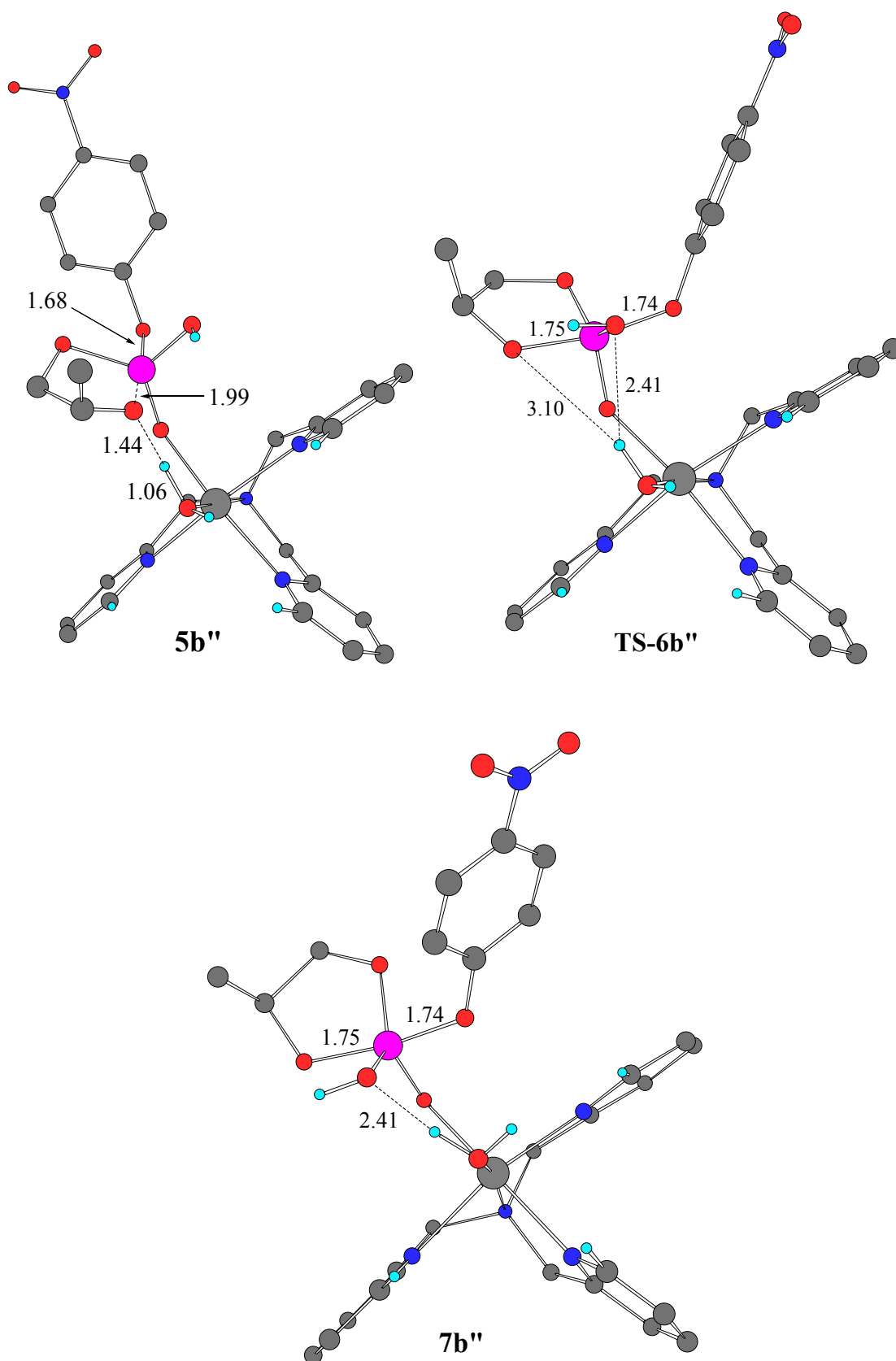


**Figure S1.** Optimized geometries of stationary points in the water-assisted proton transfer mode in the absence of catalyst. Distances are in Å. Certain hydrogen atoms are omitted for clarity.

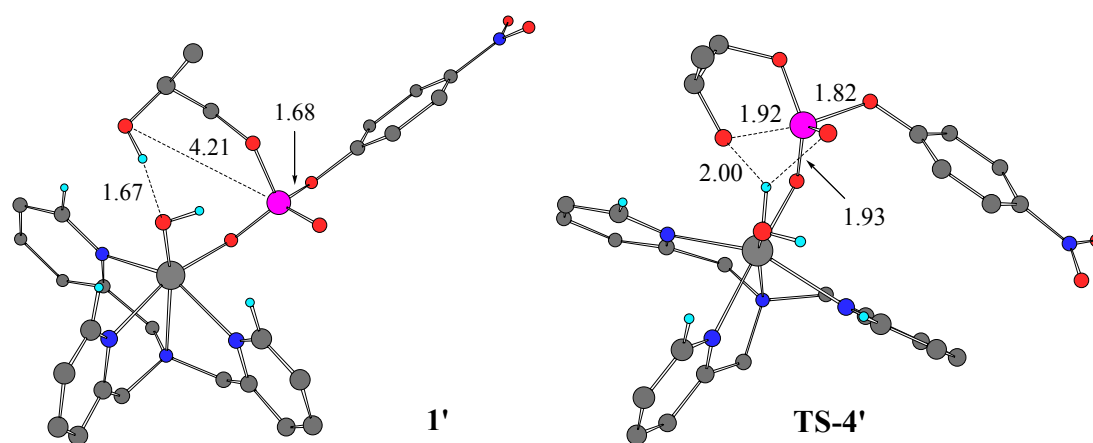


**Figure S2.** Optimized geometries of stationary points in the direct proton transfer mode catalyzed by catalyst **B**. Distances are in Å. Certain hydrogen atoms are omitted for clarity.





**Figure S3.** Optimized geometries of stationary points in the general base mode catalyzed by catalyst **B**. Distances are in Å. Certain hydrogen atoms are omitted for clarity.



**Figure S4.** Optimized geometries of the reactant and the rate-determining transition state in the general base mode catalyzed by catalyst **B**. The active catalyst is of the Zn-OH form. Distances are in Å. Certain hydrogen atoms are omitted for clarity.

## The coordinates of all species

### (1) catalyst A:

#### 1a:

N	-2.96096100	0.89678600	0.87597200
C	-2.91894100	0.40851400	2.27090900
C	-4.27321100	0.64697800	0.23013100
C	-2.52291500	2.31068700	0.75875900
C	-4.34442200	-0.62793900	-0.59843000
C	-5.51463800	-1.37161000	-0.67224700
C	-5.55699100	-2.46001800	-1.55342900
C	-3.31962500	-1.92772900	-2.23603600
C	-4.46189000	-2.73880700	-2.35621500
C	-2.15543300	2.65177200	-0.67212300
C	-2.45742300	3.88973600	-1.22247200
C	-2.04043400	4.15494700	-2.53424200
C	-1.09580100	1.94730900	-2.62322600
C	-1.35797900	3.18363300	-3.24616100
C	-2.91701700	-1.10560400	2.33717700
C	-3.67181500	-1.79519900	3.27460400
C	-3.54418900	-3.19041200	3.33277900
C	-1.91840300	-3.05652800	1.56920700
C	-2.65985100	-3.83197200	2.48452000
N	-2.08373600	-1.72624500	1.47133500
N	-3.24969100	-0.93436600	-1.33081000
N	-1.48772600	1.69598500	-1.36036100
N	-0.47106900	0.91787300	-3.31136100
N	-1.00424700	-3.63951300	0.70674400
N	-2.19318500	-2.11785300	-3.03833900
H	-0.21220500	-3.04986100	0.48542200
H	-2.34674000	-2.74293700	-3.82060900
H	-1.76719200	-1.24242800	-3.33910100
H	-3.75254800	0.81579000	2.86029200
H	-1.98310700	0.76977600	2.71131700
H	-4.47219400	1.48018200	-0.45394300
H	-5.07743400	0.65164000	0.97671300
H	-1.62595000	2.44623600	1.37548200
H	-3.29474100	3.00163200	1.12502700
H	-6.37429400	-1.10924900	-0.06493700
H	-6.45278900	-3.06953400	-1.62675100
H	-4.48500000	-3.54833100	-3.07906600
H	-2.99645200	4.63132200	-0.64291200
H	-2.25382200	5.11597500	-2.99277800



H	-1.02758800	3.35937000	-4.26519200
H	-4.33240600	-1.26273600	3.95048100
H	-4.12152100	-3.76411700	4.05176700
H	-2.51554200	-4.90702600	2.52871700
Zn	-1.40101300	-0.23164800	-0.19190000
O	0.04312300	-1.34166200	-1.42145800
H	0.03732200	1.20110000	-4.13875400
H	-0.21285900	-2.17153100	-1.85447400
H	0.03663600	0.25485300	-2.73292800
H	-0.73353400	-4.58671000	0.93568100
H	3.15817500	3.31355500	-0.38795200
C	2.51465800	2.95629300	0.42122300
O	2.00819000	1.67498900	-0.02899600
C	1.38086900	3.95448000	0.67670200
H	3.12153200	2.81434400	1.32051500
P	1.66507700	0.47428900	1.00123500
C	1.94926000	5.32672600	1.04934700
H	0.78962100	4.03850600	-0.24344200
O	0.46648400	3.47067300	1.65811600
O	2.40626500	0.57454300	2.29705500
O	2.23780700	-0.82790800	0.08040000
O	0.17308400	0.17717100	0.99209400
H	2.54519200	5.26410100	1.96657800
H	2.58603900	5.72674600	0.25201100
H	1.13107600	6.03172100	1.22118300
H	0.92525100	3.39939100	2.52269900
H	2.06704100	2.76054000	4.79282600
O	2.05884200	2.80134900	3.83022600
H	2.24519300	1.90088900	3.48153900
H	0.92627400	-1.38630700	-0.98061000
C	3.59825000	-1.05328900	-0.12650200
C	4.43036000	-1.39459300	0.94366700
C	4.08361000	-0.99064100	-1.43505300
C	5.76987100	-1.68173200	0.69427800
H	4.02886300	-1.41600400	1.95003100
C	5.42090600	-1.28461500	-1.68654900
H	3.41644800	-0.70633500	-2.24268600
C	6.24420700	-1.62677900	-0.61576300
H	6.44734700	-1.95037500	1.49548400
H	5.83339000	-1.24925300	-2.68720200
N	7.65823600	-1.94212700	-0.87903800
O	8.36121800	-2.24018400	0.08389100
O	8.04215500	-1.88837700	-2.04633900

**1a (TPSS/Gao's basis set):**

Zn	-1.41698600	-0.20152300	-0.19330600
P	1.60208000	0.68784500	1.04201700
N	-2.93332000	1.00673600	0.75629300
N	-1.97099800	-1.51663300	1.57499000
N	-3.24405100	-1.07378000	-1.18218000
N	-1.46791700	1.52656300	-1.53293400
N	-0.51804000	0.49879500	-3.40731200
N	-0.67190000	-3.38107700	1.04896700
N	-2.19336200	-2.54350900	-2.66068200
N	7.47256400	-2.14654800	-0.88275400
O	0.02520200	-1.39142000	-1.25852600
O	0.07414700	0.43352800	1.02771400
O	2.11436800	-0.80239500	0.25288800
O	2.36391100	0.85851500	2.35021800
O	2.07957400	1.70958500	-0.16167500
O	0.61325900	3.54558000	1.46493700
O	2.21816900	3.23786100	3.65637500
O	7.73806700	-2.46928000	-2.05573200
O	8.29464000	-2.11318600	0.05010400
C	-2.93150000	0.62464700	2.19150500
C	-4.24781900	0.74425500	0.10571000
C	-2.44683200	2.39948600	0.52249500
C	-4.34991700	-0.63883800	-0.52157100
C	-5.54299000	-1.36077100	-0.50386800
C	-5.59968600	-2.57685300	-1.20890900
C	-4.49470300	-3.00025800	-1.94101700
C	-3.32908300	-2.20197600	-1.92764200
C	-2.09573500	2.58149500	-0.94451500
C	-2.37417200	3.76275400	-1.62948600
C	-1.98134500	3.86215900	-2.97784000
C	-1.34321300	2.79028300	-3.59030800
C	-1.09636300	1.61969800	-2.83374600
C	-2.88421600	-0.88570600	2.35647800
C	-3.65900800	-1.56255500	3.29801600
C	-3.47065800	-2.94956500	3.44285300
C	-2.48766900	-3.59258000	2.69614700
C	-1.72078000	-2.82745400	1.78801000
C	2.62379900	3.02354000	0.18810400
C	1.49314100	4.03194200	0.43819600
C	2.05787000	5.42297200	0.76074500
C	3.46036500	-1.08293200	-0.00568300
C	4.41342800	-1.07075400	1.02655200

C	3.81072900	-1.44045000	-1.31834700
C	5.73679500	-1.41504200	0.73350900
C	5.13004700	-1.79649700	-1.60996600
C	6.07496800	-1.77568600	-0.57696500
H	0.14215300	-2.76739100	1.01334100
H	-0.40782700	-4.31812800	1.34539700
H	-2.34530800	-3.27509800	-3.35091900
H	-1.71589600	-1.73410600	-3.06365600
H	-0.01321700	0.66398700	-4.27326200
H	-0.03796700	-0.12931500	-2.75831800
H	-0.25647800	-2.32902100	-1.30178000
H	0.87721200	-1.30513300	-0.72532500
H	1.08756400	3.59474200	2.33800300
H	2.33528900	2.28971800	3.38757200
H	2.04864100	3.24777000	4.61232500
H	-3.80112500	1.04702600	2.71991700
H	-2.01598300	1.04345400	2.63023000
H	-4.36503500	1.48025200	-0.70271000
H	-5.07255200	0.90204800	0.81707200
H	-1.53481200	2.54086600	1.12105600
H	-3.19402300	3.14729000	0.83167100
H	-6.40675900	-0.98679300	0.04206600
H	-6.51113900	-3.17238600	-1.20492800
H	-4.52555200	-3.91414200	-2.53190900
H	-2.87873700	4.58463200	-1.12601100
H	-2.17982400	4.77188900	-3.54220400
H	-1.03538700	2.83744700	-4.63346600
H	-4.38418700	-1.02644600	3.90701300
H	-4.06701600	-3.51362900	4.15814000
H	-2.28354700	-4.65388100	2.82790800
H	3.22928600	3.30922800	-0.67998000
H	3.27135100	2.92193500	1.06829600
H	0.86889500	4.08091200	-0.46486000
H	2.67807700	5.39158800	1.66690500
H	2.67286100	5.80210300	-0.06852600
H	1.23415400	6.12811900	0.92908300
H	4.11636200	-0.78397300	2.03173300
H	3.05676400	-1.43142000	-2.10357400
H	6.50233100	-1.41452200	1.50486800
H	5.43557800	-2.07760400	-2.61414000

**TS-2a:**

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C	-2.68008300	0.47674400	2.33115800
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C	-3.22833700	2.09208000	0.55235600
C	-4.07468300	-1.50547700	0.07912200
C	-4.85788900	-2.58566900	0.46161100
C	-4.63431400	-3.82162200	-0.16025700
C	-2.94194300	-2.77640200	-1.50219500
C	-3.68103900	-3.92425500	-1.15993600
C	-3.25859300	2.26034400	-0.95655400
C	-4.06986100	3.20581000	-1.56395900
C	-4.00080400	3.33929000	-2.95958900
C	-2.36253300	1.57777000	-2.99694400
C	-3.15007100	2.52743600	-3.68493300
C	-2.04962200	-0.88401900	2.55595500
C	-2.33329100	-1.64271800	3.68038600
C	-1.63413800	-2.84688700	3.85922600
C	-0.41207200	-2.37333100	1.84079000
C	-0.66416900	-3.21587700	2.94636900
N	-1.14334900	-1.26251700	1.62611900
N	-3.10047700	-1.60916200	-0.85275500
N	-2.42254300	1.45796400	-1.65636400
N	-1.54306600	0.70543100	-3.68054100
N	0.57779100	-2.65812200	0.92165300
N	-1.99045200	-2.79779100	-2.52003200
H	1.08132600	-1.83844100	0.58309100
H	-2.01942000	-3.62200800	-3.10733400
H	-1.96360100	-1.94175700	-3.06771000
H	-3.51480200	0.63243600	3.02924900
H	-1.92045300	1.23839700	2.53934500
H	-4.87870100	0.43756900	-0.16937500
H	-5.00020200	-0.15616900	1.48682900
H	-2.33877500	2.59899500	0.94291800
H	-4.11390700	2.56203200	1.00308400
H	-5.62483200	-2.47074400	1.21999800
H	-5.22044100	-4.69085400	0.12296600
H	-3.51551800	-4.85867900	-1.68710800
H	-4.73339600	3.82687100	-0.97181900
H	-4.61665900	4.07411000	-3.46964300
H	-3.08167900	2.60575200	-4.76549000
H	-3.07060600	-1.30749200	4.40199800
H	-1.83543900	-3.47421600	4.72267400
H	-0.07696700	-4.11874700	3.08255100
Zn	-1.41937300	-0.05640300	-0.32026900
O	-0.02809200	-0.88325400	-1.72617300

H	-1.31276500	0.95871700	-4.63109300
H	-0.09216100	-1.84915200	-1.81612800
H	-0.78422100	0.27844500	-3.15504100
H	1.20333300	-3.40705300	1.18875900
H	3.17825700	4.02591500	-0.71485200
C	2.88604700	3.50528600	0.20027900
O	2.53915100	2.16341200	-0.17811400
C	1.65794100	4.11186400	0.87441200
H	3.73846000	3.47011100	0.88980600
P	1.47311900	1.31121400	0.72129000
C	1.95827400	5.34563300	1.71367800
H	0.90650600	4.35177400	0.10913800
O	1.13585400	3.03689200	1.65829600
O	1.92493100	0.66978900	2.06366900
O	1.95702700	-0.15333600	-0.26797500
O	0.02237800	1.26393600	0.23564500
H	2.69411100	5.12529800	2.49403100
H	2.35816100	6.14570400	1.08084700
H	1.04642600	5.71819300	2.18974900
H	1.60398000	2.91321300	2.78862700
H	1.61403400	2.33858500	4.51368000
O	2.14122100	2.38460400	3.70642100
H	2.07796800	1.41561600	3.03015500
H	0.84797700	-0.62984900	-1.29310600
C	3.26955200	-0.52304700	-0.48505000
C	4.08985900	-0.94412100	0.57186500
C	3.74793000	-0.53484200	-1.80257800
C	5.38528300	-1.37970700	0.30553700
H	3.70817000	-0.91023400	1.58541500
C	5.03851000	-0.97714700	-2.07229100
H	3.10525600	-0.18301600	-2.60380300
C	5.84166700	-1.39527000	-1.01184600
H	6.04374200	-1.71009200	1.09979800
H	5.43355200	-0.99776800	-3.08054600
N	7.20463200	-1.86767100	-1.29233600
O	7.88908100	-2.22989400	-0.33655100
O	7.57374300	-1.87376800	-2.46618700

**TS-2a:**

Zn	-1.42767700	-0.10596700	-0.32939700
P	1.41492100	1.39909800	0.62879100
N	-3.02651200	0.80302000	0.84546600
N	-1.09188600	-1.08030900	1.67486400
N	-3.08249800	-1.64928000	-0.63092400

N	-2.39350300	1.22119000	-1.80837200
N	-1.59254100	0.15331000	-3.72585200
N	0.60079200	-2.56376400	1.06802900
N	-1.99746700	-3.05087900	-2.15211700
N	7.21762500	-1.95822900	-1.15290800
O	-0.04869500	-1.05273000	-1.62022400
O	-0.02689800	1.32351600	0.03612400
O	1.80911400	0.78470500	2.03050400
O	1.94432500	-0.16567300	-0.30526800
O	2.56414900	2.17517800	-0.29973300
O	1.05408200	3.15995100	1.43765700
O	2.03259200	2.63287800	3.56098100
O	7.50496700	-2.36005400	-2.29704800
O	8.00548100	-1.94454700	-0.18814800
C	-2.56681900	0.75390700	2.25606800
C	-4.29227800	0.04395800	0.64119300
C	-3.10467800	2.19018600	0.30760200
C	-4.07014100	-1.41525500	0.27204600
C	-4.90226800	-2.42526400	0.75410500
C	-4.71329300	-3.73326200	0.27217800
C	-3.74768300	-3.97468000	-0.70054100
C	-2.96106200	-2.89258400	-1.15440400
C	-3.17693100	2.15688300	-1.21081600
C	-3.97049600	3.04683500	-1.93158700
C	-3.94221000	2.97425700	-3.33833500
C	-3.14321800	2.02528900	-3.96269500
C	-2.36678700	1.14977400	-3.16251600
C	-1.97585900	-0.60457800	2.59015600
C	-2.26130900	-1.26699700	3.78163800
C	-1.59497300	-2.48080700	4.04279000
C	-0.64315100	-2.94724400	3.14530200
C	-0.37818500	-2.19410500	1.97410000
C	2.89251400	3.54509100	0.03578100
C	1.62248100	4.19108500	0.59308800
C	1.86187600	5.48340400	1.36921600
C	3.25797400	-0.55270700	-0.48795900
C	4.18292000	-0.56687500	0.57594000
C	3.64271600	-0.99567400	-1.77005800
C	5.48470400	-1.02184500	0.35365300
C	4.94044600	-1.46061800	-1.99245400
C	5.84769700	-1.46718200	-0.92480900
H	1.12035900	-1.76690600	0.68167400
H	1.22278800	-3.29772500	1.39735700
H	-2.05270200	-3.93659000	-2.64950600

H	-1.95101700	-2.25809600	-2.79597100
H	-1.37082800	0.26831700	-4.71004300
H	-0.81849300	-0.19171500	-3.14894500
H	-0.10196400	-2.02707700	-1.52122300
H	0.83398000	-0.71521600	-1.21118900
H	1.96460300	1.62934700	2.97715100
H	1.46327000	2.63755500	4.34979300
H	1.51184900	3.10610400	2.58966900
H	-3.38176900	1.00687800	2.95345800
H	-1.77414700	1.50772700	2.35715100
H	-4.82579400	0.51752700	-0.19542800
H	-4.93830800	0.11951500	1.52932000
H	-2.17817500	2.69587600	0.61193500
H	-3.96393600	2.74233600	0.72109000
H	-5.67772000	-2.20122900	1.48380600
H	-5.33531500	-4.54905800	0.63678800
H	-3.60951600	-4.96801700	-1.12425600
H	-4.59032400	3.77785300	-1.41647400
H	-4.54584900	3.65551700	-3.93576600
H	-3.10607600	1.94502500	-5.04777300
H	-2.97846100	-0.85311600	4.48783500
H	-1.80271500	-3.03730400	4.95539600
H	-0.07761500	-3.85605700	3.34441900
H	3.24168400	4.01092900	-0.89190400
H	3.70202600	3.54343700	0.77963100
H	0.90434000	4.35665500	-0.22345200
H	2.56124700	5.32485800	2.20097500
H	2.28676000	6.24680500	0.70242700
H	0.91782100	5.87275800	1.77102400
H	3.86924300	-0.22482200	1.55836000
H	2.92560000	-0.95817900	-2.58882300
H	6.21795500	-1.04388900	1.15567500
H	5.26076000	-1.80461400	-2.97231200

**3a:**

N	-3.15215900	0.65072900	0.89314100
C	-2.76060300	0.46585800	2.30604700
C	-4.35506100	-0.14047700	0.53630000
C	-3.28788100	2.07781400	0.51856400
C	-4.05238200	-1.53415000	0.01481800
C	-4.82307700	-2.62825700	0.38246400
C	-4.56078100	-3.86115400	-0.23059400
C	-2.85893900	-2.78524600	-1.53620800

C	-3.58279900	-3.94716000	-1.20739800
C	-3.27009800	2.25487800	-0.98958600
C	-4.07788400	3.18940300	-1.61781800
C	-3.96318800	3.33444000	-3.00951100
C	-2.29232800	1.60263500	-3.00220100
C	-3.07327400	2.54394700	-3.71029400
C	-2.11482200	-0.88503400	2.54533100
C	-2.42176500	-1.65323500	3.65668600
C	-1.70839800	-2.84697800	3.85213900
C	-0.43069400	-2.34396500	1.87422500
C	-0.70491700	-3.19571100	2.96892900
N	-1.17311800	-1.24281600	1.64272300
N	-3.05535100	-1.61971800	-0.89409300
N	-2.39555500	1.47282900	-1.66464600
N	-1.43558800	0.75155400	-3.66286400
N	0.58901900	-2.60935700	0.98708900
N	-1.88483600	-2.79154700	-2.53144600
H	1.08329000	-1.78187700	0.64771900
H	-1.88458100	-3.61546400	-3.11962900
H	-1.85215200	-1.93366400	-3.07511600
H	-3.61860200	0.60519700	2.97906400
H	-2.02039900	1.23916600	2.53995300
H	-4.87697900	0.39537100	-0.26438100
H	-5.04474100	-0.19698900	1.38861900
H	-2.42489700	2.60295700	0.94284600
H	-4.19881600	2.52546500	0.94083700
H	-5.60972900	-2.52661000	1.12234100
H	-5.13595100	-4.74120500	0.04151500
H	-3.38609400	-4.87948200	-1.72756500
H	-4.77336500	3.79341200	-1.04496600
H	-4.57498500	4.06133300	-3.53560500
H	-2.96963500	2.63096400	-4.78739400
H	-3.18718300	-1.33380600	4.35583700
H	-1.92683000	-3.48204100	4.70576000
H	-0.10869000	-4.09054800	3.11844700
Zn	-1.40249500	-0.03501700	-0.30736000
O	0.01740500	-0.83017800	-1.67891200
H	-1.17782200	1.01119000	-4.60432900
H	-0.03264300	-1.79551900	-1.77929000
H	-0.69716800	0.31652300	-3.11413400
H	1.21828500	-3.35047300	1.26590000
H	2.97023900	4.01803100	-0.96267200
C	2.84407000	3.52374300	0.00367900
O	2.54148500	2.14153000	-0.25252700



C	1.66603800	4.06160100	0.81521400
H	3.77997700	3.57917000	0.57225000
P	1.45388400	1.45235000	0.77072000
C	1.98965300	5.27932500	1.66374800
H	0.82524100	4.28532300	0.14055400
O	1.30959200	2.94706200	1.63952800
O	1.92525000	0.64591600	2.08626200
O	1.93008400	-0.15080700	-0.17656200
O	0.00124300	1.31011000	0.30213700
H	2.81355700	5.06760700	2.35361200
H	2.28403800	6.11992800	1.02566900
H	1.11523100	5.59140600	2.24316700
H	1.70449000	3.00811300	3.61073100
H	1.70981600	2.37566600	5.05047200
O	2.14046600	2.35687400	4.18770700
H	2.01132800	1.20642600	2.89703000
H	0.88215400	-0.57078900	-1.19665400
C	3.22638100	-0.52636500	-0.43453900
C	4.06601800	-0.98476800	0.59364700
C	3.68654900	-0.51303500	-1.76101800
C	5.35048200	-1.43008200	0.29430700
H	3.70525600	-0.97672400	1.61535600
C	4.96582100	-0.96371400	-2.06515000
H	3.03551300	-0.13265000	-2.54221400
C	5.78396200	-1.41846500	-1.03086700
H	6.01823000	-1.78935200	1.06806000
H	5.34213800	-0.96403900	-3.08081400
N	7.13407900	-1.89987000	-1.34750200
O	7.83241100	-2.29339800	-0.41378200
O	7.48245900	-1.88266700	-2.52801300

**TS-4a:**

N	-3.17075600	0.71217500	0.86736100
C	-2.79969600	0.55136600	2.28850100
C	-4.38384500	-0.06615900	0.51403100
C	-3.28333500	2.13304700	0.46316700
C	-4.10097200	-1.47414400	0.02181900
C	-4.88856600	-2.54984500	0.40691600
C	-4.64139200	-3.79729900	-0.18331500
C	-2.92022800	-2.76917600	-1.50251000
C	-3.66175400	-3.91500200	-1.15484800
C	-3.22949500	2.28237300	-1.04706000
C	-4.01207900	3.21367000	-1.71056300

C	-3.86229200	3.33234700	-3.10181500
C	-2.21171300	1.58173000	-3.02435500
C	-2.96533500	2.52004200	-3.76700500
C	-2.18054200	-0.80464900	2.56361300
C	-2.51921300	-1.54348200	3.68485200
C	-1.83188300	-2.74715500	3.91471300
C	-0.51430600	-2.30897300	1.94478700
C	-0.82425200	-3.13278700	3.05384300
N	-1.23179700	-1.19602900	1.68131900
N	-3.10271400	-1.58978300	-0.88188100
N	-2.34736100	1.47945900	-1.68646400
N	-1.35183700	0.70951900	-3.64744600
N	0.50977400	-2.61570700	1.08438900
N	-1.94414200	-2.80670700	-2.49259400
H	1.02207000	-1.81350000	0.70139800
H	-1.95148500	-3.63713700	-3.07099800
H	-1.87995400	-1.95350600	-3.04011900
H	-3.66317900	0.71921800	2.94782000
H	-2.04995800	1.31756800	2.51503100
H	-4.88900700	0.46323800	-0.30156700
H	-5.08164800	-0.09415200	1.36112100
H	-2.42595800	2.65865900	0.89785100
H	-4.19885500	2.59738100	0.85658100
H	-5.67592500	-2.42385700	1.14225900
H	-5.22958000	-4.66421800	0.10282300
H	-3.47600500	-4.85954400	-1.65665900
H	-4.71488500	3.83487600	-1.16569700
H	-4.45378700	4.05567800	-3.65538600
H	-2.83645300	2.58549700	-4.84292700
H	-3.28882400	-1.19538000	4.36548100
H	-2.07575600	-3.36098200	4.77700300
H	-0.24926500	-4.03702500	3.22813400
Zn	-1.41359100	-0.03453900	-0.29723400
O	-0.00369600	-0.84650000	-1.61570700
H	-1.06783400	0.94276900	-4.58796300
H	-0.09332400	-1.80662100	-1.73134300
H	-0.64669500	0.25187700	-3.07019100
H	1.11483500	-3.36955600	1.38063000
H	3.11963800	3.84329400	-1.06019700
C	2.95278400	3.41119100	-0.07120100
O	2.50889900	2.05144600	-0.26466000
C	1.83921000	4.10466900	0.71528000
H	3.89406700	3.39607300	0.49022700
P	1.41305100	1.55221900	0.83426700

C	2.28665500	5.31562900	1.51335300
H	1.02000900	4.38033300	0.03577900
O	1.36524800	3.06623900	1.59698600
O	1.90348800	0.72527300	2.11053100
O	1.88717300	-0.33150900	-0.15750700
O	-0.01457400	1.34609800	0.36284400
H	3.08970100	5.05174400	2.20955900
H	2.66046500	6.09412800	0.83939700
H	1.45014100	5.73755000	2.07835700
H	1.96472900	3.15645600	3.65956000
H	2.25351200	2.43978200	5.02670900
O	2.47593300	2.45155000	4.08770600
H	2.12857400	1.29672900	2.89197700
H	0.90546600	-0.62608700	-1.09504300
C	3.16174600	-0.70201100	-0.43846100
C	4.03474100	-1.09905800	0.59339600
C	3.61553100	-0.72878200	-1.77158200
C	5.32644200	-1.52007300	0.29796300
H	3.68421100	-1.06443000	1.61897300
C	4.90318800	-1.15478800	-2.07192700
H	2.94707000	-0.40119200	-2.56241900
C	5.74775100	-1.54732300	-1.03215100
H	6.01201500	-1.83137500	1.07701600
H	5.26814700	-1.18471900	-3.09144500
N	7.10499500	-1.99891900	-1.34516100
O	7.82652400	-2.33684100	-0.40575700
O	7.44346600	-2.01536700	-2.52968800

**1a':**

N	2.92892700	0.85463800	-1.04370900
C	2.92453200	0.19180900	-2.36503000
C	4.23057900	0.71966600	-0.34620000
C	2.45451900	2.25982200	-1.11188700
C	4.31495200	-0.45918600	0.61291400
C	5.49613700	-1.16979200	0.77689000
C	5.54396700	-2.16297100	1.76428800
C	3.28846900	-1.60487400	2.36173200
C	4.44243200	-2.37959600	2.57683600
C	2.06730300	2.77389900	0.26255800
C	2.33191900	4.08003200	0.65038400
C	1.89836500	4.49780500	1.91698100
C	1.00873800	2.29563500	2.28204800
C	1.23431500	3.60807100	2.74346700

C	2.92710600	-1.31885500	-2.23908600
C	3.71647400	-2.11769000	-3.05331300
C	3.59084200	-3.50973100	-2.93970400
C	1.89325600	-3.16165300	-1.27584600
C	2.67093700	-4.04294600	-2.05451300
N	2.06077600	-1.82940100	-1.33465100
N	3.21530100	-0.70848600	1.36075100
N	1.42250300	1.89634100	1.06574100
N	0.39802500	1.34603600	3.08585000
N	0.93422100	-3.63341500	-0.39225600
N	2.15485000	-1.73386500	3.16380600
H	0.12563000	-3.03016800	-0.30800000
H	2.30414500	-2.27496700	4.00686100
H	1.70470300	-0.84283300	3.36488300
H	3.77163900	0.52489900	-2.98120500
H	1.99918600	0.48664600	-2.87201400
H	4.38522900	1.62617700	0.25029900
H	5.05385600	0.67156900	-1.07033000
H	1.56196800	2.28102000	-1.74875200
H	3.20898800	2.91915900	-1.56291600
H	6.35965300	-0.95555500	0.15639200
H	6.44873000	-2.74560900	1.91006000
H	4.46880000	-3.11178600	3.37774200
H	2.85667600	4.75626100	-0.01583400
H	2.08377600	5.51449300	2.25070700
H	0.88957100	3.90428600	3.72925700
H	4.40205100	-1.67119700	-3.76549300
H	4.19577400	-4.16712200	-3.55716000
H	2.52500200	-5.11547500	-1.97137800
Zn	1.37229100	-0.16054700	0.14377800
O	-0.09354800	-1.13565100	1.46177400
H	-0.12019400	1.71650100	3.87163400
H	0.15694800	-1.93917400	1.94424500
H	-0.09665000	0.61160600	2.58798600
H	0.67918900	-4.60512700	-0.51114000
H	-3.05309300	3.43645800	0.22314000
C	-2.60940300	2.94020400	-0.64440200
O	-1.94897800	1.76251600	-0.12729100
C	-1.63406100	3.88640800	-1.35198100
H	-3.41003200	2.63535500	-1.32660800
P	-1.66060900	0.50360200	-1.12193300
C	-2.37900500	5.08902600	-1.93515400
H	-0.89215100	4.23365100	-0.62264400
O	-0.86450000	3.20349400	-2.34527300

O	-2.39405000	0.62184300	-2.41463200
O	-2.26153100	-0.75421500	-0.15068600
O	-0.17544500	0.17171000	-1.08850200
H	-3.12225700	4.76909800	-2.67454000
H	-2.89692400	5.65577000	-1.15274400
H	-1.67166300	5.75761500	-2.43297700
H	-1.44940500	2.64396500	-2.88412700
H	-0.96348600	-1.22123100	1.00163000
C	-3.62461700	-0.96064500	0.04883800
C	-4.47468600	-1.22445500	-1.03000100
C	-4.09898500	-0.95742900	1.36365300
C	-5.81864300	-1.49176000	-0.78221500
H	-4.08336800	-1.20243000	-2.04028100
C	-5.44067000	-1.23203300	1.61235800
H	-3.41908000	-0.73525800	2.18046600
C	-6.28151000	-1.49540300	0.53298200
H	-6.50840200	-1.70163800	-1.59054600
H	-5.84335900	-1.24064800	2.61759500
N	-7.70075500	-1.78809400	0.79278500
O	-8.41932900	-2.01691500	-0.17753000
O	-8.07356200	-1.78632400	1.96509700

**TS-2a':**

N	-2.93737200	0.78882800	1.02148300
C	-2.38438800	0.56631400	2.37576200
C	-4.22090700	0.07781600	0.80811200
C	-3.01240300	2.22603900	0.66385800
C	-4.07709700	-1.30574200	0.19289800
C	-4.90164800	-2.35441100	0.57581200
C	-4.79638300	-3.56984000	-0.11405700
C	-3.12527000	-2.56909500	-1.51514400
C	-3.91543000	-3.68320200	-1.17716400
C	-3.16592300	2.40908900	-0.83604600
C	-3.98604900	3.39228200	-1.36898400
C	-4.04026200	3.52684000	-2.76416600
C	-2.48880000	1.70050400	-2.95101600
C	-3.29468300	2.68132500	-3.56550300
C	-1.82408200	-0.83435600	2.52914900
C	-2.04590400	-1.59041200	3.67056300
C	-1.41981000	-2.84081600	3.77082100
C	-0.37168400	-2.42192000	1.64935200
C	-0.57013500	-3.26206400	2.76284600
N	-1.04165900	-1.26373200	1.51263800

N	-3.17107100	-1.42695500	-0.80465900
N	-2.43466900	1.57561100	-1.61231600
N	-1.76314600	0.79338000	-3.70395700
N	0.51391700	-2.75546900	0.63118700
N	-2.23629100	-2.59767700	-2.58662700
H	1.08328600	-1.96944800	0.32917000
H	-2.34762400	-3.39259200	-3.20375000
H	-2.19071300	-1.72102800	-3.10125500
H	-3.13990400	0.76186300	3.14961600
H	-1.56268300	1.27867600	2.51734300
H	-4.82172100	0.67563100	0.11294600
H	-4.78809800	0.01326500	1.74553900
H	-2.06795900	2.68213400	0.98070100
H	-3.83138700	2.73393100	1.19206000
H	-5.61080500	-2.23049900	1.38717300
H	-5.41840600	-4.41416900	0.16795000
H	-3.84354800	-4.59971700	-1.75436000
H	-4.56392700	4.04064300	-0.71914500
H	-4.66733700	4.28980200	-3.21580400
H	-3.32070300	2.76279200	-4.64764200
H	-2.68224300	-1.21497300	4.46477000
H	-1.57744400	-3.46431300	4.64595600
H	-0.03259400	-4.20237300	2.83622500
Zn	-1.42549200	-0.01018700	-0.37942200
O	-0.06148900	-0.83368900	-1.86702300
H	-1.61398100	1.04860000	-4.67096000
H	-0.12671800	-1.79863700	-1.96147600
H	-0.94386300	0.39455400	-3.25366800
H	1.08878400	-3.56415800	0.83318700
H	3.44122800	4.05866700	0.84679900
C	2.98808700	3.20296000	1.35106800
O	2.53487100	2.31692600	0.29686600
C	1.78659000	3.58585500	2.23267900
H	3.75431800	2.67536600	1.93187800
P	1.48320900	1.15336300	0.66963700
C	2.22739100	4.11393900	3.59497100
H	1.20767500	4.36479200	1.71153000
O	0.97142000	2.43683100	2.32791100
O	1.79581600	0.34256300	1.98853200
O	2.09592100	0.00682300	-0.47721200
O	0.09065500	1.27192500	0.06798900
H	2.78895400	3.34974500	4.14418000
H	2.86300800	5.00129700	3.48926300
H	1.35362400	4.39077900	4.19159200

H	1.49055400	1.27814200	2.60165800
H	0.83541100	-0.58361900	-1.52880800
C	3.44620900	-0.28803700	-0.62979400
C	4.17388200	-0.90306500	0.39579600
C	4.03674200	-0.00851200	-1.86622900
C	5.50691800	-1.24298200	0.17541400
H	3.69924000	-1.09286300	1.35177300
C	5.36622900	-0.35295300	-2.08980100
H	3.45178400	0.48451000	-2.63609600
C	6.08264900	-0.96671200	-1.06335400
H	6.10304000	-1.71908100	0.94440900
H	5.85448700	-0.15023000	-3.03501300
N	7.48848300	-1.33607100	-1.29629600
O	8.09315100	-1.87582100	-0.37171900
O	7.96497000	-1.08315900	-2.40119900

**3a':**

N	-3.11890400	0.54219600	1.01462600
C	-2.76047400	0.13709600	2.39017000
C	-4.31417900	-0.17781500	0.51178600
C	-3.24356000	2.01127900	0.86415900
C	-4.00221200	-1.47432300	-0.21565100
C	-4.78912100	-2.60515900	-0.04606400
C	-4.51490000	-3.72997800	-0.83578000
C	-2.76991200	-2.48015100	-1.90885300
C	-3.50880800	-3.67181900	-1.78601000
C	-3.19862800	2.41889800	-0.59790100
C	-3.99040000	3.44607100	-1.08682700
C	-3.85556200	3.80006800	-2.43845100
C	-2.19609000	2.07327600	-2.67318400
C	-2.96122600	3.11689500	-3.23995100
C	-2.11458600	-1.23449000	2.42847400
C	-2.43970900	-2.16808700	3.39983200
C	-1.72818800	-3.37815300	3.41772700
C	-0.41537000	-2.57165200	1.56857200
C	-0.70771600	-3.58491500	2.50874800
N	-1.15471100	-1.44712600	1.49965400
N	-2.97971900	-1.42678100	-1.09902700
N	-2.31986200	1.74139100	-1.37302600
N	-1.33254000	1.32628800	-3.44438000
N	0.62340900	-2.69268600	0.66859700
N	-1.76613300	-2.34046800	-2.86554200
H	1.12748300	-1.82310600	0.48905300

H	-1.75035800	-3.06868200	-3.56879400
H	-1.72692500	-1.41302600	-3.27955600
H	-3.63521800	0.16758500	3.05516000
H	-2.03080000	0.86477000	2.76254600
H	-4.81952800	0.47912300	-0.20505100
H	-5.02274100	-0.36567500	1.32918800
H	-2.38717400	2.45874900	1.38080300
H	-4.16085000	2.39264800	1.33479900
H	-5.59640200	-2.61227600	0.67839500
H	-5.10262700	-4.63593300	-0.72112700
H	-3.30226800	-4.51319800	-2.44008100
H	-4.68943400	3.96169600	-0.43716900
H	-4.45456300	4.60404900	-2.85580100
H	-2.84156400	3.36625100	-4.28970400
H	-3.21822300	-1.96166200	4.12648700
H	-1.96099700	-4.13931900	4.15668600
H	-0.11293200	-4.49291700	2.52727600
Zn	-1.35274600	0.04521800	-0.24688400
O	0.11542400	-0.53001000	-1.68633600
H	-1.06069500	1.72845500	-4.33036600
H	0.07559300	-1.47160200	-1.92452200
H	-0.59576000	0.82228400	-2.95660600
H	1.24568700	-3.47214600	0.83687200
H	2.99304800	4.22729600	0.04286800
C	2.86279700	3.52672400	0.87104500
O	2.57590200	2.23369800	0.30512500
C	1.67305400	3.86212100	1.77505600
H	3.79472700	3.45562700	1.44425700
P	1.46705200	1.34157800	1.12787700
C	1.99090300	4.82572900	2.90471300
H	0.84751400	4.25933900	1.16343400
O	1.28999400	2.58822000	2.29331700
O	1.89618900	0.30339400	2.32314100
O	2.00203900	-0.05009400	-0.03227600
O	0.03360400	1.27824800	0.59078500
H	2.79463900	4.43287400	3.53580100
H	2.30524200	5.79477900	2.50121400
H	1.10847800	4.98828500	3.52997700
H	1.88813100	0.80224800	3.15634200
H	0.96178100	-0.33837700	-1.16006900
C	3.31675000	-0.35594800	-0.30550600
C	4.11080000	-1.02906200	0.63570900
C	3.83687600	-0.04767700	-1.57154300
C	5.41424900	-1.39447400	0.30935300



H	3.70174500	-1.24924700	1.61489100
C	5.13595500	-0.41531300	-1.90378000
H	3.21776100	0.49451300	-2.27937600
C	5.90954500	-1.08592600	-0.95647700
H	6.04933800	-1.91582100	1.01532900
H	5.56057000	-0.18854600	-2.87409300
N	7.28150300	-1.48022900	-1.30363700
O	7.93734000	-2.07201200	-0.44712400
O	7.68711900	-1.19602600	-2.43009900

**1a":**

N	-2.89223000	0.15066500	-1.77813300
C	-2.18617100	1.23000600	-2.50971100
C	-4.25782800	0.56607300	-1.38643900
C	-2.87568300	-1.14985500	-2.48252700
C	-4.75491300	-0.06389300	-0.10091700
C	-6.09409700	-0.39092400	0.03417200
C	-6.54698500	-0.84010200	1.28441900
C	-4.29888500	-0.60076400	2.11510300
C	-5.65594500	-0.94042800	2.33160500
C	-2.81433700	-2.33842400	-1.53567400
C	-3.54344300	-3.50174400	-1.74764900
C	-3.33228100	-4.58365000	-0.88371800
C	-1.66605300	-3.28609700	0.24979600
C	-2.37400800	-4.49060700	0.11713400
C	-1.90659400	2.42130400	-1.60656500
C	-1.83614300	3.70167200	-2.12618000
C	-1.47879000	4.75059600	-1.26162600
C	-1.34998200	3.15772500	0.53957300
C	-1.23458600	4.48771700	0.07082400
N	-1.67261300	2.14907800	-0.29711000
N	-3.85514700	-0.18258000	0.90776900
N	-1.93262400	-2.22213900	-0.52159200
N	-0.64018500	-3.10885800	1.19865000
N	-1.17784700	2.87887200	1.87106400
N	-3.39265700	-0.72604400	3.13256600
H	-0.51528200	3.47335900	2.35408800
H	-2.48754500	-0.28241800	3.03901500
H	-3.74676000	-0.83192500	4.07095400
H	-2.74945900	1.55683300	-3.39535300
H	-1.22871500	0.81909800	-2.84798400
H	-4.96846400	0.36881900	-2.20067200
H	-4.23882300	1.65059500	-1.23466600

H	-1.96875500	-1.18136400	-3.09671200
H	-3.73450000	-1.24546900	-3.16020800
H	-6.77423300	-0.28247800	-0.80377300
H	-7.59120500	-1.10084100	1.42930900
H	-5.97423400	-1.27591500	3.31372200
H	-4.25381600	-3.56789200	-2.56495800
H	-3.89398800	-5.50396000	-1.01281700
H	-2.15322700	-5.33357500	0.76436100
H	-2.04063800	3.88302400	-3.17588500
H	-1.40448000	5.76672000	-1.63763400
H	-0.97308100	5.27748800	0.76716000
Zn	-1.67251200	-0.03842000	0.06250300
O	-0.76996000	-0.32393500	2.01257400
H	-0.42812000	-3.95181200	1.72169300
H	-0.76680300	-1.29886700	2.12701600
H	0.20779100	-2.74787300	0.76464600
H	-1.09319100	1.90495200	2.12892900
H	3.88698000	2.63372500	-1.15601200
C	3.25830400	2.31426400	-0.32197700
O	2.25353400	1.44752700	-0.92748600
C	2.63072500	3.52883900	0.35605900
H	3.87114400	1.75018900	0.38780500
P	1.59295300	0.17984500	-0.19581200
C	3.69796400	4.57208600	0.68451300
H	1.90360200	3.95967400	-0.34926900
O	1.94041300	3.18681700	1.56322300
O	1.61002900	0.37346900	1.32404700
O	2.51593500	-1.10855400	-0.61446600
O	0.24274800	-0.11791600	-0.82265800
H	4.48152000	4.14461200	1.31945100
H	4.15730800	4.97270000	-0.22567100
H	3.24043100	5.40040200	1.23217000
H	1.84307000	2.21795400	1.62866700
H	0.20603100	-0.05760100	1.89078900
C	3.88568700	-1.19870300	-0.38934300
C	4.41551000	-1.15906400	0.90514100
C	4.70290600	-1.39929700	-1.50498300
C	5.78871100	-1.31591300	1.08069700
H	3.75904700	-1.00209800	1.75370600
C	6.07432600	-1.56124300	-1.32882800
H	4.25543000	-1.43244000	-2.49270900
C	6.59717800	-1.51457700	-0.03723400
H	6.23829900	-1.29215900	2.06587000
H	6.73909600	-1.72135800	-2.16873900

N	8.04771500	-1.68558600	0.15258200
O	8.47724200	-1.63674600	1.30345700
O	8.73233900	-1.86553600	-0.85228600

**TS-2a”:**

N	-2.75744100	-0.20751000	-1.87249500
C	-2.20811900	0.87842100	-2.71924900
C	-4.21253500	-0.03274400	-1.65327200
C	-2.41631700	-1.55862500	-2.36765700
C	-4.70285300	-0.45519300	-0.28183600
C	-5.96217100	-1.01038900	-0.12724000
C	-6.43273400	-1.23099700	1.17807600
C	-4.37028700	-0.31563600	2.01721400
C	-5.64881400	-0.87714400	2.25611700
C	-2.37833600	-2.59657100	-1.26012800
C	-2.95027100	-3.85136600	-1.40868300
C	-2.77592200	-4.78522000	-0.37692800
C	-1.45043100	-3.16042900	0.79610300
C	-2.01346300	-4.45107800	0.72885300
C	-2.18112400	2.20131700	-1.97057200
C	-2.43289900	3.40548200	-2.60849800
C	-2.32142000	4.58806700	-1.86006600
C	-1.72849200	3.26575000	0.05792500
C	-1.96646100	4.52953600	-0.52512700
N	-1.85462500	2.13253400	-0.65880500
N	-3.89790500	-0.14481200	0.76189600
N	-1.67942200	-2.24199000	-0.15857000
N	-0.65066300	-2.77211200	1.86385900
N	-1.29907200	3.14847400	1.36151900
N	-3.58468700	0.09598500	3.05046800
H	-1.45899800	3.93293400	1.97801500
H	-2.65391500	0.45287500	2.86614500
H	-3.86824000	-0.06964200	4.00198600
H	-2.77127100	0.98722600	-3.65695500
H	-1.17791700	0.60542500	-2.96934600
H	-4.78415600	-0.54992200	-2.43583800
H	-4.43149500	1.03649900	-1.75443100
H	-1.41088200	-1.50273600	-2.79859000
H	-3.10531200	-1.87653800	-3.16244600
H	-6.57114900	-1.25008800	-0.99219300
H	-7.41397800	-1.66766900	1.33970500
H	-5.99497700	-1.01393300	3.27588300
H	-3.50984300	-4.10140000	-2.30367500

H	-3.21677200	-5.77472800	-0.45383100
H	-1.82726200	-5.16890900	1.52177500
H	-2.70575400	3.42834000	-3.65803300
H	-2.51326500	5.54930700	-2.32752400
H	-1.86378600	5.43017100	0.07199700
Zn	-1.68350700	0.05365300	0.07134000
O	-0.85614200	0.33191200	1.93415900
H	-0.36994000	-3.52305600	2.48126800
H	-0.97257900	-0.46756800	2.47024900
H	0.12869900	-2.17028500	1.61538500
H	-1.31617700	2.22632000	1.80101900
H	4.05353700	2.49515700	-0.31400200
C	3.24868900	2.17928000	0.35450500
O	2.25003600	1.54870300	-0.50666600
C	2.63980100	3.36836200	1.09165300
H	3.63074100	1.45545500	1.07759800
P	1.58648600	0.12259500	-0.24883800
C	3.71544600	4.09833000	1.89364800
H	2.20767100	4.05209800	0.34607500
O	1.63115500	2.92310500	1.99428800
O	1.50148900	-0.15450600	1.29650700
O	2.59446500	-0.98829400	-0.85263400
O	0.27103800	-0.00115300	-0.96463000
H	4.15142500	3.43210600	2.64552700
H	4.51649200	4.46900900	1.24563400
H	3.27101000	4.94900200	2.41623500
H	0.76091300	2.93063700	1.56369100
H	0.55476400	0.18566000	1.67459400
C	3.97084500	-1.03548200	-0.62612400
C	4.47066700	-1.39451800	0.62831900
C	4.81502700	-0.78102500	-1.70826100
C	5.84948200	-1.48665000	0.80532600
H	3.78801700	-1.59434300	1.44687700
C	6.19342600	-0.87743000	-1.53222400
H	4.38826700	-0.52018300	-2.67094000
C	6.68862800	-1.22467100	-0.27636800
H	6.28034400	-1.76089500	1.76044200
H	6.88334500	-0.69079300	-2.34599200
N	8.14745700	-1.32459500	-0.08725800
O	8.55157900	-1.63336100	1.03146600
O	8.85997000	-1.08917200	-1.06014900

**3a”:**

N	-2.43762600	-0.25010400	-1.99508700
C	-1.75087100	0.78197800	-2.80709500
C	-3.90714000	-0.06948000	-2.03230700
C	-2.03282300	-1.62818000	-2.34300500
C	-4.61875700	-0.41655800	-0.73979800
C	-5.88595400	-0.97553200	-0.76208100
C	-6.56379800	-1.12454800	0.45948400
C	-4.66525500	-0.14426800	1.57067700
C	-5.96706600	-0.70161000	1.62863100
C	-2.17568400	-2.59040600	-1.17699200
C	-2.73851200	-3.85056500	-1.32058500
C	-2.73781600	-4.70725600	-0.21063000
C	-1.56409700	-3.01654300	1.02628800
C	-2.13828600	-4.30158000	0.97041300
C	-1.84799100	2.14866600	-2.14926300
C	-2.00910800	3.30076700	-2.90097900
C	-2.04719200	4.53260800	-2.22625400
C	-1.77821100	3.34939200	-0.14724100
C	-1.93252800	4.56732700	-0.85129600
N	-1.74167900	2.16831200	-0.79876800
N	-3.99566800	-0.03852300	0.39986000
N	-1.64402900	-2.16482000	-0.00973300
N	-0.89677400	-2.55411700	2.15769800
N	-1.62623600	3.33401600	1.21213300
N	-4.05516400	0.33215300	2.69051900
H	-1.89283600	4.15535800	1.73251400
H	-3.08301600	0.63242500	2.63489300
H	-4.47386200	0.17836300	3.59326800
H	-2.15417500	0.82920100	-3.82877200
H	-0.69648200	0.49716200	-2.86949100
H	-4.34306800	-0.63293700	-2.86882000
H	-4.10026000	0.99114500	-2.22960900
H	-0.97206600	-1.59794400	-2.61266000
H	-2.59105900	-2.00059200	-3.21339300
H	-6.34436200	-1.27108200	-1.69966200
H	-7.55826900	-1.56075600	0.48379000
H	-6.47530900	-0.78348200	2.58446100
H	-3.16339300	-4.16119400	-2.26908200
H	-3.18151600	-5.69592100	-0.28244400
H	-2.08062900	-4.96354500	1.82895300
H	-2.10364300	3.24755000	-3.98017200
H	-2.17180400	5.45648600	-2.78349600
H	-1.95740300	5.50589000	-0.30634800
Zn	-1.67621100	0.13324100	0.09672000

O	-1.23610000	0.55839600	2.03958600
H	-0.73860600	-3.25743500	2.86853300
H	-1.31833800	-0.26731900	2.54272300
H	-0.04547600	-2.04093300	1.94303000
H	-1.64347400	2.44343200	1.70510600
H	3.34106400	2.90759100	1.09312100
C	2.84331700	1.98102400	1.38535900
O	2.21124400	1.49694400	0.16842500
C	1.81369900	2.24632300	2.48444700
H	3.59897700	1.26405100	1.72302600
P	1.73148100	-0.01035900	-0.09408700
C	2.47462600	2.85197700	3.71911400
H	1.05086700	2.92589000	2.08531300
O	1.16979000	1.00512200	2.84243000
O	1.89642400	-0.79699900	1.27282800
O	2.77991500	-0.67709100	-1.11753000
O	0.38232600	-0.05071100	-0.73795000
H	3.23185700	2.17445300	4.12731100
H	2.95217500	3.80888800	3.48294300
H	1.72379400	3.02429100	4.49442200
H	0.18832600	0.97971900	2.56025000
H	1.65533300	-0.14837900	2.05590000
C	4.16363600	-0.69135000	-0.90343600
C	4.73141800	-1.72180900	-0.15329000
C	4.94091800	0.29502600	-1.51221100
C	6.11521100	-1.75872800	0.00319600
H	4.09616600	-2.47790200	0.29445200
C	6.32480100	0.25850400	-1.35501800
H	4.46335200	1.06971500	-2.10264900
C	6.88822700	-0.76604200	-0.59633100
H	6.60006900	-2.54037600	0.57491000
H	6.96716900	1.00156200	-1.81133800
N	8.35300900	-0.80380100	-0.42608600
O	8.81948900	-1.72209200	0.24367800
O	9.00623700	0.08744700	-0.96319600

**TS-4a”:**

N	-1.99046600	-0.52423400	-1.98963600
C	-1.44723000	0.61128400	-2.77294200
C	-3.44598500	-0.68694800	-2.19842000
C	-1.24301600	-1.78545300	-2.18955400
C	-4.21323800	-1.14807500	-0.97286500
C	-5.33369300	-1.95028400	-1.12280400

C	-6.10227100	-2.24042000	0.01417700
C	-4.56713600	-0.92016700	1.31402900
C	-5.72909200	-1.72190200	1.23746900
C	-1.31791300	-2.69679200	-0.97662800
C	-1.57146800	-4.05832300	-1.07388800
C	-1.53600200	-4.82436600	0.09916400
C	-0.92238000	-2.84582200	1.31085400
C	-1.19659700	-4.22476300	1.30333400
C	-1.99244500	1.93523200	-2.26165700
C	-2.24469600	2.98889700	-3.12513800
C	-2.69711700	4.20053900	-2.57875200
C	-2.63066400	3.18652400	-0.39854500
C	-2.89494200	4.30910600	-1.21623600
N	-2.18376400	2.02791900	-0.92310600
N	-3.81422900	-0.65382600	0.22414900
N	-1.05022100	-2.09857100	0.20357300
N	-0.49533700	-2.16278500	2.45878200
N	-2.85539000	3.23068400	0.95238600
N	-4.15390900	-0.41626600	2.52032200
H	-3.02897000	4.12477200	1.38422700
H	-3.48162500	0.33955100	2.52051300
H	-4.81085900	-0.42773300	3.28560600
H	-1.66402700	0.50710500	-3.84558200
H	-0.36050600	0.60445200	-2.63902400
H	-3.64117100	-1.36722800	-3.03855800
H	-3.84915000	0.29102400	-2.48370300
H	-0.18990600	-1.52254000	-2.33706700
H	-1.58823500	-2.31428100	-3.08860800
H	-5.61273300	-2.32847400	-2.10041800
H	-6.98848400	-2.86297300	-0.06662800
H	-6.30758600	-1.91895900	2.13467700
H	-1.78899600	-4.51327400	-2.03438500
H	-1.74376000	-5.88967400	0.06283800
H	-1.10742700	-4.80669700	2.21541200
H	-2.09131100	2.87643700	-4.19296000
H	-2.89788300	5.04984200	-3.22511900
H	-3.25274600	5.23158800	-0.76975800
Zn	-1.61859800	0.11706100	0.10362900
O	-1.46465600	0.72779800	2.14479500
H	-0.36026400	-2.77221600	3.25792300
H	-1.36723700	-0.09277800	2.66398900
H	0.35641100	-1.63089300	2.27024100
H	-2.46790500	2.50724100	1.54431800
H	2.75096100	4.01385500	0.85325600

C	2.51980600	3.09032500	1.38901100
O	2.62687300	2.01916900	0.43580600
C	1.10552800	3.06475700	1.96937400
H	3.26892100	2.92599200	2.17289500
P	1.69751000	0.69218200	0.53101200
C	0.99753000	3.79557400	3.30211400
H	0.41205400	3.51576700	1.23938500
O	0.82607600	1.68193800	2.09150100
O	2.02553200	-0.36317800	1.75597800
O	2.59592000	-0.14887800	-0.59151000
O	0.36412400	0.61384400	-0.19632200
H	1.66525800	3.34522300	4.04396200
H	1.26556700	4.85248300	3.18898700
H	-0.02486400	3.74726200	3.68970800
H	-0.51144900	1.20907200	2.17823000
H	1.87011800	0.13239400	2.58034000
C	3.96468500	-0.33281500	-0.54679000
C	4.50277700	-1.42078400	0.14985700
C	4.79108500	0.52555300	-1.28130900
C	5.87604900	-1.64684700	0.12126800
H	3.84204900	-2.07658100	0.70509600
C	6.16398100	0.30329100	-1.31308500
H	4.34731900	1.35778300	-1.81644700
C	6.68830100	-0.77989600	-0.60805700
H	6.32504600	-2.47981800	0.64810900
H	6.83056200	0.94852600	-1.87196500
N	8.13859400	-1.01847000	-0.63945700
O	8.57034900	-1.98193100	-0.00757800
O	8.82928500	-0.23957700	-1.29473300

**5a”:**

N	-1.97980000	-0.52972000	-1.98874100
C	-1.45138900	0.61348800	-2.77097800
C	-3.43321800	-0.71189000	-2.19537000
C	-1.21528500	-1.78079100	-2.18887000
C	-4.19255800	-1.18222900	-0.96817500
C	-5.30225500	-1.99943800	-1.11672400
C	-6.06505700	-2.30093600	0.02111900
C	-4.54558100	-0.96155900	1.31973800
C	-5.69659400	-1.77886100	1.24432500
C	-1.27790800	-2.69330300	-0.97593600
C	-1.50964200	-4.05888200	-1.07284400
C	-1.46397800	-4.82368500	0.10055600



C	-0.88332800	-2.83549300	1.31226200
C	-1.13574400	-4.21829200	1.30518500
C	-2.01593200	1.92948100	-2.26011900
C	-2.28236300	2.97944700	-3.12392300
C	-2.75305600	4.18433500	-2.57830900
C	-2.67547300	3.17113100	-0.39830800
C	-2.95465100	4.28984300	-1.21601700
N	-2.21090900	2.01925100	-0.92185100
N	-3.79828900	-0.68348200	0.22885200
N	-1.02158200	-2.09116000	0.20457200
N	-0.46617200	-2.14340800	2.45962600
N	-2.90333000	3.21223600	0.95279300
N	-4.13682500	-0.45533500	2.52692300
H	-3.08614000	4.10493200	1.38389600
H	-3.47766300	0.31165900	2.52861900
H	-4.79274700	-0.47806400	3.29292000
H	-1.66497200	0.50664200	-3.84399300
H	-0.36487300	0.62170000	-2.63488400
H	-3.62066400	-1.39573200	-3.03435800
H	-3.84990700	0.26017900	-2.48133500
H	-0.16576800	-1.50340600	-2.33570000
H	-1.55292600	-2.31407500	-3.08817000
H	-5.57755700	-2.38071300	-2.09418800
H	-6.94291900	-2.93529700	-0.05882900
H	-6.27056000	-1.98488000	2.14241800
H	-1.71818900	-4.51778200	-2.03346800
H	-1.65457200	-5.89219200	0.06433300
H	-1.03834500	-4.79850500	2.21751000
H	-2.12573800	2.86925300	-4.19150500
H	-2.96519600	5.03063600	-3.22496700
H	-3.32647900	5.20699000	-0.77002100
Zn	-1.61446400	0.11443900	0.10207600
O	-1.46170700	0.72260000	2.15630700
H	-0.33078900	-2.74965600	3.26133400
H	-1.34377800	-0.10514400	2.66155400
H	0.38628700	-1.61122800	2.27061300
H	-2.50093500	2.49756000	1.54486700
H	2.73777800	4.05153000	0.79787000
C	2.51958100	3.13615900	1.35288700
O	2.63245400	2.04544200	0.42471800
C	1.10603500	3.10358200	1.93478000
H	3.27209400	2.99751300	2.13854500
P	1.68274200	0.73084400	0.55299100
C	0.98815500	3.83765000	3.26404400

H	0.40718900	3.54157900	1.20231200
O	0.84008000	1.71696000	2.06655500
O	2.01417000	-0.33600600	1.77389300
O	2.57611000	-0.12933900	-0.56890000
O	0.35297000	0.64313200	-0.18590800
H	1.66112200	3.39883000	4.00799100
H	1.24403200	4.89695800	3.14580400
H	-0.03381000	3.77973200	3.65154100
H	-0.53037200	1.21045600	2.18111100
H	1.87979900	0.15569400	2.60297400
C	3.94264100	-0.31866700	-0.53164500
C	4.48323400	-1.39979200	0.17467600
C	4.76801600	0.52578600	-1.28417400
C	5.85508400	-1.63264400	0.13738800
H	3.82459800	-2.04531800	0.74415800
C	6.13942300	0.29700100	-1.32480700
H	4.32352800	1.35315600	-1.82623000
C	6.66520000	-0.77934100	-0.61024400
H	6.30482500	-2.46071600	0.67131200
H	6.80404300	0.93190300	-1.89770500
N	8.11357500	-1.02519700	-0.65119000
O	8.54661200	-1.98283200	-0.01095900
O	8.80250700	-0.25807500	-1.32238700

**TS-6a”:**

N	-2.64211500	-0.44423700	-1.78609000
C	-2.65148100	0.80904200	-2.57485500
C	-4.04347500	-0.84509000	-1.50952900
C	-1.85673900	-1.53871400	-2.40218400
C	-4.21409300	-1.78074200	-0.33838900
C	-5.08333400	-2.85609100	-0.43185300
C	-5.31867100	-3.61710600	0.72471300
C	-3.79496800	-2.16720600	1.90431600
C	-4.68180200	-3.27496900	1.89725700
C	-1.23376000	-2.46386100	-1.36788600
C	-1.19499000	-3.84090100	-1.52794800
C	-0.53508100	-4.60259800	-0.55319500
C	0.03913500	-2.56773400	0.58790800
C	0.09543600	-3.97077200	0.50786300
C	-3.05561300	1.98190000	-1.69665300
C	-3.90679100	2.98927700	-2.12603700
C	-4.14974100	4.06202700	-1.25525200
C	-2.60389600	3.08661800	0.30944900

C	-3.48951100	4.12600100	-0.03808800
N	-2.47582500	2.00230800	-0.47786400
N	-3.55961900	-1.43328100	0.79300300
N	-0.65841300	-1.84946900	-0.31227600
N	0.68540000	-1.83268300	1.58566200
N	-1.80644900	3.11954800	1.45308300
N	-3.13752500	-1.83176700	3.05008300
H	-1.93533600	3.96328700	1.99998900
H	-2.60522700	-0.97100000	3.07433100
H	-3.42150500	-2.25041600	3.92075600
H	-3.31384300	0.73652000	-3.44913300
H	-1.63384700	0.98644300	-2.94179500
H	-4.49079600	-1.28232300	-2.41381800
H	-4.59966100	0.07213700	-1.28593000
H	-1.03958900	-1.08169700	-2.97253000
H	-2.46577700	-2.11682300	-3.10986600
H	-5.58100300	-3.08579900	-1.36789000
H	-5.99810700	-4.46401800	0.69797100
H	-4.84270400	-3.83777200	2.81182300
H	-1.66905100	-4.31240300	-2.38205000
H	-0.49806000	-5.68449700	-0.63967600
H	0.64982900	-4.53616400	1.25012800
H	-4.36988300	2.94384800	-3.10596600
H	-4.82779700	4.85857800	-1.54695800
H	-3.61532100	4.97724100	0.62366600
Zn	-1.52565300	0.10511500	0.12821200
O	-1.28992800	0.19323900	2.30305700
H	1.22820700	-2.41360300	2.21557400
H	-0.45176700	-0.30500400	2.42596100
H	1.28493000	-1.10513300	1.16772300
H	-0.81088100	2.98971300	1.22900500
H	2.91921000	3.98518300	-1.71343200
C	2.79673300	3.68504500	-0.67009700
O	2.65955200	2.25692400	-0.64228500
C	1.53078000	4.24886700	-0.02055800
H	3.69444100	3.96057500	-0.10300800
P	1.61891700	1.62562400	0.45902100
C	1.70987500	5.62863600	0.59173200
H	0.72104200	4.27264700	-0.76873600
O	1.21226600	3.28338100	0.97746600
O	2.04646800	1.34534200	2.03466200
O	2.25324700	0.04336000	0.06655900
O	0.18512200	1.24918500	0.05599800
H	2.49210500	5.61278700	1.35748100

H	1.99045100	6.35633300	-0.17818100
H	0.78055100	5.97239200	1.05587500
H	-1.14789500	1.13290700	2.50668300
H	1.95969000	2.18147300	2.51978300
C	3.56308100	-0.33768900	-0.04623400
C	4.61800300	0.23490100	0.68270600
C	3.81818100	-1.40688000	-0.92074500
C	5.91105900	-0.25505600	0.52810500
H	4.42489200	1.04609300	1.37274200
C	5.10666400	-1.90359800	-1.06999900
H	2.99110200	-1.82717200	-1.48458100
C	6.14324800	-1.31854600	-0.34304900
H	6.74184600	0.17021900	1.07811700
H	5.32440300	-2.72519000	-1.74135400
N	7.50624000	-1.83615400	-0.49705600
O	8.40098500	-1.28883400	0.14704200
O	7.67101600	-2.78829500	-1.26039600

**7a”:**

N	-3.00191500	-0.26309100	-1.57977200
C	-3.22212900	1.07023900	-2.18225300
C	-4.27280600	-0.76244400	-0.99975900
C	-2.41463900	-1.21852000	-2.54912500
C	-4.10735900	-1.74726900	0.13467600
C	-4.97210300	-2.82196400	0.24142400
C	-4.87547300	-3.64094900	1.37916800
C	-3.07379100	-2.23694800	2.15830000
C	-3.93589500	-3.35049100	2.34142600
C	-1.67654300	-2.35768900	-1.87510900
C	-1.78777700	-3.66480400	-2.31796600
C	-1.00079400	-4.64345700	-1.68840800
C	-0.04225400	-2.91636300	-0.30952400
C	-0.12050200	-4.27657000	-0.68919000
C	-3.45554300	2.11458200	-1.11002100
C	-4.46207900	3.06805400	-1.20923700
C	-4.56554600	4.03081500	-0.19839800
C	-2.62749800	3.06078700	0.83589200
C	-3.63363300	4.04198800	0.82961800
N	-2.58955700	2.07628300	-0.07671700
N	-3.15666300	-1.45030600	1.05570400
N	-0.85413000	-1.99321000	-0.86590300
N	0.83521900	-2.47319900	0.64958500
N	-1.58637800	3.05397700	1.78326200

N	-2.13624700	-1.94730700	3.09479700
H	-1.67195800	3.80610000	2.45967200
H	-1.57804200	-1.10395600	3.01375700
H	-2.09008300	-2.49280000	3.93942200
H	-4.05985100	1.05665600	-2.89441300
H	-2.31675700	1.33811900	-2.73832100
H	-4.90256900	-1.19765900	-1.78823300
H	-4.81088300	0.10673400	-0.60480700
H	-1.68918700	-0.66159600	-3.15342600
H	-3.18291300	-1.60965500	-3.23050400
H	-5.71072300	-3.01429800	-0.52904500
H	-5.53767400	-4.49308300	1.50123600
H	-3.83825700	-3.95637600	3.23698600
H	-2.46186000	-3.92000000	-3.12849200
H	-1.06746200	-5.68169500	-2.00014300
H	0.52871300	-5.00576000	-0.21472000
H	-5.14874200	3.05998200	-2.04916700
H	-5.35042000	4.78047600	-0.23173200
H	-3.65498200	4.80807600	1.59857500
Zn	-1.48218000	-0.06386400	0.09300100
O	-0.87461000	0.40463800	2.18627200
H	1.49213400	-3.16433800	0.98592700
H	0.09992600	0.51453300	2.20167100
H	1.27881400	-1.57122500	0.45122400
H	-0.66720500	3.10977200	1.31043100
H	2.84879000	3.71669200	-2.19399800
C	2.68173200	3.50009600	-1.13620900
O	2.65361000	2.07277400	-0.98505700
C	1.33661500	4.01543400	-0.61847000
H	3.51708300	3.89340300	-0.54486300
P	1.54642300	1.42975100	0.03724100
C	1.37782300	5.45044500	-0.11811600
H	0.57759600	3.91540200	-1.41085500
O	1.02726800	3.10920600	0.43662400
O	1.78217700	1.28538100	1.69582800
O	2.32325100	-0.10771600	-0.14986900
O	0.19382700	0.93806600	-0.48868800
H	2.10288500	5.55675100	0.69542500
H	1.66441100	6.12959300	-0.92897500
H	0.39568900	5.76545300	0.24778500
H	-1.22892000	1.32518100	2.30220200
H	1.74739400	2.17996700	2.07226500
C	3.68058600	-0.33383300	-0.06228800
C	4.32457300	-0.41132000	1.18053200

C	4.39139700	-0.57590000	-1.24564500
C	5.68103500	-0.72309300	1.23829200
H	3.75998000	-0.22525300	2.08672000
C	5.74499900	-0.88860100	-1.19255700
H	3.86916400	-0.50842300	-2.19398300
C	6.37323600	-0.95633900	0.05152900
H	6.20679400	-0.79185100	2.18291200
H	6.31987100	-1.07876600	-2.09058800
N	7.80351800	-1.28887900	0.11268800
O	8.32720400	-1.34716000	1.22470600
O	8.38696700	-1.48915000	-0.95176400

**(2) catalyst B:**

**1b:**

C	2.90886700	2.10095600	-0.04708900
C	4.36180500	0.14383200	0.25486900
C	2.60460100	0.66201300	1.92351400
C	4.35651800	-1.32086600	-0.16349800
C	5.46831600	-2.12935100	0.08625800
C	5.48253100	-3.43769300	-0.39353000
C	3.30185900	-3.04960700	-1.29496800
C	4.37795300	-3.91005500	-1.10381400
C	2.01783900	-0.68369700	2.31302300
C	2.09509400	-1.15037700	3.62817900
C	1.43363300	-2.32872700	3.97123300
C	0.70406600	-2.49578600	1.69867800
C	0.71816700	-3.01588100	2.98912700
C	2.87172000	2.09391500	-1.56588900
C	3.32050800	3.19178800	-2.30303900
C	3.19390400	3.17638000	-3.69070100
C	2.22518800	0.99747300	-3.50362100
C	2.63600700	2.05569800	-4.30753000
H	3.72038000	2.75362400	0.30599900
H	1.96357300	2.51987100	0.31236500
H	5.01187000	0.27103700	1.13119800
H	4.82949200	0.70626900	-0.56203200
H	1.81351500	1.40771300	2.08013300
H	3.43576900	0.91739700	2.59637900
H	6.31055600	-1.73424800	0.64636400
H	6.33898400	-4.07982800	-0.21096900
H	4.34412700	-4.92228900	-1.49214300
H	2.65784100	-0.59067100	4.36927100
H	1.47696000	-2.70531200	4.98895700

H	0.18668500	-3.93427100	3.21431000
H	3.75261200	4.04656000	-1.79178300
H	3.52875800	4.02350800	-4.28173600
H	2.52147100	2.00030600	-5.38469800
Zn	1.51743900	-0.44112100	-0.66125600
H	2.40930600	-3.37976200	-1.81857500
H	0.17025500	-2.99498900	0.89498800
H	1.78831500	0.10430900	-3.94187400
N	2.33645300	1.01225300	-2.16491700
N	3.29015800	-1.78346800	-0.84288600
N	1.33891400	-1.35882300	1.36785100
N	3.02712800	0.73167500	0.50621500
O	0.02646800	-1.72951900	-1.65982000
H	-0.00678800	-2.02721100	-2.57761300
H	-2.92690900	1.02008200	3.09891200
C	-2.18465700	1.55060100	2.49502300
O	-1.75337400	0.61151900	1.48320900
C	-1.01748400	2.00194900	3.37881300
H	-2.66760400	2.40660600	2.01362300
P	-1.45177400	1.07992200	-0.03641100
C	-1.51216900	2.94636900	4.47814500
H	-0.57761700	1.10871000	3.83960700
O	0.04193000	2.57702300	2.61715700
O	-2.10326600	2.38818100	-0.37091200
O	-2.14793600	-0.20526800	-0.86968200
O	0.01246400	0.86746300	-0.38129500
H	-1.95715700	3.85082800	4.04736600
H	-2.26604600	2.46407300	5.11042300
H	-0.67460100	3.24947000	5.11228200
H	-0.26394400	3.37772600	2.13703900
H	-1.15015500	5.34200700	0.73904500
O	-0.72740300	4.47556800	0.74836600
H	-1.28205600	3.86864900	0.20540500
H	-0.82911100	-1.26861400	-1.47572400
C	-3.51700400	-0.46758700	-0.87398300
C	-3.92680400	-1.75200600	-0.50752500
C	-4.43617500	0.50185800	-1.28661200
C	-5.27759600	-2.08218100	-0.55821000
H	-3.18836000	-2.47825100	-0.18313300
C	-5.78922700	0.17377400	-1.32833500
H	-4.08926200	1.49238300	-1.55687800
C	-6.19030600	-1.11149900	-0.96701300
H	-5.63307800	-3.06754400	-0.28363900
H	-6.53332100	0.89566500	-1.64210500

N	-7.62016200	-1.45751300	-1.01993800
O	-7.93738300	-2.60253300	-0.70190300
O	-8.40292400	-0.58063600	-1.37889700

**TS-2b:**

C	2.89895900	1.94902300	0.92463900
C	4.35934500	0.06047900	0.33420900
C	2.57605100	-0.21396200	2.03875400
C	4.36103000	-1.01408200	-0.74765500
C	5.49011800	-1.81564800	-0.93643100
C	5.51049700	-2.72879600	-1.98865700
C	3.30373500	-2.00578500	-2.55900400
C	4.39534500	-2.82608400	-2.82255300
C	2.06201300	-1.62032500	1.78200600
C	2.19606600	-2.63027100	2.73767000
C	1.59383100	-3.86725700	2.50689400
C	0.80883400	-3.01305400	0.41308700
C	0.87978500	-4.06364200	1.32414000
C	2.84901000	2.62072000	-0.43706000
C	3.34069700	3.91366700	-0.62711600
C	3.19571500	4.52014900	-1.87411800
C	2.12501300	2.52211100	-2.63764100
C	2.57452000	3.81196800	-2.90334800
H	3.71200000	2.37928300	1.52739500
H	1.95217800	2.15063000	1.43667100
H	4.98273000	-0.27122400	1.17566000
H	4.85737500	0.94075300	-0.08980200
H	1.73848400	0.36641200	2.44758000
H	3.37444200	-0.23677200	2.79469700
H	6.34041500	-1.72061800	-0.26752600
H	6.37996700	-3.35854500	-2.15175900
H	4.36612200	-3.52591300	-3.65075500
H	2.75500700	-2.44402300	3.64986500
H	1.68104200	-4.66443900	3.23916600
H	0.39249100	-5.00828000	1.10758300
H	3.82351900	4.43582000	0.19340000
H	3.56547600	5.52742100	-2.04093000
H	2.44213200	4.24462100	-3.88911500
Zn	1.49637100	-0.05952000	-0.74877600
H	2.40351800	-2.06167200	-3.16439700
H	0.27252100	-3.11562600	-0.52609700
H	1.63921700	1.93210000	-3.40983000
N	2.25566200	1.93766800	-1.43573200



N	3.28631100	-1.11545000	-1.55102200
N	1.38752500	-1.82193200	0.63512900
N	3.02202100	0.47812400	0.80844400
O	-0.01636400	-0.70316200	-2.15288800
H	-0.09408500	-0.54688400	-3.10181100
H	-2.39142200	-1.35181200	3.34322700
C	-2.17343600	-0.33571200	3.00591000
O	-1.91453100	-0.44133700	1.58864900
C	-0.94080700	0.28041600	3.67247800
H	-3.05724700	0.29590200	3.15466500
P	-1.38811200	0.84591900	0.75936200
C	-1.23521800	0.74468500	5.09963800
H	-0.15514500	-0.49643200	3.71179400
O	-0.51723300	1.31613400	2.81661300
O	-2.24813600	2.13306900	0.89199600
O	-2.03900500	0.25031300	-0.72485200
O	0.05175500	0.91980100	0.27688200
H	-2.01284900	1.51530400	5.10770500
H	-1.56939400	-0.09300400	5.72375900
H	-0.33351300	1.16588200	5.55509900
H	-1.07961200	2.48874800	3.04711800
H	-1.30436400	4.20650100	2.87425900
O	-1.76536200	3.36001000	2.91037900
H	-2.08778400	2.81126700	1.76696100
H	-0.85773000	-0.37054100	-1.72249400
C	-3.39093300	-0.00772500	-0.91858100
C	-3.83933300	-1.33160200	-0.88195700
C	-4.26496400	1.04330800	-1.21312800
C	-5.17613800	-1.61377600	-1.14828900
H	-3.14044400	-2.12407100	-0.63604600
C	-5.60382800	0.76526000	-1.47526600
H	-3.89097900	2.06041500	-1.22234900
C	-6.03899700	-0.55900000	-1.44105500
H	-5.55902400	-2.62662300	-1.13011100
H	-6.31029300	1.55272700	-1.70726100
N	-7.45237500	-0.85485200	-1.72669400
O	-7.80330900	-2.03341400	-1.69143500
O	-8.19027400	0.09411400	-1.98406500

**3b:**

C	2.61752600	2.22769200	-0.71959600
C	4.33626600	0.47704000	-0.74645500
C	3.32377500	1.18789200	1.39538400

C	4.37359700	-1.03816500	-0.88680400
C	5.59440000	-1.70953900	-0.99046800
C	5.59756500	-3.08503400	-1.21562900
C	3.20683900	-3.01643300	-1.18793000
C	4.37826200	-3.75573900	-1.32051100
C	3.16147800	-0.09892100	2.18955900
C	3.85819000	-0.31259300	3.38022500
C	3.57689800	-1.45359000	4.13235400
C	1.97450800	-2.07233200	2.46402700
C	2.61239600	-2.34956800	3.67107600
C	1.98291100	1.91284100	-2.06417800
C	1.99171200	2.83979400	-3.10759800
C	1.30916000	2.54014900	-4.28686600
C	0.69897200	0.44168800	-3.31276800
C	0.64542300	1.31820700	-4.39312300
H	3.39633700	2.99530500	-0.83974100
H	1.83455000	2.63484500	-0.07096600
H	5.25496700	0.82434400	-0.25358000
H	4.35335200	0.89325600	-1.76062400
H	2.54193400	1.87514300	1.73622100
H	4.29413100	1.65242800	1.62431100
H	6.52653400	-1.15985100	-0.89882700
H	6.53573800	-3.62509200	-1.30137600
H	4.33303000	-4.82597900	-1.49134400
H	4.59976700	0.40663100	3.71518600
H	4.10318900	-1.63896000	5.06403100
H	2.35982900	-3.24494900	4.22896000
H	2.52060600	3.78135800	-2.99356400
H	1.29812100	3.24877600	-5.10959100
H	0.09928900	1.04608200	-5.28979100
Zn	1.42393900	-0.47248300	-0.28080500
H	2.23466000	-3.49811300	-1.23586300
H	1.21954200	-2.73777500	2.05475900
H	0.19621100	-0.52018100	-3.34990900
N	1.35384100	0.72717200	-2.17644400
N	3.20027600	-1.68820900	-0.98283000
N	2.24532600	-0.97446900	1.74121400
N	3.13965100	1.01032800	-0.05986100
O	-0.02654500	-1.99617800	-0.48383400
H	-0.21738400	-2.56378600	-1.23976800
H	-2.57394700	1.40333400	3.80457500
C	-2.52484100	1.89646200	2.83037000
O	-2.36913600	0.87510600	1.83440000
C	-1.31507300	2.81640100	2.67215900

H	-3.46184200	2.43446700	2.64220000
P	-1.38808500	1.23755700	0.56198200
C	-1.52148800	4.22180200	3.21339600
H	-0.43966200	2.35552400	3.15835400
O	-1.10447200	2.83258200	1.26099900
O	-1.97440500	1.89421000	-0.79460800
O	-1.92912900	-0.38939200	-0.09972400
O	0.07971400	0.77541900	0.58642000
H	-2.38838500	4.70022300	2.74485800
H	-1.69243300	4.19156500	4.29527300
H	-0.63706900	4.84102400	3.03274800
H	-1.70551300	4.43429600	0.31748300
H	-1.90521500	5.39053300	-0.91896200
O	-2.24092400	4.60039700	-0.48025800
H	-2.05457700	2.87648900	-0.77204700
H	-0.86731700	-1.42983300	-0.29983000
C	-3.23347300	-0.81798500	-0.18686600
C	-3.62772900	-1.90940700	0.60165800
C	-4.13660900	-0.23671600	-1.08936400
C	-4.91307800	-2.42720900	0.48832800
H	-2.91961000	-2.33194700	1.30777300
C	-5.42724200	-0.74631100	-1.19864500
H	-3.81693200	0.60579500	-1.68984300
C	-5.79911100	-1.83636000	-0.41215900
H	-5.24221100	-3.26890900	1.08524300
H	-6.14556200	-0.31939000	-1.88803300
N	-7.15672900	-2.38076900	-0.53815500
O	-7.44981700	-3.34906400	0.16351700
O	-7.91715600	-1.83786500	-1.33926400

**TS-4b:**

C	-2.71948300	1.81651300	1.58513800
C	-4.37413100	0.13136000	0.95020700
C	-3.40905000	1.61935200	-0.76914000
C	-4.39395500	-1.30903800	0.46447100
C	-5.60250600	-1.97525700	0.24981000
C	-5.58054500	-3.32711600	-0.09155900
C	-3.19129000	-3.23032600	-0.00558600
C	-4.35019600	-3.97245000	-0.21822100
C	-3.18799700	0.73438900	-1.98671800
C	-3.88493600	0.94011800	-3.17837100
C	-3.55117300	0.17383800	-4.29606000
C	-1.89951300	-0.93272500	-2.95978200

C	-2.53581300	-0.77722900	-4.18974000
C	-2.03625800	1.04662300	2.70383700
C	-2.05101200	1.50750400	4.02090000
C	-1.32162900	0.81570200	4.98864400
C	-0.65415300	-0.72315300	3.28119500
C	-0.60422500	-0.31984100	4.61322300
H	-3.52917600	2.43903400	1.99447300
H	-1.97478700	2.48339800	1.13888600
H	-5.30845800	0.63448300	0.66317300
H	-4.36217600	0.09913300	2.04601900
H	-2.66962500	2.42582700	-0.82139100
H	-4.40478700	2.08459400	-0.81636200
H	-6.54360100	-1.44323200	0.35334600
H	-6.50829900	-3.86560800	-0.26062500
H	-4.28581600	-5.02209200	-0.48443300
H	-4.66808400	1.69068200	-3.23062900
H	-4.07770800	0.31742500	-5.23502000
H	-2.24426700	-1.38946700	-5.03648000
H	-2.61921000	2.39580200	4.28053600
H	-1.31504100	1.15835700	6.01908300
H	-0.01956900	-0.88378500	5.33192900
Zn	-1.41529600	-0.51473500	0.16213400
H	-2.20953900	-3.68065300	-0.11905700
H	-1.10717000	-1.66092100	-2.81006200
H	-0.10745000	-1.59632400	2.93804800
N	-1.35697000	-0.06011600	2.34970000
N	-3.20933200	-1.93076500	0.33292700
N	-2.22179500	-0.19366500	-1.88705700
N	-3.19964700	0.91831000	0.51349400
O	0.02359400	-1.89390700	-0.21189500
H	0.10844500	-2.74035600	0.24057800
H	2.58259800	2.06431600	-3.30516300
C	2.55790800	2.39254700	-2.26377000
O	2.24356800	1.23992900	-1.45627300
C	1.45951000	3.41526600	-1.97209700
H	3.54461700	2.76933200	-1.97038200
P	1.33003400	1.57631500	-0.14489500
C	1.84787500	4.85709400	-2.24556100
H	0.55160900	3.15488400	-2.53623200
O	1.19395100	3.22000700	-0.57081700
O	2.04902800	1.82872400	1.25956200
O	1.87521800	-0.44754800	0.27907100
O	-0.11310200	1.10741900	-0.13188300
H	2.74434400	5.13527900	-1.68145300

H	2.05809900	4.99619000	-3.31165700
H	1.03323900	5.53571300	-1.97511400
H	1.99898400	4.68637100	0.80037200
H	2.55413700	5.06350800	2.22028800
O	2.64282500	4.44535200	1.48464700
H	2.30300500	2.77619500	1.41063400
H	1.00457800	-1.22520100	-0.00551300
C	3.13814100	-0.94042000	0.14210300
C	3.41423600	-1.91117200	-0.83740000
C	4.16310400	-0.50089000	0.99739100
C	4.69208000	-2.44520900	-0.95455400
H	2.62128100	-2.22983400	-1.50712400
C	5.44463200	-1.02545800	0.87543200
H	3.93441300	0.24344800	1.75076900
C	5.69617800	-1.99445000	-0.09718600
H	4.92750300	-3.19477800	-1.70023900
H	6.25008500	-0.70586600	1.52557100
N	7.04453700	-2.55409500	-0.21976100
O	7.23096400	-3.41283300	-1.08323100
O	7.91068600	-2.13334800	0.54805600

**1b':**

C	-2.89610800	-0.41695500	2.19759200
C	-4.32387300	0.33410900	0.34345400
C	-2.47934600	1.77391800	1.16466800
C	-4.33860500	0.13552000	-1.16832700
C	-5.45172900	0.53335700	-1.91378000
C	-5.49241300	0.26005600	-3.27939800
C	-3.33398100	-0.74598000	-3.06436900
C	-4.41232100	-0.39754000	-3.87035800
C	-1.92629800	2.40211000	-0.10381000
C	-1.97069800	3.78375400	-0.30541200
C	-1.33741600	4.32736400	-1.42301100
C	-0.70248800	2.10743700	-2.05180600
C	-0.68432700	3.47452000	-2.31367300
C	-2.91085100	-1.90633100	1.89742800
C	-3.42455600	-2.82340000	2.81646700
C	-3.33796600	-4.18641500	2.53766900
C	-2.27880000	-3.61926400	0.46928300
C	-2.75339300	-4.59614100	1.33878200
H	-3.69878700	-0.16738600	2.90648700
H	-1.94030000	-0.17996000	2.67530200
H	-4.90876900	1.22870000	0.59668400

H	-4.85883600	-0.51700300	0.78161700
H	-1.65373700	1.72284800	1.88568600
H	-3.25656900	2.42102700	1.59630200
H	-6.27475900	1.04742000	-1.42619800
H	-6.35017200	0.56023600	-3.87378100
H	-4.39940100	-0.62735100	-4.93033000
H	-2.48671300	4.42004200	0.40752900
H	-1.35501000	5.39939900	-1.59569500
H	-0.17576900	3.85584200	-3.19265400
H	-3.87604900	-2.47089600	3.73884600
H	-3.72369900	-4.91651900	3.24279000
H	-2.66703400	-5.64604900	1.08057900
Zn	-1.50803200	-0.57907300	-0.42098000
H	-2.46071500	-1.23795700	-3.48309100
H	-0.21521000	1.39979700	-2.71654900
H	-1.82021500	-3.89325000	-0.47681600
N	-2.35143400	-2.30539500	0.73837500
N	-3.29675100	-0.49302400	-1.74390600
N	-1.31040900	1.58345600	-0.97560600
N	-2.98175000	0.39615800	0.96288300
O	-0.01541500	-1.38751100	-1.81205700
H	0.01568300	-2.23114200	-2.28001800
H	2.73569900	3.15722000	1.12267000
C	2.26719200	2.36379400	1.71169800
O	1.67557600	1.45783000	0.75613600
C	1.22083000	2.96034300	2.65824900
H	3.04129500	1.83853500	2.28054200
P	1.43030600	-0.09918600	1.17127600
C	1.88237100	3.85880400	3.70408100
H	0.51111800	3.55075100	2.06538400
O	0.41738200	1.94081300	3.26373900
O	2.10335500	-0.44659700	2.45676800
O	2.12547300	-0.86330400	-0.16675400
O	-0.03181200	-0.45523200	0.94060000
H	2.59023600	3.28979800	4.31761400
H	2.42709100	4.68474800	3.23217500
H	1.12261200	4.28212000	4.36645100
H	0.99218600	1.22419200	3.58350100
H	0.83764900	-1.29449900	-1.31639600
C	3.49419900	-0.84816200	-0.42415900
C	3.91215800	-0.37809200	-1.67212100
C	4.40803900	-1.33928600	0.51352200
C	5.26486600	-0.40311600	-1.99789400
H	3.17841000	0.00615000	-2.37374000

C	5.76276800	-1.35623600	0.19055800
H	4.05522600	-1.68734300	1.47740700
C	6.17140800	-0.89119000	-1.05865700
H	5.62626300	-0.04916300	-2.95539700
H	6.50244100	-1.72916300	0.88846300
N	7.60314200	-0.91743600	-1.40023600
O	7.92706900	-0.50558800	-2.51317800
O	8.38095000	-1.34907600	-0.55222300

**TS-2b':**

C	2.20446200	2.36590900	0.36135500
C	4.18941200	1.05217300	-0.26058800
C	3.05595500	0.65288200	1.90479300
C	4.46061600	-0.21544600	-1.06363700
C	5.77247900	-0.56196300	-1.39885700
C	5.99989300	-1.66744700	-2.21541000
C	3.63452000	-2.00952400	-2.28030700
C	4.90786400	-2.40792800	-2.67153200
C	3.14285400	-0.85423800	2.08397700
C	3.84555300	-1.41829700	3.15045800
C	3.78967100	-2.79814700	3.34493700
C	2.38113000	-2.94049000	1.41507300
C	3.03852500	-3.57727600	2.46432500
C	1.60464000	2.53545600	-1.02210100
C	1.40992900	3.80220100	-1.57730500
C	0.76455900	3.91341100	-2.80726600
C	0.58250600	1.52924100	-2.84554200
C	0.34057000	2.75372400	-3.45807600
H	2.86613300	3.21375700	0.59083200
H	1.37246700	2.38235500	1.08142300
H	5.03926100	1.24633300	0.40807600
H	4.16660700	1.88249500	-0.97635900
H	2.15429300	0.99014000	2.42725500
H	3.91819600	1.13955900	2.38344000
H	6.60147900	0.03160200	-1.02503600
H	7.01244100	-1.94999800	-2.48749400
H	5.03778700	-3.27717100	-3.30717300
H	4.41574800	-0.78379400	3.82235600
H	4.32360200	-3.25718100	4.17167700
H	2.96318500	-4.65276900	2.58384400
H	1.75002900	4.68422400	-1.04357400
H	0.59585100	4.88967200	-3.25175500
H	-0.16554500	2.79490100	-4.41649000

Zn	1.52763000	-0.42221200	-0.43972300
H	2.75616500	-2.56701500	-2.59314500
H	1.78488600	-3.50065500	0.70017700
H	0.26898900	0.60036600	-3.31339400
N	1.20004600	1.41778200	-1.65722500
N	3.41122500	-0.93756200	-1.49918600
N	2.43462000	-1.61242000	1.22760700
N	2.91653400	1.07086400	0.49401200
O	0.11365800	-1.85546300	-1.31459900
H	-0.06686500	-2.18993900	-2.20148700
H	-2.99082200	1.20143400	3.86596100
C	-2.61898900	1.56615900	2.90642900
O	-2.27480900	0.37297300	2.14803900
C	-1.37920100	2.46871400	3.03356500
H	-3.42778800	2.08015000	2.37348300
P	-1.42092900	0.51533000	0.79817000
C	-1.77198700	3.87723500	3.48200400
H	-0.71748500	2.02554500	3.79965500
O	-0.71563300	2.44731000	1.79810000
O	-1.84129200	1.73987500	-0.11304900
O	-2.12233000	-0.75856300	-0.06176600
O	-0.00100600	-0.02046000	0.82906500
H	-2.42710100	4.34919400	2.74078400
H	-2.29228100	3.86391200	4.44782200
H	-0.87718100	4.49781900	3.58706200
H	-1.44942700	2.46550400	0.60485300
H	-0.75366200	-1.62649800	-0.89891300
C	-3.49397100	-0.88956600	-0.27045100
C	-4.16747200	-1.90403200	0.41445900
C	-4.15543600	-0.06549100	-1.18572300
C	-5.52477600	-2.10487200	0.17998000
H	-3.62476700	-2.51807400	1.12539100
C	-5.51421700	-0.26335500	-1.41975400
H	-3.60998600	0.72463000	-1.68851800
C	-6.17747600	-1.28017200	-0.73501200
H	-6.08118300	-2.88028800	0.69179800
H	-6.06353100	0.35363400	-2.12020300
N	-7.61291300	-1.49150400	-0.98795300
O	-8.16976400	-2.39701700	-0.37040600
O	-8.16016500	-0.74874600	-1.80073000

**3b':**

C	2.63437300	2.27543600	-0.69335400
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C	4.30694700	0.47882000	-0.70503700
C	3.29359300	1.21734700	1.42642000
C	4.30938400	-1.03724200	-0.84098500
C	5.51464900	-1.73790500	-0.93078400
C	5.48743800	-3.11382900	-1.15240100
C	3.09898000	-2.98862000	-1.14932600
C	4.25382200	-3.75581600	-1.26799500
C	3.08347800	-0.06231500	2.22205700
C	3.75686600	-0.29043200	3.42319700
C	3.43375200	-1.42008600	4.17564000
C	1.83858400	-2.00148300	2.48725900
C	2.45152600	-2.29141100	3.70413800
C	2.00804900	1.97984000	-2.04558000
C	2.04008000	2.91559300	-3.08070500
C	1.36675400	2.63497400	-4.26963000
C	0.71858000	0.53650400	-3.31981600
C	0.68944100	1.42186900	-4.39368900
H	3.43392600	3.02298000	-0.80266000
H	1.85459500	2.70237200	-0.05368400
H	5.22929400	0.80501700	-0.20462800
H	4.34307100	0.89175400	-1.72002800
H	2.53192100	1.93044700	1.75971300
H	4.27586100	1.65181800	1.66271900
H	6.45861700	-1.21024200	-0.83133800
H	6.41340500	-3.67604700	-1.22764700
H	4.18489500	-4.82511700	-1.43673700
H	4.51294200	0.40953100	3.76623300
H	3.94134400	-1.61579500	5.11553000
H	2.16634100	-3.17711300	4.26169500
H	2.57781100	3.85010000	-2.95158900
H	1.37301500	3.35115400	-5.08582500
H	0.15105900	1.16376100	-5.29919300
Zn	1.37546200	-0.39755500	-0.26999600
H	2.11614500	-3.44726600	-1.20640000
H	1.07119900	-2.64705600	2.06942400
H	0.20255000	-0.41785000	-3.37076000
N	1.36338200	0.80423900	-2.17315700
N	3.12191400	-1.66013500	-0.94766500
N	2.15000700	-0.91466000	1.76416800
N	3.11742100	1.04321400	-0.03011500
O	-0.12741800	-1.87595300	-0.50032800
H	-0.32252200	-2.43576600	-1.26100700
H	-2.65203800	1.81631900	3.70002400
C	-2.58871900	2.22431400	2.68831800

O	-2.41267500	1.12016600	1.78463700
C	-1.38140000	3.14053800	2.47273900
H	-3.52742800	2.73349200	2.43836500
P	-1.40765700	1.39261000	0.50980100
C	-1.62466300	4.59565600	2.83567400
H	-0.52258800	2.75136700	3.04480700
O	-1.11068400	3.00522400	1.08146900
O	-1.95712700	2.03760000	-0.89740900
O	-2.00528900	-0.21523300	-0.11689700
O	0.04143400	0.88196300	0.56054700
H	-2.46299100	5.00249200	2.26084100
H	-1.85432400	4.69127900	3.90289500
H	-0.73674900	5.19840200	2.62376500
H	-1.92454800	3.00300500	-0.79888300
H	-0.95186600	-1.29147400	-0.32800600
C	-3.32572800	-0.59831900	-0.19703300
C	-3.77163700	-1.62955900	0.64247100
C	-4.19323900	-0.03129700	-1.14181100
C	-5.07561500	-2.10109100	0.53883200
H	-3.08834600	-2.04191000	1.37816500
C	-5.50224200	-0.49416600	-1.24244700
H	-3.83243000	0.76283500	-1.78381700
C	-5.92647800	-1.52413200	-0.40364300
H	-5.44532100	-2.89656600	1.17410800
H	-6.19483800	-0.07745100	-1.96364800
N	-7.30433000	-2.01958400	-0.51909700
O	-7.64313100	-2.93905400	0.22569700
O	-8.03376000	-1.48616300	-1.35441400

**1b”:**

Zn	-1.69247000	-0.10201800	0.36202300
N	-2.46962200	1.91525700	-0.07565900
N	-3.70285900	-0.80052000	1.10463300
N	-1.34117700	-2.28084700	-0.07984900
N	-2.82828900	-0.41182400	-1.58489600
H	-0.57147600	-2.88439100	1.74100600
H	-3.31169000	-0.75343400	3.13432600
H	-2.15213200	2.78872200	1.76998400
O	-0.79467900	0.18887700	2.26042300
H	-0.80570700	-0.29391900	3.09383100
H	0.16925100	0.49019100	2.06087000
P	1.43501900	0.70212900	-0.10122900
O	1.46514600	0.93138200	1.41206900

O	0.05846600	0.37397300	-0.67424100
O	2.13918900	1.91359700	-0.88757600
C	1.52890100	3.21558700	-1.07821800
H	2.06376300	3.64615100	-1.92919500
H	0.47569000	3.08206900	-1.34599300
C	1.64559000	4.13387900	0.14298000
H	1.23959700	5.10214600	-0.17959700
C	3.08605400	4.32778700	0.61893000
H	3.52340000	3.37889100	0.94403900
H	3.71429100	4.73269800	-0.18211800
H	3.10554000	5.02589500	1.46000700
O	0.78369900	3.70695700	1.19843600
H	1.13247400	2.87109800	1.55915600
O	2.39976800	-0.52820800	-0.54207000
C	-2.11542600	-1.51290600	-2.26481300
C	-2.67247300	0.88668600	-2.28065800
C	-4.24643400	-0.72027200	-1.29617300
C	-1.65429900	-3.96097500	-1.75755100
C	-0.87262200	-3.22280700	0.75363900
C	-1.71737200	-2.63637500	-1.32219900
C	-1.16616200	-4.93766800	-0.88961000
C	-0.76109600	-4.56264000	0.39142000
C	-5.71589200	-1.88760000	0.40001500
C	-4.01590000	-1.09161200	2.37987700
C	-4.54353600	-1.17752200	0.12623200
C	-6.03461600	-2.19157700	1.72148700
C	-5.17150200	-1.77757900	2.73773200
C	-3.44552400	3.26444000	-1.79568900
C	-2.53952400	2.95517600	0.77038500
C	-2.89865000	2.06376000	-1.34472200
C	-3.52574100	4.34449200	-0.91347000
C	-3.05927200	4.19149200	0.39107500
C	3.76325900	-0.64010600	-0.29549000
C	4.52117200	-1.22332600	-1.31467300
C	5.88418800	-1.42431400	-1.12722300
C	6.46284600	-1.03187000	0.07908200
C	5.71335000	-0.44931200	1.09903900
C	4.34636000	-0.25371400	0.91600800
N	7.90392000	-1.24348300	0.28177500
O	8.38557900	-0.88342300	1.35465400
O	8.53455100	-1.76779400	-0.63486700
H	-3.08952900	5.00814100	1.10391600
H	-3.94450700	5.29050100	-1.24369300
H	-3.79390200	3.35425900	-2.82026300

H	-1.63873800	0.93860000	-2.63727600
H	-3.33369100	0.96413700	-3.15570100
H	-5.38400400	-1.98449500	3.78109100
H	-6.94157600	-2.74106600	1.95517300
H	-6.37064400	-2.18941300	-0.41229100
H	-4.83115100	0.19282100	-1.46153700
H	-4.63077500	-1.46355500	-2.00760100
H	-2.70064700	-1.91390400	-3.10500900
H	-1.18945600	-1.09488500	-2.67406300
H	-1.97227400	-4.21822000	-2.76340400
H	-1.10244300	-5.97354200	-1.20903600
H	-0.36905200	-5.28779100	1.09640300
H	4.03318700	-1.51118200	-2.23978200
H	6.50204100	-1.87264000	-1.89534000
H	6.20283700	-0.16298500	2.02188800
H	3.73849400	0.18801000	1.69683600

**TS-2b”:**

Zn	1.73286600	-0.00760600	-0.33983600
N	2.61457600	1.84263300	0.57104800
N	3.79003400	-0.66262100	-0.94377200
N	1.22222800	-2.19205700	-0.30394500
N	2.61977600	-0.72829100	1.65712100
H	0.64450100	-2.40271700	-2.27575000
H	3.61933700	-0.23727600	-2.96070000
H	2.67678400	3.02005800	-1.12632300
O	0.86526000	0.70248400	-2.03419300
H	1.18771400	0.64674100	-2.94047600
H	-0.39981300	0.33323900	-1.88343500
P	-1.45503900	0.49619700	0.02742300
O	-1.39664100	0.04877100	-1.46292500
O	-0.11654200	0.38916200	0.73486400
O	-2.09480500	1.95675900	0.16536400
C	-1.28810500	3.16470700	0.17565400
H	-1.73542500	3.80510000	0.94118700
H	-0.27091400	2.90920300	0.49086400
C	-1.28430200	3.90257200	-1.16476000
H	-0.66422600	4.79976100	-0.98200900
C	-2.67370000	4.34873600	-1.60807000
H	-3.32890600	3.48340800	-1.73852800
H	-3.12030200	5.02520200	-0.87183600
H	-2.60216600	4.87455200	-2.56366400
O	-0.72759500	3.14305200	-2.23146800

H	0.00578100	2.56810800	-1.95412800
O	-2.52902100	-0.42856200	0.78403700
C	1.76506000	-1.86950700	2.04937300
C	2.45577600	0.43737900	2.55426800
C	4.04062300	-1.10325400	1.47676500
C	1.28538900	-4.16317200	1.05338700
C	0.82236800	-2.93647800	-1.34678700
C	1.44079800	-2.78720500	0.88330500
C	0.87048800	-4.93659000	-0.03173700
C	0.62804700	-4.31288000	-1.25533600
C	5.74935500	-1.83594100	-0.23165500
C	4.25318700	-0.69567800	-2.20714100
C	4.52374200	-1.21636500	0.03424400
C	6.22783900	-1.86597800	-1.53855400
C	5.46652300	-1.27902800	-2.55187700
C	3.50195900	2.76240100	2.59603500
C	2.92274700	2.98262300	-0.06867200
C	2.89498300	1.72730900	1.88284500
C	3.81292400	3.95026200	1.93308100
C	3.51932700	4.06535800	0.57380500
C	-3.90361800	-0.49665900	0.55143600
C	-4.68741600	-0.80942800	1.66352000
C	-6.06388000	-0.93785400	1.51266800
C	-6.62318800	-0.74585300	0.25021300
C	-5.84372600	-0.43464000	-0.86157200
C	-4.46376400	-0.31172600	-0.71487600
N	-8.07964500	-0.87989900	0.08699100
O	-8.54302200	-0.69888700	-1.03730100
O	-8.73876700	-1.15234100	1.08863300
H	3.74918100	4.96907200	0.01951700
H	4.28222100	4.77012500	2.46862400
H	3.72188300	2.63965200	3.65228100
H	1.38815700	0.52392100	2.78000500
H	2.99269600	0.30246900	3.50447600
H	5.80053900	-1.27843700	-3.58383200
H	7.17781500	-2.34090900	-1.76471400
H	6.31882600	-2.28334800	0.57802300
H	4.66470900	-0.34617900	1.96743100
H	4.25029500	-2.04823200	1.99514000
H	2.21219600	-2.44479200	2.87294500
H	0.81741300	-1.45469400	2.40821100
H	1.47481400	-4.61736500	2.02132100
H	0.73720500	-6.00863300	0.07863100
H	0.29648700	-4.87539300	-2.12146200

H	-4.21243300	-0.94737500	2.62892300
H	-6.70568500	-1.17859000	2.35102500
H	-6.31944400	-0.29756600	-1.82484800
H	-3.83599300	-0.08440300	-1.56875700

**3b”:**

Zn	-1.91299800	0.23937400	0.41118500
N	-2.33251800	2.26578300	-0.41029400
N	-4.13136900	-0.40070000	0.46141700
N	-1.58532200	-1.94787300	0.10738100
N	-2.46215600	-0.10360500	-1.84248600
H	-1.33682800	-2.41472600	2.10087400
H	-4.33218100	-0.47431700	2.51607800
H	-2.56842500	3.21221500	1.40687500
O	-1.54662600	0.53482100	2.33969900
H	-2.25277500	0.64813700	2.98382100
H	1.39156700	-0.68437200	2.08343000
P	1.53115200	0.31600400	0.21818500
O	1.71409100	-0.95471100	1.13665200
O	0.14174000	0.54782200	-0.30797700
O	2.14779600	1.57392100	0.99705100
C	1.44805000	2.22588200	2.09679900
H	1.96957500	3.17608600	2.23317300
H	0.41562100	2.41663300	1.79087900
C	1.47749200	1.40374500	3.39211200
H	0.92498800	1.99771900	4.13588500
C	2.88300200	1.12668900	3.91289400
H	3.47148500	0.56221500	3.18395400
H	3.40739600	2.06426500	4.12412100
H	2.82665300	0.54580900	4.83700800
O	0.79728900	0.15142500	3.21570300
H	-0.18903300	0.31206600	2.95499400
O	2.52462000	0.12111200	-1.02378300
C	-1.74362200	-1.32710100	-2.24953000
C	-1.95717700	1.10783200	-2.52310200
C	-3.93093800	-0.21935100	-1.97068700
C	-1.61807700	-3.74575400	-1.46977300
C	-1.41176300	-2.83328800	1.10117700
C	-1.67808400	-2.38607800	-1.15948200
C	-1.43602400	-4.66722000	-0.43792500
C	-1.32502500	-4.20469900	0.87348100
C	-5.83231400	-1.46543000	-0.84759500
C	-4.79198100	-0.75922700	1.57419100

C	-4.64345000	-0.74100500	-0.73407200
C	-6.51882800	-1.82903700	0.31022200
C	-5.99265700	-1.46423500	1.54955100
C	-2.53626300	3.58618400	-2.39533900
C	-2.56869800	3.36014700	0.33057200
C	-2.30851400	2.36876500	-1.75140900
C	-2.77713200	4.72449300	-1.62572100
C	-2.79339300	4.61286400	-0.23493800
C	3.91158800	-0.06361900	-0.91176000
C	4.74053900	1.00987400	-1.23455000
C	6.12103100	0.83272800	-1.19482100
C	6.62815400	-0.41455800	-0.83491400
C	5.80065400	-1.49000300	-0.51763400
C	4.41946900	-1.31373400	-0.55872500
N	8.08972200	-0.60360100	-0.79168400
O	8.50652100	-1.71498800	-0.47330200
O	8.79289600	0.36317700	-1.07629300
H	-2.97952500	5.47317600	0.39905900
H	-2.95393000	5.68262800	-2.10534500
H	-2.52056500	3.63942100	-3.47981100
H	-0.86629300	1.03190400	-2.55939600
H	-2.32469200	1.18406500	-3.55746300
H	-6.49188200	-1.72582600	2.47643700
H	-7.44600700	-2.39066100	0.24537700
H	-6.21455000	-1.73418900	-1.82795300
H	-4.32657100	0.78456800	-2.16530500
H	-4.19928800	-0.83390000	-2.84195000
H	-2.17107600	-1.75889400	-3.16660800
H	-0.71241300	-1.03808600	-2.47826800
H	-1.70333400	-4.07427300	-2.50140100
H	-1.38195900	-5.72973600	-0.65607900
H	-1.17716700	-4.88728000	1.70348600
H	4.30365200	1.96332800	-1.51079900
H	6.80348500	1.63799500	-1.43666700
H	6.24172500	-2.44155700	-0.24784900
H	3.74367000	-2.12552300	-0.31533100

**TS-4b”:**

Zn	1.90229200	-0.12898700	0.41173700
N	2.44319200	-1.98394600	-0.70493000
N	4.04474600	0.47776800	0.25048000
N	1.43565000	2.08390200	0.54316800
N	2.01793300	0.57979200	-1.75694000

H	1. 70227100	2. 38878200	2. 57001100
H	4. 61893800	-0. 01446200	2. 17637700
H	3. 04665800	-3. 14398200	0. 89124500
O	1. 80965400	-0. 89358100	2. 35379000
H	2. 22448200	-0. 58006900	3. 16491500
H	-1. 57603100	0. 66015500	2. 58032400
P	-1. 45621900	-0. 49454700	0. 80280000
O	-1. 89308700	0. 80950500	1. 67333300
O	-0. 08270900	-0. 54970700	0. 14491800
O	-2. 32625200	-1. 85287400	0. 98493400
C	-1. 87119300	-2. 88994100	1. 86889100
H	-2. 74326600	-3. 50741800	2. 09469300
H	-1. 12538700	-3. 49211400	1. 33800300
C	-1. 26492200	-2. 21610400	3. 10882900
H	-0. 50618000	-2. 88299900	3. 54269200
C	-2. 30264500	-1. 86448700	4. 17558700
H	-3. 11425500	-1. 26212900	3. 75302800
H	-2. 74180800	-2. 77175300	4. 60543500
H	-1. 83451300	-1. 29752700	4. 98639100
O	-0. 63133700	-1. 05286700	2. 59601000
H	0. 75384000	-1. 01783800	2. 52778900
O	-2. 31262100	-0. 00703300	-0. 54739500
C	1. 01651300	1. 66684900	-1. 82533300
C	1. 60848900	-0. 61023300	-2. 53593100
C	3. 38838500	1. 03453800	-2. 07903400
C	0. 81446300	3. 97807700	-0. 78474700
C	1. 44567900	2. 87083300	1. 63054100
C	1. 11798000	2. 62191800	-0. 64934100
C	0. 82109300	4. 79162100	0. 34798000
C	1. 14125400	4. 22839700	1. 58357300
C	5. 70612100	1. 44051800	-1. 17477700
C	4. 95971600	0. 41058900	1. 23667100
C	4. 40546000	0. 97896800	-0. 94031800
C	6. 64821800	1. 37475700	-0. 15356300
C	6. 26961200	0. 84518400	1. 08309300
C	2. 61686300	-2. 92245900	-2. 89956600
C	2. 94026300	-3. 11914100	-0. 18967100
C	2. 27293500	-1. 88149800	-2. 03589500
C	3. 13156100	-4. 10362400	-2. 36413600
C	3. 29458700	-4. 20828800	-0. 98248000
C	-3. 68666500	0. 10915200	-0. 63123100
C	-4. 40760500	-0. 90582700	-1. 27124100
C	-5. 78129900	-0. 77462900	-1. 44548200
C	-6. 41278800	0. 37693500	-0. 97629800



C	-5.70647500	1.39753100	-0.34117800
C	-4.33168300	1.26263300	-0.16908700
N	-7.86359600	0.52107000	-1.16178300
O	-8.39184000	1.55036200	-0.74257400
O	-8.45926300	-0.39630600	-1.72526300
H	3.68930400	-5.11011400	-0.52678300
H	3.40225500	-4.92842400	-3.01663100
H	2.47548500	-2.81110000	-3.97038600
H	0.52850300	-0.72790700	-2.40009500
H	1.80092900	-0.47859200	-3.61061100
H	6.97175900	0.77065400	1.90648100
H	7.66180900	1.72827300	-0.31729600
H	5.97089600	1.84314100	-2.14852900
H	3.78392200	0.43069000	-2.90551700
H	3.35381400	2.06554600	-2.45351300
H	1.08789400	2.22348000	-2.77105900
H	0.02652800	1.20056400	-1.78220800
H	0.56749000	4.38432900	-1.76093400
H	0.58126400	5.84756400	0.26657800
H	1.15700200	4.82388800	2.49010100
H	-3.88140900	-1.78738800	-1.62104300
H	-6.36759100	-1.54215500	-1.93542900
H	-6.23680100	2.27694300	0.00299800
H	-3.75261700	2.03603200	0.32173400

**5b”:**

Zn	1.91630000	-0.22660800	0.39401200
N	2.34106500	-2.18046300	-0.58372800
N	4.06594300	0.37417700	0.15115800
N	1.54838300	2.01703500	0.36657900
N	1.99348100	0.29722600	-1.81811500
H	1.83603800	2.44655700	2.36638400
H	4.68228600	0.10225800	2.10587300
H	3.00043500	-3.23698800	1.06321900
O	1.84482100	-0.71191000	2.44337600
H	2.28472600	-0.32315400	3.20725200
H	-1.47003800	1.06841700	2.46665900
P	-1.42366100	-0.38937600	0.91366400
O	-1.78490100	1.07082900	1.54827400
O	-0.06912700	-0.62354000	0.24762900
O	-2.38766700	-1.64964900	1.27823100
C	-2.01198700	-2.55010400	2.32993000
H	-2.92873100	-3.04061900	2.66447100

H	-1.32750100	-3.29954200	1.91646600
C	-1.33285500	-1.71853700	3.42829500
H	-0.60877700	-2.34850200	3.96319800
C	-2.31684900	-1.11121500	4.42872300
H	-3.09794500	-0.53760400	3.91782000
H	-2.80381100	-1.89591900	5.01846100
H	-1.79111900	-0.44530700	5.12041300
O	-0.62958400	-0.71165500	2.70909800
H	0.80845600	-0.76363100	2.63850200
O	-2.26417900	-0.06476400	-0.50614100
C	1.09073300	1.45857600	-1.96460400
C	1.45686200	-0.91711800	-2.47486500
C	3.38988200	0.58062900	-2.21477600
C	1.06420200	3.84872900	-1.09823600
C	1.61476600	2.87791400	1.39382700
C	1.26975400	2.48777700	-0.86271300
C	1.13003000	4.73998100	-0.02772000
C	1.40794700	4.24676900	1.24745100
C	5.56720900	1.51040700	-1.32539000
C	4.96579700	0.51319300	1.14096600
C	4.36030000	0.85227400	-1.07003900
C	6.49637800	1.65452100	-0.29790100
C	6.19517100	1.13826200	0.96391700
C	2.27081300	-3.32155700	-2.68653300
C	2.80602400	-3.29831800	-0.00391100
C	2.06754800	-2.18514800	-1.90211700
C	2.75071600	-4.48421200	-2.08305000
C	3.02266700	-4.47614300	-0.71465900
C	-3.63024200	0.08544600	-0.62102800
C	-4.36803200	-0.95783300	-1.19449200
C	-5.73449300	-0.80832800	-1.40468100
C	-6.34533600	0.39035400	-1.03658500
C	-5.62361700	1.43945500	-0.46876600
C	-4.25547300	1.28663300	-0.26202900
N	-7.78816300	0.55406500	-1.25904000
O	-8.29855900	1.62337200	-0.92619700
O	-8.39675300	-0.38771400	-1.76610000
H	3.39627000	-5.35914600	-0.20732100
H	2.91206900	-5.38129600	-2.67336100
H	2.04944700	-3.29569500	-3.74925200
H	0.38138600	-0.94434300	-2.27167300
H	1.59667700	-0.88749600	-3.56523500
H	6.89102800	1.22211100	1.79177600
H	7.43978200	2.16123100	-0.47793200

H	5.77457200	1.89716900	-2.31892900
H	3.77515400	-0.29384800	-2.75335300
H	3.42587200	1.41691500	-2.92582900
H	1.20531800	1.93563400	-2.94890800
H	0.06400300	1.08289300	-1.89322700
H	0.84596800	4.19950000	-2.10239700
H	0.96708300	5.80171100	-0.18696400
H	1.46568400	4.90406500	2.10846800
H	-3.85845000	-1.87666200	-1.46433800
H	-6.33144800	-1.59744600	-1.84495700
H	-6.13715400	2.35549400	-0.20357200
H	-3.66624000	2.08363900	0.17553400

**TS-6b”:**

Zn	1.71228700	0.00545400	-0.48888200
N	3.23160400	1.44189800	0.35223800
N	3.36379000	-1.47932600	-0.75951300
N	0.41773000	-1.82368000	-0.39567700
N	1.99357100	-0.68642300	1.63120900
H	0.06836300	-2.13072700	-2.40955100
H	3.63315900	-1.31660000	-2.80271400
H	4.00285200	2.22071700	-1.39877700
O	1.56957600	0.59457700	-2.63633000
H	1.45259600	0.11664700	-3.46724400
H	-1.59088100	2.23315000	-2.63128700
P	-1.08931900	1.83984500	-0.56925900
O	-1.55939200	1.40928800	-2.11886100
O	0.39490200	1.50944500	-0.29314700
O	-2.01530900	2.49764400	0.63521600
C	-1.92949100	3.91749900	0.79961000
H	-2.89397600	4.26227200	1.18058700
H	-1.14688800	4.13833100	1.53487700
C	-1.58257000	4.48858400	-0.58396500
H	-0.92685400	5.36086400	-0.47943500
C	-2.80946300	4.86343800	-1.41558200
H	-3.51314100	4.02558500	-1.48050800
H	-3.33448300	5.71468500	-0.96747600
H	-2.50806300	5.14732200	-2.42872100
O	-0.82936200	3.45116500	-1.20119400
H	0.80091000	1.18728200	-2.54151100
O	-1.66649900	0.29062700	-0.02123400
C	0.71524400	-1.34610100	1.97406700
C	2.21375500	0.56657300	2.38769400

C	3.15914700	-1.59776700	1.70202200
C	-0.51636900	-3.40750000	1.13894900
C	-0.11066100	-2.52107800	-1.41195300
C	0.21070000	-2.24906800	0.86362100
C	-1.06418300	-4.13107300	0.07976100
C	-0.86290700	-3.67736100	-1.22359200
C	4.47229200	-3.28405200	0.35401800
C	3.89088600	-1.89958300	-1.92319200
C	3.65625700	-2.14891800	0.36900200
C	5.01375100	-3.71906700	-0.85323400
C	4.72539700	-3.00745300	-2.01936200
C	4.05857900	2.32172000	2.42057900
C	4.04565900	2.27424600	-0.31469000
C	3.22586400	1.46673100	1.69754500
C	4.90262800	3.18853100	1.72583000
C	4.89612000	3.16837400	0.33115300
C	-2.97800400	-0.07660800	0.09666300
C	-3.52718200	-0.20665700	1.38311900
C	-4.82591200	-0.67149400	1.55091800
C	-5.57521300	-1.00209800	0.42110300
C	-5.05324100	-0.87391400	-0.86585100
C	-3.75040700	-0.41222300	-1.02820800
N	-6.94263800	-1.50407000	0.59267700
O	-7.57860600	-1.78821400	-0.42256500
O	-7.36962900	-1.61568500	1.74229400
H	5.53510600	3.82764200	-0.24649200
H	5.55635300	3.86690500	2.26590800
H	4.03970600	2.31254200	3.50630700
H	1.25635700	1.09782800	2.42105400
H	2.52255400	0.36902600	3.42448200
H	5.13108800	-3.30539900	-2.98020300
H	5.65063200	-4.59799900	-0.88429600
H	4.68324200	-3.81330100	1.27871400
H	3.99588800	-1.04701700	2.14848700
H	2.94760700	-2.43429300	2.38110200
H	0.78986100	-1.90523500	2.91793800
H	-0.03425000	-0.55815300	2.10765600
H	-0.66230200	-3.72713700	2.16628300
H	-1.64211700	-5.03043800	0.26979200
H	-1.27813200	-4.20355500	-2.07636000
H	-2.92460400	0.07743600	2.23973000
H	-5.27025000	-0.77730200	2.53311200
H	-5.66853100	-1.14117000	-1.71656700
H	-3.31854600	-0.30284900	-2.01564700

**7b”:**

Zn	1.40941500	-0.10983800	-0.30875500
N	2.77974800	1.60873200	-0.80365100
N	2.94545100	-1.50780400	-1.15969400
N	0.80503400	-1.92762600	0.89368500
N	2.94951000	-0.15076400	1.34906400
H	-0.49793200	-2.84401800	-0.42488700
H	2.02245800	-1.90761700	-2.96470300
H	2.31496100	1.87866600	-2.79802000
O	0.28422800	0.02348300	-2.18072300
H	-0.34807100	-0.68978000	-2.34500400
H	-1.01153600	2.99951000	-1.34533100
P	-1.17156300	1.67416300	0.38271200
O	-1.24844700	2.05993900	-1.27186100
O	0.21531900	1.12935500	0.77326100
O	-2.40197500	1.73137700	1.47773700
C	-2.45300600	2.89996400	2.30608700
H	-3.50217300	3.08201300	2.55003400
H	-1.89293700	2.69973900	3.22635400
C	-1.81368200	4.03041500	1.48419200
H	-1.26157300	4.71124600	2.14182300
C	-2.81516600	4.82318900	0.64549300
H	-3.42891600	4.15871400	0.02717200
H	-3.48506600	5.40045300	1.29261400
H	-2.28970700	5.52495100	-0.00955700
O	-0.85818700	3.35619100	0.66773200
H	-0.29822500	0.81444400	-2.02767500
O	-1.79577800	0.09947500	-0.08036900
C	2.23430900	-0.75693100	2.49007100
C	3.25284900	1.28295400	1.56559700
C	4.13617000	-0.92405200	0.92100100
C	1.23154600	-3.04258100	2.97099000
C	-0.01396800	-2.93088800	0.54325400
C	1.41440200	-1.97266700	2.09311200
C	0.38089700	-4.08480300	2.60265300
C	-0.25924500	-4.02836600	1.36474800
C	4.83384900	-2.85034300	-0.56377500
C	2.83123400	-2.20581800	-2.30384000
C	3.93756900	-1.80923300	-0.30527900
C	4.70963500	-3.57758300	-1.74556700
C	3.69221500	-3.24450100	-2.64189300
C	4.42453300	3.05690200	0.16142900

C	2.92448700	2.24521500	-1.97669800
C	3.51346300	2.00382400	0.25376300
C	4.56496300	3.72573000	-1.05490200
C	3.80171100	3.31362500	-2.14735400
C	-3.10740600	-0.22608200	-0.28413900
C	-3.61110400	-1.33652800	0.41329800
C	-4.91170700	-1.77425500	0.19741600
C	-5.71222800	-1.08804700	-0.71612300
C	-5.23560800	0.02105300	-1.41415100
C	-3.92925100	0.45179200	-1.20147600
N	-7.08564800	-1.54634300	-0.94867700
O	-7.77102400	-0.91236600	-1.75073700
O	-7.46754400	-2.53937400	-0.32858100
H	3.88485400	3.80284200	-3.11197500
H	5.26392200	4.55146900	-1.14880500
H	5.00844800	3.34962700	1.02886000
H	2.36603300	1.73431800	2.02231600
H	4.10133700	1.42191000	2.25122900
H	3.56448700	-3.77826800	-3.57753500
H	5.39628100	-4.38977400	-1.96480900
H	5.62040900	-3.07991000	0.14921700
H	4.93368200	-0.21332700	0.67265900
H	4.51729000	-1.53332900	1.75145200
H	2.92307800	-1.01628100	3.30755000
H	1.53537700	-0.00299600	2.86771700
H	1.74147600	-3.05203100	3.92956900
H	0.22083900	-4.92545500	3.27112300
H	-0.93307200	-4.81360100	1.03909100
H	-2.96765900	-1.83454900	1.13149900
H	-5.32067300	-2.62597900	0.72716900
H	-5.88807000	0.52553400	-2.11665700
H	-3.53850100	1.30424000	-1.74472300

**(3) geometries of species in Gao's mechanism:  
1 in ref41(B3LYP/our basis set):**

Zn	1.65092800	0.10723700	-0.12636400
O	1.22736100	0.76759900	-1.96708600
H	0.31797700	0.56107900	-2.22649100
N	2.72913900	-0.35771100	1.84513600
N	1.40780600	-2.20756700	0.06572800
N	3.83151600	-0.47447200	-0.77382600
N	2.11330500	2.14067100	0.78821000
N	1.62023000	3.32844400	-1.13710900

H	1.46638300	2.40823900	-1.61320100
H	1.75093100	4.15863000	-1.69482200
N	3.41621600	-0.35077600	-3.04834600
H	3.59136800	-0.68788300	-3.98114000
H	2.49774900	0.09334100	-2.81149000
N	0.30493000	-2.58223500	-1.94410300
H	-0.26993100	-1.75064000	-1.77435000
H	-0.11351000	-3.26249200	-2.56084200
O	-1.54070500	-0.37035900	-1.31528400
O	-0.23841900	0.22895000	0.87991100
O	-1.95298600	1.83833100	-0.02776800
P	-1.50419200	0.27632900	0.05016900
O	-2.64858400	-0.38818200	1.06193700
C	-2.90718200	2.33450400	-0.98858200
C	-2.62750800	3.82101400	-1.19069100
C	-3.65852600	4.45721100	-2.11653000
O	-1.34522800	4.03291700	-1.77361500
H	-0.66543800	3.58939200	-1.23907400
H	-2.67077800	4.30819500	-0.20287100
H	-3.64488200	3.97243200	-3.09878900
H	-3.42490300	5.51613800	-2.25840600
H	-4.66723200	4.37744800	-1.69752900
H	-2.79900500	1.79161700	-1.93351700
H	-3.92085500	2.19004800	-0.59510100
C	2.22742600	-1.67247700	2.28686100
C	2.32080800	0.73582800	2.75213000
C	4.18939500	-0.34840300	1.61906200
C	2.43802000	-3.99642500	1.29802000
C	1.03669200	-3.07338500	-0.90000300
C	2.05163300	-2.67192100	1.15674800
C	2.12094800	-4.88768600	0.25987800
C	1.41225800	-4.43984300	-0.83639200
C	5.76854100	-1.60652400	0.09858900
C	4.19986800	-0.79441800	-2.03976200
C	4.60865000	-0.86311900	0.25553200
C	6.15017000	-1.95320900	-1.20945500
C	5.38067500	-1.55094900	-2.27969900
C	2.84091900	3.21955200	2.80677000
C	2.07450700	3.32931700	0.14477000
C	2.45560900	2.09597000	2.09025300
C	2.83830700	4.45497400	2.13685500
C	2.45357000	4.52306600	0.81313500
C	-3.95837300	-0.65910300	0.77875000
C	-4.84092100	-0.61832600	1.87040400

C	-6.18443600	-0.91765900	1.69286600
C	-6.64049000	-1.25494200	0.41666000
C	-5.77445900	-1.30259700	-0.67635100
C	-4.42561800	-1.00877700	-0.49970500
N	-8.05605000	-1.56852200	0.22371400
O	-8.43128500	-1.86079100	-0.91356400
O	-8.79454300	-1.52321300	1.21002400
H	1.26178300	0.58141100	2.98424600
H	2.88689800	0.71529000	3.69660200
H	4.70836500	-0.90734800	2.41267700
H	4.51988400	0.69409200	1.69031600
H	2.87086900	-2.10028200	3.07111200
H	1.23548800	-1.50618800	2.72077100
H	6.35999900	-1.90261900	0.95858700
H	7.05067200	-2.53814700	-1.37827800
H	5.65748200	-1.80067100	-3.29986700
H	2.96104700	-4.32957200	2.18816500
H	2.41569700	-5.93158200	0.32635800
H	1.12476600	-5.11533700	-1.63672400
H	3.12389800	3.14257800	3.85133100
H	3.13409000	5.35976600	2.66130400
H	2.42523100	5.46883000	0.28039100
H	-3.72955100	-1.04844100	-1.32927500
H	-6.16355500	-1.57474700	-1.65002500
H	-6.88389200	-0.89120100	2.51927300
H	-4.44939800	-0.35026700	2.84611600

**TS-4a in ref41 (B3LYP/our basis set):**

Zn	-1.47960000	0.09605800	0.02475800
H	-0.13761000	0.93397200	2.03924700
O	-0.98921400	0.41288600	2.12543000
H	-0.65299900	-0.45671500	2.42777800
N	-2.34159900	-0.88297600	-1.82267100
N	-0.40893500	-2.00564500	-0.03026300
N	-3.43663400	-1.11311700	0.84083300
N	-2.76715900	1.71255100	-0.82453900
H	-1.57198200	2.91729000	1.02858600
N	-2.58919600	3.13669200	0.98408900
H	-2.84431000	4.02638100	1.38869100
N	-3.51269400	-0.38469100	3.05516500
H	-3.62755300	-0.62910400	4.02645500
H	-2.77204100	0.27860500	2.84187500
N	0.73471900	-1.87210800	1.99055700
H	1.16119500	-0.95352500	1.70402200



H	1.33542900	-2.37586300	2.63209700
P	1.32431300	1.36025600	0.02907400
O	1.53888700	0.68433700	1.40675900
O	0.13011900	0.91273400	-0.85743300
O	2.45528400	0.34171500	-0.90736500
O	2.27238100	2.63855700	-0.41614600
C	1.85442500	3.97025100	-0.11961000
C	0.89208200	3.90193400	1.07641200
C	1.60093000	3.94161100	2.43781700
O	0.18473000	2.70745800	0.86432800
H	0.19735000	4.75782800	1.01649400
H	2.32302600	3.12441300	2.52254900
H	2.12232500	4.89667600	2.58244700
H	0.86756200	3.82531700	3.24348200
H	2.75797600	4.55581100	0.07967500
H	1.34640000	4.38031200	-1.00205500
C	-1.29270800	-1.81804300	-2.27516200
C	-2.51499400	0.26412500	-2.74311300
C	-3.62744600	-1.55726700	-1.55364700
C	-0.52304700	-4.03627200	-1.30965300
C	0.28685000	-2.64295000	0.93131000
C	-0.74864600	-2.67599200	-1.14972700
C	0.11076800	-4.72579900	-0.26588800
C	0.53198100	-4.03265900	0.85425600
C	-4.60067300	-3.11223300	0.16274700
C	-3.82947800	-1.32643300	2.11772800
C	-3.86025000	-1.97144700	-0.11274900
C	-4.96005600	-3.36141600	1.49544700
C	-4.59351300	-2.46486900	2.47748500
C	-4.23548900	2.13996000	-2.67318900
C	-3.20362400	2.82243400	-0.19414600
C	-3.22824800	1.41384200	-2.05609600
C	-4.76947600	3.24014000	-1.97978300
C	-4.25635000	3.59460800	-0.74764000
C	3.74400200	0.10454800	-0.66256200
C	4.44294600	-0.63647000	-1.64739400
C	5.77728300	-0.96399900	-1.48583000
C	6.44796900	-0.55276800	-0.32744200
C	5.78330700	0.18360100	0.65852800
C	4.44483200	0.51147600	0.49865200
N	7.84417900	-0.89854900	-0.14766000
O	8.41133900	-0.52523200	0.88643800
O	8.40266100	-1.55401300	-1.03648000
H	-3.75244700	-2.42465700	-2.21673200

H	-4.42732700	-0.85005700	-1.80374500
H	-1.51248100	0.60779900	-3.02010000
H	-3.04826900	-0.02759000	-3.66031700
H	-1.65370500	-2.45236700	-3.09907900
H	-0.45932800	-1.21056500	-2.64526500
H	-0.81650400	-4.54181500	-2.22375400
H	0.29877600	-5.79273600	-0.34827700
H	1.07502700	-4.52969100	1.65244600
H	-4.90408600	-3.77957900	-0.63694600
H	-5.53332300	-4.24774700	1.75308300
H	-4.87802700	-2.61453800	3.51471800
H	-4.59034500	1.86797300	-3.66160800
H	-5.56998700	3.82675900	-2.42235000
H	-4.62298200	4.46628200	-0.21393700
H	3.89889900	-0.93670600	-2.53778500
H	6.31598600	-1.52907700	-2.23694100
H	6.32865200	0.48748400	1.54427200
H	3.92149800	1.06174600	1.26878900

**1' in ref 22 (B3LYP/our basis set):**

Zn	1.63295300	-0.11489900	0.33096800
N	2.09484000	-2.08571600	-0.73959600
N	3.87016700	0.18516900	0.62976600
N	1.67250700	2.18390600	0.22297500
N	2.52914100	0.46340500	-1.83713600
H	1.32527400	2.49466300	2.22837500
H	3.69537100	-0.14791000	2.64493300
H	1.99995100	-3.31567700	0.91845600
O	1.34798800	-0.46611100	2.25414400
H	0.65430100	0.07809300	2.64748800
P	-1.48869000	0.27459800	0.21525100
O	-1.59000300	1.62760200	0.83689100
O	-0.25021200	-0.13643100	-0.58680800
O	-1.79628100	-0.83657200	1.36312000
C	-1.75006700	-2.25350500	1.10106600
H	-2.78110400	-2.59760300	0.94558800
H	-1.16503900	-2.45011100	0.19720200
C	-1.12638600	-3.00679300	2.28429700
H	-1.33730700	-4.06926300	2.08869400
C	-1.76325300	-2.62533700	3.62576800
H	-1.58734400	-1.56926500	3.84983500
H	-2.84730800	-2.79190000	3.61245700
H	-1.32454800	-3.23088800	4.42423500

O	0.28762100	-2.91076400	2.32150200
H	0.60555600	-1.96116600	2.38629000
O	-2.70344500	-0.01603700	-0.90227600
C	1.91105500	1.75929000	-2.15924400
C	2.02279000	-0.62817200	-2.68819000
C	4.00261900	0.50810300	-1.79115400
C	1.98630700	4.10333500	-1.17030600
C	1.51480000	2.98889700	1.28072400
C	1.88855400	2.72289600	-0.98608600
C	1.82592900	4.94249100	-0.06736700
C	1.57952700	4.37770800	1.18287900
C	5.87873300	1.17178800	-0.20553400
C	4.37296600	0.21382800	1.87447300
C	4.59714600	0.64748500	-0.39493900
C	6.41250800	1.19251700	1.08259400
C	5.65086600	0.70091400	2.14383300
C	2.62480500	-3.09507600	-2.84741200
C	2.21972600	-3.28332400	-0.14488000
C	2.27994900	-1.98934600	-2.06889800
C	2.76321900	-4.33922900	-2.23033400
C	2.55306400	-4.43712000	-0.85681800
C	-4.03958200	0.17814900	-0.69768700
C	-4.89148600	-0.41205800	-1.64698200
C	-6.26678500	-0.26917100	-1.53660500
C	-6.78767000	0.46590700	-0.46879400
C	-5.95308300	1.05897800	0.47942900
C	-4.57363900	0.92080000	0.36886200
N	-8.23513900	0.61830800	-0.34634900
O	-8.66912200	1.27231100	0.60485400
O	-8.94569000	0.08428900	-1.20234800
H	2.63914000	-5.38536500	-0.33647800
H	3.02840800	-5.21530900	-2.81580700
H	2.77323700	-2.98103100	-3.91738200
H	0.93792200	-0.49905300	-2.76121000
H	2.44345500	-0.59219100	-3.70635600
H	6.03047100	0.70544300	3.16042800
H	7.40700400	1.59464900	1.25571300
H	6.44423800	1.55506000	-1.05048800
H	4.38350900	-0.43233500	-2.20854400
H	4.38996200	1.31002100	-2.43730100
H	2.39375400	2.23539700	-3.02844500
H	0.86780100	1.55996000	-2.42647800
H	2.16986600	4.51030400	-2.16061700
H	1.88846600	6.02071200	-0.18521700

H	1.43552800	4.99362800	2.06428600
H	-4.45060600	-0.97793700	-2.46130300
H	-6.94175800	-0.71638600	-2.25578300
H	-6.39199300	1.62632800	1.29111600
H	-3.90757600	1.39160100	1.08212500

**TS-4' in ref 22 (B3LYP/our basis set):**

Zn	1.00082400	-0.23332700	-0.42053200
N	0.81921200	-1.55226900	1.48143300
N	2.91523800	0.18731900	0.78738000
N	2.23356200	-2.06262600	-0.93395000
N	-0.87439000	-1.65702800	-0.70754900
H	-1.07486300	-1.69016700	-2.76524800
H	2.86531200	-1.38478700	-2.77243600
H	3.98621700	1.15937100	-0.67686000
O	1.03329800	0.41513100	-2.51249600
H	0.85164500	1.38081200	-2.31998300
H	0.23645500	0.16011800	-2.99712100
P	-0.26368200	2.50635700	-0.33497200
O	-0.68605700	2.42725400	-1.80247500
O	-0.08266900	1.16324700	0.47452200
O	0.09523800	3.95917200	0.37837600
C	1.44104300	4.41678600	0.36725100
H	1.41552100	5.50682800	0.25946900
H	1.90709000	4.16442100	1.33052300
C	2.17159900	3.70628600	-0.78507400
H	3.24433000	3.63338800	-0.53211200
C	2.03501000	4.43017900	-2.13307100
H	0.98178200	4.52564300	-2.41266600
H	2.48872100	5.42914300	-2.08940400
H	2.54274300	3.85816300	-2.91812300
O	1.60269800	2.42604400	-0.78944600
O	-1.88302900	2.82250500	0.43708600
C	-0.64096500	-1.58152800	1.71438500
C	1.52511900	-0.79145000	2.52535000
C	1.39350000	-2.88578400	1.22942200
C	-2.60654300	-2.71434000	0.57095200
C	-1.53468100	-1.98919000	-1.82657300
C	-1.39838000	-2.02014100	0.47658300
C	-3.30275500	-3.02957000	-0.59446700
C	-2.74764200	-2.67130300	-1.82295300
C	3.31681900	-3.98227800	-0.01130500
C	3.02059600	-2.15135200	-2.01804500

C	2.36634100	-2.95937900	0.05597400
C	4.13144600	-4.07996300	-1.13796800
C	3.98047300	-3.14945000	-2.16685700
C	3.92859600	-0.06085600	2.94158100
C	4.01740200	0.81072000	0.35060600
C	2.85707400	-0.23071200	2.06055100
C	5.08071100	0.57807900	2.48516400
C	5.12749800	1.02797000	1.16515700
C	-2.90930400	1.99321400	0.36157500
C	-3.71398400	1.83192100	1.52057900
C	-4.78101700	0.95117700	1.53531800
C	-5.07742700	0.21118400	0.38125000
C	-4.33758000	0.39950900	-0.79559100
C	-3.26986000	1.27940800	-0.81231900
N	-6.11880500	-0.78458800	0.41770300
O	-6.25016400	-1.53519000	-0.56565500
O	-6.82170200	-0.87105500	1.43312100
H	0.88996100	0.06555300	2.77557700
H	1.66326800	-1.38971700	3.44045300
H	3.85202700	-0.41180300	3.96666400
H	5.92628900	0.72635100	3.15093700
H	6.00061200	1.53852800	0.77212200
H	0.56964700	-3.57242300	1.00085500
H	1.88296200	-3.28084200	2.13201000
H	3.41186600	-4.68995900	0.80745500
H	4.87612100	-4.86774800	-1.20887800
H	4.59538200	-3.18771500	-3.05998600
H	-0.90722100	-2.22417600	2.56846700
H	-0.94601900	-0.55382800	1.93987600
H	-3.00342000	-2.98210300	1.54568800
H	-4.26755200	-3.52333000	-0.54516900
H	-3.25149600	-2.89749400	-2.75670300
H	-2.68061200	1.44949200	-1.70544200
H	-4.61741100	-0.15556600	-1.68295700
H	-5.38032200	0.80353200	2.42623000
H	-3.45169300	2.40742200	2.40307100

**(4) reaction in the water-assisted mode in the absence of catalyst reactant:**

H	-1.20922800	1.15275800	-1.45635000
C	-1.99547800	0.90651800	-0.72847800
O	-2.36874800	-0.46219000	-0.90147700
C	-3.19841200	1.82158500	-0.96178400

H	-1.59451300	1.07370000	0.27943900
P	-1.67175100	-1.65396500	-0.01115800
C	-2.74178300	3.28682900	-1.02648100
H	-3.64422000	1.54486100	-1.92824600
O	-4.22197200	1.67084300	0.01056200
O	-1.50912000	-1.16638000	1.41889700
O	-0.11216900	-1.66884400	-0.73061700
O	-2.28551400	-2.95413300	-0.38911500
H	-2.23756800	3.57793600	-0.09683400
H	-2.05576900	3.46139000	-1.86528600
H	-3.61564200	3.93367800	-1.15073600
H	-3.87220500	1.28440400	0.84289800
H	-4.11421500	-0.11925900	2.68458800
O	-3.37627500	0.44207500	2.41890300
H	-2.66680200	-0.19206400	2.11587100
C	1.02583100	-1.03290600	-0.40252100
C	1.28007500	-0.41130300	0.84015500
C	2.03247100	-1.03322000	-1.39485700
C	2.50839200	0.19501700	1.06729700
H	0.50583200	-0.42834600	1.59754600
C	3.25641500	-0.43016900	-1.16314100
H	1.81769900	-1.52229200	-2.33946100
C	3.49109800	0.18674400	0.07177200
H	2.72200800	0.67541800	2.01469100
H	4.03464100	-0.42394500	-1.91655200
N	4.77181800	0.82083500	0.32011900
O	4.95761700	1.35877600	1.41843200
O	5.62266400	0.79370700	-0.57893500

**Transition state:**

H	-1.84280500	1.72134300	-2.16721900
C	-2.10739500	1.26156900	-1.20803500
O	-1.37025200	0.03327100	-1.15573900
C	-3.60548100	0.97087300	-1.05798000
H	-1.77020700	1.91434300	-0.38895400
P	-1.63209800	-1.11700200	-0.02509500
C	-4.39877600	2.27353900	-0.86960000
H	-3.94711800	0.49695700	-2.00218700
O	-3.73235000	0.08133800	-0.00940500
O	-1.49097400	-0.51815600	1.45034400
O	-0.00943600	-1.68739900	-0.13028200
O	-2.38703100	-2.35664700	-0.32886600
H	-4.08156300	2.78947600	0.04500100

H	-4.26897800	2.95611000	-1.72206900
H	-5.46561300	2.04477300	-0.77350700
H	-3.85008100	0.46644100	1.30259200
H	-4.27808800	-0.04832500	2.80677000
O	-3.67053700	0.55895100	2.36795100
H	-2.33329300	-0.15250100	1.88518700
C	1.13825700	-1.00142000	-0.05021500
C	1.26902900	0.31307900	0.45039700
C	2.29490500	-1.68432800	-0.49009900
C	2.51668200	0.91838100	0.49453600
H	0.39526400	0.83271900	0.81929300
C	3.53901300	-1.08133700	-0.44325300
H	2.17427600	-2.69408700	-0.86877200
C	3.64735200	0.22595900	0.04772700
H	2.63239100	1.92494200	0.87817600
H	4.42985900	-1.59652500	-0.78140500
N	4.94676200	0.86510000	0.09718300
O	5.01697200	2.02255200	0.53001400
O	5.93092900	0.22431000	-0.29622000

**END**