

Supporting Information (Computational Part)

Confined Acid-Catalyzed Asymmetric Carbonyl–Ene Cyclization

Luping Liu, Markus Leutzsch, Yiyang Zheng, M. Wasim Alachraf, Walter Thiel, and Benjamin List*

Max-Planck-Institut für Kohlenforschung, Kaiser Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

Table of content

1. Computational methodology
2. Analysis of selected geometries
3. Energy tables
4. References
5. Cartesian coordinates

1. Computational methodology

Density functional theory (DFT) was employed to study the carbonyl-ene cyclization. All calculations were carried out using the Gaussian 09 program package.^{S1} Geometries were optimized at the TPSS-D3/def2-SVP level,^{S2} and the same level of theory was used for frequency calculations to confirm each stationary point to be either a minimum or transition state (TS) structure. Intrinsic reaction coordinate (IRC)^{S3} calculations were also done at the same level to verify the identity of TS structures and to confirm the connection of each TS to the corresponding reactant and product. Relative enthalpies (ΔH) and free energies (ΔG) were determined at standard pressure (1 bar) and room temperature (298 K). Single-point calculations at the gas-phase optimized geometries were performed at the B3LYP-D3/def2-TZVP level^{S4} of theory with inclusion of continuum solvation.^{S5} Natural bond orbital (NBO)^{S6} analyses were carried out using the NBO 3.0 code as implemented in the Gaussian 09 program package.

2. Catalytic cycle

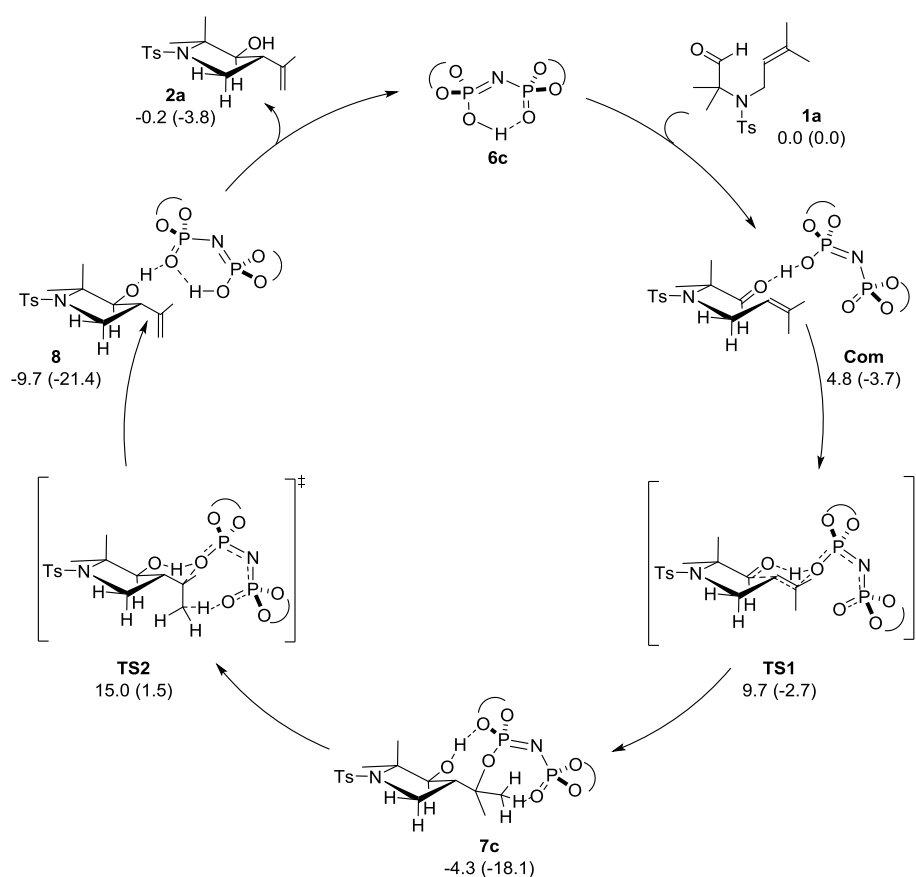


Figure S1. Predicted most favorable catalytic cycle for carbonyl-ene cyclization of **1a** and **6c**. Free energies ΔG (enthalpies ΔH) in CH_2Cl_2 solution are given at the B3LYP-D3/def2-TZVP/TPSS-D3/def2-SVP level, in kcal/mol.

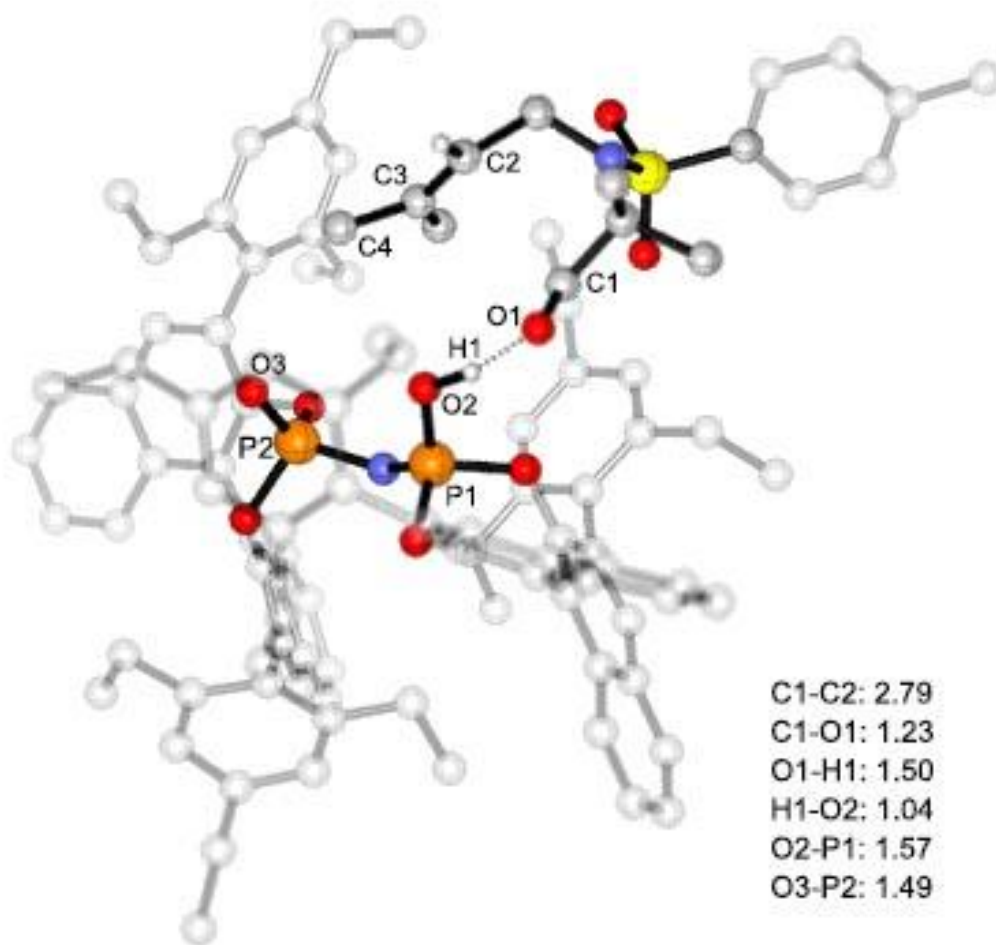
3. Analysis of selected geometries

Optimized structures for selected species in the most favorable catalytic cycle for carbonyl-ene cyclization (Figure S1) are shown in Figure S2. Key interatomic distances are given in the reactive highlighted regions. The discussion in this section refers to the geometry plots on the next four pages (S4-S7).

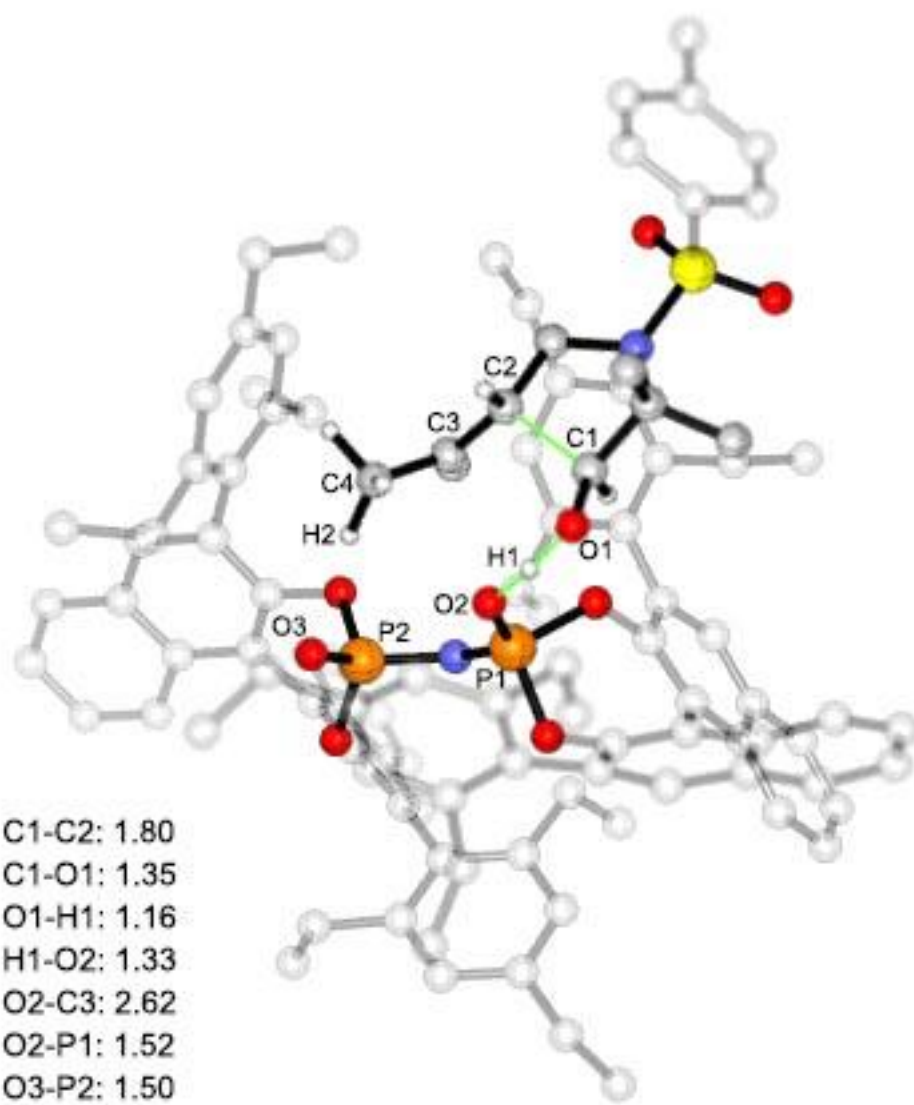
Initially, the catalyst **6c** forms a hydrogen bond (O2–H1···O1) to the aldehyde group of substrate **1a** with an H1···O1 distance of 1.50 Å (complex **Com**). Proton transfer through transition state **TS1** triggers ring formation in **1a** (new C1–C2 bond with subsequent formation of the exocyclic O2–C3 bond) and yields the intermediate **7c**. When going from **Com** to **TS1**, the proton transfer through the hydrogen bond leads to an increase of the O2–H1 distance from 1.04 Å to 1.33 Å and to a decrease of the H1–O1 distance from 1.50 Å to 2.79 Å, while the O1–C1 bond is lengthened from 1.23 Å to 1.35 Å (from a double towards a single bond). Simultaneously, the C1–C2 distance decreases from 2.79 Å to 1.80 Å (indicating the onset of covalent bonding). There is a buildup of positive charge at C3 (NBO: 0.05*e* in **Com** and 0.28*e* in **TS1**). The oxygen atoms O2 and O3 in **TS1** are both negatively charged (NBO: -1.03*e* for O2 and -1.02*e* for O3) and show similar bond lengths (O3–P2, 1.50 Å; O2–P1, 1.52 Å) in **TS1**. The presence of a positively charged C3 atom and a negatively charged O2 atom in **TS1** provides an attractive electrostatic interaction and indicates a partial ionic character of this transition state. The interatomic distance in the C3–O2 bond being formed later in this step is still very large (2.62 Å), implying that **TS1** is an early transition state with regard to C3–O2 bond formation.

On the route from **TS1** to the intermediate **7c** (see the IRC path in Figure 3c of the main paper, left side), the proton transfer within the O1–H1···O2 hydrogen bond is accompanied by the formation of the C3–O2 bond, which is longer in **7c** (1.52 Å) than a typical C–O single bond (1.43 Å) and is thus expected to be weak. In **7c** there are two new hydrogen bonds O1–H1···O4 (1.96 Å) and C4–H2···O3 (2.22 Å), with O4 and O3 acting as proton acceptors. The NBO charge of H2 (0.26*e*) is slightly more positive than that of H3 in the same methyl group (0.22*e*), consistent with its participation in the C4–H2···O3 hydrogen bond. Intermediate **7c** contains two fused eight-membered rings, each of which includes one of the new hydrogen bonds, while the C3–O2 bond belongs to both. The strain in **7c** can be alleviated by a rearrangement via **TS2** to the product complex **8**.

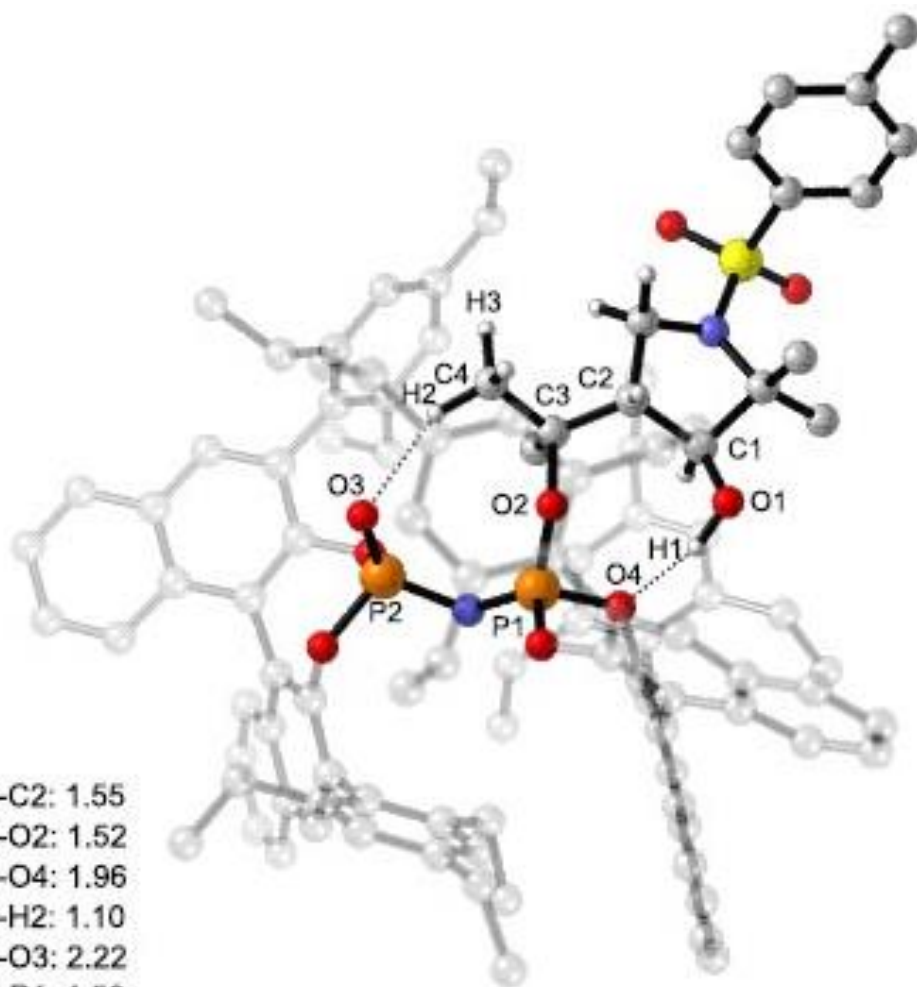
On the route from **7c** to **TS2** (see the IRC path in Figure 3c of the main paper, right side), there is initially a concomitant decrease of the O3–H2 distance (hydrogen transfer from an exocyclic methyl group of the substrate to the catalyst) and an increase of the C3–O2 distance (bond breaking) followed by a hydrogen bond rearrangement (replacing O1–H1···O4 by O1–H1···O2). In **TS2**, the migrating hydrogen atom in the C4···H2···O3 is halfway in between the heavy atoms (C4–H2 1.34 Å; H2–O3 1.32 Å), while the C3–O2 bond is already dissociated (2.69 Å), and the hydroxyl group of the substrate is engaged in a strong O1–H1···O2 hydrogen bond (1.68 Å) with the O2 atom of the catalyst. In **TS2**, the NBO charges on C3 and O2 are 0.40*e* and -1.10*e*, again suggesting a considerable ionic character of this transition state. The O2–P1–N–P2–O3 part of the catalyst moiety is negatively charged (-0.67*e* in **TS2** compared with -0.41*e* in **7c**), which facilitates the dissociation of the C4–H2 bond in the exocyclic methyl group and the transfer of H2 to the catalyst. The rearrangement via **TS2** leads to product complex **8**. The catalytic cycle is completed by an endothermic elimination from **8** which liberates the cyclic product **2a** and regenerates the catalyst **6c**.



Com

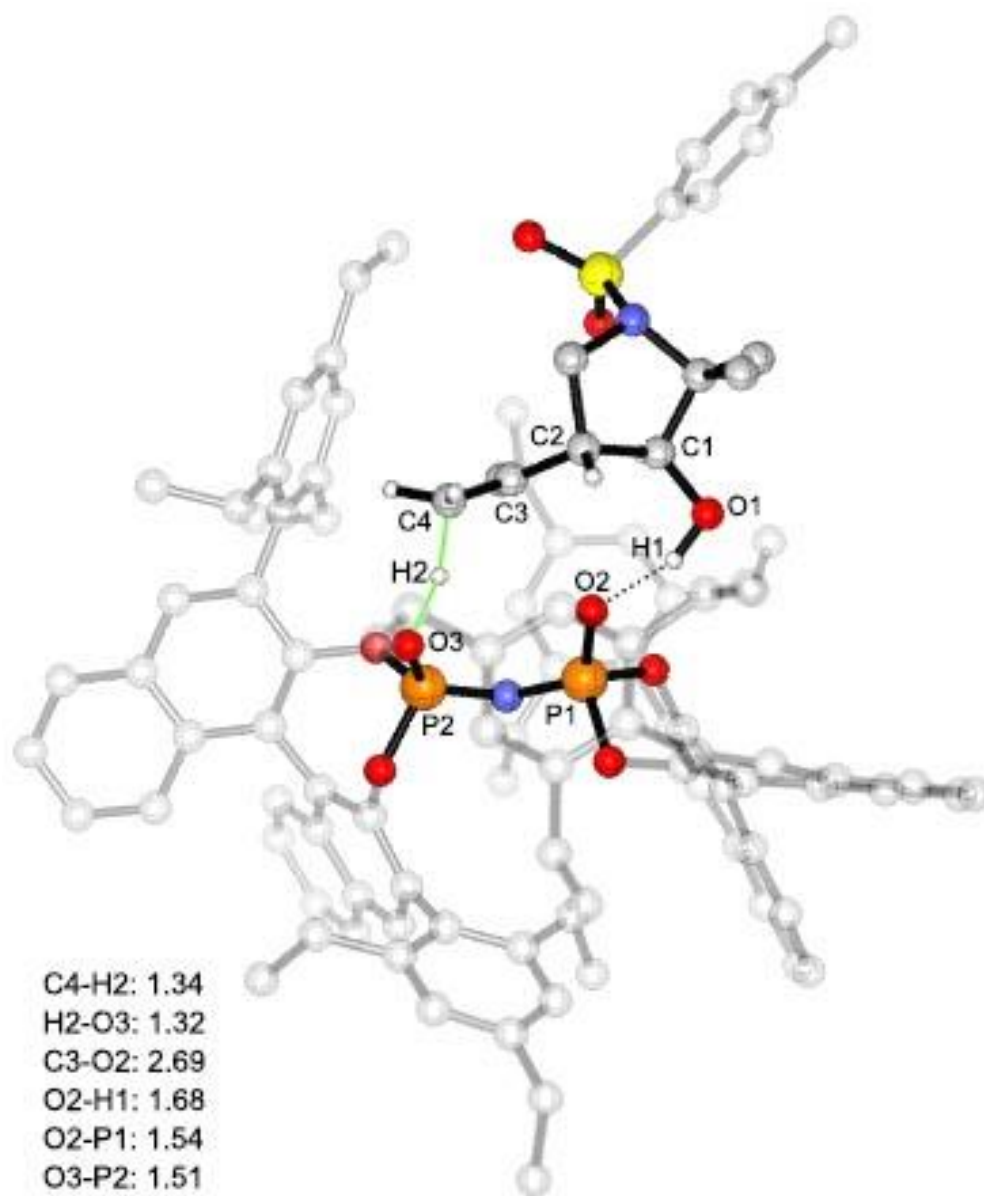


TS1



C1-C2: 1.55
C3-O2: 1.52
H1-O4: 1.96
C4-H2: 1.10
H2-O3: 2.22
O2-P1: 1.58
O3-P2: 1.49

7c



TS2

Figure S2. TPSS/def2-svp optimized structures of **Com**, **TS1**, **7c**, and **TS2** for the carbonyl-ene reaction. Selected distances in Å.

4. Energy tables

Table S1. Absolute energies ($E1$), zero-point vibrational energy corrections ($ZPVE$), enthalpy corrections (H_{corr}), and Gibbs free energy corrections (G_{corr}) on the gas-phase geometries at the TPSS-D3/def2-SVP level, and single-point solvent corrected SCF energies ($E2$) at the B3LYP-D3/def2-TZVP level. All energies are in atomic units.

Species	$E1$	$E2$	$ZPVE$	H_{corr}	G_{corr}
1a+6c	-5895.840369	-5900.732462	1.891305	2.003201	1.712026
Com	-5895.87546	-5900.745924	1.893492	2.010827	1.733202
TS1	-5895.862475	-5900.739626	1.890434	2.006051	1.734571
7c	-5895.889520	-5900.771878	1.898871	2.013786	1.744664
TS2	-5895.865516	-5900.7323845	1.890714	2.005550	1.735806
8	-5895.889874	-5900.7753182	1.89614	2.011476	1.739505
2a+6c	-5895.844879	-5900.739984	1.893969	2.004662	1.719295

Table S2. Relative energies with ZPVE correction (E), enthalpies (H), and Gibbs free energies (G) in CH_2Cl_2 solution at the B3LYP-D3/def2-TZVP//TPSS-D3/def2-SVP level. All energies are in kcal/mol.

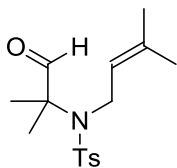
Species	E	H	G
1a+6c	0	0	0
Com	-7.08	-3.66	4.84
TS1	-5.04	-2.71	9.65
7c	-19.99	-18.09	-4.25
TS2	-0.32	1.52	14.97
8	-23.86	-21.70	-9.65
2a+6c	-3.05	-3.80	-0.16

5. References

- S1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision D.01*, Gaussian, Inc., Wallingford CT, **2013**.
- S2. (a) Tao, J. M.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. *Phys. Rev. Lett.*, **2003**, *91*, 46401. (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104. (c) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.*, **2005**, *7*, 3297. (d) Weigend, F. *Phys. Chem. Chem. Phys.*, **2006**, *8*, 1057.
- S3. (a) Fukui, K. *Acc. Chem. Res.*, **1981**, *14*, 363. (b) Hratchian, H. P.; Schlegel, H. B.; Dykstra, C. E.; Frenking, G.; Kim, K. S.; Scuseria, G. *Elsevier, Amsterdam*, **2005**, 195-249.
- S4. (a) Becke, A. D. *J. Chem. Phys.*, **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B*, **1988**, *37*, 785. (c) Miehlich, B.; Savin, A.; Stoll, H.; Preuss, H. *Chem. Phys. Lett.*, **1989**, *157*, 200.
- S5. (a) Foresman, J. B.; Keith, T. A.; Wiberg, K. B.; Snoonian, J.; Frisch, M. J. *J. Phys. Chem.*, **1996**, *100*, 16098. (b) Barone, V.; Cossi, M. *J. Phys. Chem. A*, **1998**, *102*, 1995. (c) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comp. Chem.*, **2003**, *24*, 669.
- S6. (a) Foster, J. P.; Weinhold, F. *J. Am. Chem. Soc.*, **1980**, *102*, 7211. (b) Reed, A. E.; Weinhold, F. *J. Chem. Phys.*, **1983**, *78*, 4066. (c) Reed, A. E.; Weinstock, R. B.; Weinhold, F. *J. Chem. Phys.*, **1985**, *83*, 735. (d) Reed, A. E.; Weinhold, F. *J. Chem. Phys.*, **1985**, *83*, 1736. (e) Abegg, P. W.; Ha, T.-K. *Mol. Phys.*, **1974**, *27*, 763. (f) Carpenter, J. E.; Weinhold, F. *J. Mol. Struct. (Theochem)*, **1988**, *46*, 41. (g) Reed, A. E.; Curtiss, L. A.; Weinhold, F. *Chem. Rev.*, **1988**, *88*, 899-926. (h) Weinhold, F.; Carpenter, J. E. in *The Structure of Small Molecules and Ions*, Eds. R. Naaman and Z. Vager (Plenum, **1988**) 227-236.

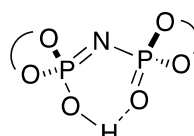
6. Cartesian coordinates (Å) for all computed species and imaginary frequencies for TS1 and TS2

1a:



C	-4.09731500	-0.21516900	-1.06794300
C	-4.61930100	0.03217300	0.20572200
C	-3.75146500	-0.03314800	1.30824700
C	-2.40495000	-0.33201600	1.14399300
C	-1.90849800	-0.56693700	-0.14035800
C	-2.74732600	-0.51479500	-1.24982600
C	-6.07686100	0.36688400	0.39838000
S	-0.20043000	-1.01682600	-0.35468900
O	-0.00625700	-2.28366900	0.33171400
N	0.63138400	0.12759900	0.51888400
C	1.61770400	-0.35320400	1.54070700
C	3.05157400	-0.08330900	1.16710800
C	3.82874100	-0.84607100	0.37783000
C	3.37824800	-2.12413600	-0.27106200
O	0.09490400	-0.92177100	-1.77563300
C	0.85993900	1.50499900	-0.01194100
C	-0.30522700	2.01561900	-0.88735800
C	2.09895700	1.50783600	-0.92838000
O	2.84285000	2.45978200	-1.04724700
C	1.02563400	2.48275800	1.15798900
C	5.23366400	-0.41666900	0.05349200
H	-4.13981100	0.15321300	2.30680200
H	-1.73699800	-0.37765700	1.99850500
H	-2.33933200	-0.70167500	-2.23737100
H	-4.75521000	-0.17240600	-1.93234500
H	-6.54127200	-0.30651200	1.12746500
H	-6.19742100	1.38883500	0.77731100
H	-6.62860500	0.28708000	-0.54204200
H	1.37739000	0.15059400	2.48225300
H	1.42261300	-1.41596500	1.67171100
H	2.19797000	0.59608100	-1.55147100
H	3.48964800	0.82919400	1.56883600
H	5.95514800	-1.18487000	0.36094600
H	5.35120800	-0.28841700	-1.03076100
H	5.49237700	0.52689800	0.54069100
H	3.31840700	-1.99056900	-1.35980100
H	4.11563600	-2.91698200	-0.09242900
H	2.40186100	-2.46586200	0.07416800
H	1.21336800	3.48055400	0.75633200
H	0.10999800	2.49963800	1.75658400
H	1.86981300	2.22426600	1.80002600
H	-0.45565100	1.40302000	-1.77710000
H	-1.22974400	2.04062300	-0.30511800
H	-0.05728500	3.03330600	-1.20060700

6c:

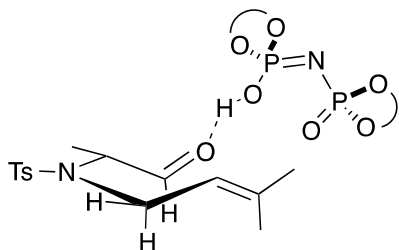


C	-4.67335400	-0.92329000	-0.00559800
C	-4.00538500	0.17105800	0.53343000
C	-4.52016300	1.01458600	1.56286100
C	-5.79010300	0.72563100	2.03648500
H	-6.23203400	1.35355300	2.81716800
C	-6.52320800	-0.40315700	1.56460500
C	-7.80223800	-0.72544100	2.10555900
H	-8.22850000	-0.06226900	2.86644300
C	-8.48735900	-1.85676700	1.69606900
H	-9.46697700	-2.09290800	2.12465900
C	-7.91014000	-2.72392100	0.73230000
H	-8.44219400	-3.63217400	0.43040600
C	-6.67461000	-2.43437000	0.17542000
H	-6.23130700	-3.11146500	-0.55981200
C	-5.95659600	-1.26266300	0.55272000
C	-4.01841000	-1.68248200	-1.10713200
C	-2.70857300	-2.14665300	-0.95480300
C	-1.99884100	-2.85723900	-1.96629100
C	-2.66353400	-3.11097300	-3.15850700
H	-2.14741800	-3.66928500	-3.94644100
C	-3.97800400	-2.62597700	-3.40483000
C	-4.61726000	-2.83035900	-4.66323200
H	-4.09055300	-3.41296500	-5.42717800
C	-5.86507300	-2.29143300	-4.92411900
H	-6.34268200	-2.45094300	-5.89651000
C	-6.51818700	-1.51113100	-3.93446600
H	-7.49192400	-1.06048300	-4.15347800
C	-5.93143700	-1.30698900	-2.69606700
H	-6.43879200	-0.69294100	-1.94793200
C	-4.66136200	-1.87515000	-2.38185100
C	-3.61257200	2.08226500	2.08191900
C	-2.96711600	1.90867500	3.33306700
C	-1.94378200	2.80549700	3.68789600
H	-1.41351900	2.66580200	4.63541200
C	-1.54857000	3.85859600	2.84721800
C	-2.23184300	4.03060500	1.63285800
H	-1.94209100	4.84608900	0.96255400
C	-3.25707000	3.16112900	1.23580900
C	-3.34220600	0.74033600	4.23289300
H	-3.46805400	-0.15055700	3.59538100
H	-4.33684500	0.93921200	4.67950600
C	-2.34464000	0.40712700	5.34540500
H	-2.23593400	1.23156300	6.07270000
H	-1.35093300	0.18060000	4.92323400
H	-2.68406900	-0.48284700	5.90295600
C	-0.37482800	4.75312500	3.19289900
H	-0.66582900	5.81128300	3.04728600
H	-0.12725100	4.63693800	4.26376300
C	0.86863400	4.44709900	2.33520000
H	1.19530500	3.40453300	2.47814700
H	1.70515400	5.11943100	2.59890500

H	0.64863500	4.57893600	1.26162000	H	2.99095100	0.95090600	-6.08411800
C	-3.99178800	3.41333300	-0.06544100	C	4.39433200	-0.58404400	-5.50709300
H	-4.18903000	2.45996400	-0.58514200	H	4.62439900	-0.87579100	-6.53689100
H	-3.33846900	4.00321500	-0.72984800	C	5.01965100	-1.25907900	-4.42576400
C	-5.32206400	4.15833200	0.14631900	H	5.72198900	-2.07439500	-4.62700200
H	-6.00215200	3.57095300	0.78787800	C	4.74079400	-0.90097100	-3.11677000
H	-5.83186900	4.34048600	-0.81688400	H	5.21439200	-1.43405100	-2.28812800
H	-5.15295000	5.13260300	0.63803000	C	3.81504500	0.14347100	-2.82609100
C	-0.57202800	-3.26038100	-1.76362400	C	3.13821700	-1.34876000	3.13938900
C	0.45390400	-2.53215300	-2.41348600	C	2.82875200	-0.34703900	4.09201400
C	1.78791400	-2.93360500	-2.24186200	C	1.92560600	-0.65279800	5.12605600
H	2.57539700	-2.35288100	-2.73376900	H	1.67429400	0.12791900	5.85528200
C	2.13741100	-4.03769300	-1.45197000	C	1.30994600	-1.90871200	5.22965300
C	1.10487300	-4.73683600	-0.80509200	C	1.62118600	-2.87854000	4.26091900
H	1.35394200	-5.59768700	-0.17194400	H	1.13728300	-3.86217400	4.30884500
C	-0.24262900	-4.35987100	-0.93325800	C	2.52075500	-2.62084800	3.21606800
C	0.17050500	-1.32710000	-3.28611200	C	3.41888100	1.04958400	4.02123100
H	0.85663400	-0.51767700	-2.98372300	H	3.67294500	1.30083300	2.97740800
H	-0.84925400	-0.95808500	-3.09697500	H	2.64116200	1.77004800	4.33056700
C	0.35401000	-1.60212100	-4.78751500	C	4.66041400	1.23296800	4.91180700
H	1.37642700	-1.95856800	-5.00222600	H	4.42764500	1.00018200	5.96599500
H	0.18458000	-0.68287500	-5.37509900	H	5.02940800	2.27275700	4.86164100
H	-0.35450400	-2.37144200	-5.14224000	H	5.48009000	0.56534500	4.59548400
C	3.58913800	-4.45490900	-1.31928800	C	0.36398900	-2.22802100	6.36886800
H	4.18275200	-3.59550800	-0.95179200	H	-0.05839300	-1.28931900	6.76855100
H	3.67367000	-5.24390100	-0.55139000	H	-0.48683200	-2.81925400	5.98310600
C	4.19760500	-4.95692900	-2.64078600	C	1.05290400	-3.00492900	7.50649800
H	5.25646300	-5.24185500	-2.50576700	H	1.46456000	-3.96114400	7.13789700
H	4.15054200	-4.17518200	-3.41909900	H	0.34177000	-3.22814700	8.32170700
H	3.64770300	-5.83742800	-3.01657600	H	1.89012100	-2.42142200	7.92836800
C	-1.31845600	-5.16863000	-0.23406100	C	2.84516600	-3.70657600	2.21238000
H	-2.09724200	-4.49249300	0.15859400	H	2.00949300	-4.42726200	2.18475400
H	-0.87059000	-5.67034000	0.64281300	H	2.90695300	-3.27125300	1.20154400
C	-1.96508100	-6.22432600	-1.14954000	C	4.15342200	-4.44785300	2.54074900
H	-1.20649500	-6.92924300	-1.53305100	H	4.10631100	-4.90416100	3.54507900
H	-2.45234700	-5.74655300	-2.01711400	H	5.01345300	-3.75601700	2.52362500
H	-2.73116400	-6.80355200	-0.60382000	H	4.34789400	-5.24916300	1.80626300
C	4.18760800	-0.01933100	-0.28817000	C	0.95527500	3.35597100	-2.09610600
C	3.47381300	-0.59395900	0.75834700	C	-0.41859800	3.34312700	-2.43383200
C	4.04299500	-0.99246800	2.00134500	C	-1.14462500	4.54693800	-2.36563900
C	5.42214300	-0.90077700	2.11862700	H	-2.20030200	4.54010100	-2.66430300
H	5.90288400	-1.21993200	3.04896500	C	-0.55956100	5.74929700	-1.94257200
C	6.22800800	-0.33983700	1.08592700	C	0.78300000	5.71365200	-1.52709900
C	7.63696500	-0.19739900	1.25081100	H	1.25551000	6.63320500	-1.15882600
H	8.09747600	-0.59177100	2.16327400	C	1.55372100	4.54211600	-1.59201200
C	8.40617500	0.44241400	0.29427900	C	-1.12771700	2.06953400	-2.84851600
H	9.48657800	0.54915700	0.43630100	H	-2.07763000	2.00816200	-2.28868200
C	7.78810700	0.98293300	-0.86300400	H	-0.53436300	1.20421700	-2.51937500
H	8.39329600	1.51681400	-1.60310100	C	-1.42202700	1.96839800	-4.35416300
C	6.42335500	0.84865300	-1.06249600	H	-1.97558000	1.03985300	-4.57913500
H	5.95919600	1.27912400	-1.95306100	H	-0.48951600	1.95980300	-4.94501800
C	5.60761000	0.16130200	-0.11635800	H	-2.03047400	2.82185400	-4.70305300
C	3.46409900	0.50614500	-1.47896500	C	-1.35221900	7.04158000	-1.89931300
C	2.42165500	1.41939000	-1.30508300	H	-0.66997000	7.88702600	-2.10394600
C	1.83643800	2.17347700	-2.36024900	H	-2.10046500	7.03523000	-2.71297100
C	2.22972600	1.85342200	-3.65411600	C	-2.06733400	7.28584600	-0.55790800
H	1.81327900	2.42171900	-4.49161400	H	-2.58697500	8.26033500	-0.56067500
C	3.16609200	0.81541400	-3.92270500	H	-1.34787000	7.28251200	0.27973400
C	3.48820500	0.43222900	-5.25754700	H	-2.81757000	6.50162100	-0.36009600

C	3.01159700	4.59531200	-1.16885800
H	3.13544800	5.44579300	-0.47472100
H	3.26899700	3.69171500	-0.59018900
C	3.99782800	4.75300000	-2.34069700
H	5.03668800	4.80610000	-1.96946700
H	3.78675700	5.67468300	-2.91085900
H	3.92901100	3.90091900	-3.03859600
N	-0.22498200	0.02043800	-0.19616600
O	-2.73320800	0.47539300	0.04225800
O	-2.04006800	-1.93920100	0.25171900
O	-1.36458600	-0.39793000	2.17605600
O	2.10592200	-0.80259600	0.58707000
O	1.92972700	1.66047100	-0.00768900
O	0.82719700	0.92212300	2.11810300
P	-1.51888500	-0.43800000	0.66704500
P	1.05653100	0.44079300	0.62993000
H	-0.06949800	0.47076800	2.40314400

Com:



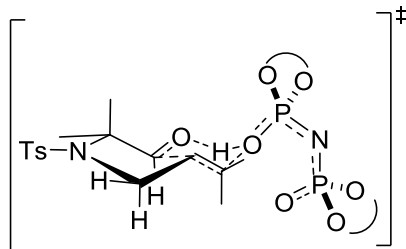
C	3.85069600	-3.21422900	-0.67500100
C	2.59739600	-3.45597300	-0.11577800
C	2.24575800	-4.70104600	0.48121000
C	3.23624300	-5.67155000	0.57462000
H	2.98492200	-6.63992700	1.02118900
C	4.56357300	-5.45049500	0.11677300
C	5.57992400	-6.43828000	0.27342200
H	5.31558200	-7.38888300	0.74992100
C	6.87432400	-6.20021800	-0.15491300
H	7.64795100	-6.96434000	-0.02512000
C	7.20375500	-4.95408200	-0.75036000
H	8.23405700	-4.75859700	-1.06597700
C	6.23604300	-3.97893900	-0.92966100
H	6.50531300	-3.01961000	-1.37798600
C	4.88770500	-4.20034100	-0.51950000
C	4.12587500	-1.93548400	-1.37926200
C	3.98827600	-0.72137800	-0.70213000
C	4.54095300	0.49531900	-1.20522400
C	5.06639500	0.47523600	-2.49346300
H	5.53139700	1.38587400	-2.88346100
C	5.06273900	-0.69190500	-3.30335700
C	5.54015200	-0.67828400	-4.64656300
H	5.90673600	0.26669200	-5.06259200
C	5.52577300	-1.82890700	-5.41605500
H	5.88552200	-1.80489000	-6.45001200
C	5.03192900	-3.04278100	-4.86834800
H	5.00368700	-3.94543300	-5.48771100
C	4.58302600	-3.09375700	-3.55863700
H	4.20144100	-4.03014600	-3.14135200
C	4.59314900	-1.92794200	-2.73793200
C	0.85890000	-5.03782600	0.93282800

C	0.54112200	-5.05107900	2.31525500
C	-0.71027900	-5.55568400	2.70972600
H	-0.96458100	-5.58820500	3.77451700
C	-1.64572700	-6.04336700	1.77880800
C	-1.32243700	-5.97507700	0.41455700
H	-2.04681800	-6.32820800	-0.32986500
C	-0.08400300	-5.47554600	-0.02695000
C	1.55174900	-4.51512100	3.31672600
H	1.76151600	-3.46439000	3.04113900
H	2.50694800	-5.05415100	3.17406100
C	1.14896600	-4.58323200	4.79126800
H	0.96157300	-5.62020700	5.12458100
H	0.23754600	-3.99266400	4.99180300
H	1.95377600	-4.16654200	5.42066900
C	-2.98684900	-6.58525300	2.23362700
H	-3.26638800	-7.44458200	1.59621800
H	-2.88921500	-6.97363400	3.26392800
C	-4.11484300	-5.53797700	2.18964300
H	-3.87404400	-4.67631100	2.83630900
H	-5.06890800	-5.97336100	2.53739700
H	-4.26844700	-5.15788000	1.16526700
C	0.24055000	-5.47723300	-1.50971700
H	0.84611200	-4.58865000	-1.75865900
H	-0.70220800	-5.38035100	-2.07363900
C	0.97125200	-6.74954300	-1.97680400
H	1.94551000	-6.85807400	-1.47086800
H	1.15357000	-6.71667100	-3.06591200
H	0.37100000	-7.64964500	-1.75517500
C	4.77720700	1.71920700	-0.37466000
C	4.19565500	2.95908300	-0.73137600
C	4.66705000	4.13805900	-0.12482400
H	4.21405800	5.09586600	-0.41138500
C	5.68672000	4.12114600	0.83600400
C	6.19243300	2.87074500	1.23424700
H	6.96249400	2.82761900	2.01524900
C	5.75709700	1.66789800	0.65505700
C	3.07184700	3.05727800	-1.74384300
H	2.28099600	3.69605900	-1.31447300
H	2.62026000	2.06217500	-1.88222400
C	3.48915900	3.64115500	-3.10359300
H	3.93493200	4.64440600	-2.98382000
H	2.61442400	3.73679700	-3.76748700
H	4.23237300	2.99965500	-3.60679900
C	6.26090900	5.40470600	1.39913400
H	5.50396300	6.20747900	1.33605400
H	6.49310200	5.26828300	2.47134300
C	7.53480200	5.84755200	0.65436900
H	7.94195100	6.78171700	1.08105100
H	7.32195300	6.01929200	-0.41541900
H	8.31605100	5.06979700	0.71828600
C	6.39639000	0.36409000	1.10295700
H	5.61988600	-0.40812100	1.22903000
H	6.83438200	0.52637800	2.10450000
C	7.49651200	-0.15285500	0.15675800
H	8.30816900	0.58890000	0.05335600
H	7.09542900	-0.35716800	-0.85019100
H	7.93058500	-1.09084600	0.54570500
C	-0.70520600	4.23151800	0.17132400
C	-0.04917800	3.51664500	1.16839100

C	-0.12058800	3.80826400	2.56749600	C	-0.62141600	-1.72640100	-3.57068600
C	-0.86005700	4.92647200	2.92810300	H	0.13868700	-2.51569500	-3.62139600
H	-0.92148200	5.21104800	3.98306500	C	-1.97795200	-2.06606100	-3.68239400
C	-1.58736600	5.69192000	1.97065600	C	-2.92706000	-1.03325300	-3.60343900
C	-2.39934700	6.79215800	2.37452800	H	-3.99245700	-1.27674500	-3.67400500
H	-2.41286200	7.06832000	3.43467400	C	-2.55458300	0.29932000	-3.37935200
C	-3.16858900	7.48704800	1.45652500	C	1.27912900	-0.08017400	-3.35038800
H	-3.79003700	8.32765100	1.78268000	H	1.81800400	-0.90587000	-2.85639200
C	-3.16651600	7.09712300	0.09215500	H	1.45294800	0.81304900	-2.73069200
H	-3.79672900	7.63110300	-0.62682800	C	1.85694800	0.15132100	-4.75701200
C	-2.37608000	6.04266500	-0.33753400	H	2.93127300	0.39092400	-4.70265600
H	-2.38586400	5.74445300	-1.38914500	H	1.34110200	0.98513200	-5.26467900
C	-1.54856600	5.32753800	0.57576700	H	1.73948000	-0.74946800	-5.38468200
C	-0.55699400	3.81202200	-1.25109500	C	-2.42896900	-3.50635700	-3.82287300
C	-0.80707600	2.49273200	-1.63340400	H	-3.11748800	-3.59356800	-4.68538300
C	-0.78672400	2.03325300	-2.98331500	H	-1.55364700	-4.14003400	-4.05441100
C	-0.46067300	2.95542200	-3.96600100	C	-3.13437400	-4.03283000	-2.55936400
H	-0.45738800	2.64150000	-5.01462900	H	-3.42226300	-5.09287100	-2.67999100
C	-0.10108000	4.29556400	-3.64594800	H	-4.04567100	-3.45649200	-2.33320600
C	0.31603600	5.20961500	-4.65755400	H	-2.47321300	-3.95344900	-1.68050200
H	0.31547600	4.87052000	-5.69926400	C	-3.62717700	1.36744900	-3.27726700
C	0.73815200	6.48737400	-4.33330100	H	-4.53589400	0.90102200	-2.86020300
H	1.06665200	7.17552400	-5.11904100	H	-3.31651000	2.14739600	-2.55913000
C	0.76689400	6.89930700	-2.97539600	C	-3.95780800	2.02511900	-4.62877200
H	1.13117400	7.89946100	-2.71859300	H	-4.76351300	2.77392100	-4.52032500
C	0.34337700	6.04423400	-1.97068000	H	-4.28542900	1.26790100	-5.36307600
H	0.37737300	6.36710000	-0.92676400	H	-3.07305000	2.53567300	-5.04640400
C	-0.12286500	4.73125500	-2.27276900	N	0.90713100	-0.05126900	-0.05250600
C	0.49247100	2.83686800	3.52188600	O	1.63652700	-2.45602200	-0.20723100
C	-0.33013200	2.06035700	4.37643400	O	3.40688500	-0.71783300	0.55462900
C	0.24071500	0.96725800	5.05472100	O	1.58685900	-1.37894200	2.22867900
H	-0.40771200	0.34455700	5.68358900	O	0.72641300	2.42066900	0.77494000
C	1.58347300	0.60544100	4.89785100	O	-1.16566700	1.54831100	-0.66622400
C	2.39734300	1.43698600	4.10813900	O	-1.01337900	0.66639300	1.66284000
H	3.45917400	1.19471600	3.98097200	P	1.80368000	-1.12265000	0.77319100
C	1.88254100	2.54929100	3.43363200	P	-0.08199800	1.03739600	0.45304800
C	-1.80835600	2.33143000	4.58180000	H	-1.91571700	1.17216200	1.75317500
H	-2.22429100	2.89280800	3.73075300	O	-3.37190700	1.51280900	1.88894400
H	-2.34484700	1.36548600	4.60703800	C	-3.98221900	0.60416300	1.31999000
C	-2.09543500	3.09365200	5.88838100	C	-5.49621800	0.44636100	1.41401500
H	-1.71953500	2.53483300	6.76347700	H	-3.47249900	-0.07122300	0.60207200
H	-3.18043500	3.25523900	6.02196700	N	-5.83246200	-0.98788600	1.20706600
H	-1.59853800	4.07992400	5.89172100	C	-6.10070600	1.37962800	0.33299500
C	2.14447000	-0.64970400	5.53040400	C	-6.02583800	0.90633300	2.78387100
H	1.31499200	-1.23961600	5.96020800	S	-5.86341600	-1.62294800	-0.37105600
H	2.57995100	-1.26577500	4.72290900	C	-5.39899000	-1.93582200	2.28229100
C	3.20205700	-0.37875300	6.61381700	H	-5.72038700	1.15378600	-0.67269800
H	4.05570700	0.18959700	6.20379500	H	-7.19869200	1.28985200	0.33839600
H	3.59423500	-1.32498200	7.02773000	H	-5.82224000	2.41458000	0.58869700
H	2.77684900	0.21107100	7.44542600	H	-5.75023700	1.96097500	2.93767900
C	2.82604100	3.47108600	2.69450600	H	-7.12309700	0.80663900	2.80542100
H	3.73971600	2.91732700	2.42563000	H	-5.59042400	0.32275100	3.60836300
H	2.38503900	3.81051500	1.74474100	C	-7.47455800	-1.13757500	-0.98677700
C	3.18896600	4.70031900	3.54648800	O	-5.86970300	-3.09693400	-0.23652300
H	3.68101100	4.39781700	4.48774800	O	-4.84729900	-0.96660300	-1.23064300
H	2.28293300	5.27486200	3.81075900	C	-4.05600700	-1.67076100	2.93125300
H	3.87279700	5.37074400	2.99896400	H	-6.17718800	-1.91000600	3.06402400
C	-1.17798400	0.61829300	-3.27646700	H	-5.43100100	-2.93521400	1.82631100
C	-0.19985700	-0.39742200	-3.38219100	C	-8.61933700	-1.41302300	-0.22442900

C	-7.56704500	-0.55192500	-2.25344000
C	-2.81412500	-2.00161600	2.47864700
H	-4.10755900	-1.27190800	3.95421600
C	-9.87188500	-1.07519200	-0.74144100
H	-8.52126300	-1.87206900	0.76364800
C	-8.83276800	-0.22330800	-2.75694700
H	-6.65767700	-0.34799900	-2.82545500
C	-2.52088200	-2.52926400	1.10184700
C	-1.62503400	-1.88022600	3.39329900
C	-10.00104200	-0.47510600	-2.01402900
H	-10.77041900	-1.27983400	-0.14843700
H	-8.91218600	0.24041600	-3.74627100
H	-1.86209900	-1.81989400	0.56623000
H	-1.95255200	-3.47277000	1.16786700
H	-3.41923800	-2.70084300	0.49323400
H	-0.78561400	-1.33877800	2.92961000
H	-1.89010200	-1.39450200	4.34626900
H	-1.25154300	-2.89877300	3.60944900
C	-11.36545100	-0.12052300	-2.55656800
H	-11.98545800	-1.02676800	-2.68311100
H	-11.90605100	0.54833800	-1.86302400
H	-11.29230300	0.38265900	-3.53395800

TS1: (imaginary frequency: 972i cm⁻¹)



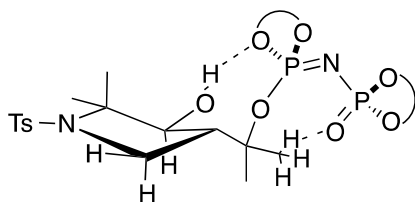
C	4.46164800	-2.89484500	-0.16161300
C	3.13879900	-3.18249700	0.17183600
C	2.73184700	-4.45047800	0.68152900
C	3.71800300	-5.40490000	0.90229300
H	3.42358200	-6.39626500	1.26194200
C	5.09583000	-5.13902600	0.67468200
C	6.09992100	-6.10942000	0.96290900
H	5.78886300	-7.08252400	1.35910000
C	7.43947900	-5.82637100	0.75963400
H	8.20287100	-6.57722300	0.98903100
C	7.82676200	-4.55188400	0.26755400
H	8.88899500	-4.32306500	0.13141400
C	6.87445800	-3.59234500	-0.03485600
H	7.18344200	-2.61084100	-0.40372600
C	5.48456400	-3.85958000	0.14162200
C	4.79427900	-1.59994500	-0.80908400
C	4.46065900	-0.39545500	-0.18450200
C	4.91167700	0.86818700	-0.67138200
C	5.64391400	0.87950800	-1.85361400
H	6.01513200	1.83684800	-2.23303300
C	5.89410100	-0.29858700	-2.60618300
C	6.55102600	-0.25401400	-3.87118900
H	6.88619300	0.71693400	-4.25239600
C	6.74367200	-1.40748400	-4.61178600
H	7.24061600	-1.36061500	-5.58647800
C	6.28112000	-2.65446800	-4.11372700

H	6.41448200	-3.56107000	-4.71343200
C	5.65654000	-2.73331200	-2.87955500
H	5.29548900	-3.69636200	-2.50810100
C	5.45521700	-1.56581900	-2.08536300
C	1.30073500	-4.82461400	0.91062100
C	0.80145300	-4.97035600	2.22622900
C	-0.48448300	-5.51862200	2.40847300
H	-0.86328800	-5.64405900	3.43120200
C	-1.29390400	-5.89763100	1.32597000
C	-0.79603500	-5.68670400	0.02685400
H	-1.41223100	-5.96421200	-0.83767300
C	0.48251400	-5.15375200	-0.20136300
C	1.60471000	-4.53596700	3.43776800
C	-2.68555900	-6.46508700	1.53187600
C	0.97520100	-4.98231200	-1.62572200
C	4.63674200	2.15833500	0.03173700
C	3.78074200	3.10993300	-0.57463000
C	3.60166000	4.35957200	0.04064600
H	2.91164600	5.07677700	-0.42115600
C	4.28232900	4.71015300	1.21561500
C	5.12923400	3.75190000	1.79782700
H	5.66510400	4.00144800	2.72226300
C	5.29977700	2.47141600	1.24511800
C	3.06850300	2.82557200	-1.87872200
C	4.11163700	6.09038600	1.81934500
C	6.23529900	1.48362000	1.91721100
C	-0.89881500	4.11227100	0.05622800
C	-0.40303000	3.47949200	1.19319900
C	-0.79568600	3.79881600	2.53808100
C	-1.61991900	4.90677100	2.69090700
H	-1.90557700	5.23039500	3.69583500
C	-2.17107500	5.60150200	1.57562400
C	-3.08836700	6.67693700	1.76389900
H	-3.30093400	7.00709000	2.78691000
C	-3.71763700	7.27651500	0.68592800
H	-4.42453800	8.09730100	0.84669300
C	-3.46335600	6.80867400	-0.62904400
H	-3.98693000	7.26042700	-1.47817200
C	-2.56054800	5.77966100	-0.84861700
H	-2.37859100	5.42330700	-1.86550600
C	-1.86606700	5.16758000	0.23498700
C	-0.48958600	3.63873500	-1.29637300
C	-0.59112900	2.28660600	-1.64238400
C	-0.42688900	1.79733600	-2.97321300
C	-0.04670600	2.70324200	-3.95178700
H	0.06216700	2.36240100	-4.98647900
C	0.21050700	4.07064200	-3.64420100
C	0.68122100	4.97794600	-4.63760900
H	0.81931800	4.60706900	-5.65919500
C	0.98313900	6.29093300	-4.31877800
H	1.35454000	6.97399300	-5.08967700
C	0.83365800	6.74616400	-2.98293200
H	1.10406300	7.77566300	-2.72581900
C	0.35205600	5.89679900	-1.99964400
H	0.24387000	6.25357400	-0.97192900
C	0.00535800	4.54687400	-2.30058400
C	-0.46912400	2.81291400	3.61105300
C	-1.52606100	2.12855700	4.27818300
C	-1.23283400	0.93310000	4.95941400

H	-2.06024800	0.38307100	5.42656600	C	-7.82137200	-1.57618000	-1.05184500
C	0.05797000	0.38980100	5.00077900	C	-8.81938200	-0.62580800	-0.79556700
C	1.10173500	1.14639100	4.44650700	C	-7.93276600	-2.89195500	-0.57727500
H	2.12700900	0.76226800	4.49236300	C	-9.93085400	-0.99907700	-0.03160900
C	0.86585900	2.35271800	3.77709700	H	-8.70784100	0.38872600	-1.18785800
C	-2.96385500	2.61289300	4.29907400	C	-9.04785100	-3.24399500	0.18932300
C	0.33959200	-0.96670800	5.61017500	H	-7.16524800	-3.63012600	-0.82746800
C	2.05684600	3.16310700	3.31188200	C	-10.06196800	-2.30723400	0.47748500
C	-0.81099700	0.38069700	-3.28438400	H	-10.71446500	-0.26102100	0.17310500
C	0.14746000	-0.65596800	-3.37036800	H	-9.14003000	-4.26886200	0.56610900
C	-0.28848100	-1.95332100	-3.70388900	H	-2.63138800	-3.63831500	-5.23917800
H	0.46169200	-2.74878400	-3.78638300	H	-1.18707300	-4.29046700	-4.44919200
C	-1.64057100	-2.25848800	-3.92112900	H	-4.19632000	0.72960400	-3.06102400
C	-2.58176500	-1.22104600	-3.78227100	H	-2.96081100	1.93573500	-2.65092200
H	-3.64885000	-1.43261500	-3.91981400	H	1.72803500	0.40711200	-2.39213400
C	-2.18987900	0.09243500	-3.47273100	H	2.05240100	-1.29970800	-2.63507000
C	1.62041200	-0.40876500	-3.12215000	C	-2.98199400	-4.32310100	-3.21702700
C	-2.08246200	-3.66563000	-4.27858500	H	-3.24929400	-5.35350300	-3.51207300
C	-3.24821700	1.17704600	-3.40010600	H	-2.46354500	-4.37529200	-2.24314400
N	1.28690300	0.16381200	0.15640200	H	-3.91763100	-3.75599700	-3.07687000
O	2.18010800	-2.20735000	-0.06046400	C	-3.48952100	1.87121900	-4.75278700
O	3.72868300	-0.43200300	0.99191400	H	-3.79652800	1.13589300	-5.51681900
O	1.77831500	-1.34056400	2.40015900	H	-4.28929700	2.62724300	-4.66341000
O	0.53256900	2.47190500	1.00479600	H	-2.57593900	2.37533600	-5.11226900
O	-0.96596000	1.34865000	-0.69550000	C	2.41796500	-0.08479100	-4.39666000
O	-0.99399000	0.40095600	1.61265800	H	3.48784700	0.04356700	-4.15975500
P	2.13321200	-0.91018000	1.01013400	H	2.32826400	-0.89625900	-5.14067000
P	0.00194100	0.96766100	0.61065700	H	2.05546400	0.84612800	-4.86644800
H	-2.44001600	0.92794800	1.85975500	H	-3.20309600	3.16641900	3.37578700
O	-3.44069200	0.78895200	1.87239500	H	-3.63041900	1.73377700	4.31319400
C	-3.70919600	0.18411400	0.70029400	H	-0.61657400	-1.49320900	5.78872200
C	-5.19827600	0.20824000	0.29974500	H	0.90396100	-1.55620500	4.86456600
H	-3.06071500	0.50031000	-0.13732700	H	1.73689400	3.95992400	2.62256500
N	-5.15695100	-0.79673200	-0.78194200	H	2.75073400	2.52031800	2.74378000
C	-5.50604000	1.61809900	-0.22616700	C	-3.26983600	3.48995900	5.52749500
C	-6.12242400	-0.13332100	1.48180400	H	-2.62569900	4.38674100	5.55529100
S	-6.33766600	-1.08869200	-1.93428100	H	-4.32360300	3.82299300	5.52392200
C	-4.26962400	-1.94759900	-0.47547700	H	-3.08763200	2.93062600	6.46200300
H	-4.86280800	1.86207400	-1.07948500	C	1.14000500	-0.89882600	6.92275800
H	-6.55596700	1.69780100	-0.55111100	H	1.34519300	-1.91152900	7.31418400
H	-5.32578700	2.34188300	0.58546700	H	2.10942600	-0.39376900	6.76680500
H	-5.86641300	0.51813500	2.33205800	H	0.58870900	-0.33450700	7.69588600
H	-7.17644500	0.02790800	1.20954700	C	2.78532100	3.79360100	4.51244500
H	-6.01385000	-1.18422000	1.79918200	H	3.13941000	3.01669000	5.21268700
O	-5.83855600	-2.27496200	-2.65660500	H	3.65944200	4.37762600	4.18059200
O	-6.64076000	0.18595600	-2.61275000	H	2.11036100	4.46538000	5.07233500
C	-3.51208800	-1.60319500	0.80851400	H	-2.79100700	-6.81054900	2.57578800
H	-4.83939300	-2.88227200	-0.32830300	H	-2.81285900	-7.35588500	0.88886000
H	-3.59457400	-2.10257500	-1.32682700	H	0.91914300	-4.01337600	4.12990100
C	-2.09785900	-1.86965900	0.92075400	H	2.35108700	-3.78620900	3.13069500
H	-4.06057500	-1.81891800	1.73587000	H	0.09743400	-4.86305800	-2.28484800
C	-1.23242300	-2.00890900	-0.27133300	H	1.55333900	-4.04621400	-1.70447400
C	-1.57329200	-2.29985100	2.23819100	C	-3.80387100	-5.45597400	1.20910800
H	-1.49496700	-1.31635900	-1.09085200	H	-4.80144700	-5.91476800	1.32850000
H	-0.16331000	-1.94991900	-0.03699400	H	-3.75125700	-4.57929300	1.87850100
H	-1.42058900	-3.03444000	-0.64818600	H	-3.71817100	-5.09357000	0.16926200
H	-0.51474400	-2.03995300	2.39118100	C	2.28067300	-5.69569000	4.18972400
H	-2.19325800	-1.92647000	3.06797600	H	2.79510600	-5.32335800	5.09292200
H	-1.65216300	-3.41251200	2.22605200	H	1.54124200	-6.45427300	4.50393000

H	3.03058500	-6.19899300	3.55655200
C	1.82674600	-6.16115900	-2.13109300
H	1.25605200	-7.10553800	-2.08906000
H	2.13986700	-5.99278000	-3.17667300
H	2.73496300	-6.28393300	-1.51759200
H	3.03316500	6.29239000	1.96660800
H	4.57428600	6.11174700	2.82222600
H	1.99762800	3.04455300	-1.74507200
H	3.14164200	1.75493300	-2.11141600
H	5.78319200	0.47737800	1.90276600
H	6.33431800	1.76380000	2.98159200
C	4.72003400	7.20577400	0.95019800
H	4.56853100	8.19727400	1.41313500
H	5.80458500	7.04944400	0.81408900
H	4.25682800	7.22224600	-0.05225300
C	7.63381500	1.43433100	1.27462900
H	7.57174500	1.12643000	0.21666400
H	8.11883900	2.42588700	1.31097900
H	8.28223700	0.71266600	1.80285700
C	3.61103100	3.64706400	-3.05939500
H	3.45722500	4.72817400	-2.89853500
H	4.69335500	3.47796600	-3.19975200
H	3.09683200	3.36938700	-3.99478400
C	-11.27902100	-2.70669100	1.27799400
H	-12.08355100	-3.06371300	0.60736500
H	-11.04805700	-3.52422900	1.98092700
H	-11.68150500	-1.85429700	1.85024000

7c:



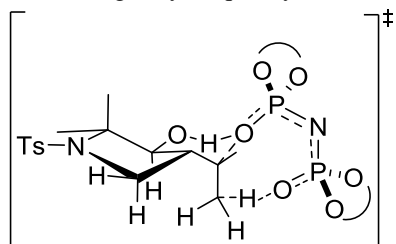
C	-4.26992700	3.29591500	0.18182200
C	-2.88423000	3.44110300	0.20726400
C	-2.22869600	4.66913300	0.51109600
C	-3.02651400	5.74940800	0.86475400
H	-2.55349200	6.71414200	1.07500800
C	-4.44188200	5.64221800	0.96514000
C	-5.24076500	6.74303400	1.39239400
H	-4.74142300	7.68746000	1.63565900
C	-6.61454300	6.62106600	1.51108300
H	-7.21696600	7.47238000	1.84492900
C	-7.24304700	5.38306400	1.21489000
H	-8.32705900	5.28265800	1.33356400
C	-6.49680800	4.29818500	0.78405200
H	-6.98883600	3.34647300	0.56719800
C	-5.08282600	4.39708700	0.62881500
C	-4.87679800	2.02569600	-0.29668000
C	-4.52848700	0.80685600	0.28893300
C	-5.18888700	-0.41945700	-0.01811500
C	-6.18223300	-0.39086100	-0.98863300
H	-6.71468300	-1.31671600	-1.22912900
C	-6.49752200	0.79108500	-1.71230900
C	-7.44733900	0.78163500	-2.77593100
H	-7.95736100	-0.15887500	-3.01203300

C	-7.70759300	1.92788800	-3.50681400
H	-8.43340800	1.90661200	-4.32645700
C	-7.01749600	3.13137600	-3.20445200
H	-7.20570900	4.02964000	-3.80184000
C	-6.10176200	3.17793800	-2.16595900
H	-5.56782000	4.10677900	-1.94826100
C	-5.82581800	2.02053700	-1.37941000
C	-0.74546100	4.81699800	0.38271300
C	0.07673900	4.87300600	1.52993200
C	1.45610900	5.11771000	1.36903000
H	2.07861400	5.16170900	2.26947400
C	2.04318600	5.29204300	0.10817000
C	1.20428100	5.19732700	-1.01970800
H	1.63995500	5.31286700	-2.01970600
C	-0.17180500	4.95657400	-0.90923800
C	-0.48060000	4.67933700	2.92766300
H	0.24242000	4.07561200	3.50595400
H	-1.40409500	4.08046500	2.88000700
C	-0.73796700	5.99920300	3.67574000
H	-1.50094000	6.60755700	3.16099800
H	0.18314400	6.60546600	3.74432600
H	-1.09694900	5.80257900	4.70157200
C	3.52640400	5.56020200	-0.08780000
H	3.92160200	4.85712100	-0.84282800
H	3.63792000	6.56581400	-0.53939500
C	4.40219600	5.47426400	1.16453200
H	4.12395100	6.23208300	1.91852800
H	5.45971400	5.62992600	0.89383000
H	4.32398400	4.48109300	1.64290900
C	-1.01997100	4.89399000	-2.16588100
H	-1.77435500	4.09404900	-2.06843500
H	-0.36705600	4.60834600	-3.00965800
C	-1.72016600	6.22322500	-2.50239800
H	-2.41109600	6.52213200	-1.69603500
H	-2.30358600	6.13193400	-3.43588600
H	-0.98114700	7.03287200	-2.63450300
C	-4.80410700	-1.70108300	0.64696300
C	-4.14244000	-2.69486700	-0.11334300
C	-3.79830700	-3.91044800	0.49903000
H	-3.26607800	-4.66040100	-0.09622000
C	-4.11597700	-4.18347400	1.83704300
C	-4.78190800	-3.18675200	2.57026000
H	-5.04261700	-3.37523900	3.61915000
C	-5.11446500	-1.94202200	2.00888900
C	-3.79689900	-2.49138600	-1.57225100
H	-2.73297700	-2.73776600	-1.71269700
H	-3.90958400	-1.43145200	-1.83911300
C	-4.64202300	-3.35137100	-2.52487500
H	-4.51172500	-4.42639500	-2.31240300
H	-4.34581500	-3.17472800	-3.57340200
H	-5.71637300	-3.11513900	-2.42748000
C	-3.74872500	-5.51909000	2.45596000
H	-2.65005000	-5.65195800	2.40569500
H	-4.01073100	-5.50928000	3.52873900
C	-4.43032900	-6.71689400	1.77142000
H	-4.12907300	-7.66765200	2.24618800
H	-4.15998300	-6.76978500	0.70192800
H	-5.52938900	-6.63207800	1.83402800
C	-5.85158400	-0.91460300	2.84668000

H	-5.42722100	0.08704700	2.66363700	H	-2.31460600	-1.98562300	3.47872300
H	-5.67319800	-1.13706800	3.91427500	H	-1.50164900	-3.49021100	3.05250800
C	-7.36771500	-0.89242800	2.57841400	C	-2.04617800	-3.36445900	5.14297200
H	-7.81963400	-1.87760000	2.78994100	H	-2.14175400	-2.61450400	5.94773100
H	-7.57740800	-0.64279300	1.52394200	H	-1.33077700	-4.13323400	5.48548400
H	-7.86730200	-0.13930300	3.21345500	H	-3.02959400	-3.84533900	5.00600600
C	0.40087900	-4.19778800	0.07820900	C	0.17428100	-0.91705000	-3.63875700
C	0.29722600	-3.38308600	1.20421500	C	-0.54091800	0.30021700	-3.57209400
C	0.95263200	-3.62661500	2.45064500	C	0.10408800	1.48432100	-3.97660600
C	1.65296300	-4.81961300	2.55829100	H	-0.44622300	2.42892300	-3.90215000
H	2.13303800	-5.07397100	3.50740400	C	1.42892400	1.49608700	-4.43672400
C	1.83278100	-5.69290200	1.44893100	C	2.10764600	0.26705200	-4.52017400
C	2.63944300	-6.86290900	1.56487000	H	3.14088800	0.24873600	-4.88805700
H	3.05545600	-7.11319000	2.54692700	C	1.50936500	-0.93916300	-4.12402100
C	2.91751000	-7.64954000	0.46061000	C	-1.97463100	0.35961100	-3.09135300
H	3.54589100	-8.54047800	0.56154100	H	-2.13306200	1.31425700	-2.56277500
C	2.40988600	-7.28155700	-0.81173000	H	-2.13996700	-0.42822600	-2.34259300
H	2.66320200	-7.88083200	-1.69241100	C	-3.00794300	0.21783100	-4.22236600
C	1.60153000	-6.16477700	-0.95364000	H	-4.03315300	0.30827400	-3.82183600
H	1.22820000	-5.88941600	-1.94240000	H	-2.91995600	-0.76363200	-4.72174600
C	1.25876600	-5.35763200	0.16996100	H	-2.87066000	0.99934400	-4.99067200
C	-0.25368600	-3.82566900	-1.20911100	C	2.13728900	2.79169700	-4.77978800
C	-0.05942800	-2.55798000	-1.75935100	H	2.58329700	2.71022700	-5.78939200
C	-0.38372800	-2.19912100	-3.10030700	H	1.39368900	3.60765500	-4.82921400
C	-1.05998100	-3.14065200	-3.86044000	C	3.24186300	3.15383500	-3.76949700
H	-1.31744600	-2.90935900	-4.89858800	H	3.71027700	4.12056500	-4.02325800
C	-1.43042500	-4.40733000	-3.32166000	H	4.04103200	2.39519400	-3.74700400
C	-2.18997900	-5.33939500	-4.08687300	H	2.83062700	3.23289200	-2.74994600
H	-2.47808000	-5.06386400	-5.10695900	C	2.29290100	-2.23403300	-4.24621200
C	-2.57660700	-6.55557600	-3.55117300	H	3.36797800	-2.00089200	-4.18154500
H	-3.16910900	-7.25691000	-4.14742200	H	2.06779800	-2.89865100	-3.39317700
C	-2.22026500	-6.88730800	-2.21787600	C	2.02792100	-2.98195400	-5.56541100
H	-2.54940400	-7.83843400	-1.78687300	H	2.64734600	-3.89424000	-5.62879500
C	-1.46144700	-6.01453300	-1.45459800	H	2.26726800	-2.34079900	-6.43172700
H	-1.19188200	-6.27558000	-0.42793400	H	0.97003400	-3.28209200	-5.65013500
C	-1.03303200	-4.76169200	-1.98195100	N	-1.34339700	-0.05364600	0.03446400
C	0.97576900	-2.54696000	3.48220700	O	-2.09787600	2.34725500	-0.14286900
C	2.21334300	-1.92338600	3.80269700	O	-3.55312900	0.77687500	1.27395900
C	2.20107300	-0.77697500	4.61631500	O	-1.31194900	1.49588400	2.26852800
H	3.15710600	-0.28886400	4.84712000	O	-0.53009400	-2.25972200	1.13837100
C	1.01072100	-0.19626700	5.07735600	O	0.61462600	-1.58576100	-1.00839000
C	-0.19396100	-0.84679600	4.77486000	O	1.18898600	-0.37299300	1.08238000
H	-1.14001200	-0.41266500	5.11935600	P	-1.96403700	1.12469300	0.97722900
C	-0.23233800	-2.02263900	4.01218800	P	-0.08747600	-0.92663100	0.33576200
C	3.55534900	-2.40112900	3.27584800	H	2.42098900	-2.13737100	-0.47064800
H	3.43009800	-2.92642000	2.31568900	O	3.38108600	-1.99435800	-0.36391000
H	4.17268300	-1.51078400	3.05499400	C	3.61814000	-0.63205500	-0.66020800
C	4.33219100	-3.27754300	4.27503900	C	5.10595800	-0.42664600	-1.06035600
H	4.51128900	-2.73234800	5.21860800	H	3.00443900	-0.30866400	-1.52148000
H	5.31037600	-3.57536400	3.85714600	N	5.12684200	1.06027800	-0.94472100
H	3.77574500	-4.19614400	4.52917100	C	5.36223300	-0.93874100	-2.47541200
C	1.01332400	1.09093800	5.87480400	C	6.04950200	-1.11471700	-0.05426300
H	1.96721900	1.62376800	5.70657500	S	6.28303800	2.09109900	-1.58323600
H	0.21083800	1.74693000	5.48911300	C	4.43747500	1.47349200	0.29224900
C	0.81221000	0.86493000	7.38435300	H	4.76869800	-0.36967400	-3.20579500
H	-0.14718300	0.35490700	7.58142200	H	6.42335300	-0.86331800	-2.75652900
H	0.80878600	1.82420800	7.93192500	H	5.05787500	-1.99834400	-2.50148300
H	1.61788600	0.23319600	7.79836600	H	5.81149500	-2.18943200	-0.01554200
C	-1.56663000	-2.71643900	3.83222400	H	7.10074800	-0.98879300	-0.35852000

H	5.93645700	-0.70386600	0.96327700	C	-5.04083700	1.68124600	-1.95383300
C	7.78834500	1.83382600	-0.64170100	H	-5.92064000	1.10020800	-2.24584800
O	5.80299700	3.45257100	-1.26324500	C	-4.54880000	2.67347300	-2.84185600
O	6.55629400	1.67273300	-2.97104900	C	-5.10789600	2.86372200	-4.14000200
C	3.41281200	0.33643300	0.53188000	H	-5.93095500	2.21349700	-4.45557900
H	5.13389200	1.56459600	1.14902700	C	-4.60996100	3.83594100	-4.99022300
H	3.97281100	2.45536600	0.12948100	H	-5.03948300	3.96747500	-5.98870400
C	7.92141600	2.42677100	0.62433200	C	-3.52589600	4.65374800	-4.57456900
C	8.79228900	1.00738200	-1.16225400	H	-3.11818300	5.40330400	-5.26075200
C	1.99065500	0.87639700	0.76481500	C	-2.97657800	4.50849800	-3.31108200
H	3.68454100	-0.22261300	1.44052000	H	-2.13921000	5.13926400	-2.99968500
C	9.06373500	2.15425900	1.38331300	C	-3.47733300	3.52769000	-2.40622200
H	7.14654700	3.10567600	0.99161900	C	1.50670800	4.56077900	1.08150900
C	9.93180400	0.75198800	-0.39018400	C	1.72214200	4.64371900	2.48224200
H	8.67479200	0.58433400	-2.16402100	C	3.01805800	4.42224400	2.98343900
C	10.08373700	1.31111400	0.89391000	H	3.17983600	4.47448400	4.06771300
H	9.17226700	2.61291100	2.37279800	C	4.09163000	4.07630800	2.14664100
H	10.72193400	0.10874400	-0.79351700	C	3.84473200	3.96102400	0.76746900
C	11.31876800	1.04205700	1.72171800	H	4.66269500	3.65529600	0.10390400
H	11.93682800	1.95455900	1.81251800	C	2.57406400	4.20853700	0.21880500
H	11.05107300	0.72775800	2.74597700	C	0.58503300	4.89607000	3.45756000
H	11.94292500	0.25445500	1.26948800	C	5.48172900	3.85719000	2.70776100
C	1.91742400	1.70385200	2.04185400	C	2.38126400	4.13807600	-1.28219500
H	0.86436000	1.91157500	2.28430900	C	-5.13171900	0.45216900	0.19508100
H	2.37473900	1.15092600	2.87616100	C	-5.25388000	-0.90472300	-0.18699400
H	2.44763500	2.65791000	1.89291300	C	-6.12370600	-1.74099400	0.53748200
C	1.40615500	1.61395400	-0.43676900	H	-6.22057200	-2.79114000	0.23415600
H	2.09658000	2.42104100	-0.72495800	C	-6.86160200	-1.27408700	1.63313700
H	1.27187200	0.95993400	-1.31300700	C	-6.66561100	0.05825000	2.03896500
H	0.44732700	2.09317900	-0.19285100	H	-7.20673000	0.43800900	2.91528800

TS2: (imaginary frequency: 1112i cm⁻¹)

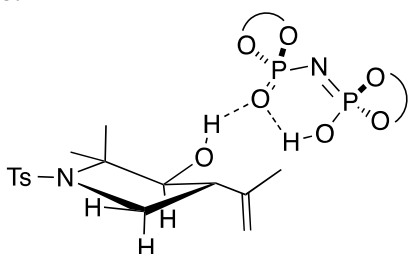


C	-2.01553900	4.34299800	-0.49293900	C	-5.81446100	0.93269700	1.34636900
C	-0.76924600	3.97282500	0.00879100	C	-4.47922100	-1.48980000	-1.35187900
C	0.16437300	4.92082400	0.52849600	C	-7.87619700	-2.15253000	2.33561300
C	-0.21153800	6.25907000	0.52614100	C	-5.72106100	2.37934300	1.80188600
H	0.50443300	7.00483300	0.88613400	C	-1.64484600	-4.30906800	-0.20197500
C	-1.49894900	6.69043900	0.11005700	C	-1.70676400	-3.51179900	0.94117900
C	-1.89032800	8.05855300	0.20020800	C	-1.63101400	-4.01403500	2.27615400
H	-1.15883600	8.78886300	0.56341700	C	-1.58837300	-5.39207400	2.43046200
C	-3.17171000	8.45303500	-0.14248500	H	-1.56235800	-5.81790900	3.43865200
H	-3.46570700	9.50475800	-0.06264500	C	-1.51386700	-6.27180800	1.31300400
C	-4.11498900	7.48586900	-0.57884000	C	-1.39570200	-7.68091700	1.49637300
H	-5.13759800	7.79494700	-0.81927400	H	-1.42787800	-8.07739100	2.51730700
C	-3.75832500	6.15233600	-0.69673500	C	-1.22159400	-8.52941000	0.41667800
H	-4.49890500	5.41856100	-1.02318800	H	-1.12672100	-9.60916100	0.57272900
C	-2.43759600	5.71635700	-0.37817300	C	-1.13939500	-7.99354000	-0.89456500
C	-2.93328400	3.33938100	-1.08833700	H	-0.96573600	-8.66137200	-1.74495800
C	-3.34566900	2.23438300	-0.34280200	C	-1.26732100	-6.63037300	-1.10914700
C	-4.46011600	1.42925900	-0.71438300	H	-1.18830600	-6.22991000	-2.12254000
				C	-1.49006100	-5.73214300	-0.02428700
				C	-1.63200400	-3.67240800	-1.54979700
				C	-0.72520800	-2.64478500	-1.82315600
				C	-0.53896000	-2.06960100	-3.11263800
				C	-1.34459100	-2.52736700	-4.14447200
				H	-1.20719600	-2.12566100	-5.15344300
				C	-2.35575500	-3.50432900	-3.92241300
				C	-3.22336800	-3.92024600	-4.97529400
				H	-3.07596300	-3.49036600	-5.97219700
				C	-4.24245700	-4.82824400	-4.74367800
				H	-4.90660500	-5.13207500	-5.55946000

C	-4.44142600	-5.34827600	-3.43823000	H	0.61118500	1.18801500	2.31024500
H	-5.26827200	-6.04096700	-3.24949100	H	2.19094300	1.07602300	3.45182200
C	-3.60238600	-4.98165700	-2.39832500	H	1.85190800	2.34966500	2.13555100
H	-3.76909400	-5.37986200	-1.39382800	C	2.43133600	0.83068500	-0.02285200
C	-2.52287700	-4.07415200	-2.60865200	H	3.44231700	1.01391100	-0.43211800
C	-1.49095500	-3.04723400	3.40825500	H	2.03099300	-0.01238200	-0.61102200
C	-0.23880400	-2.91428500	4.05883700	H	1.80773800	1.71549700	-0.18814600
C	-0.08523200	-1.91312200	5.03412300	C	7.82915600	-0.72645900	-0.59529100
H	0.89176400	-1.80432900	5.52313400	C	8.14646100	-1.03324700	-1.92217800
C	-1.12482800	-1.03647600	5.37557700	C	8.73187600	-0.97025000	0.45074700
C	-2.36181100	-1.20059700	4.73002500	C	9.39277900	-1.60878700	-2.20204600
H	-3.19524900	-0.53375800	4.98391400	H	7.41620700	-0.83633100	-2.71198800
C	-2.56459800	-2.19088600	3.75834500	C	9.96748500	-1.54754700	0.15136500
C	0.94852500	-3.80308400	3.74205500	H	8.45082300	-0.72695400	1.47902200
C	-0.90683800	0.09407700	6.36103500	C	10.32008000	-1.87431700	-1.17695400
C	-3.93707800	-2.38244700	3.15373500	H	9.64608300	-1.86382300	-3.23686000
C	0.54113600	-1.05417500	-3.30842600	H	10.67387400	-1.75504300	0.96305200
C	0.21591900	0.31197100	-3.47048700	C	11.67716000	-2.46365300	-1.48232700
C	1.25604100	1.23986400	-3.67587400	H	12.43588500	-1.66253800	-1.57308500
H	0.99756500	2.29920000	-3.80090800	H	12.01136200	-3.13627400	-0.67477100
C	2.60233400	0.85202100	-3.70854600	H	11.67091600	-3.02423500	-2.43096400
C	2.90155000	-0.50650600	-3.49648100	H	0.69174000	4.18535400	4.29767000
H	3.94911700	-0.82418300	-3.46864000	H	-0.37774600	4.65874700	2.97520200
C	1.90153000	-1.46570000	-3.28576900	H	6.02798100	3.14171500	2.06883100
C	-1.21645000	0.80778200	-3.43423700	H	5.40213800	3.40489200	3.71405400
C	2.30366800	-2.91207300	-3.05591800	H	3.12002000	3.43249700	-1.69674900
N	-0.94987300	0.12919100	-0.07990600	H	1.38675800	3.72241200	-1.51672200
O	-0.39103900	2.63411000	-0.08542900	C	2.54044600	5.50552200	-1.97051300
O	-2.69185100	1.95975000	0.86436300	H	3.53976800	5.93129800	-1.77319400
O	-0.65062700	1.47005900	2.25848700	H	2.41654500	5.40758900	-3.06380200
O	-1.83583300	-2.13391800	0.77669800	H	1.78609500	6.22287100	-1.60356100
O	0.11713500	-2.18178200	-0.82684100	C	6.28371100	5.16921300	2.80340600
O	0.61448600	-1.43359000	1.51394800	H	6.39846800	5.62894600	1.80615000
P	-1.13093100	1.43895600	0.79306800	H	5.77099700	5.90047600	3.45336500
P	-0.44876900	-1.30313900	0.45149600	H	7.29183900	4.98677700	3.21591700
H	1.86727600	-2.59658800	1.19331400	C	0.54830500	6.32775200	4.01997200
O	2.78618800	-2.95416900	1.07529200	H	1.50216400	6.58480100	4.51404800
C	3.58995400	-1.83647000	0.81843900	H	0.37535800	7.06716700	3.21971300
C	5.09615200	-2.20233400	0.91832900	H	-0.26237300	6.43416900	4.76197500
H	3.43179800	-1.45067300	-0.20865900	H	-3.96585000	-2.39707200	-0.99194900
N	5.72495000	-0.84502500	1.09352700	H	-3.68191100	-0.79380500	-1.66006700
C	5.57104500	-2.99181600	-0.30386600	H	-7.80405600	-2.00208700	3.42864000
C	5.39127900	-3.01253700	2.19259700	H	-7.63925900	-3.21448600	2.14420100
S	6.26709700	0.06684400	-0.24580400	H	-4.67072400	2.71443800	1.78677500
C	4.85274700	-0.08832500	2.01197800	H	-6.04179900	2.42652800	2.85811500
H	5.41855400	-2.42990200	-1.23698200	C	-9.31751000	-1.86414100	1.87507500
H	6.63239300	-3.27771600	-0.21799300	H	-10.03984200	-2.51455800	2.39993900
H	4.95865600	-3.90711300	-0.35041800	H	-9.59253900	-0.81342300	2.07500100
H	4.84190600	-3.96503500	2.14355500	H	-9.42231800	-2.03559800	0.78934900
H	6.47380500	-3.20912400	2.26976700	C	-5.35467000	-1.86352500	-2.55925400
H	5.06359000	-2.48809700	3.10552200	H	-4.74423600	-2.31300400	-3.35949500
O	6.52489700	1.42721000	0.28260100	H	-6.12910400	-2.59723100	-2.27494500
O	5.41636200	-0.06008200	-1.45993400	H	-5.86880000	-0.97926700	-2.97497500
C	3.40254300	-0.67064600	1.82646800	C	-6.58602300	3.34768900	0.97294400
H	5.19428000	-0.24257500	3.04846400	H	-6.48927600	4.37922200	1.35558300
H	4.92944100	0.98693300	1.79611300	H	-6.27976500	3.34847600	-0.08695000
C	2.53124600	0.47896400	1.42408200	H	-7.65122100	3.05990500	1.01605500
H	3.04481900	-1.07666300	2.78593100	H	0.83636000	-4.25300600	2.74328700
C	1.96455900	1.29087700	2.39935700	H	1.85581600	-3.17758100	3.69034900

H	-1.87524200	0.37423400	6.81442400
H	-0.25886600	-0.25450500	7.18711400
H	-4.52201100	-1.45545700	3.27704300
H	-3.85558000	-2.54476100	2.06712300
C	1.16436800	-4.91426900	4.78448500
H	2.05735500	-5.51615900	4.53774000
H	1.30278000	-4.49010600	5.79512000
H	0.29578000	-5.59436000	4.82898500
C	-0.27194900	1.33655100	5.70675700
H	-0.15719000	2.15559000	6.43992100
H	0.72671800	1.09632400	5.30144400
H	-0.88533600	1.69695000	4.86490100
C	-4.68658600	-3.56360900	3.79519200
H	-4.82924400	-3.39934800	4.87799600
H	-5.67858200	-3.70092500	3.33313200
H	-4.11946600	-4.50254800	3.66826900
H	3.36925800	-2.92687600	-2.76635800
H	1.75185300	-3.32223200	-2.19277800
H	-1.24574000	1.73980400	-2.84416200
H	-1.84839000	0.08429200	-2.89387700
H	3.30407100	2.87196000	-3.93868100
H	4.46390100	1.77028500	-3.15920600
C	3.71547600	1.84752700	-3.96943400
C	2.10513300	-3.81738300	-4.28467900
H	2.68141500	-3.43995900	-5.14800700
H	2.44133700	-4.84714900	-4.06830100
H	1.04302000	-3.86204500	-4.57987600
C	4.41616000	1.62386000	-5.32163200
H	5.22301400	2.36261600	-5.47599200
H	4.86449700	0.61572700	-5.37289100
H	3.70028200	1.71387500	-6.15771000
C	-1.80193900	1.07650500	-4.83058500
H	-2.82629500	1.47761300	-4.75432900
H	-1.18891200	1.81178900	-5.38159400
H	-1.83659700	0.15210900	-5.43315500

8:



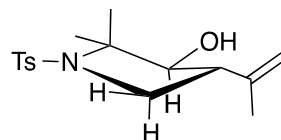
C	4.82348700	-2.68386200	-0.06859300
C	3.48691600	-3.05596900	0.04595300
C	3.06542800	-4.35689600	0.44092200
C	4.05539800	-5.25792400	0.81530200
H	3.76155200	-6.27299500	1.10056700
C	5.43223900	-4.90554000	0.84418900
C	6.42773400	-5.82044900	1.29707800
H	6.11257100	-6.81719700	1.62434200
C	7.76204400	-5.45483000	1.33471600
H	8.51754100	-6.16376100	1.68894100
C	8.15303500	-4.15192800	0.92725100
H	9.20704200	-3.86035100	0.98094000

C	7.21227800	-3.24431300	0.46903100
H	7.52009100	-2.24043300	0.16461300
C	5.83261900	-3.59657200	0.39951800
C	5.18481500	-1.38246600	-0.68396200
C	4.67506900	-0.19253500	-0.16959900
C	5.04642100	1.09332800	-0.65655100
C	5.93840900	1.13246400	-1.72240700
H	6.24945900	2.10904000	-2.10707400
C	6.42548600	-0.04213500	-2.35575200
C	7.27511500	0.02627000	-3.49893300
H	7.57263000	1.01264800	-3.87097600
C	7.70175400	-1.12648300	-4.13447600
H	8.34917000	-1.06318300	-5.01517300
C	7.28332600	-2.39595500	-3.65527000
H	7.60095100	-3.30433000	-4.17761300
C	6.47048800	-2.49671200	-2.53820400
H	6.14613900	-3.47909300	-2.18571000
C	6.03370400	-1.32894000	-1.84542300
C	1.63372400	-4.77985400	0.40332200
C	0.92542000	-4.99450700	1.60654600
C	-0.39265300	-5.48516900	1.54143600
H	-0.93592300	-5.63388300	2.47937900
C	-1.03452200	-5.73549100	0.32261200
C	-0.30697900	-5.50996200	-0.86154100
H	-0.79053000	-5.69114200	-1.82980500
C	1.01049300	-5.03386200	-0.84788000
C	1.52992700	-4.68927000	2.96587400
H	0.78517700	-4.12623500	3.55941800
H	2.39741000	-4.01929400	2.84802700
C	1.94119400	-5.94510100	3.75391200
H	2.73243900	-6.50594300	3.22704700
H	1.08283800	-6.62674800	3.88851500
H	2.32388700	-5.67339600	4.75353600
C	-2.49189600	-6.15550000	0.23921400
H	-3.05043000	-5.32518900	-0.23664600
H	-2.57534800	-7.00717200	-0.46285600
C	-3.17035800	-6.50269800	1.56604200
H	-2.64994100	-7.32669900	2.08623500
H	-4.21365200	-6.81785700	1.39236100
H	-3.19165500	-5.62858700	2.23996500
C	1.75217700	-4.84698800	-2.15846700
H	2.34645400	-3.91754500	-2.12805200
H	1.00842100	-4.71148700	-2.96329200
C	2.67080800	-6.03030700	-2.51416000
H	3.45299700	-6.17041700	-1.74810900
H	3.17025300	-5.85956800	-3.48442300
H	2.09290900	-6.96848600	-2.58326600
C	4.52635400	2.38110100	-0.10116700
C	3.51203200	3.07628800	-0.80081500
C	3.09856100	4.33083200	-0.32721000
H	2.28779100	4.84413000	-0.85485100
C	3.69218900	4.93501200	0.79112400
C	4.71520000	4.23625200	1.45306700
H	5.19317400	4.68792700	2.33095900
C	5.12217600	2.95383100	1.04790900
C	2.88670700	2.52450900	-2.06309700
H	1.79113100	2.60373900	-1.97503700
H	3.11361500	1.45208100	-2.15456900
C	3.34250400	3.25910300	-3.33410900

H	3.09179100	4.33264000	-3.28268900	H	-3.70247000	0.38426800	4.60203100
H	2.84358100	2.83697200	-4.22332700	H	-4.69997800	1.78877600	5.05004700
H	4.43411600	3.17060600	-3.47699500	H	-3.44236200	1.21563700	6.17511500
C	3.21879600	6.29424900	1.26891300	C	0.83581000	-1.09990800	5.72382800
H	2.13723800	6.23446700	1.49990700	H	-0.03579100	-1.77944800	5.68835200
H	3.72550000	6.54493600	2.21796200	H	1.64069600	-1.58545500	5.14154200
C	3.45276300	7.41840300	0.24448300	C	1.29094600	-0.92808600	7.18479700
H	3.08225200	8.38549200	0.62825700	H	2.17718400	-0.27190500	7.24506400
H	2.92955100	7.20538200	-0.70426500	H	1.55187100	-1.90135000	7.63783900
H	4.52787800	7.52568500	0.01703900	H	0.49232100	-0.46722600	7.79240500
C	6.21591300	2.23167600	1.81193900	C	2.23811800	3.09638700	3.30495800
H	6.02213400	1.14444800	1.79822300	H	3.06073700	2.47529500	2.91244900
H	6.17253000	2.54305400	2.87155500	H	1.90134600	3.72299800	2.46646500
C	7.62662500	2.50792700	1.26047800	C	2.75593800	4.00217900	4.43697700
H	7.85123900	3.58875300	1.28264200	H	3.13006200	3.40306500	5.28598300
H	7.71526700	2.16618800	0.21475300	H	1.94654300	4.65084400	4.81635100
H	8.39328900	1.98347600	1.85812000	H	3.57715900	4.64817400	4.08215300
C	-0.98496000	3.98189000	0.22148300	C	-1.20290700	0.34753500	-3.23661800
C	-0.37758600	3.33652900	1.29260100	C	-0.29467600	-0.72235000	-3.40649500
C	-0.66364000	3.60102100	2.67289500	C	-0.80058200	-1.99297700	-3.73915700
C	-1.49320700	4.68614500	2.92553600	H	-0.09156400	-2.81965100	-3.86899700
H	-1.70731300	4.96864500	3.96010000	C	-2.17212400	-2.23310400	-3.90810300
C	-2.14696800	5.40259700	1.88195600	C	-3.05728800	-1.15366100	-3.73614200
C	-3.06488100	6.45304700	2.17702900	H	-4.13704200	-1.30396700	-3.84800200
H	-3.19716000	6.75186700	3.22279900	C	-2.59609900	0.13223100	-3.41058200
C	-3.79561600	7.06497000	1.17271200	C	1.20233400	-0.52835500	-3.29199500
H	-4.50390400	7.86402900	1.41523300	H	1.63888500	-1.40437500	-2.78175700
C	-3.64689500	6.63672800	-0.17176700	H	1.40985800	0.33358900	-2.64369900
H	-4.25249500	7.09711000	-0.95926300	C	1.89565700	-0.33349800	-4.65159200
C	-2.74721500	5.63352600	-0.49630400	H	2.98679200	-0.21846300	-4.51954200
H	-2.64731100	5.30490500	-1.53386600	H	1.51697900	0.56784300	-5.16492400
C	-1.95220300	5.01032100	0.50844600	H	1.71883800	-1.19644600	-5.31801300
C	-0.68299100	3.54172000	-1.16975300	C	-2.68711100	-3.61114100	-4.28418100
C	-0.81563000	2.19878700	-1.53764500	H	-3.16919700	-3.55103100	-5.27935100
C	-0.75369700	1.73582600	-2.88755500	H	-1.82676900	-4.29614000	-4.39785400
C	-0.40552900	2.66137200	-3.86120100	C	-3.69457500	-4.20391100	-3.28454700
H	-0.36077300	2.34129200	-4.90695200	H	-4.04339000	-5.19576300	-3.62311900
C	-0.10899000	4.01680100	-3.54084600	H	-4.57635100	-3.55083600	-3.16984300
C	0.32818000	4.93696700	-4.53804800	H	-3.23192900	-4.32906000	-2.29028200
H	0.42641900	4.58081200	-5.56923600	C	-3.59592000	1.27049100	-3.34486800
C	0.64075400	6.24564700	-4.21234700	H	-4.54577900	0.89621000	-2.93337600
H	0.98413200	6.93935100	-4.98665600	H	-3.23717300	2.05626400	-2.65881500
C	0.52875800	6.68652300	-2.86763900	C	-3.86642400	1.89565200	-4.72535900
H	0.79689500	7.71598500	-2.60835200	H	-4.62383100	2.69531200	-4.64726300
C	0.08654800	5.82295900	-1.87843400	H	-4.24261000	1.13361200	-5.42996600
H	0.00955100	6.16890400	-0.84428700	H	-2.94705300	2.33034000	-5.15532200
C	-0.25507100	4.47203600	-2.18290900	N	1.34490200	0.20786000	-0.17916200
C	-0.23820600	2.59342000	3.69292700	O	2.49313800	-2.12472700	-0.31292500
C	-1.23769800	1.85763000	4.39916100	O	3.77343200	-0.27536300	0.91290400
C	-0.85506800	0.67776000	5.05667900	O	1.74149100	-1.24395800	2.04981400
H	-1.62114600	0.07355400	5.55187100	O	0.57548500	2.36644600	0.98278600
C	0.47054600	0.21228800	5.06098100	O	-1.09254800	1.23780800	-0.55536000
C	1.45225200	1.02065200	4.47246900	O	-0.53731500	0.08110200	1.69384500
H	2.50388700	0.70953900	4.50557900	P	2.25887500	-0.80248900	0.61236900
C	1.12121500	2.20852100	3.80202700	P	0.06601100	0.87711500	0.54961600
C	-2.69252000	2.30915500	4.42204000	H	-2.26326900	0.22132600	2.20828300
H	-2.74298800	3.29266000	4.92545000	O	-3.24681800	0.32314800	2.17795600
H	-3.02294200	2.47990000	3.38301800	C	-3.65427200	-0.17201300	0.93395900
C	-3.68293900	1.36329000	5.10689100	C	-5.05613300	0.34660100	0.52648100

H	-2.95713900	0.14213700	0.13567200
N	-5.30506200	-0.62342100	-0.59177700
C	-4.95478300	1.80558200	0.06915300
C	-6.07129400	0.21474200	1.67462900
S	-6.61285500	-0.62464200	-1.61844500
C	-4.54974900	-1.89996200	-0.44037400
H	-4.25399500	1.89944800	-0.77244500
H	-5.93122800	2.20719600	-0.23858100
H	-4.56293200	2.39753000	0.91387700
H	-5.68787400	0.75245000	2.55678600
H	-7.03820300	0.65784100	1.38694700
H	-6.24494300	-0.83777300	1.95401500
C	-7.96442000	-1.45579400	-0.77320300
O	-6.23939000	-1.50934000	-2.74713900
O	-7.02972400	0.77536500	-1.83558800
C	-3.78559700	-1.71287600	0.87439500
H	-5.22939800	-2.76943600	-0.40379700
H	-3.87720000	-2.02322200	-1.30262800
C	-8.02930100	-2.85700800	-0.77839700
C	-8.93442700	-0.69379900	-0.10577800
C	-2.43303900	-2.36244600	1.03057200
H	-4.42358900	-2.01019100	1.72387200
C	-9.05445800	-3.49429100	-0.06804000
H	-7.30242900	-3.43258100	-1.35790700
C	-9.95619600	-1.34666000	0.58960300
H	-8.88681000	0.39758900	-0.15693200
C	-10.02689700	-2.75500800	0.63280400
H	-9.10941300	-4.58880900	-0.07067900
H	-10.72020100	-0.75247300	1.10395600
C	-11.11815900	-3.44679200	1.41628800
H	-12.09435600	-2.95438100	1.26472800
H	-11.21369700	-4.50596100	1.12604700
H	-10.90099600	-3.41398500	2.50072000
C	-2.03519800	-2.73756400	2.26253700
H	0.80025100	-0.85549400	2.16563200
H	-2.71288900	-2.67738000	3.12217400
H	-1.01315200	-3.07743900	2.44901500
C	-1.51460300	-2.39023600	-0.16242500
H	-1.86608500	-3.10270700	-0.92841500
H	-1.47338900	-1.40726700	-0.66479800
H	-0.49428400	-2.68949200	0.11996800

2a:



C	4.45520900	-0.65533300	-0.51073200
C	3.79789300	0.36742500	-1.23025500
C	2.56858600	0.87469000	-0.80461100
C	1.98083000	0.34180700	0.35266900
C	2.60620700	-0.66614800	1.09216800
C	3.84291700	-1.15858100	0.65204700
H	4.26230800	0.77198500	-2.13681400
H	2.05631600	1.66724300	-1.35759800
H	2.12057400	-1.04979000	1.99424100
H	4.34045500	-1.95030600	1.22300700
C	5.78708700	-1.18739500	-0.98604500
H	5.71135000	-1.58101300	-2.01580300
H	6.54885700	-0.38669200	-1.00006400
H	6.15393600	-1.99710600	-0.33481900
S	0.43605000	1.04014100	0.94561600
N	-0.53089600	0.78091400	-0.44252100
O	0.61716200	2.49635100	1.10193500
O	-0.01265300	0.22627900	2.10731600
C	-1.91460200	1.36756400	-0.48818800
C	-0.64354000	-0.66741300	-0.80123400
H	-0.26771000	-0.81166400	-1.82834300
H	-0.00994400	-1.26815300	-0.13282900
C	-2.77102200	0.16206500	-0.00009100
C	-2.13339300	-1.06604500	-0.67862100
C	-2.44112300	-2.36644400	0.05146800
O	-4.15037000	0.24155400	-0.32879700
C	-1.75194900	-2.76331300	1.13756200
C	-3.63648700	-3.11809500	-0.47884800
H	-3.46988200	-3.43524400	-1.52660900
H	-3.86539200	-4.01056200	0.12626500
H	-4.51901500	-2.45143700	-0.48744400
C	-2.21139200	1.72140700	-1.95440200
H	-3.27770500	1.97648400	-2.06638600
H	-1.59145000	2.57915900	-2.26253100
H	-1.99175300	0.87742300	-2.62955100
C	-2.14822500	2.59147200	0.40150800
H	-1.95253000	2.37230500	1.46341800
H	-1.51920500	3.44350400	0.10521800
H	-3.21001700	2.87814900	0.29075500
H	-2.57676900	-1.12227000	-1.68895200
H	-2.02430300	-3.67948600	1.67459000
H	-0.92375300	-2.17267600	1.54733600
H	-4.58633100	0.78938800	0.34646500
H	-2.62365400	0.07264800	1.09423800