Electronic Supplementary Information

For

Theoretical Study on the Hydroboration of α,β-Unsaturated Carbonyl Compounds Catalyzed by Metal-Free Complex and Subsequent C–C Coupling with Acetonitrile

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1. The scanning result of C–C bond formation via step-wise mechanism.

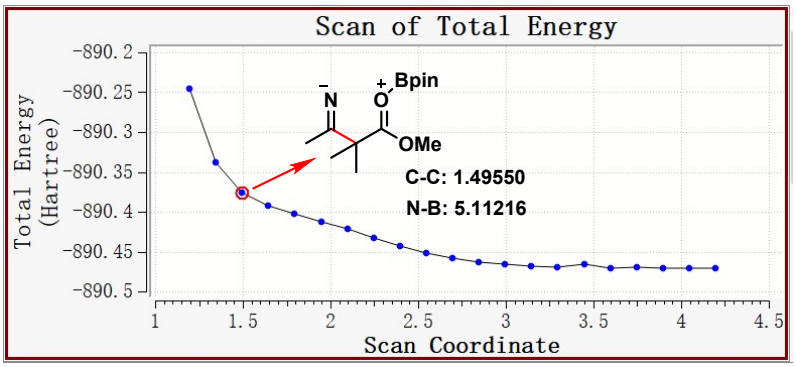


Figure S1. The scanning result of the direct formation of the C–C bond. The key bond lengths were given in Å.

2. The direct 1,4-hydroboration and 1,2-hydroboration without DAP catalysis.

In Figure S2, the theoretical study was performed on the direct 1,4-hydroboration and 1,2-hydroboration reactions of **1a** with HBpin without the participation of DAP and expressed by path C and path D, respectively.

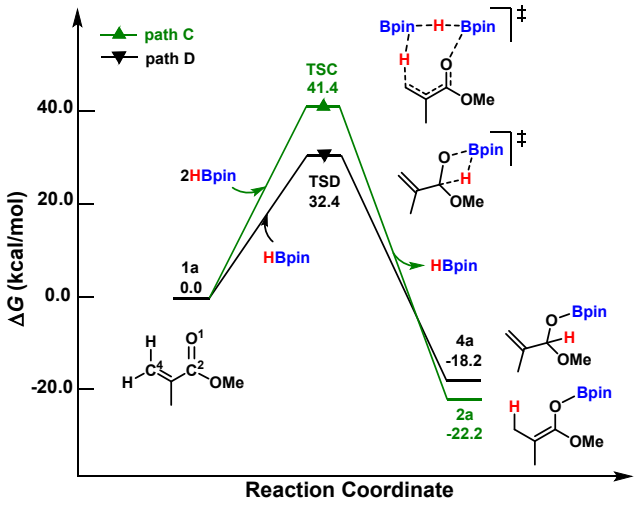


Figure S2. The Gibbs free energy profiles of catalyst-free pathways. Path C is 1,4-hydroboration mode and path D is 1,2-hydroboration mode.

The different of the chemoselectivity is mainly determined by the different properties of DAP and HBpin in the first hydrogen transfer step. In order to further

explore the effect of DAP on the reaction, IRC analysis was performed on **TSD** and **TSB1**, and the results are shown in Figure S3. In the IRC analysis of **TSD**, only Bpin is transferred to O atom at first, and then the C−H and O−B bonds are formed at the same time. This is completely different from the IRC analysis of **TSB1**, in which the C−H bond is formed at first and then the O−B bond is formed (a concerted but asynchronous process). This may be due to the weak nucleophilicity of the hydride in HBpin. Therefore, the empty orbital contained in the B atom coordinate with a pair of lone electrons of the O atom firstly, thus shortening the distance between the two molecules and making the reaction easier. However, for DAP the nucleophilicity of hydride is much stronger than that in HBpin, so hydride is easier to transfer first.

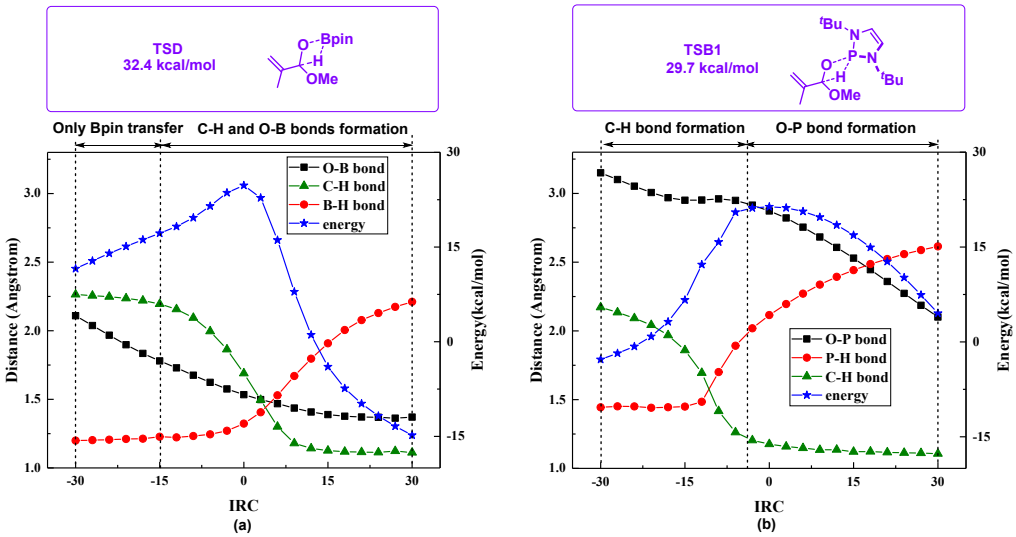


Figure S3. IRC analysis of (a) The transition state of path D and (b) The transition state of the first hydrogen transfer step in path B.

3. The Gibbs free energy profiles of DAP catalyzed 1,4-hydroboration and 1,2-hydroboration of 1,1,1-Trifluoro-3-methyl-3-buten-2-one.

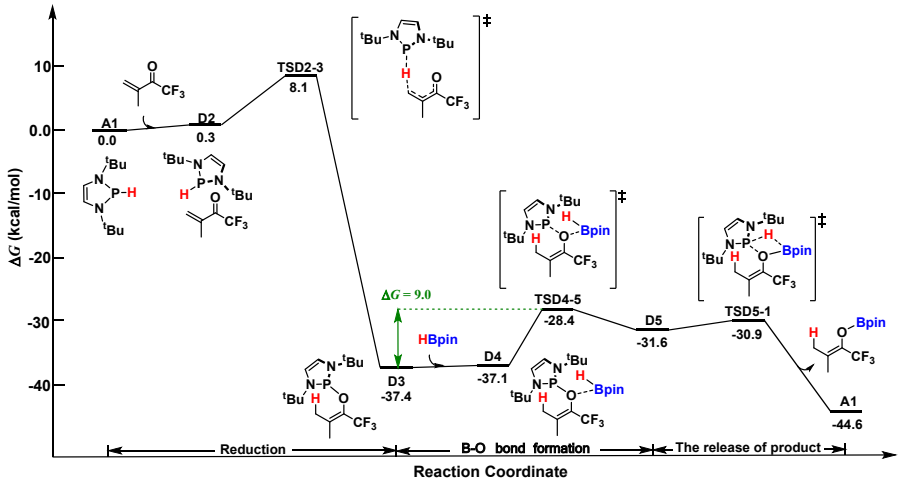


Figure S4. The Gibbs free energy profile of DAP catalyzed 1,4-hydroboration of 1,1,1-Trifluoro-3-methyl-3-buten-2-one.

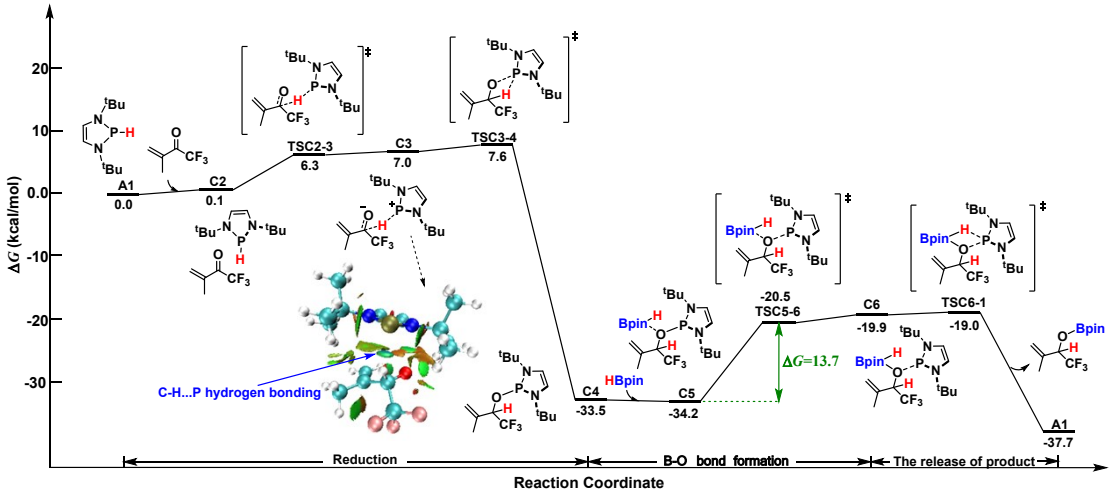


Figure S5. The Gibbs free energy profile of DAP catalyzed 1,2-hydroboration of 1,1,1-Trifluoro-3-methyl-3-buten-2-one. And the NCI analysis of **C3** using RDG method. (Pink: F, blue: N, light blue: C, red: O, gray: H, brown: P)

Figure S4 and Figure S5 show the Gibbs free energy profiles of 1,4- and 1,2-hydroboration, where the -R in substrate is $-CF_3$. Due to the inductive effect of the $-CF_3$ group, the energy barriers of the first hydrogen transfer steps of 1,2- and 1,4-

hydroboration are reduced, and the energy barrier of 1,2-hydroboration (6.3 kcal/mol) is lower than that of 1,4-hydroboration (8.1 kcal/mol). In the whole reaction pathway, the total energy barrier of 1,4-hydroboration is 9.0 kcal/mol lower than that of 1,2-hydroboration (13.7 kcal/mol), so that the 1,4-hydroboration pathway is still more favored. However, the first hydrogen transfer step is irreversible, so the chemoselectivity of hydroboration is determined by the first hydrogen transfer step.

In addition, the strongly electron-withdrawing substituents could make the first HT step change from a concerted mechanism to a stepwise mechanism. As shown in Figure S5, firstly, hydrogen is transferred to C^2 via **TSC2-3** to form intermediate **C3**. The electron withdrawing effect of $-CF_3$ group makes the H atom connected with C^2 more positive, thereby there is a strong C−H...P hydrogen bonding interaction, which helps to stabilize intermediate **C3**. Then the P−O bond is formed via **TSC3-4**. The tendency to reduce through a stepwise mechanism is another reason for the lower energy barrier of the first HT step in 1,2-hydroboration of substrates with electron-withdrawing substituents.

4. Hirshfeld charge and NBO charge.

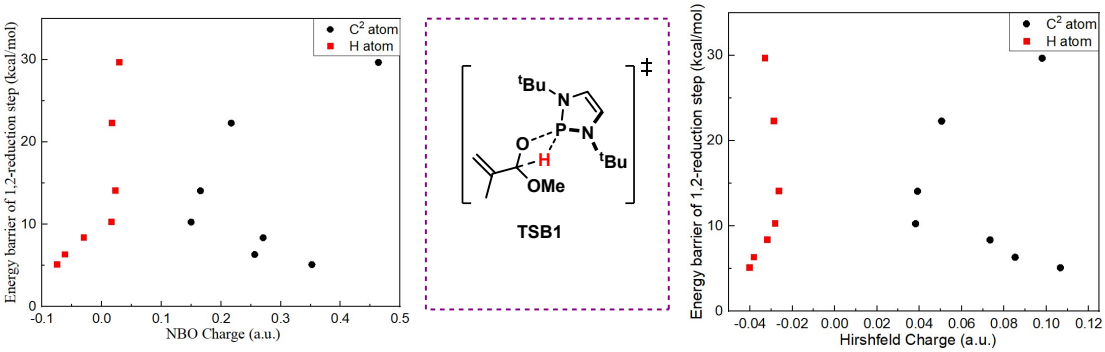


Figure S6. Correlation between the Hirshfeld charge and NBO charge with the energy barrier of the first hydrogen transfer of 1,2-hydroboration pathway for different substrates.

5. IRC of TSA1 and TSB1.

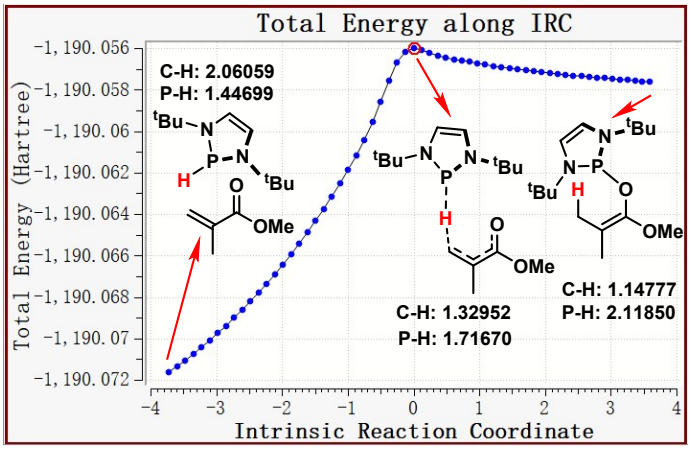


Figure S7. IRC of **TSA1**. The key bond lengths are given in Å.

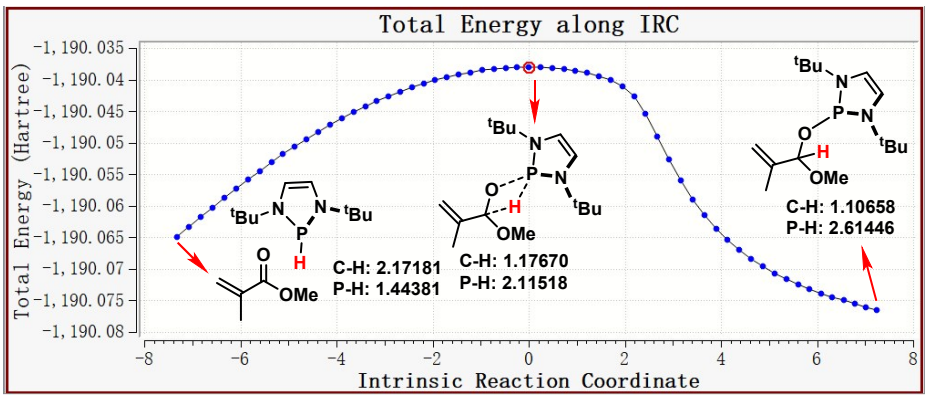


Figure S8. IRC of **TSB1**. The key bond lengths are given in Å.

6. Functional and basis set test.

Table S1: The relative Gibbs free energies (in kcal/mol) of key intermediates and transition states were calculated with different DFT functionals.

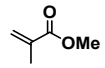
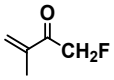
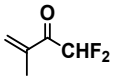
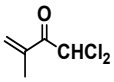
Complex	ωB97X-D	B3LYP	B3LYP-D3	PBE0
A1	0.0	0.0	0.0	0.0
TSA1	15.0	11.7	6.6	10.4
TSA2	-4.6	9.5	-8.6	5.5
2a	-22.2	-18.8	-21.9	-22.7
TS2-3a	-4.1	6.4	-6.8	-3.9
TSB1	29.7	29.4	23.1	29.6
TSB2	7.3	19.7	-2.6	12.1

Table S2: The relative Gibbs free energies (in kcal/mol) of key intermediates and transition states were calculated with different basis sets under ωB97X-D level.

Complex	6-31G(d)	6-31G(d,p)	6-31+G(d)	6-31++G(d,p)
A1	0.0	0.0	0.0	0.0
TSA1	15.0	14.8	16.6	16.4
TSA2	-4.6	-4.8	1.6	1.3
2a	-22.2	-22.2	-19.7	-19.7
TS2-3a	-4.1	-4.4	0.6	0.4
TSB1	29.7	27.5	28.3	27.6
TSB2	7.3	-0.6	5.8	5.0

7. Statistical table of free energy barriers for 1,4- and 1,2-reduction of different substrates.

Table S3. The energy barriers of the first hydrogen transfer steps in different pathways with different substrates.

substrate	NAO of C_4 atoms	$\Delta G_{1,4\text{-hydroboration}}$ (kcal/mol)	NAO of C_2 atoms	$\Delta G_{1,2\text{-hydroboration}}$ (kcal/mol)
	-0.23405	15.01505	-0.06186	29.67555
	-0.23137	13.30006	-0.09986	22.31236
	-0.26003	9.94916	-0.14839	14.07567
	-0.27303	8.30132	-0.19439	10.28551
	-0.27518	7.409	-0.22196	8.37976
	-0.28686	8.06287	-0.24295	6.34098
	-0.29094	6.38177	-0.25600	5.12362

8. The sum of the valence NAO of hydride in HBpin and DAPs.

Table S4. The sum of valence NAO of hydride.

substance	the valence NAO of hydride
DAPs	-0.13318
HBpin	-0.00725

9. Potential energy and free energy of stable points and transition states.

Table S5. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) (Calculated at 298.15 K and 1 atm).

Complex	*E*	*G*	Δ*G*
A1	-844.3923739	-844.118421	0.0
HBpin	-411.7566063	-411.585482	/
1a	-345.6797191	-348.711421	/
2a	-757.4853531	-757.197208	/
3a	-889.900908	-890.2381312	/
4a	-757.19094	-757.479094	
TSA1	-1190.056005	-1189.670918	15.0
A2	-1190.113157	-1189.720671	-16.2
A3	-1601.881821	-1601.306914	-16.7
TSA2	-1601.867948	-1601.2876	-4.6
A4	-1601.873445	-1601.293121	-8.0
TSA3	-1601.86989	-1601.291909	-7.3
TS2-3a	-890.1783087	-889.845261	-4.1
TSB1	-1190.103718	-1189.647555	29.7
B1	-1601.875797	-1189.709486	-9.2
B2	-1601.849212	-1601.298997	-11.7
TSB2	-1601.850515	-1601.268664	7.3
B3	-1601.848628	-1601.270534	6.1
TSB3	-1190.084696	-1601.26712	8.3
TS1-4a	-757.3968562	-757.110213	32.4
TS1-2a	-1169.150284	-1168.681427	41.4

10. Atomic cartesian coordinates of intermediates and transition states in the most favored path A (presented in Å).

TSA1

	Coordinates (Angstroms)		
	X	Y	Z
C	-2.77757900	0.69720200	-0.88690200
C	-1.95545200	1.75866300	-0.94412400
H	-3.67642100	0.54256500	-1.46575300
H	-2.06090700	2.62465900	-1.58080500
N	-2.38734600	-0.22598100	0.08278200
N	-0.91518600	1.67758700	-0.01880600
P	-0.86456500	0.16128500	0.73645800
C	0.10289200	2.74942100	0.12250400
C	-3.07160500	-1.52771900	0.25191200
C	1.03133600	2.40920800	1.29037000
H	1.59870100	1.49160000	1.09642700
H	1.76499900	3.21351900	1.40424900
H	0.48142100	2.31855600	2.23362000
C	0.92760000	2.84022400	-1.16808200
H	1.62402800	3.68380500	-1.10662400
H	1.51960200	1.93047000	-1.30560000
H	0.28653100	2.99746600	-2.04272800
C	-0.61774100	4.07304400	0.40813600
H	-1.25268800	3.98411400	1.29589600
H	0.11895700	4.86295000	0.58658400
H	-1.24306900	4.39182500	-0.43252100
C	-2.39078300	-2.31250900	1.37669700
H	-2.90614000	-3.26831500	1.51178300
H	-1.34350600	-2.53948000	1.14123700
H	-2.42864200	-1.77268700	2.32867300
C	-4.53717900	-1.27150800	0.62250300
H	-5.05723400	-2.22292900	0.77537600
H	-4.60410300	-0.68605700	1.54523400
H	-5.06655100	-0.72881900	-0.16770800
C	-2.97537300	-2.32972500	-1.05380700
H	-3.46533600	-1.81137200	-1.88461200
H	-1.92840900	-2.49864400	-1.32534000
H	-3.46042500	-3.30432900	-0.93409000
H	0.11991700	-0.69763900	-0.37713600
C	3.14210200	-0.83351800	-0.29376300
O	4.18864400	-1.44591900	0.33705800

O	3.15650800	0.38748600	-0.48149700
C	5.24548300	-0.58850800	0.72955900
H	5.99310400	-1.23114900	1.19993100
H	5.68782100	-0.07586500	-0.13055300
H	4.90420100	0.16587600	1.44627400
C	2.10642900	-1.74375200	-0.67256500
C	2.12762400	-3.17641400	-0.21392600
H	3.09511800	-3.65470500	-0.40389300
H	1.93656800	-3.28573500	0.86566800
H	1.36090900	-3.76027900	-0.73788700
C	0.96556400	-1.18620600	-1.27924400
H	0.28199700	-1.87632100	-1.78147400
H	1.10462300	-0.25355500	-1.82902500

A2

Coordinates (Angstroms)			
	X	Y	Z
C	-0.46066700	1.80106300	1.19038200
C	-1.65715200	1.20419700	1.26789600
H	-0.02450000	2.47603400	1.91262600
H	-2.37674100	1.29901800	2.06850700
N	0.22159700	1.46548700	0.00760500
N	-1.93427200	0.40566900	0.14675200
P	-0.54234600	0.18922800	-0.80529100
C	-3.16121800	-0.41334300	0.06368700
C	1.41684100	2.21550400	-0.43814700
C	-3.18177100	-1.16519100	-1.27066700
H	-2.35575500	-1.88195600	-1.34140200
H	-4.11621200	-1.72935000	-1.35311200
H	-3.12587200	-0.47639400	-2.12019900
C	-3.18389900	-1.42876500	1.21603900
H	-4.05872900	-2.08370800	1.13477300
H	-2.27833000	-2.04252300	1.19417500
H	-3.23243600	-0.92735500	2.18856700
C	-4.38250100	0.51200600	0.13486600
H	-4.35673500	1.24503400	-0.67808600
H	-5.30679300	-0.07000900	0.05166900
H	-4.42249500	1.05830100	1.08308700
C	1.89482400	1.67882600	-1.79025500
H	2.79329500	2.22647100	-2.09275800
H	2.15243100	0.61494900	-1.74096200
H	1.13864600	1.81801000	-2.57020900
C	1.04695300	3.69775200	-0.58807800

H	1.91207200	4.27270500	-0.93584600
H	0.23560100	3.81719400	-1.31392800
H	0.71841600	4.13092500	0.36243500
C	2.54081100	2.04476700	0.59267600
H	2.24455400	2.41497700	1.57999600
H	2.80628200	0.98749900	0.68447200
H	3.42941900	2.60487500	0.28106400
H	0.62882400	-0.69245200	2.35251400
C	1.35876300	-1.55600100	0.00586200
O	1.85814000	-1.84949700	-1.23495300
O	0.04468100	-1.24584300	0.05097500
C	1.06357400	-2.72548000	-2.02020800
H	1.67521600	-2.99885400	-2.88293500
H	0.80109200	-3.63159000	-1.46024400
H	0.14717600	-2.23957400	-2.37257400
C	2.15079200	-1.56139400	1.08707400
C	3.58278200	-2.01356800	1.02620000
H	3.84396300	-2.41188400	0.04350000
H	4.26981700	-1.18479100	1.24981800
H	3.77764900	-2.79104700	1.77781800
C	1.64489000	-1.08730700	2.42040200
H	2.29294700	-0.29568500	2.82224600
H	1.65041000	-1.90101400	3.15930100

A3

Coordinates (Angstroms)

	X	Y	Z
C	0.11925100	-2.71716000	0.73524400
C	0.43659800	-1.43314800	0.96132500
C	-0.47160700	-3.17758700	-0.56672800
H	-1.39302800	-3.74824000	-0.39033900
H	-0.72317500	-2.34374900	-1.22410700
H	0.21592700	-3.85449200	-1.09411500
C	0.35684700	-3.78000600	1.77211000
H	-0.57564900	-4.31395000	2.00112000
H	1.06675300	-4.53511500	1.40575300
H	0.75526600	-3.36477900	2.69987500
O	0.14944900	-0.43634800	0.08186400
O	1.07808300	-1.05870800	2.10301500
C	0.42176600	-0.05683600	2.86056900
H	-0.54229400	-0.42543900	3.23781400
H	1.07679400	0.17040000	3.70438800
H	0.26271500	0.85205100	2.27392100

C	2.71585700	1.66344100	1.03631000
C	3.38074700	0.54194100	0.73605600
H	2.93535300	2.35008900	1.84151500
H	4.24058600	0.14102800	1.25326900
N	1.60754100	1.86523000	0.19524300
N	2.81279400	-0.14936800	-0.34354400
P	1.31691400	0.52054200	-0.80867300
C	3.53718200	-1.24553900	-1.02348400
C	0.99473700	3.20509200	0.04926500
C	3.80098600	-2.38203700	-0.02636300
H	2.85763000	-2.75193400	0.38587700
H	4.31688100	-3.20964300	-0.52601300
H	4.43222200	-2.05470300	0.80625000
C	2.68642400	-1.78133900	-2.17692600
H	3.20878000	-2.61573800	-2.65604800
H	1.72015100	-2.15362500	-1.82101000
H	2.50569600	-1.01671500	-2.93953400
C	4.86117900	-0.70276800	-1.57897300
H	5.50764000	-0.32489900	-0.77950500
H	5.40819400	-1.49247600	-2.10595300
H	4.67312600	0.11769300	-2.27980400
C	0.41574500	3.65315100	1.39919900
H	-0.00597000	4.66056000	1.31180300
H	-0.38437500	2.97643400	1.71704700
H	1.17700400	3.68049900	2.18594900
C	2.06535300	4.19847700	-0.42453200
H	1.62867300	5.19192700	-0.57516600
H	2.87582600	4.29422200	0.30588600
H	2.50082600	3.86308800	-1.37174600
C	-0.14130300	3.15614800	-0.97411800
H	0.21939600	2.90422100	-1.97629100
H	-0.91473700	2.43551400	-0.69133500
H	-0.61629800	4.14122700	-1.02987800
B	-2.51811800	0.35304900	-1.83124700
O	-2.88360100	-0.91134200	-1.48487900
O	-3.10184000	1.32714800	-1.07108400
C	-3.74708300	0.66967400	0.04660700
C	-3.66077600	-1.87841300	0.58247200
H	-4.38407700	-1.78885100	1.40075500
H	-3.78117200	-2.86949500	0.13414100
H	-2.64981100	-1.81026900	0.99206200
C	-5.24253500	-1.06346100	-1.17679600
H	-5.20557200	-2.04341100	-1.66210700
H	-6.07826400	-1.06145000	-0.47006500

H	-5.43630400	-0.31342500	-1.95048600
C	-5.05335700	1.39081800	0.34691600
H	-5.59555400	0.88679500	1.15462800
H	-4.84062800	2.41454000	0.67059400
H	-5.70329000	1.44420600	-0.52954600
C	-2.79236700	0.79668100	1.23307200
H	-2.61844300	1.85933100	1.43250300
H	-3.21180600	0.34532700	2.13804900
H	-1.83048100	0.32907000	1.00803700
C	-3.91018100	-0.80890400	-0.47159700
H	-1.77749000	0.59440900	-2.73285400

TSA2

Coordinates (Angstroms)

	X	Y	Z
C	-0.38878900	-2.04141500	1.30020800
C	-0.04616300	-0.75773300	1.12159600
C	-0.91034700	-2.91442300	0.19427900
H	-1.84147300	-3.40272900	0.51327500
H	-1.12798000	-2.34717600	-0.71216300
H	-0.20606700	-3.72536500	-0.03999000
C	-0.30995500	-2.67972600	2.66046600
H	-1.31192100	-2.87053600	3.07006500
H	0.19137400	-3.65476900	2.59577300
H	0.24080100	-2.06054400	3.37183800
O	-0.08123700	-0.11488000	-0.07739800
O	0.42789400	0.00829700	2.15077400
C	-0.57430900	0.74067000	2.84183200
H	-1.20810200	0.06690600	3.43401600
H	-0.05259400	1.41980400	3.52096900
H	-1.20110000	1.31206700	2.15065800
C	3.08298800	1.09598700	0.92582900
C	3.33444500	-0.20790500	0.75869800
H	3.44950300	1.72793000	1.71953100
H	3.96404500	-0.83468300	1.37211200
N	2.22185600	1.59468600	-0.05885900
N	2.63748900	-0.74036200	-0.33407800
P	1.54927400	0.36246400	-0.99855700
C	2.99011200	-2.06369900	-0.90654200
C	1.83609300	3.02691200	-0.13728300
C	2.88395500	-3.13352800	0.18715700
H	1.90213400	-3.09205100	0.66490300
H	3.02884900	-4.12814100	-0.24745800

H	3.64577500	-3.00181300	0.96274600
C	2.02772300	-2.39896100	-2.04835700
H	2.25483600	-3.39917300	-2.43008000
H	0.98626500	-2.39486700	-1.71341600
H	2.12730800	-1.69577200	-2.88165800
C	4.42289600	-1.99730200	-1.45107000
H	5.13947600	-1.74836200	-0.66121800
H	4.71343000	-2.96329700	-1.87824300
H	4.50009400	-1.23485700	-2.23349400
C	0.67321500	3.30168800	0.82207400
H	0.41032100	4.36562300	0.80495200
H	-0.21235200	2.72463200	0.54086900
H	0.94935900	3.03427100	1.84726300
C	3.04530700	3.89633000	0.23340700
H	2.80666600	4.94656400	0.03824500
H	3.30679100	3.81910200	1.29326600
H	3.92295700	3.62764500	-0.36420500
C	1.42561900	3.36021300	-1.57572000
H	2.23690800	3.13835100	-2.27745100
H	0.53228500	2.81112600	-1.88754600
H	1.19244200	4.42733400	-1.64639600
B	-1.60613000	0.62990000	-0.91118500
O	-2.29274900	-0.45526500	-1.48443300
O	-2.40490500	1.24432600	0.06782300
C	-3.63807700	0.52047200	0.18126100
C	-4.31067300	-1.68709700	-1.03524600
H	-5.36796900	-1.60977000	-0.75673700
H	-4.25182600	-2.20142600	-2.00011600
H	-3.79835200	-2.30470500	-0.29474300
C	-4.33659800	0.45552300	-2.31092300
H	-4.17201900	-0.09948300	-3.23978200
H	-5.41572100	0.57186000	-2.16562800
H	-3.89246600	1.44857300	-2.43517200
C	-4.76823300	1.53528700	0.33059400
H	-5.74469000	1.03756800	0.33999000
H	-4.65499700	2.07214900	1.27845000
H	-4.75806200	2.27328300	-0.47467400
C	-3.59837200	-0.36184300	1.43013500
H	-3.42885300	0.26569800	2.31064800
H	-4.54716000	-0.89019300	1.57274200
H	-2.78918900	-1.09422400	1.37759700
C	-3.67515700	-0.30723200	-1.15633000
H	-0.92870200	1.34359000	-1.60541700

A4

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.44656600	-2.78262500	0.44220200
C	-0.12052600	-1.49294900	0.63235200
C	-0.90758100	-3.31608600	-0.88408800
H	-1.94801200	-3.66128900	-0.83436400
H	-0.86303500	-2.56326900	-1.67100600
H	-0.29547800	-4.18298200	-1.17534200
C	-0.33819900	-3.79104800	1.55383900
H	-1.29994700	-4.29860500	1.71223700
H	0.38998200	-4.57720500	1.30594000
H	-0.03234700	-3.33150500	2.49600900
O	-0.20005200	-0.52064200	-0.29508600
O	0.51450400	-1.11437500	1.78824600
C	-0.09366200	-0.06767300	2.52866500
H	-0.80892300	-0.48505200	3.24952800
H	0.70342000	0.44145900	3.07816100
H	-0.61389700	0.63472100	1.87315200
C	2.63388000	1.53975600	1.17142500
C	3.19457900	0.32316600	1.01653900
H	2.73446300	2.20104600	2.01880700
H	3.84172300	-0.18828500	1.71232100
N	1.86394300	1.89406100	0.07680300
N	2.84530100	-0.25317800	-0.18837000
P	1.74910600	0.66842300	-1.05425000
C	3.42164600	-1.55285900	-0.64983500
C	1.22304500	3.24458900	-0.02607100
C	3.26507800	-2.60915800	0.44777900
H	2.21229800	-2.74486900	0.70419300
H	3.66382200	-3.56080400	0.08195000
H	3.81717200	-2.35094600	1.35663200
C	2.67142100	-2.00900200	-1.90234100
H	3.07145600	-2.97443000	-2.22564600
H	1.60261200	-2.13765900	-1.70189800
H	2.79756300	-1.30769400	-2.73510500
C	4.90095400	-1.31563600	-0.97214000
H	5.45446600	-0.98944000	-0.08493200
H	5.35845900	-2.24237100	-1.33302900
H	5.01153300	-0.55035400	-1.74771000
C	0.12895900	3.36535300	1.03823100
H	-0.28574400	4.37888500	1.01252500
H	-0.68302400	2.65567600	0.84551700

H	0.52681800	3.19492700	2.04485800
C	2.31689900	4.30069200	0.17464300
H	1.88478000	5.29625800	0.03462000
H	2.74903600	4.26879800	1.17954500
H	3.12318900	4.16943800	-0.55494600
C	0.60915900	3.41446700	-1.41584600
H	1.36617300	3.34036600	-2.20522600
H	-0.18272800	2.68252900	-1.60307600
H	0.15948000	4.40984800	-1.47948700
B	-1.47309200	0.16751000	-0.83246200
O	-2.48393800	-0.79590400	-1.20407800
O	-2.09245800	1.03149800	0.17575200
C	-3.41519000	0.57925200	0.42545300
C	-4.74280000	-1.37792600	-0.67034200
H	-5.70994600	-0.99879300	-0.31832400
H	-4.90795200	-1.89412400	-1.62247500
H	-4.37256200	-2.11360400	0.04831900
C	-4.21103100	0.65272700	-2.02400400
H	-4.21502500	0.06437700	-2.94773300
H	-5.22146000	1.04553800	-1.86244700
H	-3.52809300	1.49590500	-2.16825700
C	-4.31513300	1.79103200	0.65490200
H	-5.36638100	1.49528900	0.75612100
H	-4.02052300	2.30213000	1.57885500
H	-4.23257100	2.51116200	-0.16335300
C	-3.42587500	-0.29815600	1.68325100
H	-3.02728900	0.27637800	2.52603500
H	-4.43915700	-0.62154700	1.94843500
H	-2.79823900	-1.18441600	1.54500200
C	-3.74055200	-0.24469500	-0.86881600
H	-1.00741600	0.82049800	-1.77083400

TSA3

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.96406100	-3.03746700	0.66163400
C	-0.37675900	-1.83877300	0.82010700
C	-1.43314800	-3.53389800	-0.67693000
H	-2.52555800	-3.63605500	-0.71363200
H	-1.15117000	-2.86008200	-1.48630700
H	-1.01205500	-4.53140300	-0.87632600
C	-1.13995100	-3.99206600	1.81169600
H	-2.19354800	-4.28833200	1.91697600

H	-0.57300200	-4.92117300	1.64990400
H	-0.81105400	-3.55844500	2.75853400
O	-0.15257500	-0.92476800	-0.13096000
O	0.24341400	-1.55378800	2.01955800
C	-0.24552000	-0.40742200	2.68956300
H	-1.15430100	-0.65355700	3.25624800
H	0.52755800	-0.08938800	3.39639700
H	-0.47547400	0.39724900	1.98652700
C	2.37928800	1.18627700	1.36710400
C	2.93191400	-0.01074400	1.05015400
H	2.32705500	1.63617900	2.34643700
H	3.38457800	-0.71601700	1.73022600
N	1.84949900	1.81253700	0.26862800
N	2.84278700	-0.27000200	-0.29173100
P	2.00883900	0.91086500	-1.12983500
C	3.37375400	-1.52962300	-0.90325900
C	1.24189800	3.18456400	0.33822100
C	2.68295200	-2.73121500	-0.25504700
H	1.61079500	-2.71373800	-0.45813000
H	3.10693000	-3.65127700	-0.67008700
H	2.82396900	-2.75485700	0.82924100
C	3.07275900	-1.51970100	-2.40245000
H	3.45336300	-2.44619100	-2.84191700
H	1.99463300	-1.48256700	-2.59546500
H	3.56305100	-0.68545000	-2.91773000
C	4.88751100	-1.55906800	-0.66972400
H	5.13296000	-1.60958200	0.39595600
H	5.31373700	-2.44515900	-1.15001100
H	5.36653500	-0.67093500	-1.09502400
C	0.21217900	3.22515100	1.46960900
H	-0.21861000	4.23081600	1.51437300
H	-0.58900500	2.50883900	1.26362800
H	0.65676100	3.01930600	2.44867700
C	2.38219600	4.17832900	0.57844500
H	1.98061600	5.19589600	0.61097000
H	2.88834000	3.98666800	1.53082100
H	3.12499800	4.12573600	-0.22484800
C	0.53333600	3.47872400	-0.98468700
H	1.22758700	3.49288900	-1.83339000
H	-0.26420600	2.75101500	-1.16688800
H	0.07812700	4.47157000	-0.92316900
B	-1.16101500	-0.02955600	-0.79385500
O	-2.32482300	-0.73812100	-1.28880300
O	-1.69664400	1.01251200	0.10744500

C	-3.10693500	0.88484500	0.18048800
C	-4.70399000	-0.75712700	-1.06159600
H	-5.59249200	-0.15066500	-0.84685000
H	-4.86260500	-1.26091800	-2.02151200
H	-4.61144500	-1.52801000	-0.29207800
C	-3.54122200	1.03515300	-2.35459900
H	-3.55282500	0.42399900	-3.26332900
H	-4.45007100	1.64823100	-2.34158400
H	-2.67302700	1.69950600	-2.41142700
C	-3.72960400	2.27606300	0.27489000
H	-4.82413300	2.22788600	0.22112700
H	-3.46287300	2.74153600	1.23099200
H	-3.37058000	2.92940900	-0.52507200
C	-3.47415100	0.08374500	1.43575500
H	-3.05834200	0.58752000	2.31530900
H	-4.55871900	0.00551900	1.57477800
H	-3.04955400	-0.92401200	1.38776700
C	-3.44555600	0.10310600	-1.13569600
H	-0.47677400	0.50530000	-1.69158400

TS2-3a

Coordinates (Angstroms)

	X	Y	Z
N	0.56714400	-1.12417500	-0.90798400
C	1.71902700	-1.28663400	-1.07322300
C	2.88838800	-1.86672100	-1.73116000
H	3.49197800	-1.07289200	-2.17722700
H	3.49918700	-2.40887200	-1.00583900
H	2.55082300	-2.55529200	-2.51174100
C	2.88508900	-0.10963700	0.70886400
C	2.66633700	-1.22035200	1.70546300
H	3.17306700	-0.98819000	2.65298700
H	1.60745000	-1.37781900	1.92143900
H	3.09052600	-2.17052300	1.35340200
C	4.31334300	0.20033300	0.34799900
H	4.83509800	0.68661000	1.18436600
H	4.86845000	-0.71990200	0.12625500
H	4.38935800	0.86621600	-0.51564900
C	1.88978000	0.80104400	0.46333800
O	0.64489700	0.59518100	0.79580600
O	2.18925200	1.93106700	-0.20775000
C	1.11935800	2.83371800	-0.48765900
H	0.33128300	2.35868400	-1.07592800

H	0.68804000	3.22277200	0.43994600
H	1.57584400	3.65098300	-1.04856500
B	-0.37966500	-0.18412300	0.00106100
O	-1.20381000	-0.92211400	0.88044800
O	-1.19426400	0.59295200	-0.87384000
C	-2.51436400	0.57950800	-0.32989200
C	-3.49045900	-0.86265000	1.60509500
H	-4.52611000	-0.67497200	1.29872000
H	-3.44805100	-1.85739100	2.06142800
H	-3.21265600	-0.13259400	2.36918400
C	-2.83295300	-1.96933300	-0.53895900
H	-2.62370100	-2.90860100	-0.01688500
H	-3.87810300	-1.98546100	-0.86670000
H	-2.19068800	-1.92500700	-1.42449100
C	-3.52068000	0.71912200	-1.46473200
H	-4.54697600	0.62093400	-1.09235800
H	-3.42311300	1.70647500	-1.92900900
H	-3.35629800	-0.03280100	-2.24065700
C	-2.64861200	1.76513900	0.63290700
H	-2.41321700	2.68818800	0.09249100
H	-3.66326800	1.85659400	1.03582400
H	-1.94692600	1.67404300	1.46748900
C	-2.54630100	-0.80154200	0.41109000

3a

Coordinates (Angstroms)

	X	Y	Z
N	0.71379200	-1.16834300	-1.03034100
C	1.94150500	-1.16200200	-0.74003000
C	2.91149300	-1.96867700	-1.56238400
H	3.65532100	-1.32027900	-2.03844800
H	3.45881300	-2.68077500	-0.93344300
H	2.36702400	-2.51601900	-2.33377400
C	2.49445000	-0.40070100	0.48796900
C	2.13361200	-1.21044300	1.74131400
H	2.49482100	-0.70419400	2.64138900
H	1.05238300	-1.34041300	1.83053300
H	2.60078200	-2.19994700	1.69154600
C	4.01303800	-0.16051800	0.43381200
H	4.32459000	0.43280500	1.30042900
H	4.55713000	-1.10878700	0.47352100
H	4.31188700	0.37802600	-0.46913300
C	1.80271000	0.96046700	0.53725000

O	1.12074000	1.36732500	1.45020500
O	2.06137900	1.66670600	-0.56741600
C	1.36214300	2.90515700	-0.69993800
H	0.29582600	2.70842100	-0.83144500
H	1.52197500	3.54042600	0.17427200
H	1.76950300	3.37903900	-1.59318100
B	-0.50991300	-0.65788000	-0.52714000
O	-1.25070500	-1.31358500	0.43098600
O	-1.15553600	0.43721300	-1.05878200
C	-2.37392900	0.62250400	-0.30498200
C	-3.18839900	-0.75833500	1.74985000
H	-4.18084900	-0.29465600	1.73723100
H	-3.29711100	-1.77885100	2.13056000
H	-2.55172500	-0.20506000	2.44381300
C	-3.38656700	-1.75156600	-0.53688300
H	-3.33583200	-2.75558400	-0.10463300
H	-4.43936300	-1.46121200	-0.61058200
H	-2.96639100	-1.80164700	-1.54679900
C	-3.47394600	1.05162100	-1.26669800
H	-4.43375300	1.13561200	-0.74487900
H	-3.23274000	2.03236700	-1.68874100
H	-3.58687100	0.34861300	-2.09510200
C	-2.12224600	1.72572800	0.72198900
H	-1.84544300	2.64689500	0.19947000
H	-3.02225200	1.93357500	1.30961100
H	-1.30350500	1.46714500	1.39790800
C	-2.59190200	-0.79139600	0.35006800

2a

	Coordinates (Angstroms)		
	X	Y	Z
C	-2.18863200	0.27725700	-0.08157600
O	-2.77951600	1.19807200	0.71749700
O	-1.09459000	0.76570800	-0.75261300
C	-3.07082300	2.43918400	0.08606500
H	-3.65588900	3.01740600	0.80361100
H	-2.15708200	2.98725200	-0.16450500
H	-3.66128700	2.28505600	-0.82581600
C	-2.63908300	-0.97266700	-0.21121300
C	-3.87271000	-1.43953400	0.50877700
H	-3.62675900	-2.23540000	1.22459500
H	-4.35671600	-0.62866800	1.05662000
H	-4.59858900	-1.86187500	-0.19883900

C	-1.89158900	-2.00375500	-1.01163400
H	-1.31226800	-2.66965500	-0.35830900
H	-2.59249000	-2.63279200	-1.57383500
H	-1.20160000	-1.55616900	-1.73248300
C	2.42123600	0.53417600	-0.31320700
C	1.90081000	-0.66230300	0.56243600
C	2.78987900	1.76497300	0.51525200
H	3.71456600	1.60733200	1.07935900
H	2.93935500	2.61412900	-0.15847400
H	1.99287100	2.02735000	1.21875700
C	1.99162500	-2.01060000	-0.15286200
H	3.02867300	-2.34748900	-0.24721800
H	1.43958200	-2.75829000	0.42441100
H	1.55045800	-1.96199100	-1.15377200
C	3.55296900	0.18106900	-1.26595600
H	3.25044600	-0.58719000	-1.98101100
H	3.85155500	1.06945500	-1.83126500
H	4.42760700	-0.17831900	-0.71307800
C	2.52059500	-0.75901800	1.94773500
H	2.34165600	0.14529500	2.53346600
H	2.08463700	-1.60476700	2.48834400
H	3.60126800	-0.92286100	1.87535300
O	0.49464700	-0.35310100	0.69940400
O	1.25189100	0.88037400	-1.08936000
B	0.17497500	0.43421500	-0.37364800

TSB1

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.30090900	1.87226300	1.34591200
C	1.03228600	1.64281100	1.41170500
H	-0.92523000	2.29064200	2.12068600
H	1.67652600	1.82838200	2.25749000
P	0.29233600	0.78896100	-0.87655100
N	-0.82359500	1.53342100	0.11869500
N	1.51933200	1.13561500	0.23054600
C	-2.26214400	1.79328700	-0.22498800
C	2.92635600	0.65296300	0.07505100
C	-2.48253500	1.50545200	-1.70994900
H	-2.26328900	0.45478700	-1.92767500
H	-3.53328700	1.69819600	-1.94772000
H	-1.87154000	2.16108400	-2.34280600
C	-3.12723300	0.85793500	0.61970000

H	-2.88770000	-0.17517200	0.35472600
H	-2.95795100	1.00902300	1.69172800
H	-4.18513700	1.05178900	0.41340100
C	-2.56204000	3.26723100	0.06872600
H	-2.49325900	3.50595600	1.13495800
H	-1.88162900	3.92525800	-0.48239900
H	-3.58552800	3.48920700	-0.24856300
C	3.24651300	0.53801200	-1.41757900
H	2.63561300	-0.22271000	-1.91437500
H	3.10721600	1.49557100	-1.93080200
H	4.29118100	0.23607400	-1.53616200
C	3.05172600	-0.71620000	0.75375100
H	2.36405900	-1.44480600	0.31086600
H	4.07436900	-1.09119600	0.64134500
H	2.83306900	-0.64404400	1.82450800
C	3.87628600	1.67167100	0.71179600
H	3.72084600	2.67065300	0.29139800
H	3.76494000	1.72583400	1.79885400
H	4.90891200	1.37223200	0.50928100
H	0.13270800	-1.10260500	0.05645100
C	-0.65905700	-1.91236600	-0.26295900
O	-1.51846000	-1.42971400	-1.09538700
O	0.23029500	-2.96818900	-0.76740200
C	0.60506000	-2.75747800	-2.09471400
H	-0.26065000	-2.68289700	-2.76292600
H	1.19833900	-1.83251900	-2.22057600
H	1.23228800	-3.60418100	-2.39549800
C	-1.16456700	-2.49045200	1.06674100
C	-2.46424400	-2.72225200	1.23193700
H	-3.15259700	-2.50947700	0.41844500
H	-2.86999500	-3.13849300	2.15225700
C	-0.12890700	-2.75864400	2.12043500
H	0.61145300	-3.47907200	1.75465800
H	0.41760700	-1.83767900	2.36756300
H	-0.57076500	-3.14967700	3.04339500

B1

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.13357700	-1.12340900	-1.52500500
C	1.09186700	-0.58750500	-1.58223100
H	-0.73368500	-1.43023400	-2.37128200
H	1.64835900	-0.37163800	-2.48353600

P	0.38057800	-0.40102500	0.90510700
N	-0.65225200	-1.18834200	-0.22271400
N	1.58134100	-0.18714100	-0.32152000
C	-1.71308200	-2.16419000	0.11589800
C	3.02421700	-0.34344400	0.00047600
C	-2.07065700	-2.04356700	1.59951100
H	-2.38505800	-1.02400600	1.84653800
H	-2.90121300	-2.71935600	1.82822800
H	-1.23089000	-2.31705900	2.24600800
C	-2.96697600	-1.85639700	-0.71501000
H	-3.31657400	-0.84010900	-0.51049300
H	-2.78256300	-1.95196300	-1.79020400
H	-3.76758900	-2.55918200	-0.45915200
C	-1.21388000	-3.58605100	-0.17738700
H	-0.98752900	-3.71711100	-1.24137000
H	-0.30042700	-3.79403200	0.39095800
H	-1.97078700	-4.32832600	0.09938900
C	3.36937400	0.52217700	1.21629400
H	3.18325500	1.57998500	1.00610200
H	2.78920300	0.23918100	2.10083000
H	4.42905100	0.40167700	1.46565200
C	3.86699100	0.13520100	-1.18818600
H	3.56882800	1.14141500	-1.50232000
H	4.92168000	0.16857200	-0.89621700
H	3.79249300	-0.53851400	-2.04764600
C	3.34091300	-1.81779900	0.29375700
H	2.81297900	-2.15767300	1.19188100
H	3.03033700	-2.45051100	-0.54552500
H	4.41475600	-1.96594100	0.45616900
H	-0.32802600	1.51268000	-0.94195000
C	-0.78044100	1.88337100	-0.00950200
O	-0.27988200	1.12455100	1.07998500
O	-0.44524600	3.22501500	0.16094800
C	0.94150000	3.47340700	0.08620100
H	1.46429600	3.06953600	0.96046600
H	1.38040300	3.04048500	-0.82490800
H	1.06841600	4.55863700	0.06264100
C	-2.29301700	1.82085400	-0.10682400
C	-3.04679800	1.59751800	0.96640900
H	-2.59943600	1.42811100	1.94094700
H	-4.13242700	1.58634200	0.90419600
C	-2.84228200	2.07004200	-1.48149200
H	-2.48807100	3.03242500	-1.87084300
H	-2.49973600	1.29532300	-2.18029700

H	-3.93622200	2.07727200	-1.48615400

B2

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.88956000	0.21988300	0.24920600
C	-3.41259700	1.41969200	0.60237200
H	-4.79335200	-0.25112800	0.60849100
H	-3.85505000	2.11263400	1.30335500
P	-1.56604100	0.38808400	-0.90660700
N	-3.04942000	-0.43462200	-0.66729400
N	-2.20222300	1.71817600	-0.04046300
C	-3.42565100	-1.72985100	-1.26806400
C	-1.56100000	3.04258100	0.09499500
C	-2.36517700	-2.15970500	-2.28600200
H	-1.38543000	-2.29283600	-1.81449400
H	-2.65627800	-3.11957700	-2.72479600
H	-2.26537100	-1.43200900	-3.09776700
C	-3.52114900	-2.80061800	-0.17038500
H	-2.54567500	-2.94804900	0.30557200
H	-4.24546700	-2.52110100	0.60226300
H	-3.84163300	-3.75788900	-0.59695900
C	-4.77543800	-1.57861600	-1.98368500
H	-5.57627200	-1.31366400	-1.28530000
H	-4.71708500	-0.79510700	-2.74641100
H	-5.05717500	-2.51864500	-2.47065700
C	-0.21377200	3.04373300	-0.63460100
H	0.47683600	2.30100300	-0.22187700
H	-0.33166100	2.85028900	-1.70573600
H	0.25320700	4.02822300	-0.52425100
C	-1.32124300	3.34480900	1.58137200
H	-0.77953300	2.51748600	2.04741500
H	-0.74352800	4.26908200	1.69299400
H	-2.26345200	3.48036400	2.12371400
C	-2.47538200	4.10730700	-0.52611300
H	-2.63586600	3.90229600	-1.58994300
H	-3.45349400	4.12893900	-0.03328000
H	-2.02843800	5.10303100	-0.42685300
H	-1.88151300	-0.82859200	1.59933900
C	-0.79469100	-0.79320400	1.45806000
O	-0.48044500	-0.39828800	0.15010500
O	-0.36278000	0.15363300	2.40648800
C	1.03241500	0.38212400	2.40499000

H	1.58835400	-0.50582800	2.74058600
H	1.39261900	0.67790100	1.41401900
H	1.21678700	1.19448900	3.11262100
C	-0.21932700	-2.17186200	1.74656600
C	0.44858000	-2.86649400	0.82714200
H	0.62950900	-2.46269100	-0.16365100
H	0.84312900	-3.85649200	1.04448800
C	-0.49174600	-2.68144100	3.13476000
H	-0.07934700	-2.00366200	3.89081800
H	-1.57190400	-2.73836800	3.32282300
H	-0.06567700	-3.67726900	3.28704400
B	2.27755400	0.09116000	-1.51634800
O	3.10102600	-0.98714000	-1.66592600
O	2.76559200	1.03747100	-0.65585100
C	4.13715100	0.67817500	-0.36230900
C	5.46122300	-1.35447300	-1.31193600
H	6.30114600	-1.19741200	-0.62622500
H	5.38598500	-2.42751100	-1.51425300
H	5.68015100	-0.84856400	-2.25499700
C	3.78183300	-1.73606800	0.49941600
H	3.63524800	-2.76322300	0.15184100
H	4.56627300	-1.73945800	1.26293900
H	2.84560600	-1.40349000	0.95589500
C	4.44537300	1.02991800	1.08578500
H	5.47716400	0.75794700	1.33431700
H	4.33465800	2.10869400	1.23297300
H	3.77701500	0.52359300	1.78500200
C	5.01385600	1.51419700	-1.29569900
H	4.80476400	2.57476000	-1.12599200
H	6.07833400	1.34035800	-1.11040800
H	4.80279000	1.29457600	-2.34729500
C	4.16361900	-0.85766700	-0.69060300
H	1.25691100	0.21506100	-2.11235400

TSB2

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.58610900	-0.37676700	0.38642400
C	-3.38308900	0.92809300	0.61520600
H	-4.32007700	-1.01848100	0.85083000
H	-3.92161300	1.56156700	1.30336000
P	-1.52990300	0.24838100	-1.05234500
N	-2.67547100	-0.88600700	-0.54870800

N	-2.31847500	1.42909800	-0.14028400
C	-2.73758300	-2.29466100	-1.01433900
C	-1.98603500	2.87911800	-0.17464100
C	-1.61134000	-2.55146200	-2.01920300
H	-0.62467400	-2.38277200	-1.57509100
H	-1.65576500	-3.59577200	-2.34359000
H	-1.70709400	-1.92253900	-2.91056000
C	-2.56316500	-3.23241300	0.18633800
H	-1.59382900	-3.06746300	0.66816200
H	-3.35111700	-3.08920700	0.93382500
H	-2.60885400	-4.27530600	-0.14535800
C	-4.09336300	-2.52589100	-1.69270700
H	-4.92426100	-2.38527800	-0.99332200
H	-4.22800200	-1.83052000	-2.52782100
H	-4.15267500	-3.54848800	-2.07997300
C	-0.61582900	3.06988400	-0.83110200
H	0.17478900	2.54762600	-0.28400100
H	-0.60413100	2.72244600	-1.87013300
H	-0.37377300	4.13746200	-0.84402200
C	-1.92781800	3.42410100	1.25768200
H	-1.26488000	2.80259700	1.86532400
H	-1.54552300	4.45012500	1.24156200
H	-2.91559600	3.45590000	1.72979400
C	-3.06725700	3.60194900	-0.98581300
H	-3.09613300	3.22338700	-2.01338600
H	-4.05783400	3.45648400	-0.54035200
H	-2.86581100	4.67820800	-1.01886000
H	-1.32732200	-0.49715500	1.50235900
C	-0.24412000	-0.35351200	1.42906500
O	0.03967100	-0.24031000	0.03932600
O	-0.05264400	0.83907500	2.13647800
C	1.28230600	1.24392100	2.38048400
H	1.82206500	0.51500000	3.00098100
H	1.81763900	1.40293400	1.44205100
H	1.21535400	2.18442800	2.93426000
C	0.35402200	-1.56335200	2.12697900
C	0.98300900	-2.55062300	1.49445700
H	1.23713500	-2.48816200	0.44287800
H	1.30531100	-3.43617300	2.03888400
C	0.00222500	-1.63289500	3.59169500
H	0.44056400	-0.80413500	4.15798300
H	-1.08427400	-1.56597000	3.73495700
H	0.34763800	-2.57194200	4.03349500
B	1.45691600	-0.10224800	-0.99087500

O	2.34453600	-1.21105600	-0.91783200
O	2.17589500	1.06866400	-0.59532700
C	3.55778500	0.78977000	-0.80072900
C	4.67540600	-1.48786200	-1.38889600
H	5.68646800	-1.10877600	-1.19830800
H	4.66472600	-2.55635900	-1.14785000
H	4.45919700	-1.38486700	-2.45486400
C	3.89435900	-1.09691500	0.93722200
H	3.77086500	-2.17427400	1.08580100
H	4.91169700	-0.82666800	1.24210600
H	3.18330100	-0.59144900	1.59289300
C	4.39180300	1.64939900	0.14311800
H	5.46104000	1.44581500	0.01421300
H	4.22066200	2.70850400	-0.07712500
H	4.13487300	1.47871500	1.19173300
C	3.89815400	1.16057800	-2.25069900
H	3.64111300	2.21215000	-2.41379000
H	4.96273900	1.02881800	-2.47197000
H	3.31701900	0.56134100	-2.95858700
C	3.64186600	-0.75791200	-0.53353100
H	0.81959500	-0.05415100	-2.01920300

B3

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.59000000	-0.06111500	0.49236800
C	-3.22322000	1.18781800	0.82781800
H	-4.35309200	-0.66724800	0.95720000
H	-3.62656200	1.79511600	1.62378100
P	-1.63323300	0.51592100	-1.07172300
N	-2.82626900	-0.55195400	-0.56372500
N	-2.19681100	1.65987100	0.01616700
C	-3.05481800	-1.90356200	-1.15132300
C	-1.63601300	3.03445700	0.17580400
C	-2.00298300	-2.16390900	-2.23277000
H	-0.98738400	-2.10870400	-1.82558300
H	-2.14729500	-3.17089300	-2.63548100
H	-2.09022900	-1.45924600	-3.06691200
C	-2.92030600	-2.96649300	-0.05504600
H	-1.90520800	-2.97971900	0.35326600
H	-3.63050700	-2.80680200	0.76278200
H	-3.12441900	-3.95417000	-0.48115900
C	-4.45817000	-1.92791800	-1.76597100

H	-5.23490200	-1.77865300	-1.00830100
H	-4.56042000	-1.14384000	-2.52336400
H	-4.63927000	-2.89625100	-2.24350400
C	-0.49388400	3.23946500	-0.82246800
H	0.35532900	2.57612600	-0.62313900
H	-0.82440100	3.10142300	-1.85831200
H	-0.13292000	4.26869100	-0.72998700
C	-1.09613100	3.18556600	1.60094100
H	-0.38476700	2.38552600	1.82154300
H	-0.59507400	4.15370200	1.70238300
H	-1.89846800	3.14849400	2.34617400
C	-2.75693400	4.04181600	-0.10167100
H	-3.15420300	3.91367200	-1.11425200
H	-3.58355500	3.93618000	0.60899300
H	-2.36784700	5.06086300	-0.00819200
H	-1.26763500	-0.86444700	1.31505100
C	-0.17361000	-0.79604900	1.27998200
O	0.10888500	-0.35042400	-0.02607200
O	0.08848300	0.13671200	2.29486700
C	1.42935800	0.28308900	2.72922200
H	1.88247500	-0.68531600	2.98076900
H	2.02703700	0.78156100	1.96382500
H	1.38832900	0.89125000	3.63778600
C	0.30885300	-2.19511300	1.63521400
C	0.97376600	-2.98995800	0.79992400
H	1.32922600	-2.63608700	-0.16238800
H	1.21562500	-4.01140500	1.08897800
C	-0.18299200	-2.66178700	2.98225900
H	0.24635600	-2.07332300	3.80078100
H	-1.27292600	-2.54865300	3.05865700
H	0.06241900	-3.71448700	3.15008600
B	1.38324700	0.04967400	-0.84256500
O	2.28342100	-1.04263600	-1.16647900
O	2.18331900	1.02928200	-0.12283800
C	3.51918000	0.85491500	-0.56244200
C	4.56237400	-1.12182000	-1.90101000
H	5.58967100	-0.79956700	-1.69131000
H	4.56516100	-2.21386700	-1.99155900
H	4.25586500	-0.71082900	-2.86601700
C	3.97895300	-1.46162500	0.49269400
H	3.85058200	-2.53540600	0.32000900
H	5.02143000	-1.28672500	0.78340900
H	3.32820700	-1.18142000	1.32419200
C	4.47289300	1.39997600	0.49688600

H	5.51820500	1.23454100	0.21077600
H	4.32005700	2.47883800	0.61126700
H	4.30737000	0.93333600	1.47166600
C	3.71270900	1.64943300	-1.86311700
H	3.45492600	2.69716700	-1.67433900
H	4.74665600	1.61076500	-2.22367900
H	3.05320100	1.28069300	-2.65419300
C	3.60576100	-0.70068600	-0.78559500
H	0.84517200	0.49404900	-1.85614900

TSB3

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.26979000	-0.02161500	0.79441200
C	-2.67918200	1.08689300	1.30073400
H	-3.91212200	-0.71311900	1.31929900
H	-2.75609700	1.46118200	2.31012700
P	-1.85330400	0.91919600	-1.09564400
N	-2.93819500	-0.21630700	-0.52701400
N	-1.90916800	1.72970000	0.36027900
C	-3.39537200	-1.40135400	-1.31693100
C	-1.15856100	2.99230000	0.65625000
C	-2.87857000	-1.27085800	-2.75156600
H	-1.78322900	-1.25633900	-2.79139000
H	-3.21292300	-2.14032400	-3.32490700
H	-3.26978200	-0.37590300	-3.24841600
C	-2.81735500	-2.67099400	-0.68477800
H	-1.72401200	-2.63978200	-0.69609200
H	-3.15853900	-2.80203400	0.34751900
H	-3.14828800	-3.54397100	-1.25643000
C	-4.92635800	-1.41893900	-1.31330700
H	-5.33399900	-1.55658900	-0.30658200
H	-5.32864300	-0.48753500	-1.72523900
H	-5.28229100	-2.25046000	-1.92929500
C	-0.39178800	3.41481500	-0.59821500
H	0.34625500	2.65538200	-0.88069500
H	-1.06130900	3.62402300	-1.44122000
H	0.15477100	4.33698600	-0.37810200
C	-0.15858900	2.72134800	1.78200800
H	0.57784000	1.98607300	1.45062600
H	0.35690000	3.65617700	2.02755000
H	-0.64872300	2.35678400	2.68952200
C	-2.18190100	4.06317500	1.04385600

H	-2.92268000	4.20219800	0.24893800
H	-2.71026000	3.80921700	1.96900900
H	-1.66912000	5.01610600	1.20650400
H	-1.19891700	-1.54997700	1.25532000
C	-0.11740500	-1.37084200	1.17910000
O	0.05719400	-0.78501900	-0.06258100
O	0.08968300	-0.51810300	2.29324300
C	1.42507100	-0.30291900	2.70020200
H	1.94790000	-1.24709700	2.90882400
H	1.97974700	0.25882500	1.94494200
H	1.37561500	0.27345000	3.62983500
C	0.51765800	-2.74058500	1.39897300
C	1.26160600	-3.36230400	0.48704600
H	1.54604800	-2.87188500	-0.43847100
H	1.63399800	-4.36954900	0.66915500
C	0.11246500	-3.39347300	2.69682800
H	0.43310800	-2.80856000	3.56636200
H	-0.98096700	-3.47722100	2.76761900
H	0.53421800	-4.39937000	2.78532300
B	1.17585800	-0.17815700	-0.84750200
O	2.23194500	-1.07780900	-1.31757600
O	1.88631600	0.88274900	-0.11340800
C	3.19281000	0.95281800	-0.64872500
C	4.43398500	-0.73135700	-2.19772100
H	5.40625100	-0.25157300	-2.02953000
H	4.61215700	-1.79874300	-2.37002200
H	3.99254700	-0.31759700	-3.10805700
C	4.08448300	-1.32699800	0.19202600
H	4.10309700	-2.39385300	-0.05544700
H	5.10920400	-1.01606500	0.42855200
H	3.46582800	-1.20839100	1.08461700
C	4.13032300	1.56973200	0.38655100
H	5.16530300	1.58456200	0.02409000
H	3.83003900	2.60439400	0.58863800
H	4.10659000	1.02374300	1.33341900
C	3.17057800	1.85494600	-1.89358600
H	2.78397100	2.83945600	-1.60585100
H	4.16781200	1.99653200	-2.32521100
H	2.50994200	1.44804500	-2.66472500
C	3.50256200	-0.55091900	-0.99764800
H	0.55344700	0.28011900	-1.83124500

4a

	Coordinates (Angstroms)		
	X	Y	Z
B	-0.26395900	-0.49960800	0.03527800
O	-1.25699100	-1.41834700	-0.17435200
O	-0.71854200	0.77266500	0.27717900
C	-2.14883400	0.66544500	0.45421900
C	-3.62485900	-1.47390800	0.27945500
H	-4.55727900	-0.89897200	0.26031900
H	-3.77698800	-2.38466400	-0.30811100
H	-3.41756300	-1.77043900	1.31010500
C	-2.70587800	-0.45074000	-1.81052800
H	-2.73034800	-1.42456900	-2.30839600
H	-3.65427000	0.05923300	-2.00637500
H	-1.89506200	0.13496200	-2.25596400
C	-2.80789300	1.91232700	-0.11560500
H	-3.89915300	1.82566200	-0.07180700
H	-2.51444300	2.78784000	0.47238100
H	-2.51255700	2.08801400	-1.15242400
C	-2.40795900	0.57278600	1.95804800
H	-1.96911000	1.44680900	2.44891300
H	-3.47951800	0.55609200	2.18101500
H	-1.94958700	-0.32309900	2.38958700
C	-2.48117300	-0.66517100	-0.31357900
O	1.04772400	-0.86975500	0.03410900
C	2.02495100	0.12269300	0.16731700
H	1.75787900	0.81794300	0.97855800
C	3.35758100	-0.53450700	0.44752700
C	4.10419600	-0.10699400	1.46454200
H	3.75928300	0.67591200	2.13677600
H	5.08461000	-0.52983400	1.67054600
O	2.05794700	0.82228800	-1.05451700
C	2.60792600	2.11387900	-0.93911900
H	3.64383000	2.09084500	-0.57209000
H	2.59801400	2.55267400	-1.93918200
H	2.00657200	2.74494300	-0.26773200
C	3.77601900	-1.61212800	-0.51045400
H	3.08959100	-2.46379200	-0.45489500
H	3.74112500	-1.24001400	-1.54033000
H	4.78920300	-1.96439500	-0.29757100

TS1-4a

	Coordinates (Angstroms)		
	X	Y	Z

H	0.89875000	0.21105800	0.95226400
C	2.06295000	0.21027900	-0.27187300
O	1.10653600	0.16528800	-1.16072400
B	0.04746500	0.09286800	-0.05351900
O	-0.87216700	1.17337900	-0.12571000
O	-0.64419400	-1.13944600	0.05300900
C	-2.12386900	0.65453100	0.32724600
C	-2.03519500	-0.84934100	-0.11105300
C	-2.19633800	0.82046300	1.84907900
H	-2.02945700	1.87382600	2.09687100
H	-3.17249600	0.52505100	2.24823300
H	-1.42367100	0.22889900	2.35108500
C	-2.84658500	-1.80901100	0.75031600
H	-3.91287400	-1.55586900	0.72383100
H	-2.73422500	-2.83112800	0.37338200
H	-2.50925500	-1.79593500	1.78976200
C	-2.38910700	-1.04992400	-1.58825600
H	-2.10588700	-2.06519800	-1.88430900
H	-3.46153100	-0.92535300	-1.77458200
H	-1.83923000	-0.34765600	-2.22252000
C	-3.24784100	1.44287000	-0.33305900
H	-4.22373300	0.99854200	-0.10659500
H	-3.25085300	2.47249000	0.04071000
H	-3.12277000	1.47957500	-1.41799500
O	2.70378400	1.33402000	-0.04240600
C	2.05011600	2.55880600	-0.41675300
H	1.11661100	2.65858200	0.14239800
H	2.75117700	3.34773900	-0.14871000
H	1.84287800	2.56880500	-1.48735000
C	2.83896300	-0.99690400	0.11697600
C	2.52800700	-2.14308200	-0.48996400
H	1.72608000	-2.19268700	-1.21839800
H	3.06417100	-3.05982800	-0.26207700
C	3.90344100	-0.83204300	1.16223100
H	4.68578400	-0.14187700	0.83060600
H	3.47943000	-0.42327700	2.08668100
H	4.36484900	-1.79589100	1.39161000

TS1-2a

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.24189600	2.70969100	-0.12096400
O	-0.09722100	3.70175200	0.74083900

O	-1.20854100	1.88808700	0.13781800
C	-0.89415000	3.68796200	1.93067900
H	-0.79184300	2.73448700	2.45309100
H	-0.50325100	4.50132100	2.54163000
H	-1.94538400	3.86690600	1.69436000
C	0.63099200	2.70456700	-1.21484500
C	1.83995600	3.60552800	-1.18558300
H	2.37950000	3.53882400	-2.13503500
H	1.57026100	4.65502500	-1.02822300
H	2.53344600	3.31505700	-0.38814300
C	0.44749500	1.76752200	-2.23707000
B	-1.26980700	0.41582000	-0.08675700
O	-1.59410600	-0.32649100	1.06037200
O	-2.08192100	0.05447300	-1.17245600
C	-2.70647600	-1.19046500	-0.82587400
C	-3.97546700	-0.34810800	1.26329000
H	-4.90200800	-0.91640700	1.12877500
H	-3.84274600	-0.15721100	2.33298700
H	-4.08285600	0.61806800	0.75989600
C	-2.64291500	-2.45605900	1.44748900
H	-3.46816700	-3.11811500	1.16137700
H	-1.69887400	-2.95326900	1.21167900
H	-2.68671500	-2.31106500	2.53203300
C	-1.82648800	-2.33124100	-1.34014600
H	-2.29793600	-3.30652100	-1.17719600
H	-1.67682700	-2.20143200	-2.41715300
H	-0.84016700	-2.32869400	-0.86870200
C	-4.07238400	-1.24892400	-1.49734700
H	-3.94703800	-1.30227700	-2.58376900
H	-4.62475000	-2.13970300	-1.17757700
H	-4.67189500	-0.36400500	-1.27072800
C	-2.75353500	-1.11038500	0.74358500
H	0.03255900	0.11285600	-0.34164300
H	1.02709600	1.89465600	-3.14969200
H	-0.52083800	1.29201600	-2.37724900
B	1.25679000	-0.19639600	-0.81926500
O	2.24965800	0.38644900	-0.02535700
O	1.38085500	-1.58550500	-0.88307200
C	2.56559600	-1.92860000	-0.13981500
C	1.88329900	-0.74860400	2.05546300
H	2.25158400	-1.49977400	2.76236000
H	1.91208800	0.22768800	2.55042200
H	0.83707600	-0.97098000	1.81976000
C	4.19419400	-0.37442000	1.16525100

H	4.23067200	0.50812400	1.81246300
H	4.64398400	-1.21214300	1.70999000
H	4.79950800	-0.16717400	0.27945600
C	3.70614500	-2.09194700	-1.14613100
H	4.62755400	-2.43709200	-0.66527800
H	3.41269700	-2.83222000	-1.89682800
H	3.91300300	-1.14917500	-1.66255700
C	2.31650600	-3.24061000	0.59053300
H	1.41082000	-3.19215200	1.19991500
H	2.19265300	-4.05116600	-0.13502600
H	3.16255200	-3.49322800	1.23983300
C	2.75079800	-0.68208900	0.79454300
H	1.10950300	0.44864000	-1.94862100