

Supporting Information

**Mechanistic Insights into L-Proline-Catalyzed Transamidation of  
Carboxamide with Benzylamine from the Density Functional  
Calculations**

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College of Chemistry,

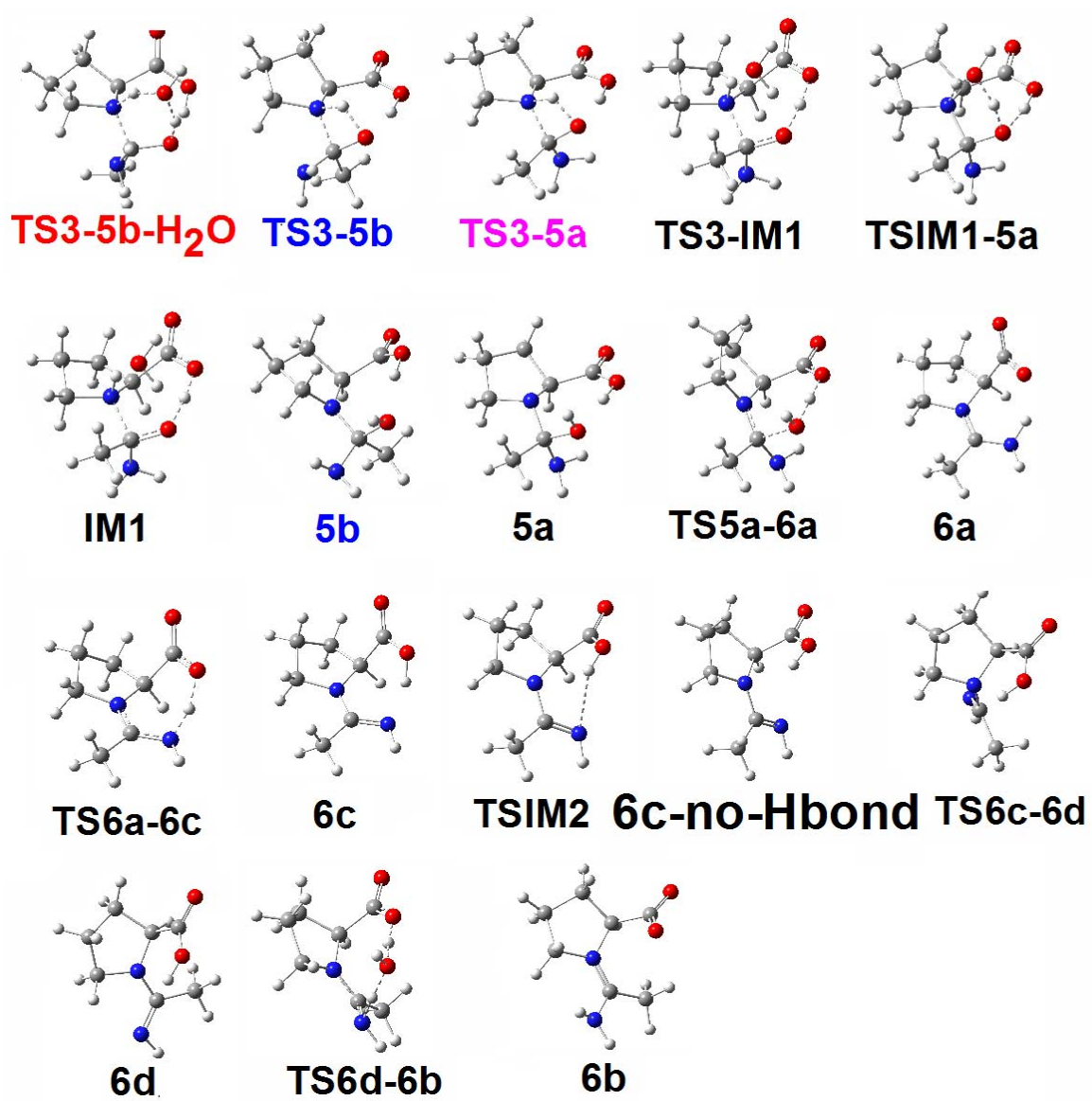
Key Lab of Green Chemistry and Technology in Ministry of Education,

Sichuan University, Chengdu 610064,

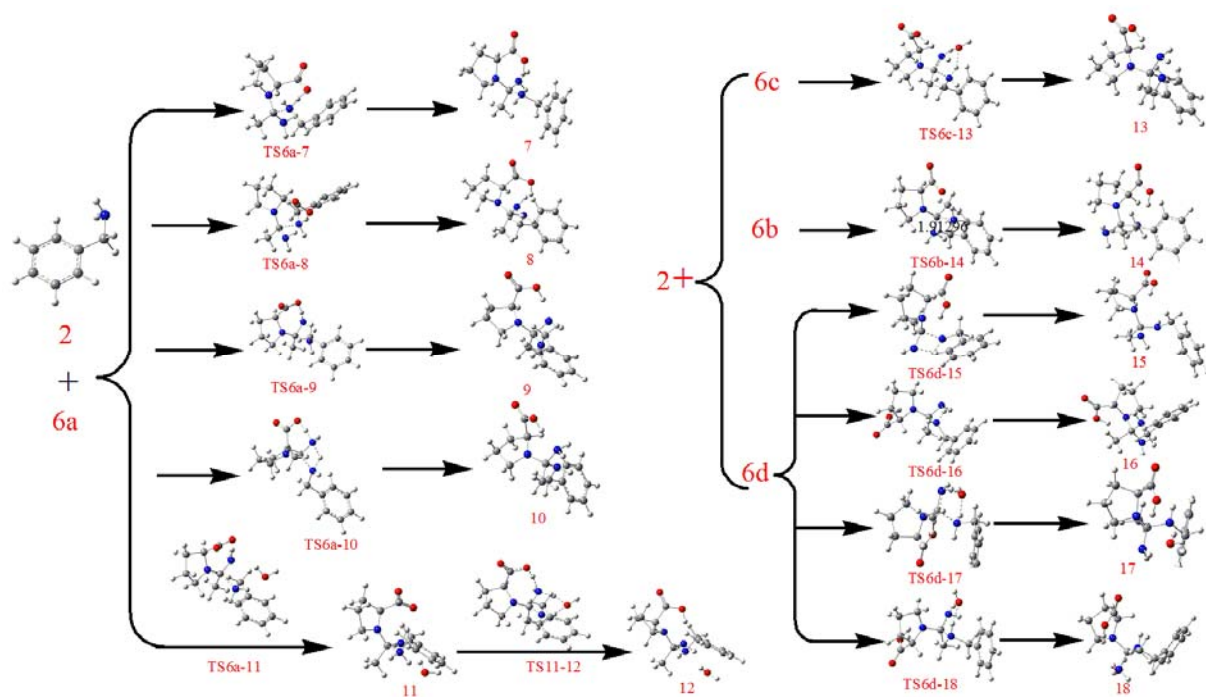
People's Republic of China

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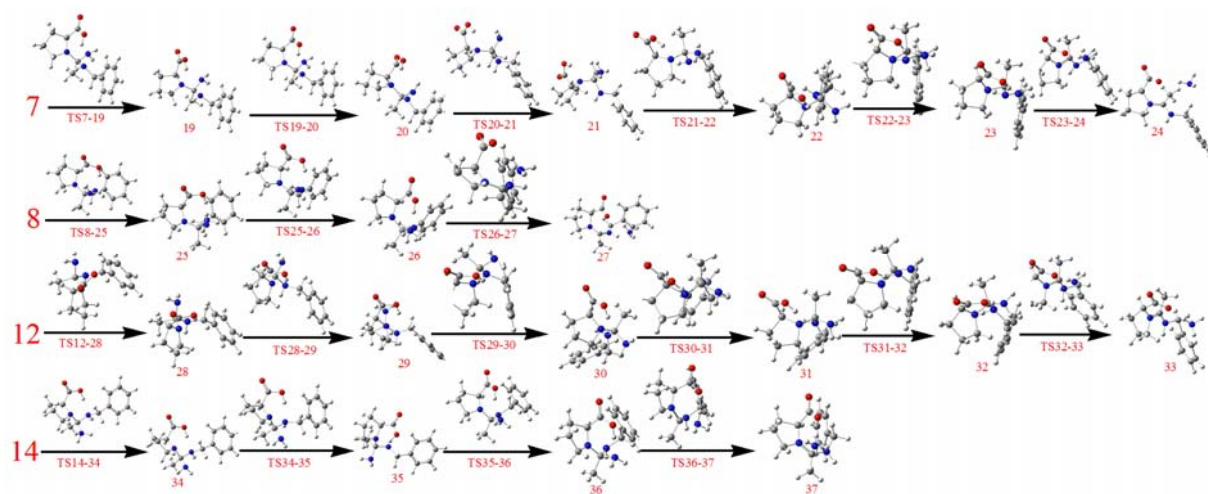
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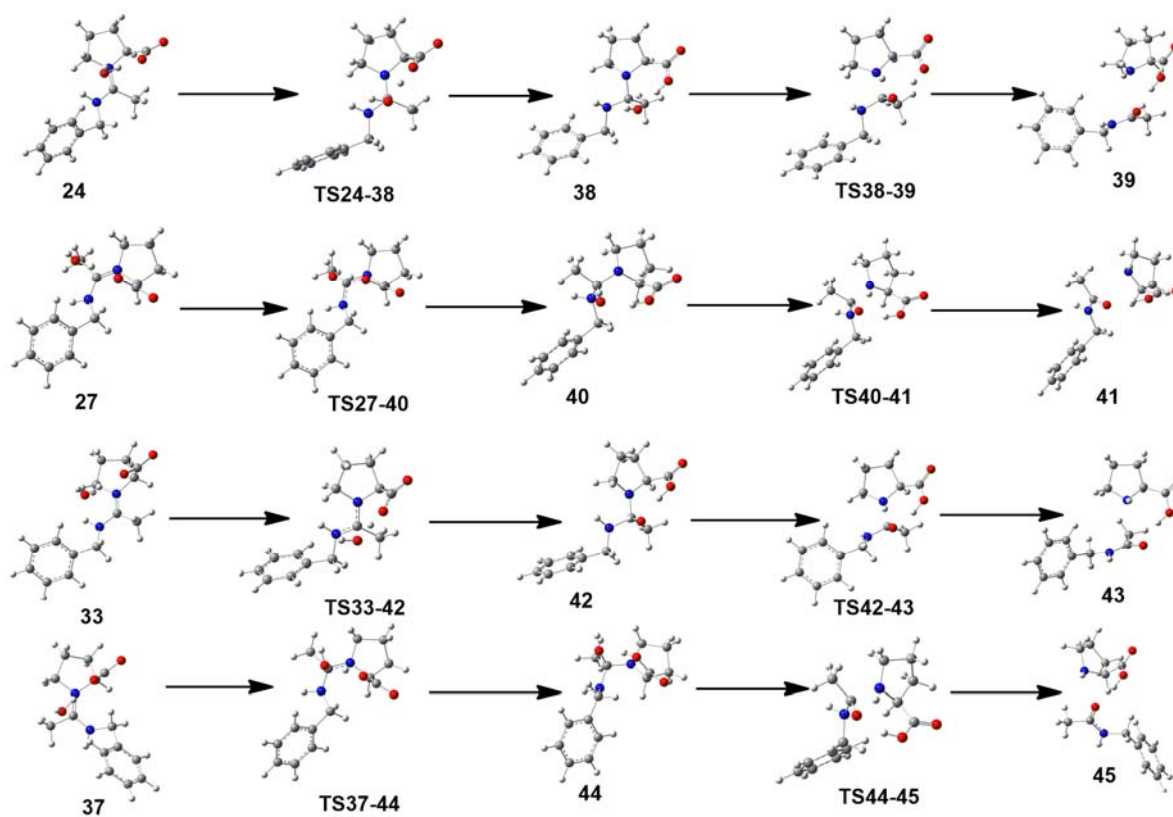
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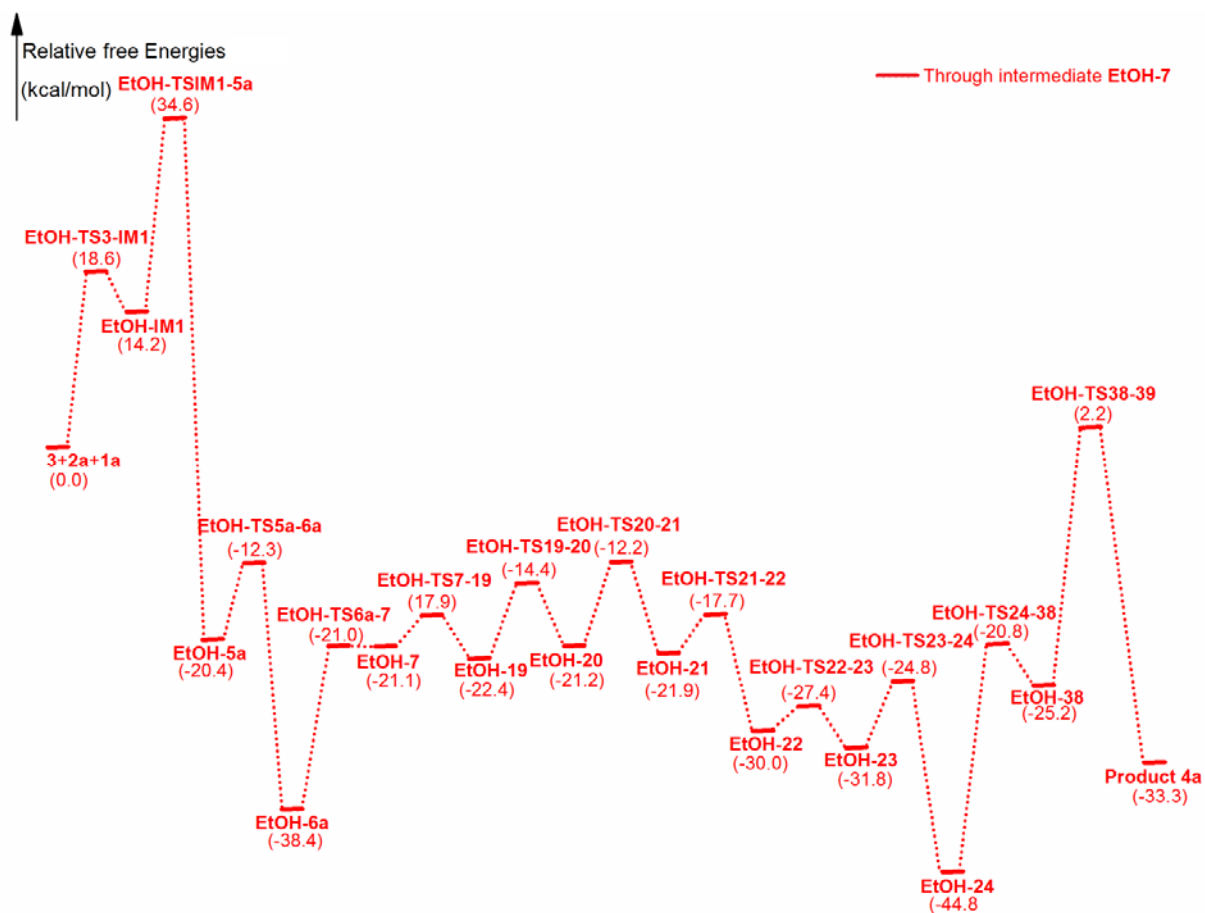
**Figure S2.** Schematic structures of the species in the trasamidation of **1a** with **2a** in step “C-N bond formation”.



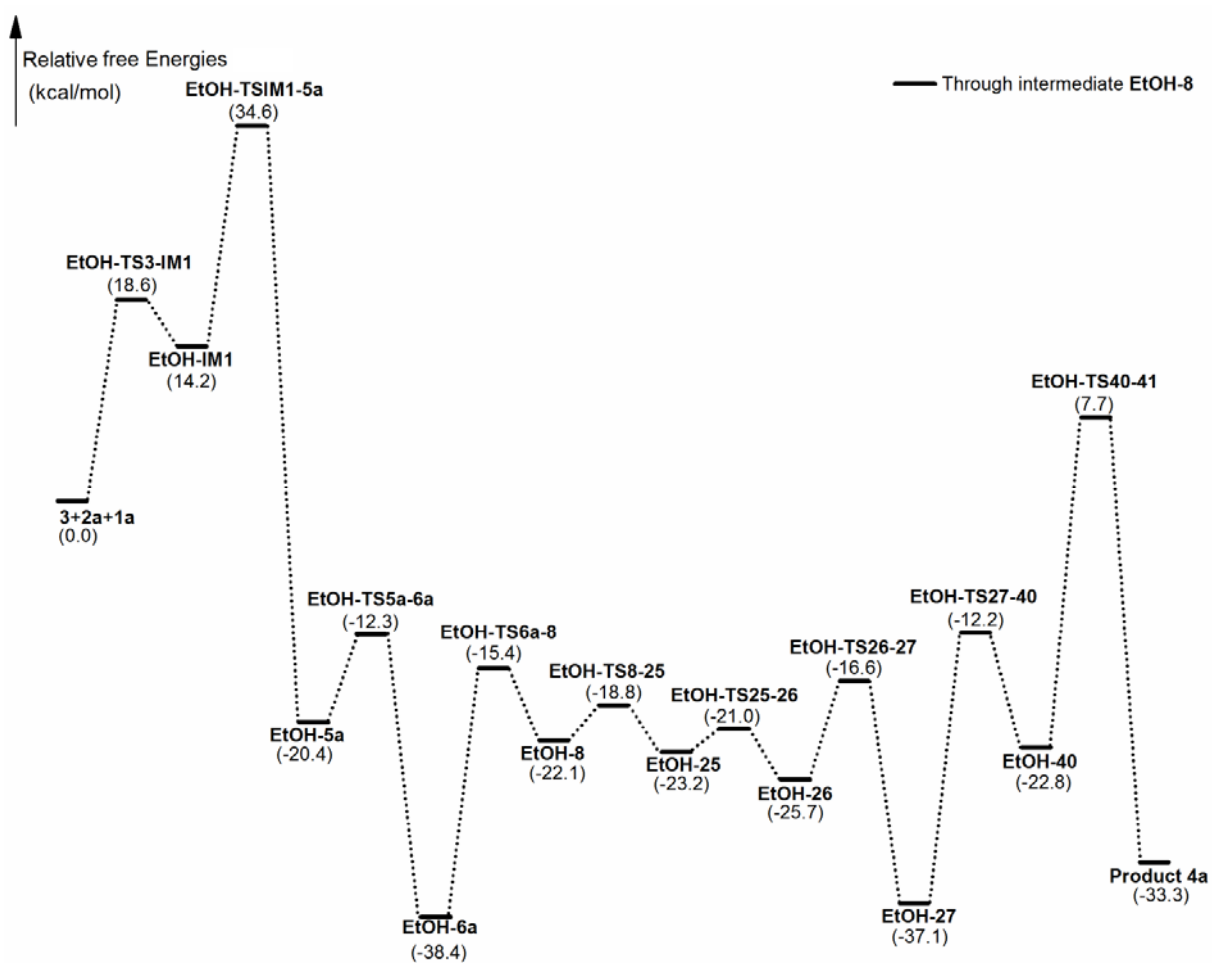
**Figure S3.** Schematic structures of the species in the trasamidation of **1a** with **2a** in step “elimination”.



*Figure S4.* Schematic structures of the species in the trasamidation of **1a** with **2a** in step “hydrolysis”.

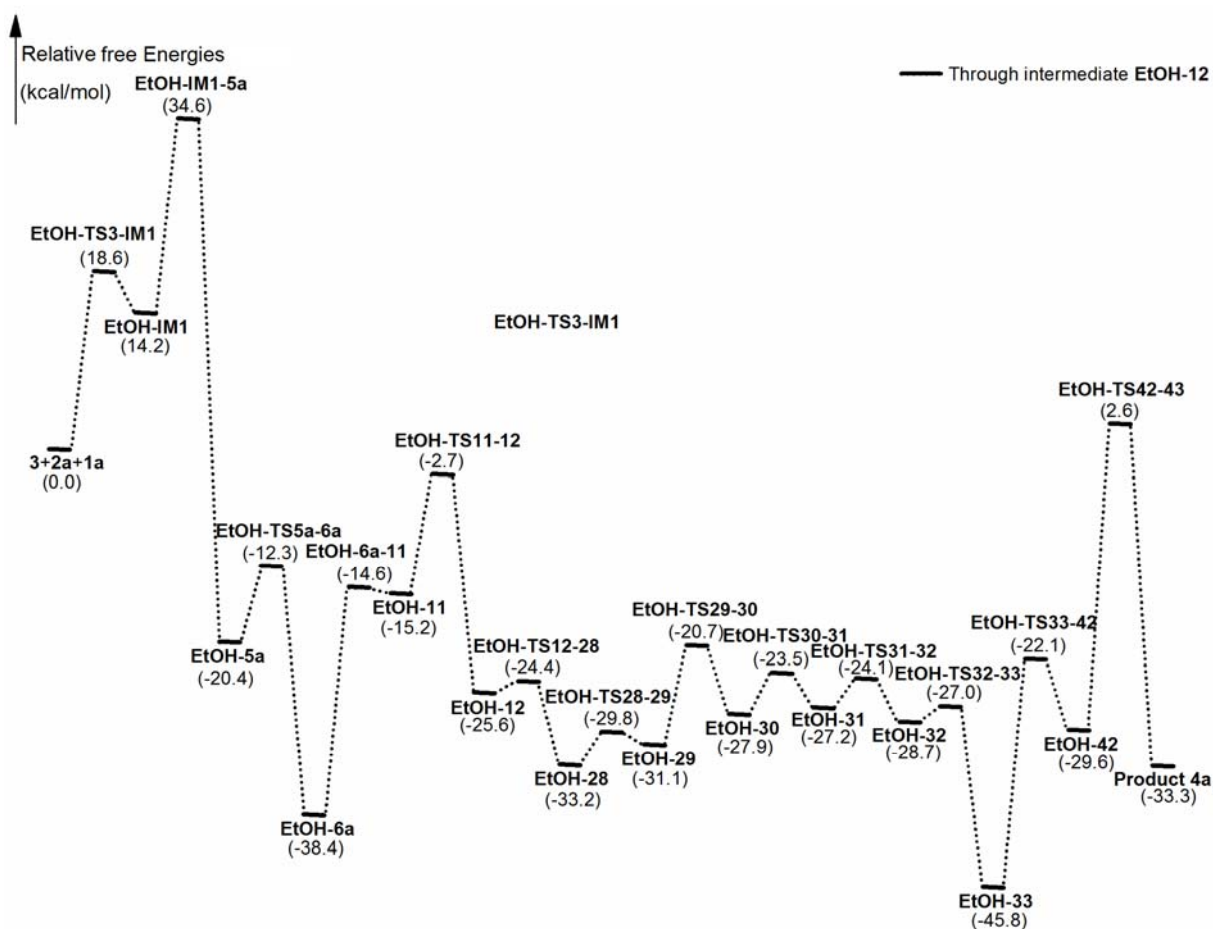


**Figure S5.** Energy profile through intermediate **EtOH-7** of L-proline-catalyzed trasamidation of **1a** with **2a** in EtOH . The relative free energies at M06/6-311+G(2d,p)//M06/6-31+G(d,p) level are given in kcal/mol.

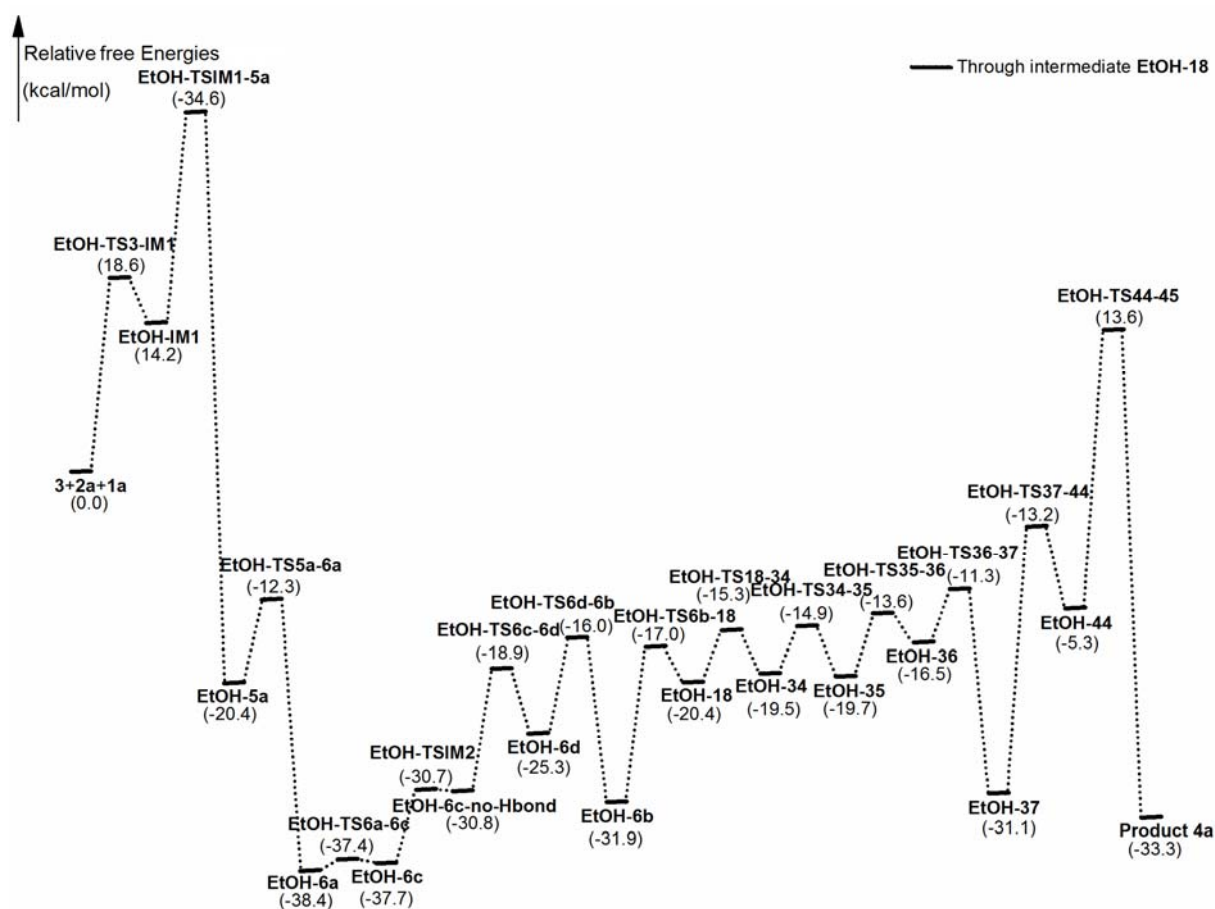


**Figure S6.** Energy profile through intermediate **EtOH-8** of L-proline-catalyzed trasamidation of **1a** with **2a** in EtOH. The relative free energies at M06/6-311+G(2d,p)//M06/6-31+G(d,p) level are given in kcal/mol.

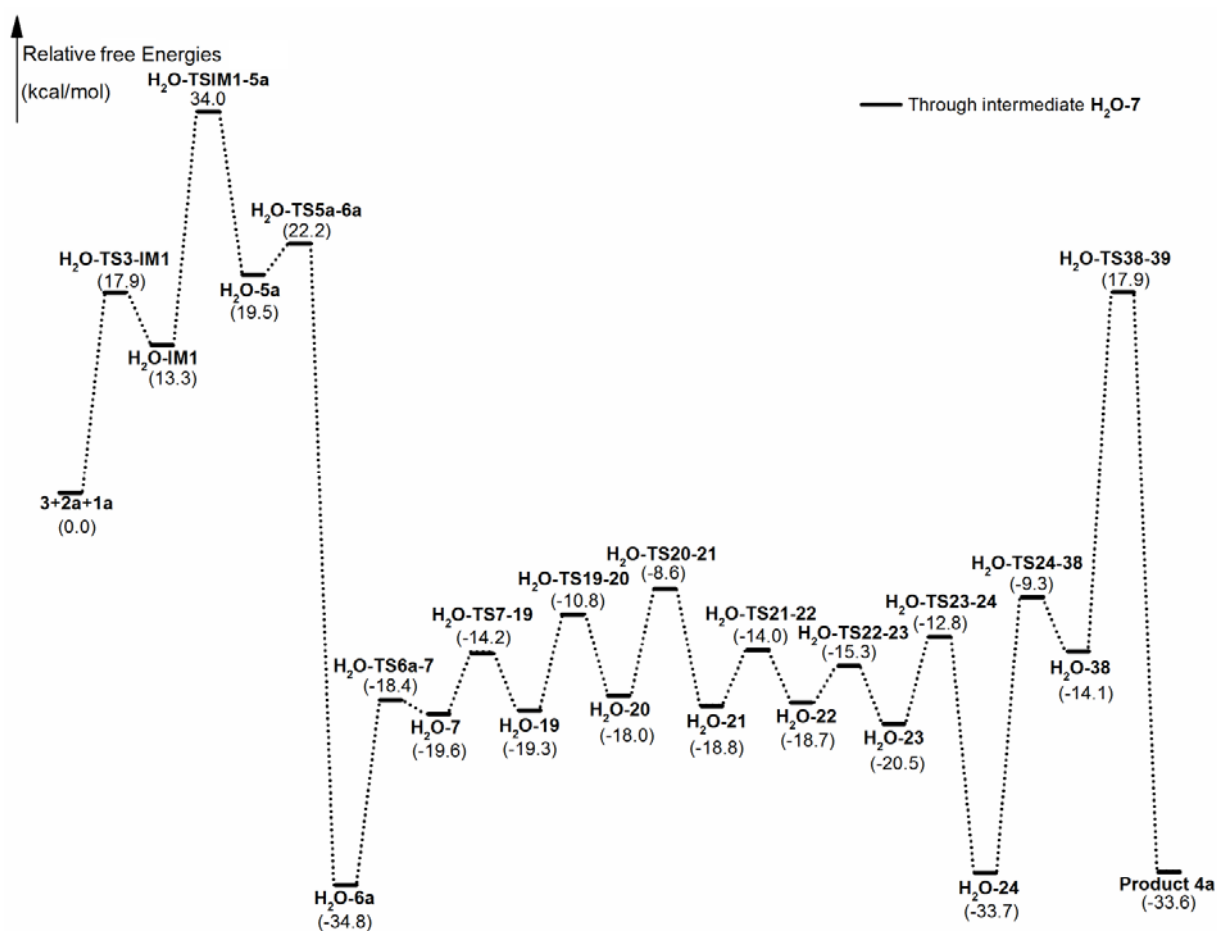




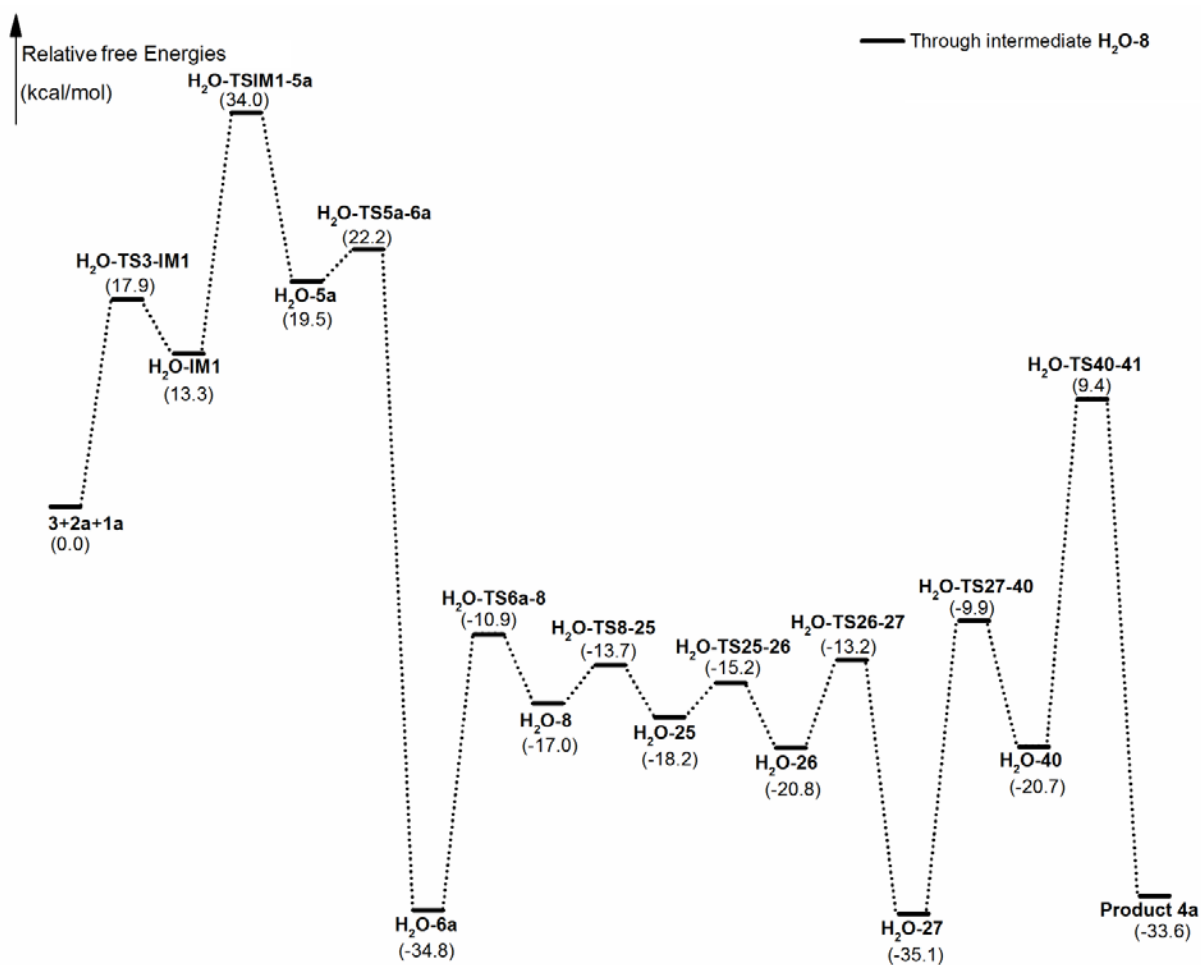
**Figure S7.** Energy profile through intermediate **EtOH-12** of L-proline-catalyzed trasamidation of **1a** with **2a** in EtOH. The relative free energies at M06/6-311+G(2d,p)/M06/6-31+G(d,p) level are given in kcal/mol.



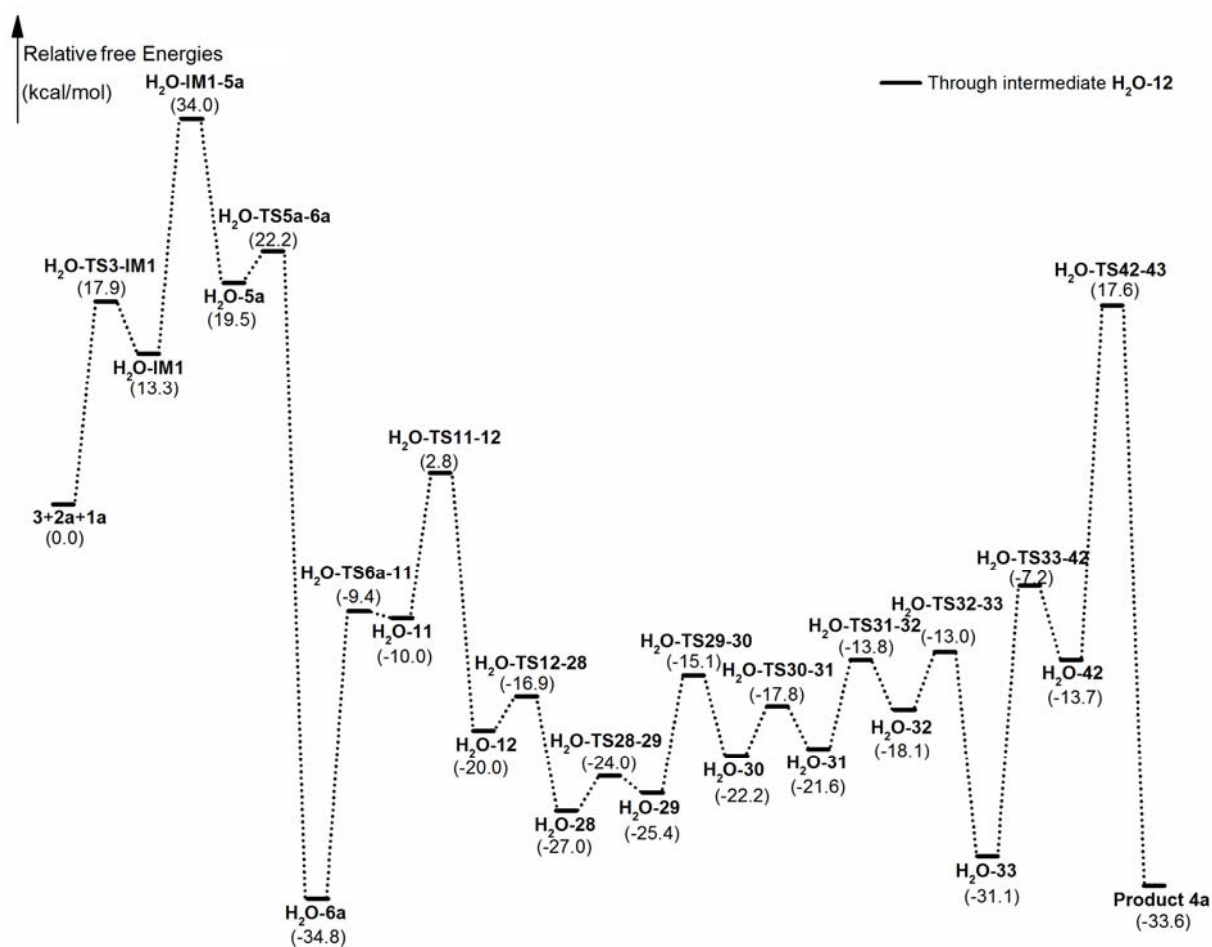
**Figure S8.** Energy profile through intermediate **EtOH-18** of L-proline-catalyzed transamidation of **1a** with **2a** in EtOH. The relative free energies at M06/6-311+G(2d,p)/M06/6-31+G(d,p) level are given in kcal/mol.



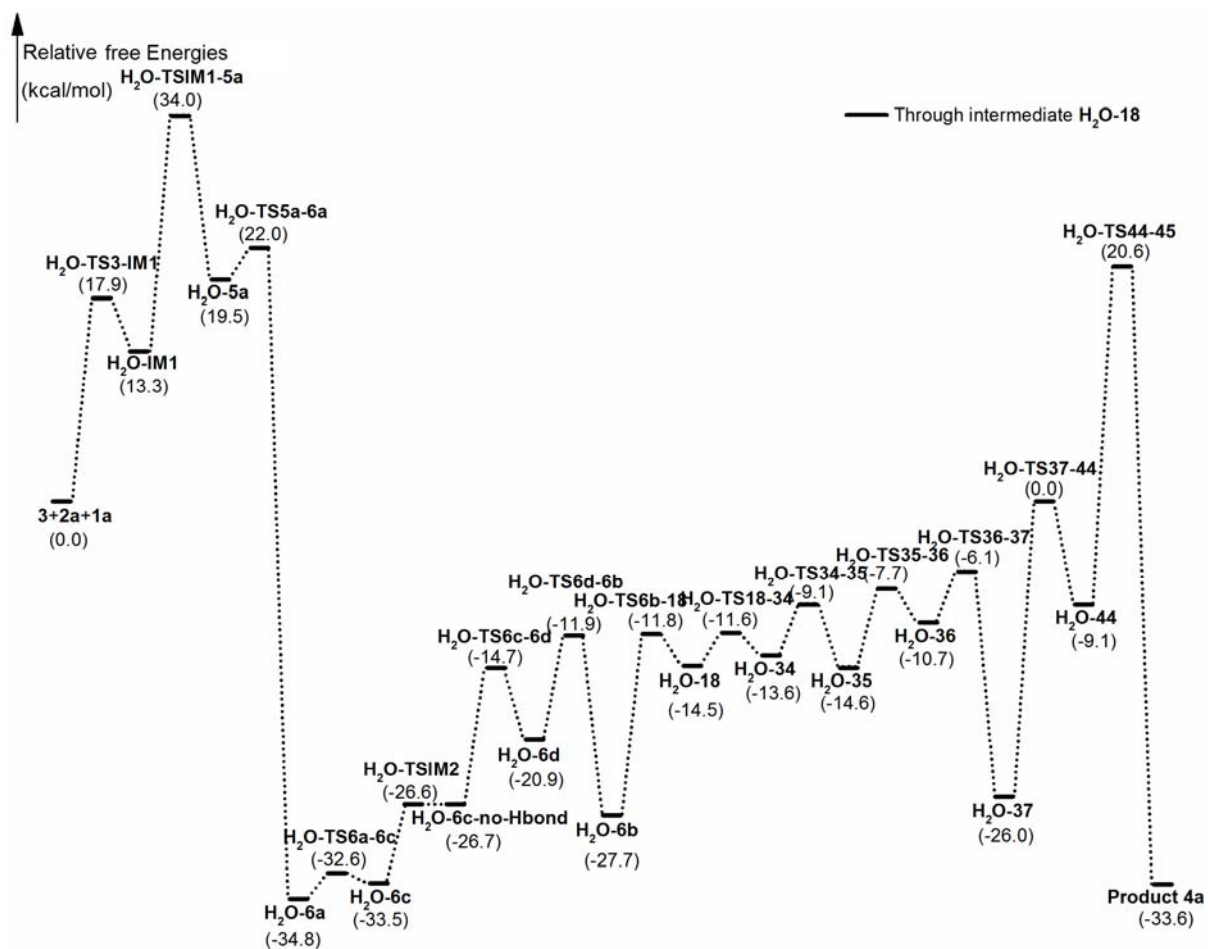
**Figure S9.** Energy profile through intermediate  $\text{H}_2\text{O-7}$  of L-proline-catalyzed trasamidation of  $1a$  with  $2a$  in  $\text{H}_2\text{O}$ . The relative free energies at M06/6-311+G(2d,p)/M06/6-31+G(d,p) level are given in kcal/mol.



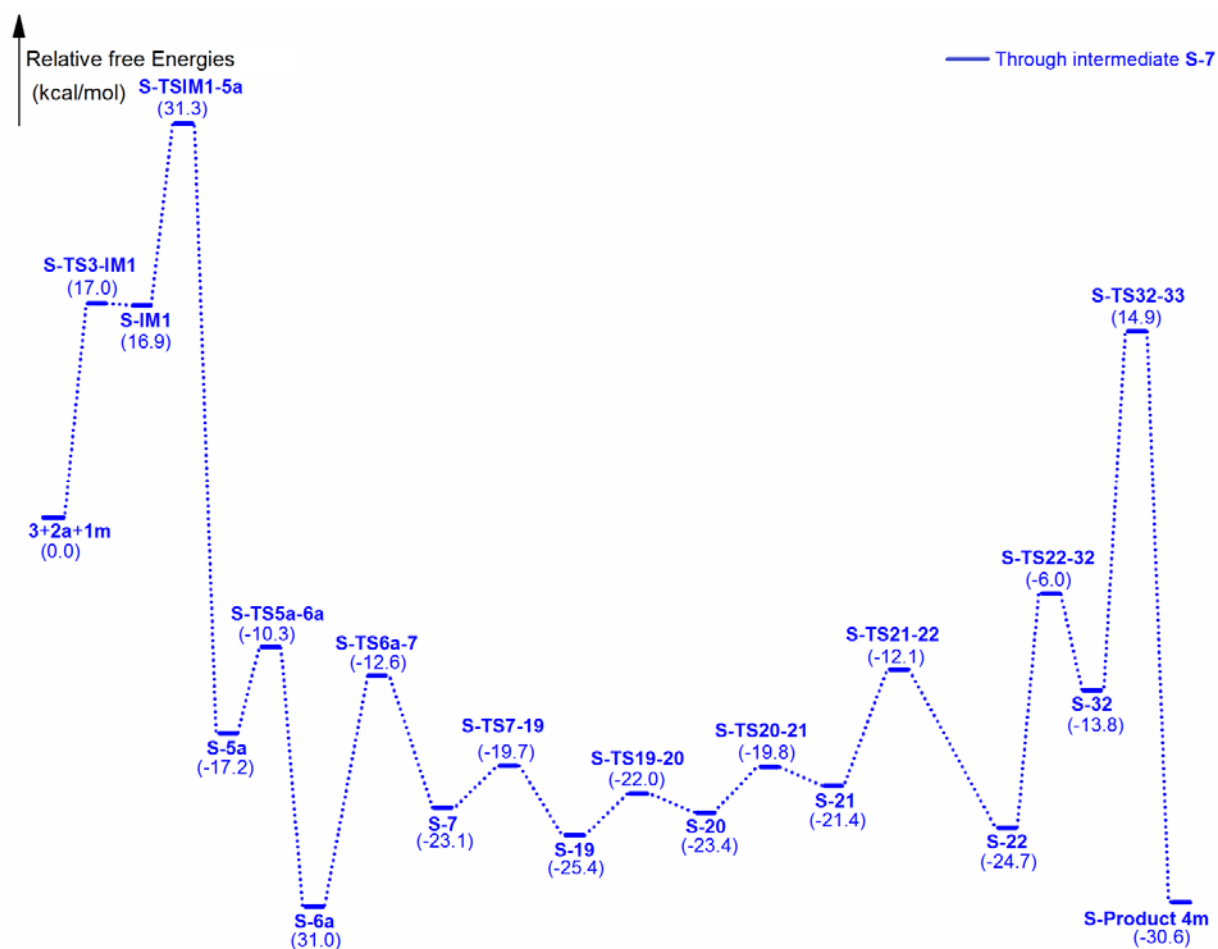
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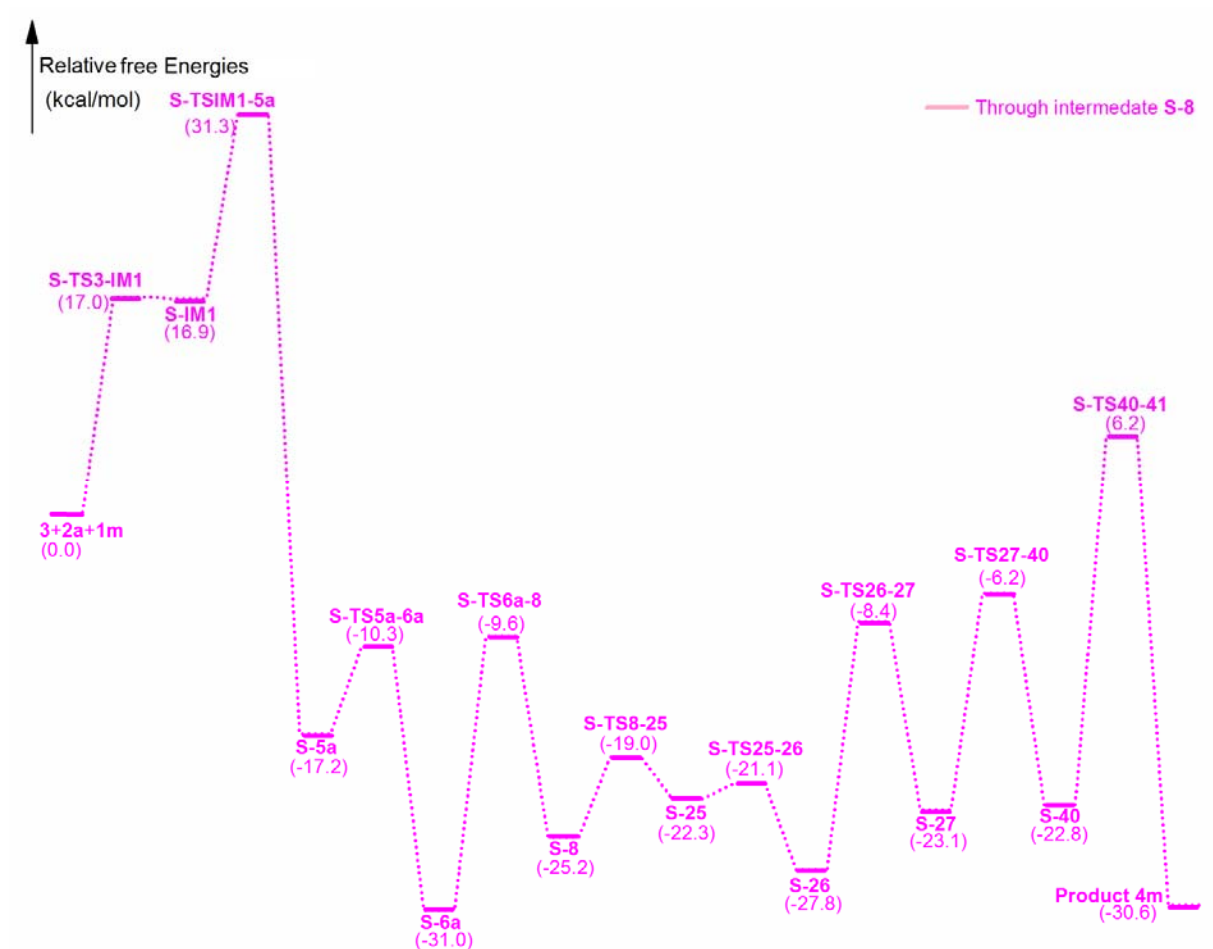
**Figure S11.** Energy profile through intermediate **H<sub>2</sub>O-12** of L-proline-catalyzed transamidation of **1a** with **2a** in H<sub>2</sub>O. The relative free energies at M06/6-311+G(2d,p)//M06/6-31+G(d,p) level are given in kcal/mol.



**Figure S12.** Energy profile through intermediate **H<sub>2</sub>O-18** of L-proline-catalyzed trasamidation of **1a** with **2a** in H<sub>2</sub>O. The relative free energies at M06/6-311+G(2d,p)//M06/6-31+G(d,p) level are given in kcal/mol.

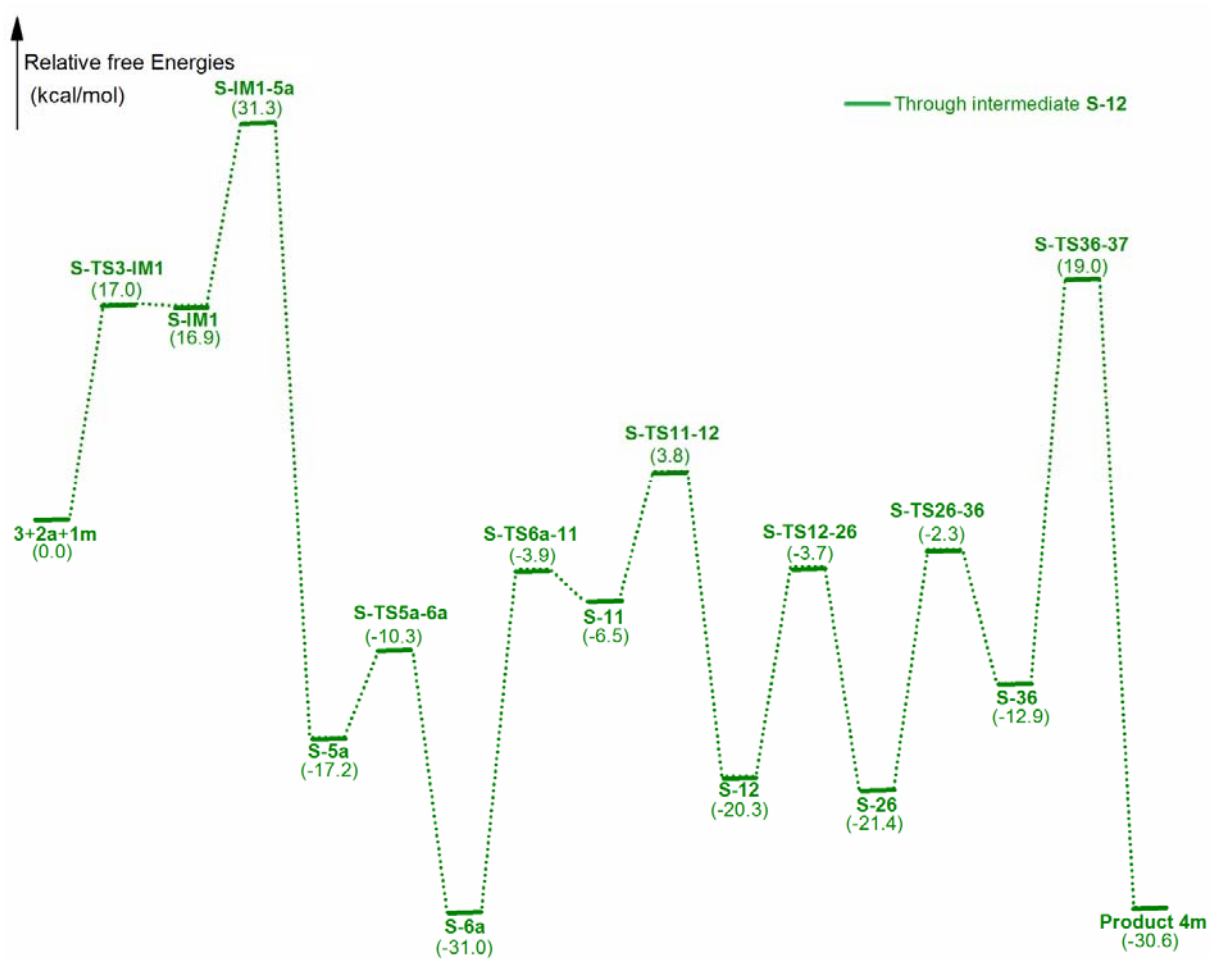


**Figure S13.** Energy profile through intermediate **S-7** of L-proline-catalyzed transamidation of **1m** with **2a** in toluene. The relative free energies at M06/6-311+G(2d,p)/M06/6-31+G(d,p) level are given in kcal/mol.



**Figure S14.** Energy profile through intermediate **S-8** of L-proline-catalyzed trasamidation of **1m** with **2a** in toluene. The relative free energies at M06/6-311+G(2d,p)/M06/6-31+G(d,p) level are given in kcal/mol.





**Figure S15.** Energy profile through intermediate **S-12** of L-proline-catalyzed trasamidation of **1m** with **2a** in toluene. The relative free energies at M06/6-311+G(2d,p)/M06/6-31+G(d,p) level are given in kcal/mol.

### Cartesian Coordinates of all stationary points

#### 5a

C	-0.72898400	2.57489100	-0.30353000
C	-1.76168500	1.47355000	-0.03946000
C	-0.92690300	0.23742100	0.34337900
C	0.60498800	1.92356300	0.02246700
H	-0.75226600	2.87956300	-1.35539900
H	-0.89639100	3.47117000	0.30164300
H	-2.35803600	1.26088000	-0.93270800
H	-2.46591500	1.71444200	0.76068700
H	-0.81942900	0.22391400	1.44619100
H	0.85449500	2.05966500	1.09263300
H	1.42678400	2.32938200	-0.57362500
N	0.38863900	0.49784500	-0.27502200
C	-1.71629400	-1.02310500	0.01060100
O	-2.87329700	-1.09674200	0.36669500
O	-1.14260300	-2.03392500	-0.62898000
H	-0.18069900	-1.88298700	-0.80946300
C	1.50280600	-0.37981900	0.07759000
C	2.85378600	0.27948100	-0.13563900
H	3.03794300	1.06875800	0.59780700
H	3.62855800	-0.48637700	-0.02894100
H	2.92863200	0.70267900	-1.14308800
N	1.42786400	-0.86950400	1.42159100
H	0.65125800	-1.51038500	1.55932400
H	2.27685800	-1.37167100	1.66365100
O	1.44282300	-1.51884300	-0.82903700
H	1.57100900	-1.17721900	-1.72656100

#### 5b

C	0.94302900	2.46562100	0.01868900
C	1.87425800	1.30527400	-0.31037900
C	0.93392400	0.11217100	-0.63204000
C	-0.25435300	1.75925200	0.62984100
H	1.40086500	3.19605400	0.69286700
H	0.62673200	2.98590100	-0.89324300
H	2.48881200	1.06278500	0.56651800
H	2.56196700	1.50504200	-1.13575900
H	0.95011200	-0.11759400	-1.70660200
H	-1.15507700	2.38367900	0.60243000
H	-0.05578300	1.49450600	1.68803600
N	-0.38311600	0.58911400	-0.22715300
C	1.54760000	-1.10712600	0.05623100
O	2.56188800	-1.59804200	-0.38975900
O	1.00999400	-1.55565700	1.18869800
H	0.08727100	-1.23235000	1.32964600
C	-1.54207400	-0.24440700	-0.17218900
O	-1.61613600	-0.93793500	1.13169700
H	-1.97794600	-0.32375400	1.78395700
C	-1.49110200	-1.36361900	-1.19261200

H	-1.35287800	-0.94509900	-2.19297600
H	-0.69351200	-2.08108300	-0.97981600
H	-2.43825400	-1.91013100	-1.16530200
N	-2.73048300	0.53166600	-0.39476700
H	-3.55773300	-0.04288900	-0.26735900
H	-2.80305100	1.34955000	0.20071300

**6a**

C	1.44946700	1.79611200	0.75893800
C	1.90193900	1.28432300	-0.60390200
C	0.92299200	0.15778800	-0.87643800
C	-0.06668000	1.80482500	0.63730600
H	1.76073300	1.08678400	1.53570400
H	1.84461100	2.78344900	1.01330100
H	2.92723800	0.90904200	-0.60118500
H	1.80354500	2.07034000	-1.36482600
H	0.74732400	-0.01891100	-1.94718600
H	-0.42721800	2.74543400	0.19685100
H	-0.58521600	1.63343300	1.58662300
N	-0.33783200	0.69247800	-0.29480800
C	1.32069000	-1.20829000	-0.22973000
O	2.44492200	-1.31206200	0.26453900
O	0.40759300	-2.09282900	-0.29914100
H	-0.60294400	-1.78794100	1.23853400
C	-1.55021500	0.25726000	-0.56548800
C	-2.73660400	0.96568800	-0.01717300
H	-2.62923800	2.05214800	-0.06539900
H	-3.64233200	0.67226300	-0.55261700
H	-2.84739200	0.67037000	1.03376400
N	-1.72006500	-0.82003700	-1.32958500
H	-0.95885300	-1.52311100	-1.25938100
H	-2.66444000	-1.15411500	-1.45766400
O	-1.19087100	-1.32372900	1.86940900
H	-1.06322300	-1.76355200	2.71470700

**6b**

C	0.83227100	2.48909900	-0.28522200
C	1.79308400	1.34054400	-0.00411000
C	1.09947000	0.10337600	-0.58686500
C	-0.52324800	1.84989200	-0.03710800
H	0.99999800	3.35849000	0.35667700
H	0.90981700	2.81534700	-1.33055900
H	1.90554500	1.20874700	1.08131800
H	2.79057900	1.47577900	-0.42890300
H	1.41786100	-0.08346700	-1.62087700
H	-1.35513100	2.33275800	-0.56266900
H	-0.75850700	1.78643600	1.03510000
N	-0.32805200	0.49111800	-0.57164400
C	1.40612800	-1.14516200	0.28518100
O	2.48920200	-1.68845100	0.02389400
O	0.55858300	-1.43846200	1.17080900
H	-0.75287600	-0.56057500	1.91733000
C	-1.30573200	-0.33803400	-0.84502600

O	-1.53138500	-0.04565400	2.24546900
H	-1.62305900	-0.26744500	3.17585100
C	-1.05011500	-1.63044900	-1.52961900
H	-0.26973700	-1.53994700	-2.28922000
H	-0.70917300	-2.35395300	-0.77867500
H	-1.96458200	-2.00571200	-1.99504000
N	-2.56565400	-0.01153700	-0.52688000
H	-3.27606800	-0.71300800	-0.68170500
H	-2.70107400	0.55442200	0.30627700

**6c**

C	-0.94263800	2.12855000	-0.30925400
C	-1.41506400	1.29276800	0.87595000
C	-0.67999000	-0.02541600	0.68895900
C	0.53526800	1.77975700	-0.40133700
H	-1.46380600	1.81188600	-1.22127000
H	-1.10712600	3.20190800	-0.17892000
H	-2.49766500	1.15099200	0.90344600
H	-1.09487500	1.75457600	1.81854000
H	-0.42963600	-0.51736900	1.64120900
H	1.13195800	2.40884700	0.27884500
H	0.94064000	1.89293200	-1.41334400
N	0.57466300	0.37751200	0.02916200
C	-1.46430100	-1.04163100	-0.15519600
O	-2.57604200	-0.82387800	-0.58654200
O	-0.84439900	-2.19357800	-0.36242300
C	1.69675100	-0.38559100	0.10102400
C	2.97408300	0.25617300	-0.34952800
H	3.14638700	1.21062400	0.15988400
H	3.82099900	-0.40461400	-0.15187900
H	2.94296000	0.45970800	-1.42616800
N	1.59329800	-1.60699200	0.52633200
H	0.07900100	-2.17635800	0.04343600
H	2.49431500	-2.07479000	0.54578300

**6c-no-Hbond**

C	0.63687900	2.19430400	0.30642700
C	1.24849000	1.40303800	-0.84496800
C	0.67026800	-0.00205000	-0.64600200
C	-0.78388700	1.65607500	0.35783000
H	1.16117300	1.97476700	1.24687500
H	0.66620600	3.27693000	0.15409200
H	2.34169000	1.39856100	-0.85945000
H	0.89834000	1.80298100	-1.80447100
H	0.51091000	-0.53410400	-1.59185100
H	-1.41539700	2.15873600	-0.39245800
H	-1.25617000	1.78089300	1.33872700
N	-0.61147900	0.23309000	0.02634300
C	1.61803300	-0.87694300	0.16820800
O	2.70584700	-1.19853600	-0.24665800
O	1.19594400	-1.24031600	1.38328300
C	-1.67219500	-0.62720400	-0.21829200
C	-3.01081400	-0.15924100	0.27578000

H	-3.33012400	0.75142600	-0.24437700
H	-3.76561100	-0.93094000	0.10822100
H	-2.98274800	0.06938500	1.34741900
N	-1.43013500	-1.74589700	-0.79885500
H	0.29441900	-0.88584100	1.49829700
H	-2.28636100	-2.29020500	-0.88033400

**6d**

C	0.78286700	2.16667600	0.19597800
C	1.23551900	1.29798000	-0.97224900
C	0.59607500	-0.06009000	-0.65232200
C	-0.65704300	1.72606300	0.40234000
H	1.38645200	1.95235000	1.08891600
H	0.86472600	3.23783100	-0.00830000
H	2.31998700	1.22065100	-1.09053400
H	0.81498500	1.67607200	-1.91206500
H	0.39503900	-0.62663000	-1.56891800
H	-1.35001500	2.23973900	-0.28012700
H	-1.03374400	1.87791000	1.41871600
N	-0.62614000	0.28946000	0.07495600
C	1.55337800	-0.91237600	0.17999100
O	2.56988800	-1.37288700	-0.28121500
O	1.20848800	-1.09912600	1.45778200
C	-1.82842300	-0.38979000	-0.06338800
C	-1.74440700	-1.78225900	-0.62521800
H	-0.97061500	-2.38534500	-0.13609200
H	-2.70196100	-2.29271000	-0.49808200
H	-1.51557900	-1.76095700	-1.69731300
N	-2.90436900	0.20156800	0.30956400
H	0.34882600	-0.65318000	1.59587400
H	-3.69934700	-0.42404800	0.19296600

**7**

N	0.32049700	-0.61502500	-0.21517500
H	-0.32934600	0.94438500	-0.19603900
H	0.54907900	-0.89179000	0.74056800
C	2.71115800	-0.22258200	-0.38882400
C	2.86018600	1.16679200	-0.34338300
C	3.67021900	-1.02812300	0.22596100
C	3.94880600	1.73860400	0.30580800
H	2.11340700	1.80103500	-0.82091700
C	4.76350100	-0.45801500	0.87602300
H	3.56063800	-2.11187000	0.19054200
C	4.90341100	0.92608100	0.91722500
H	4.05541700	2.82035200	0.33316700
H	5.50650500	-1.09667800	1.34803700
H	5.75612100	1.37345000	1.42248500
C	1.50836800	-0.83069900	-1.05226900
H	1.69590700	-1.90079600	-1.24648600
H	1.33316700	-0.34852300	-2.02368400
C	-3.38280000	-0.43493400	2.03088900
C	-3.72290500	0.67180000	1.03179500
C	-2.81013900	0.40896300	-0.19876200

C	-1.95876400	-0.80300400	1.64929700
H	-3.47811600	-0.10664200	3.07094900
H	-4.03055200	-1.30717400	1.88404600
H	-3.49726700	1.65592500	1.45909900
H	-4.77859700	0.68726100	0.74853600
H	-3.40635600	0.16681600	-1.08816700
H	-1.66623300	-1.79988200	2.00000000
H	-1.24655900	-0.06901800	2.08028600
N	-2.02273500	-0.75019400	0.19712100
C	-2.10356300	1.72649000	-0.54168700
O	-2.76066000	2.67225200	-0.92705100
O	-0.78713900	1.82328700	-0.39277700
C	-0.95852200	-1.29955500	-0.62116400
C	-0.86515000	-2.80758800	-0.41478500
H	-1.81184600	-3.27349600	-0.70338500
H	-0.06260700	-3.23766800	-1.02510200
H	-0.65468100	-3.05615400	0.62988300
N	-1.26605100	-1.05819400	-2.00845900
H	-1.09095800	-0.10032300	-2.29937100
H	-0.73954900	-1.67501600	-2.61698100

**8**

C	3.64041100	0.00701900	-1.69622300
C	2.86154000	-1.28936400	-1.44679500
C	1.68371500	-0.90197000	-0.53708100
C	3.21433900	0.89444300	-0.54195700
H	4.72260500	-0.15325200	-1.73093100
H	3.33574000	0.46833000	-2.64346500
H	3.48162700	-2.02482700	-0.92566100
H	2.50907100	-1.74876700	-2.37527200
H	0.71851800	-1.14674400	-1.00751600
H	3.34150900	1.96109000	-0.75701300
H	3.78198100	0.66614400	0.37835200
N	1.79826000	0.56195400	-0.40654300
C	1.72185600	-1.67513600	0.79449600
O	2.67013600	-2.31174400	1.19454100
O	0.59431400	-1.60727300	1.51203200
C	1.02002100	1.32562400	0.55902800
C	1.02958100	2.80408200	0.16698300
H	0.24044000	3.33824100	0.71177500
H	1.98617400	3.26805000	0.42461300
H	0.86083200	2.92828000	-0.90642400
N	1.55808300	1.24360700	1.90754900
H	1.36159000	0.36090200	2.37105100
H	1.23915000	2.00563500	2.49696000
N	-0.35491600	0.75750200	0.53442500
H	-0.00119600	-0.90645500	1.12129700
H	-0.86729400	1.17871000	1.30976800
C	-2.49641200	0.31658600	-0.51690100
C	-2.66219400	-1.06985000	-0.58353600
C	-3.60333000	1.11382800	-0.22310500
C	-3.90733300	-1.64626200	-0.35704500
H	-1.80628600	-1.70247300	-0.81951300

C	-4.85328600	0.54107000	0.00368800
H	-3.48351300	2.19623900	-0.17622700
C	-5.00630300	-0.84083300	-0.06091900
H	-4.02206000	-2.72614800	-0.41281900
H	-5.70756800	1.17484900	0.22992100
H	-5.98027900	-1.29145900	0.11461900
C	-1.14032400	0.93750900	-0.69756000
H	-1.25641300	2.00127500	-0.96019500
H	-0.59392600	0.46259600	-1.52235600

**9**

C	-2.47137300	-2.01890300	-1.13886900
C	-3.56935100	-0.97615000	-0.97389300
C	-2.89546600	0.06993500	-0.09516700
C	-1.24252800	-1.14597100	-1.33588800
H	-2.37709500	-2.61152700	-0.21921700
H	-2.63939900	-2.70680600	-1.97295400
H	-4.48999100	-1.35987800	-0.52755900
H	-3.80802900	-0.52775300	-1.94857100
H	-3.30007900	1.07538900	-0.30257300
H	-1.18456000	-0.82235300	-2.39226700
H	-0.30303700	-1.66719700	-1.09896800
N	-1.46479500	-0.02384600	-0.42450400
C	-3.11057200	-0.19525400	1.40314700
O	-3.93121500	-0.98101900	1.82677100
O	-2.34166800	0.50897200	2.22667700
C	-0.70049900	1.20355600	-0.66656900
C	-1.00749600	1.83841900	-2.02211700
H	-0.47548900	2.79053200	-2.12156400
H	-0.70561400	1.19233200	-2.85415500
H	-2.08503300	2.02491400	-2.11948300
N	-1.02838600	2.13722300	0.43043700
H	-1.74035200	1.11484600	1.70891000
H	-1.77177400	2.77321100	0.14894200
N	0.72588100	0.95123400	-0.59665200
H	1.04953800	0.50527100	-1.45176800
H	-0.20948300	2.71718300	0.60022600
C	2.66508500	-0.10112400	0.41156400
C	3.10161900	-1.41579900	0.24518000
C	3.60957600	0.92989500	0.40028900
C	4.45677400	-1.69975600	0.07870600
H	2.37103700	-2.22483900	0.25351700
C	4.96127800	0.65190400	0.23408000
H	3.27142500	1.95806900	0.52322200
C	5.38872800	-0.66640300	0.07338500
H	4.78294100	-2.72993900	-0.04508600
H	5.68615400	1.46285800	0.23278600
H	6.44634300	-0.88552100	-0.05394900
C	1.20522200	0.21226300	0.57463400
H	1.05480200	0.84014700	1.46454200
H	0.63589300	-0.71451900	0.75251400

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C	-2.42416800	-0.71192100	2.20930100
C	-1.76227800	-1.66336700	1.21855600
C	-1.81306300	-0.85279900	-0.07125100
C	-1.84302400	0.64182400	1.82018400
H	-3.51161200	-0.71881700	2.05337100
H	-2.23305200	-0.96164500	3.25742000
H	-2.27017100	-2.62571000	1.12134500
H	-0.71648500	-1.84844000	1.49923700
H	-0.99640500	-1.12276400	-0.76093300
H	-0.88833100	0.80604700	2.34982700
H	-2.51057400	1.47251200	2.08616900
N	-1.66974100	0.53777400	0.36775100
C	-3.13182800	-1.09698600	-0.82569900
O	-3.76509300	-2.12708100	-0.71774500
O	-3.53727100	-0.12622300	-1.63401000
C	-0.82644200	1.44111100	-0.38895700
C	-0.84672600	2.82241900	0.25813200
H	-0.23404400	3.50862300	-0.33862500
H	-1.87058900	3.21091000	0.30594900
H	-0.44040500	2.80875100	1.27348900
N	-1.37805000	1.55842600	-1.75402000
H	-2.86947600	0.61636000	-1.65992100
H	-1.45164100	2.52404200	-2.05876000
N	0.52999500	0.89483100	-0.56510900
H	-0.79302000	1.05480000	-2.41721300
H	1.06569900	1.51164200	-1.17486200
C	2.64484900	0.03651700	0.26385000
C	2.72182600	-1.21496500	-0.35566300
C	3.82284800	0.73910700	0.51352600
C	3.95263700	-1.75239500	-0.71398000
H	1.80185700	-1.76483600	-0.55534900
C	5.05996100	0.20449000	0.15430800
H	3.77087200	1.71389300	0.99815600
C	5.12651600	-1.04195300	-0.46019200
H	4.00023900	-2.72916900	-1.19009400
H	5.97085200	0.76324000	0.35696900
H	6.08949600	-1.46259200	-0.74012000
C	1.30636300	0.60957300	0.63698100
H	1.45618600	1.49520600	1.28216000
H	0.74926500	-0.12677300	1.23089700

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C	-1.20228400	1.27555500	-0.68393400
N	-1.41449100	2.16220700	0.42151700
H	-2.22708800	2.74369500	0.23620500
N	0.39559600	0.91696400	-0.61232400
H	0.67069700	0.52587500	-1.51712400
H	0.90485800	1.81131200	-0.48974500
C	2.25357300	-0.42824700	0.23085200
C	2.55081700	-1.60336900	-0.46311100
C	3.29782200	0.39282200	0.66352300
C	3.87303300	-1.95169400	-0.72559600
H	1.73771200	-2.25679700	-0.78101800



C	4.61963800	0.04603500	0.40271200
H	3.06735200	1.30482000	1.21384300
C	4.90820600	-1.12588600	-0.29437900
H	4.09555000	-2.87295400	-1.25839500
H	5.42671300	0.68704900	0.74891300
H	5.94148100	-1.39914800	-0.49405000
C	0.82609200	-0.03500800	0.45923900
H	0.66008800	0.46026400	1.42185000
H	0.15716100	-0.90192800	0.42015000
O	1.05639900	3.50685200	0.30434700
H	1.54456000	3.85382900	1.05718800
H	0.14366500	3.30859500	0.60904200
C	-1.31389300	2.02809100	-2.00061100
H	-0.68501400	2.92483700	-1.99381200
H	-1.03461300	1.40769600	-2.85804500
H	-2.35762200	2.33151400	-2.13839700
N	-1.92607400	0.07993900	-0.64330300
C	-2.55424700	-2.11054400	-1.16506800
C	-3.55767800	-1.52747000	-0.17697700
C	-2.80926400	-0.36646400	0.46602600
C	-1.90902400	-0.86568600	-1.75503000
H	-1.80903500	-2.69443400	-0.61140500
H	-3.00783700	-2.74856600	-1.93017200
H	-3.88445200	-2.25159600	0.57325200
H	-4.44005900	-1.14929400	-0.71249200
H	-3.49386200	0.45045700	0.73730500
H	-2.48595100	-0.48861400	-2.61763000
H	-0.88227700	-1.06192700	-2.10935700
C	-1.97484300	-0.74666900	1.72221900
O	-1.69287200	-1.94740100	1.89092800
O	-1.60185300	0.23918800	2.42416400
H	-1.56833700	1.62364900	1.29795900

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C	-0.77253300	1.01311400	-0.72805700
N	-1.05271000	2.00750700	0.32179500
H	-1.81212500	2.61790000	0.02647300
N	0.65188800	0.68519700	-0.64481600
H	0.91813000	0.12690000	-1.45438400
H	1.58805500	2.38138800	-0.59655200
C	2.50468800	-0.44339900	0.44832400
C	2.79845500	-1.68400000	-0.12304500
C	3.55877500	0.37986200	0.85062700
C	4.11799900	-2.09336600	-0.29520800
H	1.97990200	-2.33981800	-0.42249200
C	4.87980000	-0.02642900	0.68380900
H	3.33511000	1.34219200	1.31141000
C	5.16185300	-1.26375600	0.10826500
H	4.33149900	-3.06470000	-0.73538800
H	5.69143800	0.62000000	1.00982600
H	6.19322300	-1.58435700	-0.01787500
C	1.07899500	0.00292200	0.58947000
H	0.98850300	0.71292400	1.42198900

H	0.42318100	-0.85028400	0.82398300
O	1.63783600	3.31831200	-0.31098700
H	2.56877100	3.55362000	-0.26251700
H	-0.24036300	2.61761800	0.43049400
C	-1.03994400	1.59638400	-2.11507500
H	-0.48640900	2.53248500	-2.24483800
H	-0.74146700	0.91070500	-2.91598300
H	-2.11166600	1.80288700	-2.23525700
N	-1.58607600	-0.16722900	-0.43315700
C	-2.70678500	-2.13926800	-1.03438500
C	-3.75205100	-1.04883400	-0.83966100
C	-2.99313200	-0.00412000	-0.03160100
C	-1.45668800	-1.32282900	-1.31975800
H	-2.58603100	-2.71274800	-0.10596200
H	-2.94598200	-2.83923600	-1.84050200
H	-4.65948600	-1.38419400	-0.33195400
H	-4.02878200	-0.61837400	-1.81226000
H	-3.37231600	1.00785200	-0.25236300
H	-1.43879600	-1.03389600	-2.38748200
H	-0.53033200	-1.87831000	-1.11064300
C	-3.13351100	-0.21364800	1.48495400
O	-3.94500900	-0.96762900	1.97865000
O	-2.30621200	0.50012600	2.23939500
H	-1.72420700	1.07884600	1.66710800

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C	2.44305400	-0.05960500	-2.44797600
C	1.75493600	-1.22357600	-1.74359600
C	1.81298500	-0.78126200	-0.28601300
C	1.89458300	1.16138800	-1.71640900
H	3.52942600	-0.13483100	-2.30434300
H	2.25082200	-0.01914100	-3.52441400
H	2.24227500	-2.18807700	-1.90252300
H	0.70741200	-1.30588100	-2.06518700
H	1.01284500	-1.23723900	0.31839400
H	0.96718500	1.50755300	-2.20487100
H	2.60246700	2.00148700	-1.73140000
N	1.66232600	0.67363000	-0.35433300
C	3.14266900	-1.21056700	0.36175800
O	3.76135200	-2.18623700	-0.01049000
O	3.57794700	-0.46595600	1.36913500
C	0.86977500	1.38195600	0.62142500
C	0.94804600	2.88133100	0.36030500
H	0.36065800	3.41396500	1.11766500
H	1.98735400	3.22412900	0.41497500
H	0.55003600	3.14859100	-0.62274600
N	1.41634700	1.11799200	1.96317200
H	2.91661900	0.24588500	1.59914200
H	1.44256000	1.95356600	2.53820500
N	-0.53497400	0.88606400	0.64285600
H	-0.68980000	-0.76663400	1.70710400
H	-1.04887700	1.42586800	1.34199200
C	-2.60735000	0.25217500	-0.45316100

C	-2.67644700	-1.14299100	-0.38365200
C	-3.78231900	0.99395300	-0.33570700
C	-3.89646100	-1.78327000	-0.19789000
H	-1.76073300	-1.72730300	-0.48607700
C	-5.00824200	0.35598900	-0.15007800
H	-3.73618600	2.08116600	-0.39721300
C	-5.06644600	-1.03268600	-0.07975300
H	-3.93867300	-2.86904700	-0.15404900
H	-5.91825900	0.94525300	-0.06451400
H	-6.02234800	-1.53168500	0.06078000
C	-1.27479100	0.92509800	-0.62110600
H	-1.41782100	1.95131500	-1.00443500
H	-0.68137100	0.38020200	-1.36468100
O	-0.36911400	-1.36153700	2.41511900
H	-1.13488600	-1.83822200	2.74937000
H	0.88796900	0.39752900	2.45797100

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C	-3.71657800	-0.70862000	1.36979400
C	-3.94317500	-0.44111000	-0.11254300
C	-2.59446200	0.14725600	-0.54005700
C	-2.29884100	-1.25696500	1.37580400
H	-3.76880900	0.22880000	1.94029300
H	-4.43845700	-1.40622900	1.80469900
H	-4.77913400	0.22794800	-0.33642500
H	-4.10926700	-1.38711800	-0.64558700
H	-2.39790500	-0.04800700	-1.60228300
H	-2.32358200	-2.32800200	1.10523600
H	-1.79766500	-1.16682400	2.34558500
N	-1.59296000	-0.45902600	0.35240200
C	-2.60836300	1.66955000	-0.38991900
O	-3.29427300	2.38862000	-1.08104100
O	-1.82247000	2.13222800	0.57861000
C	-0.42501200	-1.11462400	-0.31034200
C	-0.87425000	-2.20534200	-1.28786200
H	0.00767700	-2.73389500	-1.66380700
H	-1.52854900	-2.93287400	-0.79276800
H	-1.41363500	-1.80214000	-2.15365400
N	0.41304100	-1.63415500	0.76093200
H	-1.37549600	1.32126100	0.93298200
H	-0.00355600	-2.45900000	1.18407300
N	0.37883900	-0.16881500	-1.04920000
H	1.30184100	-1.92298500	0.35806100
H	-0.09263300	0.17601400	-1.87553100
C	2.56636000	0.54037300	-0.10139200
C	3.31338200	-0.13608000	-1.06776100
C	3.20249300	0.95708700	1.06879800
C	4.66957300	-0.38462500	-0.86984000
H	2.81632800	-0.47667600	-1.97466000
C	4.55880800	0.71327300	1.26984900
H	2.62317500	1.47128000	1.83556400
C	5.29754300	0.04016800	0.29939900
H	5.23859100	-0.91265100	-1.63230600

H	5.03724300	1.04108800	2.19021700
H	6.35590700	-0.15626100	0.45513400
C	1.10525500	0.85989900	-0.31803500
H	1.02643000	1.79966800	-0.88239600
H	0.64660000	1.05235900	0.66271500

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C	2.42246300	2.15308300	1.04509700
C	2.11174000	2.05354300	-0.44278800
C	2.15993500	0.54034800	-0.68537900
C	1.63243800	0.98610600	1.61243000
H	3.49819400	2.01405900	1.22185200
H	2.13130500	3.11090000	1.48624900
H	2.80036600	2.59890100	-1.09467000
H	1.09473900	2.41866100	-0.63857900
H	1.49947700	0.25441600	-1.51529300
H	0.56976700	1.26045100	1.71659100
H	2.00178900	0.64001600	2.58370500
N	1.79300000	-0.07793100	0.59909100
C	3.56652200	0.10485000	-1.10528800
O	4.06406100	0.43320400	-2.15873000
O	4.19899800	-0.64591400	-0.20793700
C	0.74669900	-1.11477400	0.59625100
C	1.16256200	-2.25928200	-0.32280800
H	2.11128000	-2.69369800	0.00934900
H	0.40475200	-3.05061800	-0.30820100
H	1.26919100	-1.93019800	-1.36183200
N	0.65674200	-1.63706700	1.94498400
H	3.53975800	-0.75939300	0.52469800
H	0.26214200	-2.57126900	1.95783500
N	-0.52303500	-0.47179700	0.20447400
H	0.07452300	-1.03780200	2.52464800
H	-0.40126100	0.06450400	-0.65279800
C	-2.93604100	-0.48456600	-0.11548900
C	-3.29676300	0.45434200	0.85634300
C	-3.73796800	-0.62357300	-1.24751400
C	-4.43881500	1.23089600	0.70066900
H	-2.66353800	0.57244200	1.73513200
C	-4.88382900	0.15511800	-1.40907800
H	-3.46199300	-1.34943500	-2.01206400
C	-5.23668200	1.08331600	-0.43485300
H	-4.71063900	1.95485200	1.46569100
H	-5.49773500	0.03659100	-2.29896800
H	-6.12926800	1.69223800	-0.55750200
C	-1.69925000	-1.32222700	0.06675200
H	-1.62840400	-2.04441500	-0.76724000
H	-1.79393900	-1.91504300	0.98881200

**16**

C	3.57946600	-1.01800500	-1.51958900
C	3.02780300	-1.93510400	-0.43685500
C	2.09819900	-0.98922000	0.33419400
C	2.34610900	-0.22889000	-1.92705900

H	4.34523800	-0.35031600	-1.10057900
H	4.02843400	-1.55540900	-2.36024200
H	3.78142400	-2.39648800	0.20796400
H	2.42543400	-2.73428800	-0.88980200
H	1.28568800	-1.55634300	0.81044400
H	1.74190100	-0.80906000	-2.64370900
H	2.57704900	0.73058700	-2.40042800
N	1.62348500	-0.01800500	-0.65658100
C	2.86602300	-0.31794900	1.47345000
O	3.25832200	-0.94217100	2.43577400
O	3.10055600	0.98115500	1.32971900
C	0.16571700	0.19451100	-0.76228200
C	-0.56927700	-1.09539000	-1.13619500
H	-1.63301400	-0.91301000	-1.32208100
H	-0.13639100	-1.52403600	-2.04667300
H	-0.50562400	-1.84017900	-0.33483000
N	-0.02984100	1.15470400	-1.81264900
H	2.63015800	1.28941800	0.51682200
H	-1.00210500	1.23579800	-2.08621200
N	-0.24361500	0.74280600	0.56445600
H	-0.11912700	0.04162700	1.29206300
H	0.82057600	2.32371200	0.61121800
C	-2.78022000	0.48938600	0.49713400
C	-3.00356400	-0.62018500	1.31699100
C	-3.69789800	0.76818100	-0.51632800
C	-4.09848200	-1.45088000	1.10713400
H	-2.30630400	-0.84155900	2.12599100
C	-4.79949300	-0.05876600	-0.72995800
H	-3.54459300	1.64114000	-1.15163300
C	-4.99741600	-1.17565800	0.07649100
H	-4.25569500	-2.31360500	1.75036700
H	-5.50138300	0.16890700	-1.52891300
H	-5.85262100	-1.82597500	-0.09029600
C	-1.56646100	1.36274100	0.70409900
H	-1.59145400	1.77960900	1.72070200
H	-1.61297700	2.22549300	0.02642000
O	1.34682200	3.06004400	0.22832700
H	0.34462700	2.06791200	-1.56115300
H	1.56191400	3.65868500	0.95005300

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C	-2.69847100	0.67416000	2.20697800
C	-2.28191900	-0.77347300	1.97824500
C	-2.17477500	-0.85098200	0.44917500
C	-1.84137100	1.40766400	1.19139700
H	-3.76550100	0.80911600	1.98244900
H	-2.52466300	1.01858200	3.23058600
H	-2.96969900	-1.52142500	2.38366000
H	-1.29066600	-0.94976500	2.41731200
H	-1.42282400	-1.59408800	0.14861600
H	-0.81794300	1.52673100	1.58108300
H	-2.22072900	2.40003800	0.92608500
N	-1.86981400	0.51973300	0.01312000

C	-3.49855200	-1.32842400	-0.15241500
O	-3.89555000	-2.46538000	-0.03306100
O	-4.18686300	-0.38376100	-0.78777100
C	-0.82843400	0.72332000	-1.00210800
C	-1.16495600	-0.10232000	-2.24076200
H	-2.16527000	0.15529600	-2.60139400
H	-0.45691100	0.10712800	-3.04882500
H	-1.12583900	-1.17918000	-2.04277300
N	-0.84594700	2.11862600	-1.37889700
H	-3.60444300	0.41655200	-0.74918900
H	-0.40422200	2.26087600	-2.28081900
N	0.48620000	0.35233700	-0.39416900
H	1.13606700	1.88618800	0.61344000
H	0.39914300	-0.54357000	0.08650400
C	2.83891300	-0.25497100	-0.58126700
C	3.76743800	0.61009900	0.00200900
C	3.02393300	-1.63388300	-0.45020300
C	4.85693900	0.10455900	0.70686800
H	3.62723500	1.68567500	-0.09834200
C	4.10914300	-2.14270000	0.25821700
H	2.31105900	-2.31471800	-0.91763500
C	5.02845200	-1.27177300	0.83912000
H	5.57712800	0.78812200	1.15088100
H	4.24196600	-3.21820300	0.34949500
H	5.88091000	-1.66518400	1.38783900
C	1.63366800	0.26667200	-1.31243500
H	1.42963700	-0.39100500	-2.17401900
H	1.83274800	1.27314200	-1.70589900
O	1.33933100	2.83740700	0.74163900
H	1.62576200	2.94049800	1.65388700
H	-0.36141100	2.70050900	-0.69668700

**18**

N	-0.34822200	-0.81377500	0.34530700
H	-0.86474900	-1.28411400	1.08716300
H	-0.11252900	0.97289700	0.44275600
C	-2.56805200	-0.22940500	-0.47141000
C	-3.54035000	-1.13579700	-0.03890500
C	-2.88189200	1.13084900	-0.50880700
C	-4.79949800	-0.69513900	0.35871200
H	-3.30664500	-2.20128000	-0.02268100
C	-4.14202900	1.57438300	-0.11510800
H	-2.13149800	1.84562900	-0.84325200
C	-5.10178900	0.66407200	0.32166700
H	-5.54609100	-1.41267300	0.69137800
H	-4.37428600	2.63617500	-0.14953500
H	-6.08491100	1.01290800	0.62891700
C	-1.20350500	-0.73479100	-0.85076300
H	-0.72164600	-0.06079300	-1.57215300
H	-1.31197100	-1.71726700	-1.33892000
C	4.12854600	0.28979800	-0.65483600
C	3.70591700	0.81174400	0.71070100
C	2.19005400	0.68208400	0.66249700

C	3.19768500	-0.89439300	-0.83278200
H	3.94110100	1.05011700	-1.42423600
H	5.18343300	0.00281900	-0.70731900
H	4.02376400	1.83685100	0.91752800
H	4.09907400	0.15540100	1.49948500
H	1.77712000	0.46360800	1.65885200
H	3.58130900	-1.76631300	-0.27434700
H	3.08830500	-1.20236100	-1.87765600
N	1.91121300	-0.42524700	-0.28411800
C	1.50013700	1.95986700	0.18557300
O	2.08057700	2.96685100	-0.15438400
O	0.16942100	1.89525800	0.19037200
C	0.98487800	-1.46328000	0.17843800
C	1.35470800	-2.07433400	1.53177200
H	1.19971500	-1.37080500	2.35626000
H	0.74006300	-2.96047600	1.73237400
H	2.40284400	-2.38953900	1.52810500
N	1.04212100	-2.52661800	-0.80029100
H	0.39479900	-3.27421400	-0.57109000
H	0.83816700	-2.18790000	-1.73630800

**19**

N	-0.63820200	-0.31488400	0.16395200
H	1.63063500	1.51232000	-0.91626500
H	-0.68706300	-0.84161500	-0.70441100
C	-3.06775100	-0.15817100	0.33217800
C	-3.21981700	1.17778200	-0.05209400
C	-4.11787600	-1.04708300	0.10573500
C	-4.39979000	1.61441500	-0.64270600
H	-2.39654900	1.87157200	0.11334000
C	-5.30316300	-0.61378900	-0.48815900
H	-4.00731600	-2.09063900	0.39984300
C	-5.44655600	0.71818800	-0.86295700
H	-4.50613700	2.65725200	-0.93314000
H	-6.11240500	-1.32020900	-0.65882600
H	-6.36943500	1.06005200	-1.32577100
C	-1.79626300	-0.61533700	0.99475500
H	-1.88930700	-1.68605500	1.25314800
H	-1.67162800	-0.07528100	1.94619100
C	3.13254800	-1.94168200	-1.27117500
C	3.90821600	-0.66661200	-0.98044700
C	3.02238400	0.02746900	0.06269800
C	1.69747100	-1.43432100	-1.30344500
H	3.43383700	-2.43546900	-2.20058300
H	3.26220200	-2.65868400	-0.44790400
H	3.97395900	-0.05028900	-1.88940900
H	4.92442800	-0.82095500	-0.60771800
H	3.29271400	-0.30145400	1.07662600
H	0.96940000	-2.22012700	-1.06935400
H	1.44461700	-1.04766900	-2.30220000
N	1.65303400	-0.33637700	-0.31371100
C	3.23836200	1.52833200	0.00824700
O	4.20455200	2.07582300	0.48814400

O	2.31453600	2.18905900	-0.69553300
C	0.67997300	-0.44509300	0.79596900
C	0.86753800	-1.73888500	1.59517300
H	1.88044400	-1.79325100	2.00995400
H	0.16337400	-1.79194100	2.43337200
H	0.69960400	-2.62320000	0.97144100
N	0.92193400	0.66997000	1.68483200
H	0.43145100	1.49979500	1.36133600
H	0.65145500	0.47455000	2.64131200

**20**

N	-0.63873800	-0.32176300	0.16824500
H	1.63365700	1.48878900	-0.96336200
H	-0.66988700	-0.83189700	-0.70955000
C	-3.06845100	-0.17326400	0.33032400
C	-3.22652200	1.17584800	-0.00318500
C	-4.11082400	-1.05876200	0.05880800
C	-4.40362900	1.62748700	-0.58826900
H	-2.41008200	1.86715900	0.20130600
C	-5.29383200	-0.61039000	-0.52877600
H	-3.99607800	-2.11227000	0.31351000
C	-5.44258500	0.73412600	-0.85328300
H	-4.51481200	2.68043400	-0.83797900
H	-6.09718000	-1.31452800	-0.73382400
H	-6.36356700	1.08813400	-1.31087500
C	-1.80061100	-0.64667000	0.98717200
H	-1.89132800	-1.72577700	1.20915400
H	-1.66681500	-0.13289600	1.94923800
C	3.14826400	-1.94071200	-1.25036900
C	3.91692400	-0.66066500	-0.96405100
C	3.01646300	0.03932000	0.06466400
C	1.71200200	-1.43925800	-1.29523200
H	3.45873800	-2.43723200	-2.17517100
H	3.27668500	-2.65283900	-0.42294300
H	3.98720100	-0.05026500	-1.87631100
H	4.93018200	-0.80589800	-0.58008200
H	3.29958700	-0.28438700	1.07977900
H	0.98394700	-2.22510900	-1.06351200
H	1.46574400	-1.05623400	-2.29691700
N	1.65300600	-0.33495000	-0.30950700
C	3.22584000	1.54234200	-0.01439100
O	4.17132500	2.10708400	0.48629600
O	2.30710300	2.17905000	-0.74352900
C	0.66779700	-0.44975500	0.80651400
C	0.87178600	-1.74718400	1.59668000
H	1.88693000	-1.79994300	2.00952100
H	0.17233000	-1.79564600	2.43656400
H	0.71332900	-2.63203900	0.97103100
N	0.76453000	0.64453200	1.73739900
H	1.59213900	0.62822500	2.32236300
H	0.65453400	1.54565000	1.28331500

**21**



N	-0.48485200	-0.35540700	0.10380100
H	3.57452600	-0.37896700	1.05454100
H	-0.28530400	-0.02237700	-0.83605200
C	-2.91562000	-0.54823600	-0.12353600
C	-3.22855000	0.56028700	0.66938700
C	-3.84476800	-0.97936100	-1.07009000
C	-4.44516000	1.21676100	0.52301700
H	-2.49901900	0.90560800	1.40151800
C	-5.06671300	-0.32429400	-1.22048600
H	-3.60813900	-1.83950300	-1.69618600
C	-5.37001300	0.77535000	-0.42394100
H	-4.67668300	2.07608300	1.14879100
H	-5.77972000	-0.67359000	-1.96407200
H	-6.32153600	1.28910400	-0.54026200
C	-1.61429100	-1.27903500	0.07577300
H	-1.51570200	-2.06229500	-0.69723700
H	-1.62794600	-1.79325000	1.04602700
C	1.52879700	2.52887300	-0.08514100
C	2.70203600	1.91487900	-0.83032700
C	2.41888300	0.40985300	-0.70793400
C	1.37239600	1.59113200	1.10266400
H	1.70055900	3.56890400	0.20996300
H	0.62436200	2.49903500	-0.70865000
H	3.64480900	2.15923400	-0.31893500
H	2.79962900	2.22356600	-1.87481000
H	1.79423500	0.08197100	-1.55445300
H	0.34263400	1.57397600	1.47471800
H	2.03262100	1.89018400	1.92999900
N	1.77288900	0.25146300	0.60233800
C	3.73389200	-0.34703100	-0.79010900
O	4.28648100	-0.60518700	-1.83394300
O	4.26645100	-0.63557700	0.39977900
C	0.74786300	-0.81534100	0.74432400
C	1.28707100	-2.12327300	0.16941700
H	2.21311800	-2.43044700	0.66945600
H	0.54524800	-2.91144100	0.32678000
H	1.48119200	-2.05260900	-0.90668400
N	0.42560800	-1.05285600	2.13534000
H	1.25074300	-1.34983300	2.64793800
H	0.05647200	-0.21302200	2.57247100

## 22

N	-0.47778800	-0.36555100	0.12944100
H	3.55558700	-0.44116900	1.00623500
H	-0.29782200	-0.01791900	-0.81035000
C	-2.90707300	-0.53811300	-0.11778600
C	-3.21230600	0.59009800	0.64985300
C	-3.83584100	-0.98285500	-1.05811200
C	-4.42414200	1.25142300	0.48635000
H	-2.48111100	0.94862000	1.37397000
C	-5.05185900	-0.32139500	-1.22665400
H	-3.60357600	-1.85741100	-1.66550900
C	-5.34941700	0.79642000	-0.45348700

H	-4.65087600	2.12561300	1.09285600
H	-5.76491200	-0.68030800	-1.96548300
H	-6.29692900	1.31428200	-0.58300900
C	-1.61268500	-1.27676800	0.10314400
H	-1.51874800	-2.07847600	-0.65193100
H	-1.65872500	-1.77845800	1.08142300
C	1.52397500	2.53248400	0.02451500
C	2.67307400	1.94663600	-0.77924800
C	2.39103100	0.43709400	-0.71123500
C	1.39676100	1.54633200	1.17611900
H	1.70855600	3.55919700	0.35648200
H	0.60210400	2.52956300	-0.57420400
H	3.63079500	2.16803400	-0.28570600
H	2.74174300	2.29784900	-1.81247000
H	1.75451100	0.13950200	-1.56076800
H	0.37858800	1.51715700	1.57735600
H	2.08151000	1.80087200	1.99785800
N	1.77483400	0.23293800	0.60106400
C	3.70694500	-0.31489500	-0.83761100
O	4.25225600	-0.52151400	-1.89750700
O	4.24424000	-0.66226200	0.33237100
C	0.77505300	-0.83836600	0.74757800
C	1.29521100	-2.13327700	0.13025700
H	2.22422100	-2.45617200	0.61141800
H	0.55238300	-2.92786000	0.26247500
H	1.46896100	-2.03108500	-0.94642200
N	0.59015200	-1.07033600	2.16823600
H	-0.06621800	-0.40454300	2.56742700
H	0.24522400	-2.00535200	2.35616100

## 23

N	-0.70956700	-0.23429700	-0.16574700
H	2.55715600	-0.94530500	1.46406400
H	-0.75980500	0.23451900	-1.06795400
C	-3.13257500	-0.46944300	-0.01403300
C	-3.35641800	0.61797600	0.83564300
C	-4.16635200	-0.89634800	-0.84711600
C	-4.58989200	1.25961600	0.85447600
H	-2.54642400	0.96065800	1.47809200
C	-5.40472200	-0.25577500	-0.83141300
H	-3.99939200	-1.73912300	-1.51739000
C	-5.61902700	0.82373200	0.01950200
H	-4.75151500	2.10300300	1.52212500
H	-6.19981200	-0.59908600	-1.48937800
H	-6.58292300	1.32714100	0.03237500
C	-1.80400300	-1.17959200	-0.01332000
H	-1.82320900	-1.96711500	-0.78877700
H	-1.67487100	-1.69596800	0.95059300
C	2.21616500	2.59814700	-0.35592900
C	3.39174800	1.73801900	-0.82847900
C	2.88834300	0.26724700	-0.74631000
C	1.40382000	1.63311100	0.48876600
H	2.54163700	3.48445300	0.19814500

H	1.60950900	2.93099300	-1.20656500
H	4.25882400	1.87040400	-0.17169600
H	3.72386800	1.98691900	-1.83995100
H	2.92164000	-0.20700300	-1.73641900
H	0.35433500	1.91894700	0.60949600
H	1.85265400	1.53411800	1.49783400
N	1.51153100	0.40366300	-0.29137100
C	3.89860200	-0.51879600	0.09910600
O	5.02356000	-0.68521000	-0.32644900
O	3.54653600	-0.96715100	1.29739500
C	0.65810200	-0.72050200	0.02732300
C	1.00210500	-1.91611000	-0.85451800
H	2.01215200	-2.29757700	-0.67070200
H	0.30463000	-2.73858600	-0.66275700
H	0.91711800	-1.63604600	-1.91010900
N	0.84875400	-1.11992100	1.43797200
H	0.34229300	-0.47982400	2.04742200
H	0.51096900	-2.06043800	1.62582100

## 24

N	-0.47905100	-0.36200900	0.75232100
H	0.53553600	2.54957400	-0.88664700
H	-0.70776300	-1.14059400	0.14544200
C	-2.84675000	0.08258000	0.43895700
C	-2.88066300	0.24637100	-0.94990100
C	-3.97295100	-0.41678000	1.09245300
C	-4.02118600	-0.09040000	-1.67093700
H	-2.00516400	0.64517700	-1.46227700
C	-5.11972100	-0.74619400	0.37242100
H	-3.95268000	-0.54500900	2.17388200
C	-5.14429700	-0.58636000	-1.00975800
H	-4.03746000	0.04101800	-2.75015900
H	-5.99291500	-1.13214700	0.89293700
H	-6.03723600	-0.84615700	-1.57317400
C	-1.61126800	0.45706300	1.20532900
H	-1.77129300	0.31330800	2.28253000
H	-1.36081300	1.51129700	1.01181400
C	2.85758000	-2.69889300	-0.40660500
C	3.74974500	-1.48081100	-0.61040700
C	3.14122000	-0.38839800	0.27965600
C	1.47882700	-2.07623000	-0.27452000
H	2.91004100	-3.41792800	-1.22911000
H	3.11501300	-3.22327400	0.52264200
H	3.70130400	-1.15701900	-1.65892900
H	4.80072700	-1.65677600	-0.36877100
H	3.66656500	-0.31430300	1.23999900
H	0.76029900	-2.71467400	0.25384300
H	1.06648800	-1.80243300	-1.26032800
N	1.75438900	-0.86320400	0.50024200
C	3.18503400	0.98113500	-0.45680600
O	4.29514600	1.53939800	-0.41409800
O	2.12464800	1.32873800	-1.03210400
C	0.80379400	-0.06958100	0.96256200

C	1.12282000	1.10192400	1.81935100
H	2.19617800	1.23728300	1.94550000
H	0.69667600	2.00792400	1.37466200
H	0.66777100	0.95609400	2.80647800
N	-0.29529400	3.04217900	-0.54115000
H	-0.93188500	3.15156300	-1.32561100
H	0.00884400	3.98066000	-0.29578500

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C	3.89566000	-0.29893300	-1.09479700
C	2.75588300	-1.19016800	-1.57459900
C	1.62770800	-0.85979500	-0.60883800
C	3.19097900	0.97435300	-0.62655900
H	4.40517700	-0.78182700	-0.25341500
H	4.64233300	-0.10234900	-1.87036100
H	3.00853300	-2.25375500	-1.57327300
H	2.43963100	-0.90646100	-2.58616700
H	0.64798100	-1.06951800	-1.06674000
H	3.25803600	1.77830000	-1.37550600
H	3.64948400	1.35456700	0.30149300
N	1.79063700	0.58669800	-0.42686800
C	1.69743300	-1.69556500	0.67851900
O	2.62285700	-2.41726600	0.97749100
O	0.63079200	-1.58417000	1.47721600
C	1.00373900	1.37669700	0.51622900
C	1.03157100	2.83869600	0.07323100
H	0.32124600	3.41872300	0.67268000
H	2.02617900	3.27461700	0.21975900
H	0.78041300	2.93508500	-0.98732600
N	1.42315800	1.35503500	1.91603700
H	2.28669200	1.86921500	2.05283300
H	1.55189300	0.41030200	2.26847600
N	-0.35658100	0.80572100	0.53646200
H	0.03502400	-0.85863000	1.13559800
H	-0.83099200	1.22806900	1.33459200
C	-2.51716200	0.32657700	-0.46925900
C	-2.62580100	-1.06681400	-0.42575800
C	-3.66657500	1.09653100	-0.28963200
C	-3.85631000	-1.67597700	-0.20836900
H	-1.73594900	-1.68070200	-0.56371400
C	-4.90307300	0.49048500	-0.07309500
H	-3.59096800	2.18311000	-0.32166900
C	-4.99935300	-0.89698200	-0.03097800
H	-3.92552300	-2.76069400	-0.17783200
H	-5.79038500	1.10399600	0.06414800
H	-5.96244500	-1.37279000	0.13815300
C	-1.17974800	0.98433900	-0.66672700
H	-1.33026100	2.04889100	-0.90757900
H	-0.64548400	0.54050300	-1.51741800

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C	-3.56483100	0.51386700	-1.42425200
C	-2.26931300	1.24151400	-1.76144700

C	-1.36567700	0.84647300	-0.59010700
C	-3.08014200	-0.83043500	-0.88493200
H	-4.09977600	1.06247200	-0.63657900
H	-4.24504500	0.40750100	-2.27459900
H	-2.37347600	2.32521000	-1.85392800
H	-1.83754400	0.84962500	-2.69116300
H	-0.30894000	0.95522400	-0.86963300
H	-3.07097300	-1.60200400	-1.67188300
H	-3.74290500	-1.19510400	-0.08232900
N	-1.72231300	-0.55488600	-0.41107100
C	-1.56221100	1.84471900	0.56281400
O	-1.35144200	3.02568000	0.36570200
O	-1.97240700	1.41379300	1.74489200
C	-1.10162300	-1.42924200	0.55210900
C	-1.22356900	-2.88458900	0.09467200
H	-0.67710800	-3.53307000	0.79081500
H	-2.26835600	-3.21475100	0.07579600
H	-0.81117300	-3.02115600	-0.91110200
N	-1.74924300	-1.25742900	1.88400800
H	-1.21245400	-1.70375600	2.62554500
H	-2.65945700	-1.71271400	1.88349700
N	0.27141100	-0.98854000	0.73739100
H	-1.94056900	0.41299900	1.84174200
H	0.65137700	-1.35247800	1.60736200
C	2.47962400	-0.49026800	-0.21793200
C	2.52136500	0.77073500	0.38267000
C	3.66135100	-1.02933800	-0.73222900
C	3.71812600	1.47868900	0.45772300
H	1.60810200	1.19307300	0.79774700
C	4.85810500	-0.32189100	-0.66170000
H	3.64140800	-2.01746000	-1.19209200
C	4.88971800	0.93690700	-0.06560000
H	3.73286400	2.45989800	0.92671800
H	5.76914500	-0.75699300	-1.06674500
H	5.82362700	1.49102000	-0.00623300
C	1.18982900	-1.25752900	-0.35914400
H	1.42438200	-2.33139900	-0.47403800
H	0.68416300	-0.96360400	-1.29181300

## 27

C	4.12698500	-0.54347300	-0.00517200
C	3.23962800	-1.56083600	-0.70652800
C	1.84833200	-0.94325400	-0.59612500
C	3.56275000	0.77372000	-0.50540200
H	4.00144800	-0.61643600	1.08256400
H	5.19019000	-0.65291900	-0.23851800
H	3.25085700	-2.55641700	-0.25533100
H	3.53215900	-1.65847300	-1.76083800
H	1.22023600	-1.29138500	-1.42187900
H	3.96958200	1.02984300	-1.49387700
H	3.76036300	1.61114700	0.16592400
N	2.11233400	0.51888200	-0.65320500
C	1.14238600	-1.33044300	0.74874400

O	0.79144800	-2.52496500	0.79052000
O	1.00575100	-0.42381200	1.60451800
C	1.19920700	1.38992700	-0.21329600
C	1.59826400	2.56095000	0.62471100
H	0.70836400	3.07871000	0.98928300
H	2.18985200	2.22612000	1.48218500
H	2.18783200	3.27535400	0.03954200
N	-1.35311200	1.52142800	2.05915300
H	-0.67412600	0.76121200	2.17708100
H	-1.33603500	2.08316800	2.90522000
N	-0.09036100	1.32939300	-0.52084700
H	-2.27376100	1.09084900	2.01240500
H	-0.69610900	1.78780000	0.17781600
C	-2.11376300	0.03430700	-0.93922100
C	-2.17268400	-1.15368500	-0.20582700
C	-3.26926500	0.80151600	-1.09757100
C	-3.37631500	-1.56151200	0.36246000
H	-1.27464300	-1.75673700	-0.05838200
C	-4.47217800	0.39551100	-0.52525500
H	-3.22403500	1.72614200	-1.67332800
C	-4.52590900	-0.78853600	0.20666600
H	-3.41199300	-2.48601100	0.93351000
H	-5.36687800	0.99996200	-0.65485500
H	-5.46403600	-1.11173400	0.65206900
C	-0.81142900	0.52543700	-1.51055200
H	-1.00540800	1.16936000	-2.37978900
H	-0.19954900	-0.30503500	-1.86261000

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C	0.66695600	1.15284900	0.63075600
N	0.93520300	2.10752500	-0.44055700
H	1.84531200	2.54676600	-0.32937900
N	-0.75005000	0.86406500	0.58522400
H	-1.04884700	0.36652400	1.41997500
C	-2.73964000	-0.05752300	-0.44254700
C	-3.20616800	-1.36447700	-0.29970400
C	-3.65688500	0.99624400	-0.38690200
C	-4.56419800	-1.61933200	-0.11153800
H	-2.49690200	-2.19147600	-0.34282300
C	-5.01154700	0.74737100	-0.19971900
H	-3.29448100	2.01824500	-0.49066500
C	-5.46904400	-0.56345900	-0.06168100
H	-4.91404500	-2.64372100	-0.00550200
H	-5.71542300	1.57581900	-0.16366900
H	-6.52905300	-0.75901900	0.08295100
C	-1.27423600	0.22266000	-0.61902700
H	-1.10954700	0.90319300	-1.46444100
H	-0.75331500	-0.71968300	-0.86615800
H	0.24216000	2.84907600	-0.37379800
C	0.97946800	1.72404100	2.01574600
H	0.41860500	2.65300300	2.16214900
H	0.70672700	1.03520600	2.82456000
H	2.04840600	1.94908200	2.11262900

N	1.46659600	-0.06080100	0.33507300
C	2.46451700	-2.07394200	1.03575600
C	3.54865000	-1.00413800	1.02947600
C	2.91881600	0.09660800	0.16771900
C	1.20382000	-1.23772500	1.17657700
H	2.45724200	-2.62077800	0.08269000
H	2.57758200	-2.80563900	1.84115900
H	4.51726200	-1.33257900	0.64194800
H	3.70078000	-0.61993100	2.04719700
H	3.28587800	1.08420400	0.48279000
H	1.05740200	-0.96234800	2.23609000
H	0.29808100	-1.76307800	0.84412400
C	3.32855200	-0.05889000	-1.29903000
O	4.47724500	0.05574000	-1.66521300
O	2.33377100	-0.35262700	-2.12851300
H	1.52143900	-0.32500600	-1.56550200

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C	0.66695100	1.28845800	0.37037800
N	0.95056700	2.10036400	-0.79218300
H	0.98008400	1.56034300	-1.65180000
N	-0.75274200	0.99792300	0.40629400
H	-1.00733600	0.53297600	1.27399600
C	-2.75449900	-0.05090600	-0.46593300
C	-3.16458900	-1.37647300	-0.32183600
C	-3.70077300	0.96903400	-0.32695300
C	-4.49803400	-1.68276900	-0.05084400
H	-2.43191100	-2.17677800	-0.42927900
C	-5.03047400	0.66788300	-0.05620600
H	-3.37985400	2.00463600	-0.43049700
C	-5.43296600	-0.66098700	0.08181800
H	-4.80434600	-2.72103000	0.05496200
H	-5.75846600	1.46957600	0.04568400
H	-6.47363600	-0.89713400	0.29171900
C	-1.31703800	0.29267800	-0.73705900
H	-1.25533000	0.95823100	-1.61020600
H	-0.76718200	-0.63294900	-0.99370800
H	1.82268400	2.60928500	-0.70154000
C	1.00434100	2.09728300	1.61681300
H	0.45667400	3.04320900	1.58726900
H	0.71396100	1.56371300	2.52804600
H	2.07737800	2.31407600	1.67984300
N	1.44108600	0.00078900	0.30836600
C	2.37466000	-1.86571700	1.41440900
C	3.47261000	-0.81966100	1.27266700
C	2.90471600	0.10401100	0.18952100
C	1.12039500	-1.01106800	1.33209300
H	2.41070600	-2.57612000	0.57693700
H	2.43341900	-2.43968900	2.34386600
H	4.45648000	-1.21740900	1.00691100
H	3.57391200	-0.25377400	2.20858600
H	3.27389500	1.12997800	0.31736100
H	0.92528300	-0.54803200	2.31568200

H	0.22580500	-1.58232100	1.04971800
C	3.36975500	-0.33809900	-1.19821800
O	4.52072500	-0.25895000	-1.56163400
O	2.40144700	-0.83574100	-1.96801400
H	1.58769400	-0.75879100	-1.40761600

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C	-0.80549700	1.39402000	0.21422300
N	-0.73374700	2.30731100	1.33098200
H	-0.44337500	1.85162200	2.19099300
N	0.55045900	0.96052600	-0.12852700
H	0.54834000	0.04768700	-0.57411500
C	2.84495400	0.34515700	0.27739500
C	3.19404200	-0.91380200	0.76836700
C	3.59457600	0.89628700	-0.76506900
C	4.27893100	-1.60916800	0.23622600
H	2.61333000	-1.34874800	1.58267500
C	4.67864500	0.20689700	-1.29805100
H	3.31564400	1.87402800	-1.15597000
C	5.02384400	-1.04836400	-0.79699000
H	4.54339300	-2.58721300	0.63180000
H	5.25822400	0.64913500	-2.10515700
H	5.87304800	-1.58620300	-1.21195800
C	1.65039300	1.07344000	0.82512900
H	1.88098000	2.13731900	0.96751700
H	1.42474900	0.66148400	1.82669700
H	-1.64634800	2.72273200	1.49288900
C	-1.39197800	2.16426700	-0.96431400
H	-0.78363200	3.05889000	-1.11942600
H	-1.36427500	1.57942900	-1.88877400
H	-2.42991200	2.46359300	-0.77201500
N	-1.71064300	0.23977900	0.52240100
C	-2.02953700	-1.90252100	1.46061000
C	-1.81045900	-2.09746500	-0.03313800
C	-2.02707200	-0.68309300	-0.58830400
C	-1.33660700	-0.57253200	1.69535300
H	-3.10133200	-1.82417200	1.68959200
H	-1.61271800	-2.70865000	2.07157100
H	-2.46920600	-2.83269700	-0.50438200
H	-0.77268300	-2.40583300	-0.22077700
H	-1.40791700	-0.51863400	-1.47999500
H	-0.24489300	-0.73555300	1.73677800
H	-1.64688600	-0.08184600	2.62525700
C	-3.47699300	-0.50330700	-1.04141600
O	-3.93843400	-1.08015900	-1.99942000
O	-4.19358800	0.31610600	-0.27504700
H	-3.54429800	0.64384800	0.39842400

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C	-0.83304500	1.42907200	0.15322200
N	-0.90667400	2.36512900	1.25519300
H	-0.43441800	3.22846400	1.00170400
N	0.55629100	1.06118100	-0.17564200



H	0.60493600	0.23280400	-0.76249500
C	2.80447000	0.31985200	0.29418300
C	3.02526800	-1.01030900	0.65627700
C	3.67548300	0.92847000	-0.61244200
C	4.10177700	-1.72053600	0.12956800
H	2.34799200	-1.48917300	1.36465000
C	4.75294600	0.22358100	-1.13963900
H	3.49896600	1.96370900	-0.90246500
C	4.96838700	-1.10318900	-0.76871100
H	4.26619100	-2.75466100	0.42342900
H	5.42849200	0.70928500	-1.83998000
H	5.81195500	-1.65357100	-1.17850800
C	1.61402000	1.06254500	0.83131500
H	1.89683800	2.10246900	1.05520000
H	1.32622400	0.60211700	1.79251000
H	-0.46054700	2.01196300	2.09703500
C	-1.42123300	2.12342600	-1.07042900
H	-0.85160900	3.03808400	-1.26246900
H	-1.34052600	1.50439100	-1.96986200
H	-2.47107600	2.38605400	-0.90620800
N	-1.68796900	0.27123200	0.50833000
C	-2.04060900	-1.79662800	1.57688000
C	-1.75915200	-2.08926300	0.10862600
C	-1.95949600	-0.71717100	-0.54829600
C	-1.35702000	-0.45211000	1.74804200
H	-3.12072700	-1.70685800	1.75573200
H	-1.64789900	-2.55843400	2.25686200
H	-2.39400200	-2.85934000	-0.33911100
H	-0.71181100	-2.39782500	-0.01624700
H	-1.31101200	-0.61398400	-1.42889100
H	-0.27082600	-0.61842300	1.84376900
H	-1.70314300	0.10633500	2.62545500
C	-3.39603400	-0.57600500	-1.05778500
O	-3.81877800	-1.20424000	-2.00187500
O	-4.14674400	0.26753000	-0.35432900
H	-3.52593200	0.64706500	0.31948800

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C	-0.66685600	-1.02839900	0.16460300
N	-1.00477600	-1.66296400	-1.12319400
H	-0.68301900	-2.62771000	-1.15452500
N	0.78022800	-0.82053800	0.29058400
H	0.95073200	-0.15143700	1.03789000
C	2.98168500	-0.12436800	-0.42386900
C	3.40389900	1.20433800	-0.48000200
C	3.85072100	-1.08983000	0.09157200
C	4.67484200	1.56547700	-0.03528400
H	2.73060000	1.96172300	-0.88186800
C	5.11973500	-0.73434100	0.53430100
H	3.51981900	-2.12640300	0.14334300
C	5.53480200	0.59617500	0.47169100
H	4.99211900	2.60442600	-0.08675500
H	5.79015100	-1.49501300	0.92786400

H	6.52813700	0.87404700	0.81618800
C	1.60140900	-0.51186900	-0.87646900
H	1.66908200	-1.40965300	-1.50894000
H	1.20223700	0.29981400	-1.51228100
H	-0.57949700	-1.17825500	-1.90971700
C	-1.08297600	-1.99174700	1.26947900
H	-0.48693200	-2.90501700	1.18367300
H	-0.87606800	-1.54465100	2.24763700
H	-2.14383000	-2.25959200	1.21752000
N	-1.38192100	0.22627500	0.30607200
C	-2.22143200	2.33644300	-0.37129600
C	-2.87195700	1.87635300	0.92962800
C	-2.73405300	0.35681800	0.82727500
C	-1.06610700	1.35112300	-0.57660000
H	-2.94478000	2.24429500	-1.19281500
H	-1.88679800	3.37771200	-0.34696100
H	-3.91164300	2.19301500	1.04034600
H	-2.30017200	2.22260200	1.79874300
H	-2.82386000	-0.10957400	1.81795100
H	-0.09614000	1.79152600	-0.29702000
H	-0.99582400	1.05588300	-1.63825000
C	-3.90250000	-0.20580400	-0.00516000
O	-5.04742600	0.06883600	0.29027100
O	-3.63580200	-0.99007400	-1.04135900
H	-2.67049000	-1.24944700	-1.12676000

### 33

C	-0.68990600	-0.08531100	0.96706500
N	0.01298100	-2.05874200	-1.61489400
H	0.05745100	-3.07324300	-1.66755000
N	0.60455800	0.14044900	0.72169700
H	0.84189100	0.83789000	0.02625200
C	2.96941500	-0.31100300	0.44711800
C	3.22350700	-0.50674700	-0.91329700
C	3.90484600	0.36594000	1.23007900
C	4.40138200	-0.03103100	-1.48167300
H	2.48430500	-1.04349100	-1.50864700
C	5.08541200	0.83955500	0.66222000
H	3.70873200	0.51770700	2.29094500
C	5.33389600	0.64181500	-0.69373400
H	4.59668300	-0.19178100	-2.53933200
H	5.81241900	1.36149600	1.27970300
H	6.25685900	1.00920200	-1.13608700
C	1.68079900	-0.80999800	1.03313600
H	1.77152500	-0.91650300	2.12133600
H	1.41739800	-1.78039900	0.58973400
H	0.14989500	-1.73221500	-2.56843900
C	-1.04138500	-1.21256100	1.86886700
H	-0.38464100	-1.22961800	2.74305700
H	-2.07713700	-1.17256600	2.20168000
H	-0.90801100	-2.15053300	1.31598500
N	-1.60888300	0.69062700	0.43246200
C	-2.66145400	2.07216000	-1.16867200

C	-3.60588300	1.81976100	0.00042200
C	-3.06895700	0.52320700	0.59622100
C	-1.29767100	1.68084400	-0.61128800
H	-2.92019000	1.41586500	-2.00769300
H	-2.67400700	3.10503400	-1.52750500
H	-4.65167900	1.70543600	-0.29402300
H	-3.53801200	2.63529200	0.73313600
H	-3.31905700	0.43663200	1.65902700
H	-0.77325400	2.53665800	-0.16101200
H	-0.64840700	1.22685000	-1.37314700
C	-3.61642900	-0.73759200	-0.14754700
O	-4.83716100	-0.91036500	0.01691900
O	-2.78905700	-1.41078100	-0.80586800
H	-0.95905700	-1.82913000	-1.37419900

### 34

N	-0.36220900	-0.85157700	0.43581900
H	-0.90597700	-1.34111700	1.14535500
H	-0.06737800	0.90653400	0.63177600
C	-2.53247200	-0.21929100	-0.47893800
C	-3.54747100	-1.12527600	-0.15771300
C	-2.82051600	1.14740800	-0.46510600
C	-4.82294100	-0.67917100	0.17828000
H	-3.33396600	-2.19477500	-0.18260800
C	-4.09578600	1.59710700	-0.13249000
H	-2.03689800	1.86174400	-0.71220800
C	-5.09881900	0.68604700	0.19132800
H	-5.60305500	-1.39721700	0.42101500
H	-4.30698100	2.66391900	-0.12842800
H	-6.09487100	1.03890000	0.44848800
C	-1.15691100	-0.73043000	-0.80437300
H	-0.62184400	-0.04485200	-1.47305000
H	-1.23461500	-1.69157400	-1.33078200
C	3.96365000	0.29981900	-1.00682100
C	3.78978400	0.81428100	0.41466500
C	2.29028400	0.66720200	0.63810900
C	3.03700800	-0.90066700	-1.01047500
H	3.61532400	1.05264100	-1.72612900
H	4.99584100	0.03583100	-1.25683800
H	4.12893900	1.84205100	0.56437800
H	4.32681600	0.16101100	1.11661000
H	2.06906300	0.45017300	1.69414900
H	3.55178800	-1.75010900	-0.51490100
H	2.74021300	-1.22394100	-2.01340700
N	1.87052400	-0.44279300	-0.24602900
C	1.51757700	1.94537100	0.30471200
O	2.04032100	2.98885300	-0.02054800
O	0.19682400	1.84933400	0.43734100
C	0.97204400	-1.45923500	0.30564700
C	1.38812300	-1.95405500	1.69894300
H	1.24954800	-1.20114900	2.48270100
H	0.79271100	-2.83212700	1.97751900
H	2.44366000	-2.25373800	1.68936000

N	0.92673400	-2.56590800	-0.65034200
H	1.81482800	-3.06158800	-0.66643300
H	0.23302900	-3.23882800	-0.33166000

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N	-0.27417500	-1.12260600	0.48713000
H	-0.70324500	-1.59681800	1.27577900
H	0.99082700	0.70051500	-1.50112800
C	-2.47437000	-0.43922900	-0.30286400
C	-3.68404800	-1.12183700	-0.43267100
C	-2.49172800	0.88124900	0.15798200
C	-4.89168900	-0.50189700	-0.11306200
H	-3.67982000	-2.15101000	-0.79138100
C	-3.69316500	1.50271300	0.47780700
H	-1.55405700	1.42560800	0.25821300
C	-4.89798100	0.81191100	0.34405000
H	-5.82642700	-1.04786400	-0.22056300
H	-3.69059800	2.53232800	0.82806500
H	-5.83754200	1.29954700	0.59400300
C	-1.17528600	-1.10886400	-0.66138200
H	-0.68535000	-0.56149200	-1.47635700
H	-1.38294800	-2.11578700	-1.06037900
C	3.96062300	0.65307900	-0.52589600
C	3.33252100	1.19863200	0.75090300
C	1.85817400	0.82927800	0.56511100
C	3.23974100	-0.67598800	-0.68873600
H	3.73998000	1.31578200	-1.37396800
H	5.04679600	0.53593000	-0.46723700
H	3.47661400	2.27122700	0.91087000
H	3.72968700	0.66548400	1.62546600
H	1.33961800	0.69618700	1.52139100
H	3.72363000	-1.43245900	-0.04480500
H	3.25070200	-1.05309000	-1.71762400
N	1.85792100	-0.39795300	-0.25031400
C	1.11259200	1.95098800	-0.15490200
O	0.90881200	3.03301500	0.34882000
O	0.72015500	1.64749400	-1.39048600
C	1.09701100	-1.54408200	0.30023100
C	1.63522900	-1.98392600	1.66654000
H	1.51243100	-1.20594100	2.42910600
H	1.10090000	-2.87947300	2.00615000
H	2.69834600	-2.24025100	1.60331800
N	1.19095600	-2.61412700	-0.69660600
H	2.13616000	-2.98797900	-0.74366700
H	0.59390600	-3.38388100	-0.40205900

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N	-0.41219100	1.13017000	-0.22049600
H	-0.96400000	1.85038200	-0.67320200
H	1.63384400	0.11252600	1.81553700
C	-2.51333300	0.07445900	0.33656900
C	-3.61112700	0.93123500	0.42655600
C	-2.67247900	-1.16795700	-0.28127800

C	-4.84891400	0.55741800	-0.09337100
H	-3.49494000	1.89769900	0.91841600
C	-3.90740700	-1.54785100	-0.79654200
H	-1.82124900	-1.84542300	-0.34668100
C	-4.99796500	-0.68378000	-0.70594200
H	-5.69773700	1.23272600	-0.01359900
H	-4.02176300	-2.52224400	-1.26592500
H	-5.96404500	-0.98219600	-1.10634700
C	-1.17040500	0.50190000	0.85977200
H	-0.62841500	-0.37609700	1.22999500
H	-1.31908700	1.16550100	1.73082000
C	3.88013400	-0.64742200	-0.93171800
C	2.67644400	-1.47354300	-1.37893400
C	1.56480800	-0.90042000	-0.49768900
C	3.29678200	0.74699300	-0.67011900
H	4.28795100	-1.06635300	-0.00177300
H	4.69231400	-0.62963700	-1.66467000
H	2.80581400	-2.55021000	-1.24369400
H	2.43080300	-1.27281100	-2.42837600
H	0.56806600	-1.09537300	-0.91696700
H	3.51176500	1.43495200	-1.50194200
H	3.74098800	1.18907200	0.24017500
N	1.85857700	0.51613300	-0.55217500
C	1.60546700	-1.60451800	0.87099500
O	1.51414400	-2.81336700	0.94017000
O	1.75326400	-0.87005900	1.96959800
C	0.96714700	1.54515700	-0.05197600
C	1.17798500	2.82876800	-0.84915400
H	0.94111500	2.66174600	-1.90602800
H	0.53447200	3.62346100	-0.45343100
H	2.21408800	3.17537400	-0.78068600
N	1.26936100	1.76534300	1.39423700
H	2.15294700	2.26404900	1.48445200
H	0.56476900	2.35611900	1.83180900

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N	0.00422500	1.76090500	-0.65990700
H	0.03891100	2.73757100	-0.91488900
H	-3.27337500	0.24035000	-1.40403300
C	2.18930300	0.52278800	-0.61953300
C	2.81621000	1.40929000	0.25794800
C	2.74588500	-0.74167800	-0.82566300
C	3.98552400	1.03876900	0.91697600
H	2.38517200	2.39410300	0.43414700
C	3.91758500	-1.11008800	-0.17073300
H	2.23577600	-1.45122900	-1.47735300
C	4.54084200	-0.22059000	0.70123200
H	4.46378800	1.73586200	1.60124900
H	4.33591100	-2.10053600	-0.33256200
H	5.45255500	-0.51015800	1.21827900
C	0.95028100	0.90852400	-1.38636800
H	0.42826600	0.03120400	-1.77504500
H	1.23428000	1.49267800	-2.27015900

C	-2.53203200	-1.40198200	1.74925700
C	-1.08259500	-1.84937400	1.61405500
C	-0.57761300	-0.98545800	0.46486900
C	-2.44035100	0.10779100	1.59654300
H	-3.13549700	-1.82862600	0.93780300
H	-2.99236300	-1.68474800	2.70033200
H	-0.96141400	-2.90973800	1.38025100
H	-0.52478500	-1.62934900	2.53472000
H	0.50672500	-0.84320200	0.51673900
H	-2.24857900	0.59497100	2.56326800
H	-3.32562800	0.55829700	1.13524600
N	-1.26133400	0.30501300	0.71591900
C	-0.93496900	-1.61034600	-0.91820700
O	-0.31543000	-2.66437800	-1.15367400
O	-1.75839600	-0.99077200	-1.63404200
C	-0.98988100	1.48090400	0.19533800
C	-1.85626100	2.63736300	0.57185400
H	-1.95666500	2.72066400	1.65796500
H	-1.45776000	3.57882400	0.18753600
H	-2.85217300	2.46368400	0.13735100
N	-4.03743000	0.90797400	-1.23638200
H	-4.86492900	0.35584700	-1.02621700
H	-4.22740200	1.36200000	-2.12570700

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N	0.70442200	-0.07889300	0.25537500
H	0.90020800	0.27323900	-0.68046800
C	3.10925400	-0.42552400	0.26373600
C	3.93453800	-1.13455300	-0.60905700
C	3.53943700	0.81603200	0.74332200
C	5.17186800	-0.61971100	-0.99359100
H	3.60603600	-2.10213100	-0.98712400
C	4.77137500	1.33405600	0.35929300
H	2.89661100	1.37393800	1.42307700
C	5.59199700	0.61551800	-0.51033500
H	5.80648800	-1.18604500	-1.67126500
H	5.09703700	2.29870300	0.74197700
H	6.55665500	1.01916700	-0.80875700
C	1.77668100	-0.97862300	0.68531700
H	1.74753400	-1.05513100	1.78108800
H	1.65591700	-1.99918600	0.28509000
C	-2.31207000	2.69079100	-0.45069400
C	-3.49318700	1.71721500	-0.49801100
C	-2.95544900	0.44300700	0.16714600
C	-1.13863300	1.85356700	0.05371400
H	-2.10330000	3.10067300	-1.44427000
H	-2.49874600	3.53888600	0.21589100
H	-3.77665700	1.49129600	-1.53291900
H	-4.39039300	2.07076100	0.01543500
H	-3.05692200	0.56031600	1.26447700
H	-0.98760300	2.00403400	1.13873300
H	-0.19834500	2.10810300	-0.43844800
N	-1.53195500	0.45623400	-0.22178000

C	-3.88378700	-0.71164900	-0.19159500
O	-5.06116600	-0.60572200	0.08003200
O	-3.42328700	-1.79120700	-0.80624500
C	-0.64046900	-0.57414400	0.32183200
C	-0.98671700	-1.04431300	1.72229700
H	-1.99359400	-1.46940200	1.75858300
H	-0.29991600	-1.82805000	2.05038400
H	-0.92936400	-0.20446900	2.42292200
O	-0.79700700	-1.75224100	-0.51693500
H	-0.46208100	-1.51047400	-1.39341200
H	-2.43418000	-1.82226800	-0.81122200

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C	-3.63928300	1.20156800	1.23578200
C	-2.98088800	-0.07939300	1.72590000
C	-2.18863600	-0.53506700	0.50795900
C	-2.51280100	1.82899600	0.43914800
H	-4.49067700	0.96585200	0.58390100
H	-3.99322900	1.84963200	2.04347200
H	-3.68371600	-0.84250000	2.06943200
H	-2.28048200	0.14928900	2.54024300
H	-1.26024000	-1.03411600	0.81806600
H	-1.78934000	2.29433000	1.13417500
H	-2.85436100	2.59232500	-0.26961700
N	-1.90011600	0.69437900	-0.27375100
C	-2.95943700	-1.52691400	-0.36131300
O	-4.07425500	-1.92773700	-0.12007700
O	-2.29516100	-1.96746300	-1.43659000
C	-0.50581800	0.88768400	-0.67272200
C	-0.33426500	2.25284000	-1.31998300
H	0.64529000	2.28675900	-1.80891600
H	-1.11445400	2.42366900	-2.06985800
H	-0.38247300	3.06229200	-0.58518500
N	0.44178500	0.76106300	0.41203900
H	1.08402300	1.54408500	0.42756300
C	2.63630300	-0.38283000	0.45297600
C	3.12163000	-0.11115800	-0.83154100
C	3.54659700	-0.54608400	1.49685000
C	4.48851900	-0.00732400	-1.06282900
H	2.41020300	0.00858900	-1.64840400
C	4.91815000	-0.44342000	1.26800500
H	3.17613300	-0.75556200	2.49987700
C	5.39153200	-0.17299500	-0.01200600
H	4.85455300	0.19733500	-2.06658700
H	5.61632100	-0.57223400	2.09194600
H	6.46075800	-0.09199200	-0.19331000
C	1.15376800	-0.48775800	0.69996400
H	0.98290500	-0.78422300	1.74640400
H	0.74801900	-1.29063100	0.07305900
O	-0.21243700	-0.12042900	-1.66250500
H	-1.43762500	-1.49702600	-1.51514400
H	-0.64070400	0.16218500	-2.48291000

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C	-0.61501300	-0.67845800	0.22229200
N	0.73926100	-0.19660100	0.20068500
H	0.87013400	0.55071300	-0.47468800
C	3.15331900	-0.45140300	0.06964600
C	4.05357000	-0.69182700	-0.96813300
C	3.50532600	0.45773900	1.07276400
C	5.28773600	-0.04395700	-1.00469300
H	3.78725800	-1.39722700	-1.75473800
C	4.73427700	1.10729900	1.03824200
H	2.80184800	0.65184800	1.88074800
C	5.62983400	0.85747100	-0.00151600
H	5.97992600	-0.24296000	-1.81959700
H	4.99727400	1.80959900	1.82607700
H	6.59098800	1.36553500	-0.02800300
C	1.82923700	-1.16412400	0.11950200
H	1.79390500	-1.80063200	1.01462100
H	1.74730500	-1.84184600	-0.74731500
C	-0.88515300	-1.50444500	1.46441900
H	-0.75798300	-0.88368700	2.35575600
H	-1.89590100	-1.92245300	1.45100400
H	-0.19296400	-2.34807000	1.50956400
N	-1.50487800	0.43421900	0.12049200
C	-3.23867300	1.93594500	0.42190400
C	-2.84012700	0.48266800	0.69030300
C	-1.35341500	1.41236000	-0.96006500
H	-4.31651600	2.09211000	0.50888700
H	-2.72770100	2.58125900	1.14628000
H	-2.82957000	0.27406400	1.76852600
H	-0.52361000	2.10475500	-0.74677900
H	-1.14890100	0.93343700	-1.93249400
C	-3.91259700	-0.44348600	0.09209900
O	-5.06400500	-0.36303300	0.46113700
O	-3.55844700	-1.31354900	-0.85060500
O	-0.85567700	-1.62748700	-0.88845600
H	-2.58013200	-1.38464600	-0.97369300
H	-0.43388900	-1.28142900	-1.68633700
C	-2.68827100	2.15673800	-0.98270100
H	-3.36329800	1.70187100	-1.72018000
H	-2.57413300	3.21187300	-1.24685800

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N	-0.43272200	1.03102800	-0.29085400
H	-1.02541500	1.83897800	-0.45759000
H	1.66725900	-0.00005800	1.78631000
C	-2.54257400	-0.05885700	0.21107300
C	-3.60751300	0.27103300	1.04894300
C	-2.81647600	-0.59011600	-1.05337900
C	-4.92444800	0.07060900	0.63768800
H	-3.40247300	0.68596500	2.03518400
C	-4.12834300	-0.79055300	-1.46742200
H	-1.98719600	-0.84458700	-1.71209900
C	-5.18717500	-0.45976100	-0.62163000



H	-5.74484900	0.33117400	1.30248500
H	-4.32742000	-1.20950800	-2.45131400
H	-6.21350300	-0.61738500	-0.94500700
C	-1.12152500	0.14860300	0.65681300
H	-0.61577900	-0.82568200	0.68767800
H	-1.10670900	0.54311100	1.68395400
C	4.01670800	-0.41996000	-0.79373900
C	2.91982600	-1.30541100	-1.37869600
C	1.70424800	-0.88266400	-0.55042500
C	3.30450900	0.90495500	-0.50372600
H	4.39121500	-0.86213000	0.13915400
H	4.87379900	-0.29340000	-1.46148300
H	3.12668900	-2.37576100	-1.30288700
H	2.73107000	-1.05501200	-2.42922300
H	0.76415700	-1.13680100	-1.05797500
H	3.50353600	1.64708300	-1.29101300
H	3.64916300	1.33803800	0.45176900
N	1.88324400	0.55236300	-0.48163300
C	1.72400000	-1.65800800	0.77813300
O	1.69622200	-2.86903000	0.79111100
O	1.80737100	-0.96725500	1.91665400
C	0.90417000	1.48420300	-0.00566000
C	1.10522700	2.85017000	-0.64236000
H	0.98115000	2.77500300	-1.72702200
H	0.37272400	3.55750600	-0.23935900
H	2.10459800	3.24721200	-0.43831500
H	1.69733200	2.31999400	1.64392300
O	1.03430800	1.64466800	1.45430400

**Product**

N	1.54135300	-0.70931400	0.33754800
H	1.43929700	-0.96681400	1.30974700
C	-0.83149500	-0.46577000	-0.27902500
C	-1.94043800	-1.23891000	0.06160600
C	-0.96407300	0.92566600	-0.32907800
C	-3.16497800	-0.63718400	0.34979100
H	-1.84489900	-2.32372100	0.10050500
C	-2.18268300	1.52882400	-0.04059600
H	-0.10148100	1.53314500	-0.60239200
C	-3.28748200	0.74779100	0.30048700
H	-4.02212400	-1.25214600	0.61457900
H	-2.27527000	2.61152300	-0.08673800
H	-4.24115600	1.22024200	0.52421400
C	0.49502300	-1.10809300	-0.58799600
H	0.84664600	-0.81450500	-1.58372100
H	0.39630500	-2.20121600	-0.57959800
C	2.58719200	0.08622500	-0.01996000
C	3.55667900	0.42139000	1.08200500
H	3.29912700	-0.02051800	2.04907600
H	4.55300300	0.07907800	0.78679400
H	3.60575500	1.50928000	1.18712800
O	2.74360700	0.50390200	-1.16322900

**TS3-5a**

C	-0.83219900	2.60386200	-0.16809000
C	-1.80564600	1.42298200	-0.02578400
C	-0.92476100	0.23179800	0.36799500
C	0.55836100	1.99486200	0.00958700
H	-0.92927000	3.07118100	-1.15301300
H	-1.01060500	3.38446900	0.57740400
H	-2.30803800	1.21127000	-0.97672600
H	-2.58816100	1.58297500	0.71933900
H	-0.76835700	0.20882600	1.45852200
H	0.91573900	2.11030200	1.04494800
H	1.31174500	2.41431400	-0.66169500
N	0.38377600	0.55247100	-0.24967500
C	-1.61695000	-1.08658600	0.03279200
O	-2.72708800	-1.26584400	0.48786800
O	-1.03150700	-1.99138300	-0.73270600
H	-0.08076300	-1.76712900	-0.98517500
C	1.56912400	-0.46861400	0.04822100
C	2.88408800	0.27445100	0.12805800
H	2.97203000	0.87857500	1.03895300
H	3.68153700	-0.47570600	0.12211200
H	3.02578000	0.91214400	-0.74857600
N	1.32267500	-1.23496700	1.22145500
H	1.02848000	-2.18226000	1.01140600
H	2.10214700	-1.24925500	1.86690700
O	1.39153100	-1.13044700	-1.15242000
H	0.64698000	-0.05738300	-1.29547400

**TS3-5b**

C	1.40694400	2.10967100	0.94122300
C	2.00663300	1.42914000	-0.28640300
C	1.05148300	0.27614800	-0.60138600
C	-0.08012100	1.91117600	0.72889200
H	1.72294300	1.60053700	1.86154700
H	1.68037800	3.16486300	1.03057200
H	3.01773700	1.04791700	-0.12224000
H	2.03555900	2.12745600	-1.13060100
H	0.70067600	0.33765700	-1.64024000
H	-0.45967700	2.55580900	-0.07533700
H	-0.69934800	2.03600300	1.62111800
N	-0.17566900	0.50648600	0.24902800
C	1.62256300	-1.13640500	-0.39926400
O	2.80548900	-1.30398800	-0.16010800
O	0.76182900	-2.10177200	-0.55334500
H	-0.27529900	-1.74085600	-0.68530500
C	-1.59456200	0.05332100	-0.52534300
C	-2.70059900	0.53922400	0.39471100
H	-2.77892500	1.63175700	0.42527300
H	-3.63975000	0.13381400	0.00434500
H	-2.56442000	0.15940800	1.41246300
N	-1.56997000	0.74953500	-1.77220300
H	-1.59005800	0.08786400	-2.53969400
H	-2.30559300	1.43730600	-1.87897000

O	-1.50617400	-1.26410400	-0.62597300
H	-0.16629000	-0.12328100	1.07043000
O	-0.94124900	-1.60060700	2.11259100
H	-0.36364100	-2.33063600	2.36005000
H	-1.32802700	-1.84765500	1.24890700

**TSIM1-5a**

C	0.90496700	2.62238500	0.08211800
C	1.86657400	1.43233600	0.11604300
C	1.05298600	0.27221300	-0.44617800
C	-0.48409100	2.00465300	-0.10071700
H	0.96498000	3.21133700	1.00187700
H	1.12999200	3.29828000	-0.74874300
H	2.16610400	1.19135700	1.14426000
H	2.78363200	1.58589400	-0.45560100
H	0.96675900	0.37051100	-1.54156500
H	-0.85738500	2.15215500	-1.12254500
H	-1.22663100	2.38666500	0.60478400
N	-0.31123800	0.54156100	0.11355500
C	1.75117900	-1.07113000	-0.20738800
O	2.96389900	-1.09163800	-0.24991600
O	1.04844600	-2.17442300	-0.05656000
H	0.04913600	-2.01383400	0.03857000
C	-1.48571900	-0.33471500	-0.41600600
C	-2.80338500	0.34562500	-0.08611700
H	-2.98024100	1.24669600	-0.68090800
H	-3.59546500	-0.37964500	-0.29707200
H	-2.85516900	0.59130800	0.97898000
N	-1.33581300	-0.47928500	-1.83463600
H	-0.79185800	-1.30803500	-2.06107700
H	-2.24049800	-0.57776500	-2.28299000
O	-1.38255700	-1.52607800	0.27883200
H	-0.35330800	0.23985100	1.28240300
O	-0.77543700	-0.45768700	2.31232900
H	-0.09694900	-0.86897700	2.85804700
H	-1.18361200	-1.19132800	1.40114300

**TS3-5b-H<sub>2</sub>O**

C	0.68724900	2.64313000	0.09551200
C	1.77766000	1.59141500	0.01464700
C	1.01412900	0.36286100	-0.44496800
C	-0.46459000	1.88181700	0.72829900
H	0.97079800	3.52088800	0.68313800
H	0.41379000	2.99033800	-0.91046100
H	2.22054100	1.39793300	1.00022200
H	2.59461000	1.83439100	-0.66983100
H	0.79562400	0.45530800	-1.51941300
H	-1.45938300	2.22159600	0.43620700
H	-0.41526300	1.90356700	1.82328900
N	-0.29249800	0.44457200	0.30352800
C	1.82146000	-0.93347400	-0.28283700
O	2.97288500	-0.90082200	0.08943600
O	1.24968000	-2.05961400	-0.67555500

H	0.25920600	-1.95259100	-0.77064100
C	-1.52886800	-0.21742500	-0.38275900
O	-1.28173600	-1.57637700	-0.33714100
H	-0.25625100	-0.26732800	1.23493600
O	-0.64781700	-1.35908900	1.95288800
H	0.03155400	-1.90506900	2.35984700
H	-1.04627700	-1.73581700	0.76417800
C	-1.70622100	0.25381300	-1.80797400
H	-2.66565400	-0.12122700	-2.17827100
H	-1.71534500	1.34723800	-1.87499300
H	-0.93167500	-0.15081100	-2.46519400
N	-2.65402700	0.19804500	0.41569700
H	-3.50896300	-0.11336300	-0.03526100
H	-2.61064800	-0.24898400	1.33113200

**TS5a-6a**

C	1.36480000	1.93222500	0.61748900
C	1.81722800	1.29353100	-0.69106600
C	0.91297900	0.06654400	-0.77577700
C	-0.15133700	1.74232800	0.60942700
H	1.80735100	1.39049700	1.46363900
H	1.64947800	2.98384300	0.711164700
H	2.87258200	1.01418800	-0.70786500
H	1.61090300	1.95683700	-1.54006900
H	0.82030600	-0.28108500	-1.81333500
H	-0.67666800	2.63162700	0.23451200
H	-0.53770000	1.51818700	1.61424800
N	-0.36299700	0.61191600	-0.30609300
C	1.50044100	-1.09869900	0.05377600
O	2.64226600	-1.44843300	-0.21445600
O	0.77087300	-1.64694600	0.97383300
H	-0.34275500	-1.36946200	1.11000500
C	-1.54254600	-0.06028000	-0.35320300
C	-2.79541300	0.73208700	-0.12218100
H	-2.93174800	1.42710400	-0.95838600
H	-3.65658300	0.06151500	-0.07143500
H	-2.75425200	1.30813200	0.80432900
N	-1.65796200	-1.02035900	-1.33690300
H	-0.86779200	-1.64684200	-1.43436100
H	-2.51620600	-1.55211300	-1.25900300
O	-1.56411000	-1.10779300	1.16004800
H	-1.75935400	-0.60436300	1.96086700

**TS5b-6b**

C	-1.04504000	2.48230200	-0.03025500
C	-1.91610300	1.23815900	0.03096400
C	-0.98319100	0.13661400	0.56494200
C	0.29367400	1.92455400	-0.48170000
H	-1.43280800	3.24695600	-0.70943500
H	-0.93639800	2.93057600	0.96563400
H	-2.24691400	0.96803400	-0.98203000
H	-2.80905000	1.33825600	0.65202200
H	-1.07120500	0.04910000	1.65747800

H	1.12972500	2.57041800	-0.19122400
H	0.32110200	1.77744100	-1.57645500
N	0.35834500	0.64228400	0.21882500
C	-1.46418400	-1.19409400	-0.03376400
O	-2.50386300	-1.63990300	0.43663100
O	-0.82332200	-1.71831300	-1.02726000
H	0.29769000	-1.43651700	-1.17732900
C	1.49691300	-0.08876400	0.31060600
O	1.50223600	-1.17874600	-1.18505400
H	1.70405700	-0.62077100	-1.94717900
C	1.52885100	-1.19742200	1.32061500
H	1.47498400	-0.75856900	2.32289400
H	0.70217900	-1.89828100	1.19420300
H	2.45982300	-1.76027600	1.22367700
N	2.68569300	0.60926400	0.21069800
H	3.49676000	0.00398400	0.18926700
H	2.73585400	1.31641000	-0.51116400

#### TS6a-6c

C	1.38282400	1.84820700	0.74030800
C	1.85016100	1.33840200	-0.61908800
C	0.86894200	0.21943600	-0.91801800
C	-0.13413400	1.83953000	0.61403000
H	1.69721500	1.14465800	1.52116700
H	1.76994800	2.83910200	0.99362100
H	2.87708100	0.96666700	-0.60781500
H	1.76087500	2.12615600	-1.37845200
H	0.68790500	0.07456300	-1.99311100
H	-0.50723900	2.77799900	0.17768200
H	-0.64421100	1.66410800	1.56768500
N	-0.38613200	0.72226900	-0.30906100
C	1.27434500	-1.14987800	-0.32101200
O	2.35241000	-1.28848500	0.24135800
O	0.38006600	-2.07568000	-0.47152100
H	-0.41721600	-1.88005000	1.33293600
C	-1.58747400	0.19712700	-0.54519700
C	-2.79059000	0.88586200	0.00073600
H	-2.75650900	1.96668800	-0.16405200
H	-3.70038900	0.48446500	-0.45076100
H	-2.83739800	0.70533100	1.08168600
N	-1.66175200	-0.92832000	-1.22308700
H	-0.70655200	-1.60887000	-1.01952800
H	-2.59395100	-1.29490300	-1.36622900
O	-0.85877300	-1.37414600	2.03780800
H	-0.46843700	-1.68917400	2.85848800

#### TS6d-6b

C	1.37848600	1.91205900	0.38129000
C	1.97188000	1.04231800	-0.72260800
C	0.97733100	-0.11171700	-0.79877100
C	-0.12560600	1.83871400	0.13852300
H	1.62020800	1.48272100	1.36227400
H	1.74543600	2.94214700	0.36888100

H	2.98333500	0.68640300	-0.51241400
H	1.98439700	1.58304800	-1.67779600
H	1.00712200	-0.61493300	-1.77108200
H	-0.48784300	2.64475000	-0.51399500
H	-0.70144800	1.87478000	1.06511400
N	-0.30557500	0.56062800	-0.58308900
C	1.27218300	-1.18190600	0.28596300
O	2.30580000	-1.82577300	0.12137200
O	0.44871100	-1.32363800	1.25927300
C	-1.49158600	-0.00444200	-0.81720300
C	-1.57720900	-1.10286000	-1.82494300
H	-2.62113900	-1.32246800	-2.06015200
H	-1.04416400	-0.85579700	-2.74777600
H	-1.12911700	-2.01402000	-1.40845200
N	-2.52458500	0.38562400	-0.09258800
H	-0.59193900	-0.69705100	1.66731200
H	-3.39173000	-0.06860700	-0.35880300
O	-1.55571300	-0.24552300	2.06095300
H	-2.17274000	0.24739200	1.08575400
H	-1.41251500	0.29435300	2.84458800

#### TSIM2

C	0.73986100	2.13626600	0.37960900
C	1.26100000	1.39081000	-0.84391800
C	0.66383000	-0.00235700	-0.65668800
C	-0.69835500	1.65001800	0.47587900
H	1.30316300	1.83372600	1.27368500
H	0.80671700	3.22439400	0.29355600
H	2.35017600	1.35777100	-0.92202900
H	0.86034500	1.83817500	-1.76203100
H	0.47967700	-0.52634700	-1.60461300
H	-1.35042200	2.23968200	-0.18820700
H	-1.10469000	1.70967900	1.49209900
N	-0.61218700	0.25724200	0.01557900
C	1.60903300	-0.90238600	0.13953900
O	2.78638800	-0.98404800	-0.11995800
O	1.07661200	-1.60544600	1.14291600
C	-1.70743600	-0.54713400	-0.22043100
C	-3.02577100	-0.00634900	0.25331200
H	-3.27116800	0.93683200	-0.24828900
H	-3.82345300	-0.72415700	0.04981400
H	-3.00769600	0.19306300	1.33095300
N	-1.51822100	-1.69128100	-0.77954500
H	0.11639400	-1.45792700	1.16386000
H	-2.40316300	-2.18387900	-0.87851300

#### TS6c-6d

C	0.84902100	2.01428400	0.70118200
C	1.21101200	1.45036900	-0.66736300
C	0.57981100	0.05491300	-0.63012300
C	-0.58403500	1.53989800	0.86255700
H	1.49237900	1.58566400	1.48243100
H	0.93426200	3.10352300	0.75773300

H	2.28368700	1.41064400	-0.87729500
H	0.72459700	2.03880700	-1.45500500
H	0.24823800	-0.26148800	-1.62717900
H	-1.26257300	2.16835500	0.26670900
H	-0.93530400	1.52619400	1.90068700
N	-0.56198000	0.16081400	0.31178500
C	1.57368100	-0.99484400	-0.13640200
O	2.57588900	-1.28295900	-0.74895900
O	1.25024300	-1.56224000	1.02538700
C	-1.82576000	-0.26994300	-0.23831900
C	-2.39833700	-1.47098100	0.44100000
H	-2.51074000	-1.27241300	1.51404100
H	-3.36595500	-1.76214400	0.02306400
H	-1.70215900	-2.31516600	0.34954600
N	-2.31618500	0.37535700	-1.21468400
H	0.40373500	-1.12207100	1.28796200
H	-3.20441700	-0.03369000	-1.50901200

### TS6a-7

N	-0.36151900	0.82846300	0.06730000
H	-0.12164000	-0.17707100	-0.09410600
H	-0.47888200	0.99825600	1.06615600
C	-2.77515500	0.37871500	-0.20733300
C	-2.77136800	-1.01295100	-0.35347200
C	-3.88016300	1.00407500	0.36943300
C	-3.86257200	-1.76172600	0.07352900
H	-1.90472500	-1.50811400	-0.79518100
C	-4.97536300	0.25309900	0.79322200
H	-3.88652500	2.08791100	0.48246400
C	-4.96687900	-1.13051300	0.64607200
H	-3.85183400	-2.84262800	-0.04288600
H	-5.83320300	0.75055200	1.23973600
H	-5.81982200	-1.71894700	0.97574300
C	-1.58778800	1.18230200	-0.66373700
H	-1.78296700	2.25622800	-0.54620600
H	-1.38816200	0.98956300	-1.72631600
C	3.16928600	-0.43246300	1.96107000
C	3.88340500	-0.80661900	0.66820100
C	2.81729200	-0.53627500	-0.38443300
C	2.43130700	0.84639200	1.58381200
H	2.44744700	-1.21944300	2.22035100
H	3.83768100	-0.29154600	2.81562000
H	4.21414400	-1.84652400	0.63120600
H	4.74891200	-0.14949200	0.50835700
H	3.26925000	-0.29428800	-1.35755700
H	3.05484700	1.73695400	1.76300900
H	1.50385900	0.97172700	2.16202800
N	2.16942900	0.67916300	0.15239100
C	1.87006900	-1.74711600	-0.63296300
O	2.39103900	-2.86872300	-0.62234000
O	0.65562500	-1.46356600	-0.89451300
C	1.26404200	1.45459700	-0.52388300
C	1.19364300	2.90513400	-0.12299600

H	2.13455300	3.39320300	-0.39962800
H	0.37275100	3.41153700	-0.64144200
H	1.04552300	3.02512000	0.95335100
N	1.25619000	1.25282000	-1.89826600
H	1.08340800	0.28132900	-2.15574900
H	0.67483400	1.90094800	-2.41323900

**TS6a-8**

C	2.63389900	-0.12550800	2.47003900
C	2.76291100	1.12784500	1.61334600
C	1.69819900	0.90504000	0.56400100
C	2.35487200	-1.24318900	1.46200700
H	3.51865400	-0.34037300	3.07695400
H	1.78282400	-0.01946900	3.15594800
H	3.74202200	1.19278900	1.12281300
H	2.60301100	2.05598400	2.16983800
H	0.70478800	1.02538400	1.04230200
H	1.62050600	-1.96288100	1.85312300
H	3.27047700	-1.80016900	1.22004800
N	1.87169500	-0.54104600	0.25971600
C	1.67319100	1.86592100	-0.64487500
O	2.58179000	2.69699800	-0.75109600
O	0.67230400	1.69803700	-1.41495000
C	1.56065300	-1.20452000	-0.89504500
C	1.64047600	-2.70500000	-0.83552400
H	1.25730200	-3.13469200	-1.76572400
H	2.68648900	-3.01148400	-0.72765500
H	1.06920600	-3.11698500	-0.00054600
N	2.00499100	-0.69693800	-2.10347000
H	1.82050200	0.29403600	-2.25456700
H	1.74450200	-1.25545800	-2.90702200
N	-0.33026000	-0.91405600	-1.02949000
H	-0.24744600	0.10770800	-1.20851800
H	-0.72853100	-1.35084200	-1.86070700
C	-2.45428500	-0.46914900	0.19375200
C	-2.50121000	0.91686900	0.00797900
C	-3.64118200	-1.16522000	0.42259700
C	-3.71814900	1.58875500	0.05263600
H	-1.58352700	1.47572100	-0.18674200
C	-4.86016300	-0.49125300	0.47208500
H	-3.61164400	-2.24531900	0.56351200
C	-4.90008200	0.88727400	0.28721900
H	-3.74297700	2.66552600	-0.09594000
H	-5.77843600	-1.04577200	0.65101500
H	-5.84990300	1.41549200	0.32219800
C	-1.13520700	-1.19706800	0.16413900
H	-1.29788300	-2.27990900	0.23357900
H	-0.52120200	-0.91006500	1.03104100

**TS6a-9**

C	2.68973300	0.13537600	2.20343700
C	3.63663100	-0.42899000	1.14866100
C	2.80054200	-0.45654600	-0.12605700



C	1.96112500	1.22559500	1.43555200
H	1.98248000	-0.64466300	2.51207000
H	3.20119600	0.51720500	3.09265600
H	4.00415300	-1.42776900	1.39638900
H	4.49486500	0.24459800	1.01716300
H	3.41926400	-0.23558200	-1.01079200
H	2.54991600	2.16160700	1.42786100
H	0.97091500	1.46264100	1.85893100
N	1.83855300	0.64906900	0.10266300
C	2.04870300	-1.79106300	-0.38414000
O	2.00433200	-2.63602100	0.52000900
O	1.49781100	-1.86314100	-1.53080500
C	1.04330500	1.26753700	-0.86623400
C	1.18449400	2.77575500	-0.95301100
H	0.52924800	3.18595600	-1.72959900
H	0.92934300	3.25050500	-0.00050100
H	2.22276500	3.02843600	-1.19502000
N	1.12442700	0.66983300	-2.21928700
H	1.36793400	-0.36588600	-2.15312800
H	1.70414500	1.17879000	-2.88159400
N	-0.49275700	0.97537000	-0.75354400
H	-1.02907300	1.78360700	-0.43519600
H	-0.15805500	0.78073400	-2.01268100
C	-2.38523100	-0.24746100	0.16384600
C	-2.96021300	0.41177900	1.25338100
C	-3.21664700	-0.86799500	-0.77013400
C	-4.34324000	0.45552500	1.40543600
H	-2.31382300	0.88232100	1.99590200
C	-4.59989200	-0.83019000	-0.61849900
H	-2.77083000	-1.39223100	-1.61446400
C	-5.16537500	-0.16607500	0.46791200
H	-4.77978200	0.96524900	2.26116200
H	-5.23792100	-1.32449500	-1.34717400
H	-6.24566400	-0.13972000	0.58849200
C	-0.89690800	-0.24691800	-0.01825400
H	-0.55679800	-1.11780800	-0.59263500
H	-0.37515600	-0.27809200	0.94832100

#### TS6a-10

C	-2.67884200	0.13178400	2.27190900
C	-1.98795300	-1.12738900	1.76065400
C	-1.82942100	-0.85358200	0.27198300
C	-1.97835700	1.24074500	1.50046200
H	-3.74261800	0.10246000	2.00319800
H	-2.60357100	0.26439400	3.35537600
H	-2.56263300	-2.03983100	1.93344000
H	-1.00146100	-1.23689600	2.23353600
H	-0.92911700	-1.34286200	-0.13667300
H	-1.05111500	1.55076200	2.01662000
H	-2.60772600	2.13183400	1.38442700
N	-1.70146500	0.61955300	0.20526700
C	-3.02162700	-1.35476900	-0.57918800
O	-3.88330800	-2.07004800	-0.07900300

O	-2.99489700	-0.97994500	-1.81659700
C	-0.98194200	1.26926700	-0.80294200
C	-1.23113400	2.75850200	-0.85931400
H	-0.67918400	3.20157200	-1.69597700
H	-2.29933100	2.94296000	-1.01511300
H	-0.91960900	3.26227100	0.06254700
N	-1.05384400	0.54607000	-2.05977300
H	-2.05560100	-0.25900200	-2.02373800
H	-1.12659700	1.18954400	-2.84514700
N	0.63380700	1.02806400	-0.66687200
H	0.27414600	0.34700900	-1.61710900
H	1.13411400	1.83162400	-1.05315800
C	2.63934400	0.04798300	0.34123300
C	2.78822700	-1.15615000	-0.35287900
C	3.77704600	0.72862900	0.77382700
C	4.05349900	-1.67005900	-0.61039900
H	1.90191400	-1.69387300	-0.69098800
C	5.04760300	0.21480300	0.51829200
H	3.66757600	1.66564800	1.31904000
C	5.18704700	-0.98336500	-0.17478300
H	4.15775600	-2.60966200	-1.14750000
H	5.92798000	0.75278600	0.86170700
H	6.17717800	-1.38647600	-0.37318200
C	1.26455800	0.60080300	0.59278000
H	1.31042000	1.44687300	1.29286000
H	0.61536700	-0.16020200	1.04046600

#### TS6a-11

C	-1.46700000	1.22628600	-0.79173700
N	-1.75290000	2.10277900	0.25615900
H	-2.40944300	2.83007400	-0.00363800
N	0.41348000	1.05629700	-0.69383800
H	0.77179900	0.71988900	-1.58890900
H	0.78049300	2.00387400	-0.53901100
C	2.29257100	-0.26539200	0.19856400
C	2.58879800	-1.56924100	-0.20105900
C	3.33814600	0.64424900	0.38346900
C	3.90887000	-1.96113100	-0.41382900
H	1.77717100	-2.28550300	-0.32814500
C	4.65653700	0.25605000	0.17069600
H	3.11036000	1.66230300	0.70089200
C	4.94372800	-1.04887400	-0.22929500
H	4.12877400	-2.98224600	-0.71625200
H	5.46276600	0.96981000	0.32294400
H	5.97488200	-1.35399900	-0.39070800
C	0.86635900	0.16047500	0.39107200
H	0.71514100	0.69222800	1.33781200
H	0.20318400	-0.71334600	0.41238000
O	0.68574700	3.63110200	0.54460600
H	1.06481000	3.88615100	1.39173800
H	-0.20787900	3.28132200	0.73060100
C	-1.53577700	1.87903500	-2.14988700
H	-0.99796700	2.83301100	-2.14117100

H	-1.12332400	1.24940100	-2.94196000
H	-2.58902000	2.07082400	-2.39030100
N	-1.93381400	-0.05098100	-0.68202900
C	-2.15544000	-2.35235800	-1.07949200
C	-3.26480700	-1.90140200	-0.13623000
C	-2.75933400	-0.58425300	0.43778400
C	-1.71230600	-1.04987500	-1.72881000
H	-1.33603400	-2.78487600	-0.49379700
H	-2.48240700	-3.09086500	-1.81797300
H	-3.46260700	-2.62523600	0.65790400
H	-4.19314600	-1.72998000	-0.69879900
H	-3.58265800	0.11963900	0.62282400
H	-2.31685600	-0.82267300	-2.62189000
H	-0.65528300	-1.06924600	-2.03716400
C	-1.92701100	-0.71276500	1.74886600
O	-1.45117200	-1.82680100	2.02697600
O	-1.78556900	0.37422300	2.37964000
H	-1.95218300	1.62976800	1.16012600

#### TS11-12

C	-0.97180300	1.19958000	-0.72904200
N	-1.33626700	2.06718600	0.36142700
H	-2.15389000	2.60769500	0.08428400
N	0.56954000	0.98984500	-0.56701400
H	0.95725800	0.63580200	-1.44392500
H	0.93974500	1.99701000	-0.35599200
C	2.41030200	-0.34569700	0.35826500
C	2.67410200	-1.66554000	-0.01214200
C	3.47519800	0.54569000	0.51926300
C	3.98411300	-2.09291100	-0.21556800
H	1.84603100	-2.36489500	-0.12716700
C	4.78353900	0.12129200	0.31339600
H	3.27163400	1.57621000	0.81089900
C	5.03916900	-1.19946700	-0.05338300
H	4.18043500	-3.12513000	-0.49509900
H	5.60592300	0.82011200	0.44497900
H	6.06258700	-1.53242800	-0.20817400
C	0.99705600	0.11062000	0.56065600
H	0.88427700	0.70063700	1.47690900
H	0.30195400	-0.73431800	0.61258300
O	0.75430900	3.39390400	0.24269600
H	1.20436100	3.67930400	1.04256700
H	-0.40217500	2.84838800	0.45778200
C	-1.13309000	1.86817000	-2.08998200
H	-0.63324900	2.84274200	-2.08731500
H	-0.73123100	1.26709700	-2.91402800
H	-2.20305000	2.02164100	-2.27752000
N	-1.59191600	-0.08917100	-0.62377900
C	-2.31055100	-2.22167800	-1.20325600
C	-3.50770800	-1.46607100	-0.63771800
C	-2.87052600	-0.28465600	0.08617300
C	-1.43109200	-1.08001000	-1.68119400
H	-1.80506800	-2.77731500	-0.40117500

H	-2.57014400	-2.92319000	-2.00159100
H	-4.12795300	-2.06248400	0.03507000
H	-4.13458600	-1.09566300	-1.45974800
H	-3.50998800	0.61091800	0.01795200
H	-1.78550200	-0.71562800	-2.66314700
H	-0.37439600	-1.37174300	-1.79477900
C	-2.62007400	-0.56108700	1.58070000
O	-2.99555700	-1.58297300	2.12559000
O	-1.97417500	0.38856700	2.22191100
H	-1.70088400	1.15483100	1.55363400

**TS6c-13**

C	2.35045900	2.30828400	-0.97336800
C	1.93135700	1.12611100	-1.84202200
C	2.03307500	-0.04525700	-0.87625600
C	1.70597100	2.01051400	0.37799500
H	3.44337100	2.32415800	-0.87728300
H	2.03842300	3.27770200	-1.37325000
H	2.56688500	0.98558400	-2.71874200
H	0.89170600	1.23675700	-2.17811500
H	1.37727900	-0.88572400	-1.15610600
H	0.71938500	2.49502600	0.45320000
H	2.31550900	2.37851500	1.21427300
N	1.59529500	0.54812500	0.39883500
C	3.47281800	-0.59102200	-0.81070700
O	4.27934400	-0.39526600	-1.69749800
O	3.78297500	-1.30396600	0.25966200
C	0.98041500	-0.17471400	1.42262300
C	0.97982100	0.55120400	2.74971400
H	0.47998400	-0.05735400	3.51080600
H	2.01600000	0.70998300	3.06670500
H	0.47913400	1.52381700	2.70169700
N	1.42838800	-1.51278500	1.48557000
H	2.97227500	-1.44026900	0.84981500
H	1.25322300	-1.90736000	2.40506700
N	-0.70241800	-0.33439600	1.05576200
H	-0.70962800	-1.23240900	0.48119300
H	-1.20091600	-0.52485600	1.92735000
C	-2.78619500	0.37677300	-0.06151400
C	-3.03121900	-0.73925300	-0.86937600
C	-3.86077000	1.14238700	0.39058900
C	-4.33478600	-1.08005400	-1.21298100
H	-2.19217000	-1.34432000	-1.21842000
C	-5.16683200	0.80306400	0.04160700
H	-3.67472200	2.01478000	1.01632600
C	-5.40517600	-0.30943100	-0.75958000
H	-4.51742400	-1.94861700	-1.84115800
H	-5.99698100	1.40874200	0.39724400
H	-6.42338300	-0.57654600	-1.03211100
C	-1.37556100	0.74486500	0.30724700
H	-1.36259700	1.66494400	0.90406300
H	-0.76987500	0.91654600	-0.59167000
O	-0.00152600	-2.44533900	-0.32481800

H	-0.26204300	-3.36813500	-0.37872600
H	0.86111600	-2.14182600	0.65407100

#### TS6d-14

C	-2.68473200	1.12798500	1.65683000
C	-3.10030700	1.23346900	0.19428900
C	-1.80794800	0.80477700	-0.50562200
C	-1.83000400	-0.13747200	1.68968800
H	-2.09895500	2.01114300	1.94655100
H	-3.53246300	1.06301700	2.34568600
H	-3.43646600	2.22859500	-0.11120800
H	-3.89604800	0.51413000	-0.03843400
H	-1.97740500	0.48219700	-1.53971800
H	-2.43965800	-1.02290200	1.91012100
H	-1.04085700	-0.10683600	2.45076900
N	-1.23865900	-0.26439300	0.32684900
C	-0.87612600	2.01657600	-0.59051300
O	-1.14651800	2.99085400	-1.25646300
O	0.23656700	1.94564400	0.13686100
C	-1.25600300	-1.65196800	-0.16289800
C	-2.51411400	-2.02146200	-0.93862200
H	-2.44201900	-3.05651500	-1.29221400
H	-3.37493200	-1.96634000	-0.26111800
H	-2.72026600	-1.38027000	-1.80331600
N	-0.82731400	-2.58270800	0.79813100
H	0.27234300	1.03924900	0.51906700
H	-1.50212100	-3.33896300	0.88794900
N	0.02127100	-1.85999900	-1.15731800
H	0.21438600	-2.59775700	-0.27168600
H	-0.30250600	-2.40741600	-1.95494400
C	2.03885500	-0.45731000	-0.61207000
C	2.02222100	-0.85203600	0.72692200
C	3.07224200	0.36963000	-1.06410400
C	3.02320700	-0.41327800	1.59556800
H	1.22396700	-1.48994100	1.10830900
C	4.06444500	0.80751500	-0.19659600
H	3.08678200	0.68595500	-2.10724100
C	4.04157000	0.41739000	1.14190100
H	2.99768300	-0.72640700	2.63685600
H	4.85520100	1.45740400	-0.56370800
H	4.81447400	0.76101400	1.82518000
C	0.97503900	-0.83379900	-1.61096000
H	1.45905500	-1.21461300	-2.51935400
H	0.42226300	0.06287500	-1.92723800

#### TS6d-15

C	-2.76024900	-0.29980500	2.33753600
C	-2.29332000	-1.46186500	1.46794900
C	-2.14399800	-0.80948800	0.08412600
C	-1.91878600	0.85140200	1.81574700
H	-3.82869800	-0.10211800	2.17414800
H	-2.61331400	-0.47599000	3.40706400
H	-2.96772900	-2.32315300	1.44784600

H	-1.31187600	-1.81669000	1.81059000
H	-1.33310700	-1.27948600	-0.49287400
H	-0.90688500	0.81551200	2.25084300
H	-2.32266300	1.84559400	2.01970000
N	-1.88870400	0.60788200	0.35937900
C	-3.42103300	-1.00766200	-0.73028000
O	-3.73367100	-2.07746400	-1.19919200
O	-4.18242700	0.07950900	-0.85465900
C	-0.91320800	1.30581600	-0.42139800
C	-1.16890100	1.19756100	-1.90591700
H	-2.08752100	1.74716600	-2.14049100
H	-0.35538900	1.66059200	-2.47121400
H	-1.28744800	0.16705200	-2.26098500
N	-0.54372700	2.52940800	0.12735200
H	-3.68195000	0.80773700	-0.42026300
H	-0.31849300	3.18335000	-0.62037600
N	0.60468500	0.54548400	-0.04894700
H	0.55828000	1.64753400	0.43770100
H	0.57142900	-0.29140300	0.54048300
C	2.94070800	-0.02247100	-0.53542300
C	3.67334200	0.87030900	0.25240200
C	3.44770000	-1.30264000	-0.75961600
C	4.89014100	0.48817700	0.80561600
H	3.28024300	1.87171900	0.42997800
C	4.66787100	-1.68826600	-0.20747300
H	2.88340100	-2.00128600	-1.37674700
C	5.39016300	-0.79385300	0.57699600
H	5.45352100	1.19169700	1.41409200
H	5.05429800	-2.68785300	-0.39217800
H	6.34285500	-1.09224700	1.00785400
C	1.61222500	0.39110900	-1.10359500
H	1.27488900	-0.33954100	-1.85361700
H	1.70321600	1.36609600	-1.60524100

#### TS6d-16

C	3.71445800	-0.40341700	-1.46662600
C	2.70253900	-1.54175300	-1.47230200
C	1.73557100	-1.10241200	-0.36974600
C	2.83056600	0.82297300	-1.30117700
H	4.39984100	-0.50769000	-0.61382200
H	4.32216100	-0.35659300	-2.37498200
H	3.12374000	-2.53372500	-1.28599300
H	2.16423900	-1.56918100	-2.42924900
H	0.73914200	-1.54017100	-0.52663500
H	2.42540600	1.14416100	-2.27346700
H	3.34275400	1.68478900	-0.86373300
N	1.73862700	0.36451900	-0.40974400
C	2.22121300	-1.60542800	0.99462600
O	2.27882800	-2.78252800	1.26904200
O	2.57451200	-0.65108300	1.85329000
C	0.48220100	1.09696800	-0.56582600
C	-0.38384900	0.60895000	-1.71313800
H	-1.26716900	1.24242900	-1.83999500

H	0.20580200	0.67522900	-2.63500800
H	-0.72850500	-0.42457300	-1.59579500
N	0.73733200	2.44916300	-0.54223200
H	2.42115300	0.20944000	1.38959200
H	-0.01696600	2.98755000	-0.95408800
N	-0.27939600	0.69703000	0.86199000
H	-0.25262900	-0.30471600	1.05633400
H	0.35184300	1.22347700	1.54039600
C	-2.71913400	0.30493300	0.48701400
C	-2.78718800	-1.03924300	0.86540700
C	-3.66365500	0.79953800	-0.41234900
C	-3.76157600	-1.87790700	0.33260600
H	-2.08354500	-1.44148000	1.59583900
C	-4.64754600	-0.03370400	-0.93860700
H	-3.62407500	1.84760800	-0.70784000
C	-4.69302000	-1.37639800	-0.57399000
H	-3.79787500	-2.92208500	0.63306600
H	-5.37540600	0.36615800	-1.64047900
H	-5.45533000	-2.03037400	-0.98990100
C	-1.65869900	1.20768300	1.05153400
H	-1.79971100	1.35123900	2.13019100
H	-1.69407300	2.20671700	0.59980000
O	1.13944500	2.60909000	1.88168200
H	1.05803200	2.72680400	0.60863800
H	1.99167100	2.82147900	2.27036200

#### TS6d-17

C	-2.84835800	1.00771400	2.05041000
C	-2.42126300	-0.45513700	2.07457500
C	-2.25671600	-0.78272100	0.58379600
C	-1.96058900	1.58322100	0.96141500
H	-3.90854100	1.09472600	1.77563400
H	-2.71007900	1.51126200	3.01132700
H	-3.12257000	-1.13285300	2.57010100
H	-1.44719900	-0.55321900	2.57286200
H	-1.49808800	-1.56422700	0.43509000
H	-0.95637100	1.80464400	1.35507500
H	-2.34240100	2.49958300	0.50116300
N	-1.91417800	0.49767500	-0.04144600
C	-3.55902300	-1.35293900	0.01924800
O	-3.94634600	-2.46673800	0.28425900
O	-4.24978000	-0.51953300	-0.75872000
C	-0.96537000	0.56613500	-1.10614000
C	-1.18312800	-0.49950400	-2.15705000
H	-2.15352200	-0.32963000	-2.63509500
H	-0.41606600	-0.42912200	-2.93342100
H	-1.17064100	-1.51906900	-1.75674400
N	-0.78126900	1.84541900	-1.57806200
H	-3.70162900	0.29384200	-0.84036600
H	-0.42921800	1.82895000	-2.53023500
N	0.55214200	0.12021700	-0.32189700
H	0.79206500	1.04123200	0.13971200
H	0.42942900	-0.60458500	0.38739900

C	2.96649300	-0.40141700	-0.44726100
C	3.56747800	0.69952900	0.17334100
C	3.56273100	-1.65887400	-0.34202100
C	4.74902800	0.53428300	0.88777500
H	3.08577400	1.67665800	0.09634100
C	4.74803900	-1.82168000	0.37247800
H	3.09959300	-2.51659100	-0.82968600
C	5.34196400	-0.72437300	0.98904800
H	5.21368700	1.39316300	1.36680400
H	5.20604200	-2.80529100	0.44601700
H	6.26763800	-0.84770700	1.54637700
C	1.68231700	-0.23026000	-1.21046100
H	1.43888500	-1.15172700	-1.75171600
H	1.76408300	0.58746200	-1.93806100
O	0.97599100	2.71123700	-0.04584800
H	0.81348800	3.44935800	0.54735000
H	-0.03177200	2.44636700	-0.87853400

#### TS6b-18

N	0.42263500	-0.75662300	-0.73239000
H	0.94556600	-1.03957000	-1.56194700
H	0.14089500	0.24978500	-0.79924000
C	2.59699800	-0.27786300	0.33663400
C	3.76125600	-1.04537500	0.35842000
C	2.69097000	1.10845200	0.16575100
C	5.00929100	-0.44125700	0.21374700
H	3.69157200	-2.12458100	0.49394000
C	3.93597700	1.70985300	0.01940500
H	1.78061100	1.70979500	0.14274300
C	5.09704700	0.93721200	0.04336500
H	5.91124500	-1.04868700	0.23331200
H	4.00152900	2.78723000	-0.11194100
H	6.06931700	1.41093100	-0.07083600
C	1.24259100	-0.91838100	0.47473800
H	0.68538500	-0.44357900	1.29372700
H	1.34645100	-1.98804400	0.70722300
C	-2.81736700	0.39810600	2.07854900
C	-3.67979300	0.80322100	0.88956500
C	-2.76015700	0.52743900	-0.30098900
C	-2.17050900	-0.89111000	1.59427400
H	-2.04567300	1.15868900	2.25563800
H	-3.37995400	0.25676100	3.00605700
H	-4.00136000	1.84715400	0.90337500
H	-4.57170500	0.16402900	0.83592600
H	-3.34888100	0.30327100	-1.19961200
H	-2.81687200	-1.76074400	1.79665800
H	-1.19638800	-1.07128300	2.06972300
N	-2.04425500	-0.68433500	0.14709200
C	-1.88814100	1.77536000	-0.62346800
O	-2.54027400	2.75263800	-1.02234200
O	-0.63633500	1.69468100	-0.45305500
C	-1.33394700	-1.51064200	-0.65957300
C	-1.62575800	-1.44442700	-2.13421200



H	-1.49917700	-0.43486200	-2.53309400
H	-0.96398000	-2.12176100	-2.68267700
H	-2.65948100	-1.76391600	-2.30520200
N	-1.16362400	-2.80865700	-0.19220300
H	-0.55545800	-3.38388500	-0.76105100
H	-0.97481600	-2.92150600	0.79571800

**TS7-19**

N	-0.43817700	-0.65353700	0.09252700
H	0.67834700	1.19597400	-0.33630300
H	-0.44532100	-0.97386500	-0.87542700
C	-2.86051100	-0.35879200	0.21056700
C	-2.85928900	1.03768500	0.13553500
C	-3.99260200	-1.05573200	-0.21068600
C	-3.97084600	1.72035000	-0.34543700
H	-1.97145400	1.58515600	0.45174000
C	-5.10924700	-0.37441400	-0.69391300
H	-3.99972200	-2.14432100	-0.16059900
C	-5.10049000	1.01514700	-0.76195800
H	-3.95728600	2.80663600	-0.39695300
H	-5.98411500	-0.93227100	-1.02034100
H	-5.96893900	1.54948300	-1.14014000
C	-1.66270900	-1.08794600	0.75777300
H	-1.83394200	-2.17699300	0.68770200
H	-1.55531400	-0.85751700	1.82861100
C	3.68420800	-0.99934000	-1.63557100
C	3.79929300	0.42155700	-1.10446100
C	2.88166500	0.40320400	0.12848800
C	2.20300900	-1.29657500	-1.44589500
H	4.01603400	-1.10436100	-2.67338500
H	4.28003600	-1.68172800	-1.01382400
H	3.40740900	1.13134100	-1.84814700
H	4.81524000	0.73361500	-0.84749500
H	3.44537600	0.12732400	1.03306100
H	2.01083100	-2.37157500	-1.34516400
H	1.62099500	-0.94101200	-2.31596600
N	1.86258900	-0.56304200	-0.22916100
C	2.34719300	1.80576000	0.36505900
O	3.02558100	2.68487900	0.84672800
O	1.09413400	2.04039800	-0.04580400
C	0.85080900	-1.02977300	0.71859800
C	0.97487600	-2.52658800	1.00488200
H	1.98276500	-2.75653000	1.37053000
H	0.24898400	-2.83352400	1.76673700
H	0.77894800	-3.12843300	0.11231300
N	1.01727100	-0.31554300	1.96531500
H	0.45974200	0.53298100	2.00130700
H	0.80972400	-0.88497600	2.77571000

**TS19-20**

N	-0.66187700	-0.17567400	0.19025600
H	1.75482400	1.60442200	-0.85042300
H	-0.68136600	-0.47225400	-0.78060700

C	-3.10405900	-0.18010300	0.28411100
C	-3.28019500	1.18590900	0.04258100
C	-4.14485400	-1.05684500	-0.02207300
C	-4.47538600	1.66228000	-0.48514200
H	-2.46553700	1.87191400	0.26910900
C	-5.34477100	-0.58302300	-0.55057400
H	-4.01499100	-2.12383800	0.15747500
C	-5.51282600	0.77863000	-0.78255900
H	-4.60030000	2.72789100	-0.66455200
H	-6.14634900	-1.28029200	-0.78351300
H	-6.44713700	1.15241400	-1.19504000
C	-1.82770200	-0.69273300	0.89634500
H	-1.86678000	-1.79637100	0.93570600
H	-1.77135300	-0.35439000	1.94294800
C	2.97171000	-1.98604100	-1.18329000
C	3.90943000	-0.85694600	-0.79050000
C	3.03483200	0.02131000	0.12573800
C	1.65526700	-1.24467100	-1.35069700
H	3.28534900	-2.50863800	-2.09276300
H	2.89375500	-2.72609900	-0.37526500
H	4.20680300	-0.28728100	-1.68238600
H	4.82505200	-1.17375300	-0.28455500
H	3.20941600	-0.24391600	1.17828100
H	0.77954500	-1.89851500	-1.28844800
H	1.61970000	-0.74794700	-2.33175400
N	1.63816500	-0.21324400	-0.28396100
C	3.42932900	1.48033900	-0.06112600
O	4.49172700	1.92495000	0.30785300
O	2.52348400	2.21278800	-0.70953100
C	0.65074500	-0.41454900	0.79962600
C	0.78483900	-1.79975900	1.44130700
H	1.79613400	-1.92729500	1.84331900
H	0.09684500	-1.89077400	2.28722800
H	0.57410900	-2.61305900	0.73582300
N	0.85163800	0.57785000	1.86819300
H	1.56256100	1.26227300	1.63392600
H	-0.00560600	1.11828600	1.95501200

#### TS20-21

N	-0.68513600	-0.31102300	0.04463600
H	2.79947000	-0.29194800	1.62467200
H	-0.85289300	0.33705100	-0.72412600
C	-3.10348700	-0.51166300	0.08848500
C	-3.38331600	0.44390600	1.07137300
C	-4.05867100	-0.76080300	-0.89695000
C	-4.59406200	1.12772300	1.07073500
H	-2.63688600	0.64510200	1.83856200
C	-5.27487800	-0.07855900	-0.90031700
H	-3.84921200	-1.50085800	-1.66881200
C	-5.54480300	0.86747300	0.08353400
H	-4.79980300	1.86481400	1.84387100
H	-6.01008100	-0.28564900	-1.67468300
H	-6.49202400	1.40182500	0.08340600

C	-1.79796100	-1.25861900	0.10279800
H	-1.79152100	-1.99121000	-0.72369300
H	-1.70533100	-1.83966900	1.02722500
C	1.84266400	2.44034400	-0.70130400
C	3.21791600	1.79488900	-0.76464100
C	2.90393100	0.29836500	-0.53841100
C	1.20126400	1.65189600	0.42707000
H	1.88082300	3.51875800	-0.51436700
H	1.29170700	2.27064300	-1.63893700
H	3.84496000	2.17906700	0.05280600
H	3.76292900	1.95154000	-1.69943000
H	2.86664700	-0.20855300	-1.50916200
H	0.11666700	1.73134200	0.49790100
H	1.60696700	1.99951400	1.39246900
N	1.62825000	0.25781100	0.18351600
C	4.03676400	-0.33757900	0.25237100
O	5.11904600	-0.59301700	-0.22342200
O	3.75220500	-0.53714000	1.54255300
C	0.65841300	-0.86095400	-0.09118700
C	0.87014000	-1.47447600	-1.47605900
H	1.82318700	-2.00771300	-1.57254800
H	0.07804700	-2.20582500	-1.66180000
H	0.82187300	-0.70120600	-2.25295000
N	0.77876900	-1.93342400	0.87889900
H	1.67048200	-2.41109800	0.78964800
H	0.70730800	-1.55987200	1.82257100

#### TS21-22

N	-0.50418300	-0.31370000	0.13518000
H	3.55998600	-0.41888300	1.09696400
H	-0.31737900	0.02308600	-0.80764300
C	-2.93058400	-0.53853200	-0.11693900
C	-3.25466200	0.57249500	0.66756300
C	-3.85494900	-0.99086200	-1.05797400
C	-4.48084800	1.21062700	0.51874300
H	-2.52655000	0.93598700	1.39236600
C	-5.08523900	-0.35272300	-1.21146200
H	-3.60833600	-1.85296400	-1.67738100
C	-5.40128700	0.74891000	-0.42246000
H	-4.72219700	2.07238800	1.13725600
H	-5.79490200	-0.71682500	-1.95098800
H	-6.35968100	1.24911100	-0.54100200
C	-1.61969500	-1.25316600	0.08527800
H	-1.50409800	-2.03031300	-0.69118200
H	-1.65956300	-1.79607400	1.04172000
C	1.55620900	2.51875500	-0.17045400
C	2.74053400	1.87628500	-0.87359900
C	2.44828500	0.37652000	-0.71191500
C	1.38018400	1.62304000	1.04522100
H	1.72679200	3.56756800	0.09221300
H	0.66196400	2.47061500	-0.80737300

H	3.67403000	2.13231900	-0.35104800
H	2.86077900	2.15086400	-1.92504300
H	1.83753400	0.02868400	-1.56001700
H	0.35107600	1.61577700	1.41777900
H	2.04517200	1.94357300	1.86142800
N	1.77266200	0.26370000	0.58598200
C	3.76092700	-0.38799900	-0.74915900
O	4.33965700	-0.65193200	-1.77730800
O	4.26182600	-0.67386800	0.45413900
C	0.75411300	-0.78208800	0.74654600
C	1.23361400	-2.10068400	0.14151200
H	2.18361400	-2.41273400	0.58659900
H	0.50269200	-2.87953600	0.38042200
H	1.33500600	-2.05958300	-0.95008400
N	0.57114000	-0.99280900	2.18573600
H	0.99933200	-0.23927500	2.71246400
H	-0.41407800	-1.00118300	2.43420600

### TS22-23

N	-0.63356400	-0.30977700	0.01823000
H	3.07742600	-0.62983600	1.33070700
H	-0.58680500	0.14487300	-0.89318200
C	-3.06532900	-0.51083400	-0.05310500
C	-3.34009700	0.58221400	0.77441600
C	-4.03664900	-0.92629300	-0.96361500
C	-4.56265700	1.23994500	0.69619200
H	-2.57701100	0.91504200	1.47696300
C	-5.26374700	-0.26921800	-1.04563000
H	-3.82911200	-1.77382300	-1.61640800
C	-5.52942900	0.81524800	-0.21572800
H	-4.76485500	2.08744100	1.34749300
H	-6.00996100	-0.60453000	-1.76241600
H	-6.48474600	1.33110100	-0.27918100
C	-1.75134100	-1.23901500	0.05827600
H	-1.70890900	-2.02131300	-0.72208200
H	-1.71599500	-1.76257000	1.02580500
C	1.80191500	2.58197600	-0.26249500
C	3.07120900	1.89522400	-0.74737300
C	2.70096200	0.39523500	-0.73559900
C	1.30618000	1.61667500	0.80243900
H	1.98171000	3.59369900	0.11528500
H	1.06371000	2.64365000	-1.07478500
H	3.88625000	2.07977200	-0.03281600
H	3.42040400	2.21560500	-1.73256800
H	2.41671900	0.06545200	-1.74717300
H	0.23184000	1.69556100	0.99890500
H	1.84257600	1.78063000	1.75501900
N	1.62500600	0.30729500	0.22963400
C	3.93768200	-0.39867400	-0.33427000
O	4.86366800	-0.59221800	-1.08913100
O	3.95884200	-0.81693700	0.93441900
C	0.70795500	-0.81108400	0.36536900

C	1.12673700	-1.98530200	-0.51406200
H	2.13450100	-2.34487500	-0.28354700
H	0.44183000	-2.82391500	-0.34823400
H	1.07117000	-1.72055500	-1.57532700
N	0.76585000	-1.25376100	1.75917300
H	0.30309400	-0.57243900	2.35844600
H	0.30470000	-2.14860500	1.89863900

**TS23-24**

N	-0.67444600	-0.15707100	-0.33303300
H	1.74701500	-0.98275300	1.79017000
H	-0.83427100	0.68271500	-0.87498300
C	-3.08428700	-0.45879300	-0.16506300
C	-3.26807400	0.42455200	0.90282400
C	-4.16207800	-0.73623000	-1.00544200
C	-4.50665800	1.01637900	1.12530500
H	-2.42795700	0.65004100	1.55893900
C	-5.40567700	-0.14830700	-0.78238000
H	-4.02603300	-1.41858700	-1.84363900
C	-5.58020500	0.72985400	0.28293500
H	-4.63668700	1.70221800	1.95917300
H	-6.23670900	-0.37335100	-1.44654900
H	-6.54879900	1.19266500	0.45593200
C	-1.75290000	-1.12589800	-0.38643500
H	-1.77673700	-1.68751500	-1.33543900
H	-1.58138400	-1.86606000	0.41006400
C	2.36487000	2.63416800	-0.55395700
C	3.56739800	1.70092800	-0.49676900
C	2.98678700	0.28499200	-0.64910300
C	1.29091000	1.82802300	0.15359000
H	2.54649300	3.60173900	-0.07609100
H	2.05987700	2.81769700	-1.59278900
H	4.05001800	1.78641700	0.48597500
H	4.32509500	1.90588200	-1.25759100
H	3.07782600	-0.06968400	-1.68467500
H	0.27752900	2.16846700	-0.07782200
H	1.42007000	1.86819200	1.24876000
N	1.55047500	0.46931600	-0.33201300
C	3.78654000	-0.67125200	0.27086700
O	4.76379200	-1.21323600	-0.27139400
O	3.41213500	-0.75382200	1.47557300
C	0.66107700	-0.54625400	-0.24674100
C	1.06824100	-1.84141600	-0.89551500
H	2.04241100	-2.19583100	-0.55025100
H	0.33259700	-2.62540400	-0.70554600
H	1.12244700	-1.67946300	-1.97953400
N	0.72897500	-1.12732800	1.60350400
H	0.16127900	-0.49462300	2.16228800
H	0.46780300	-2.08518800	1.82627600

**TS8-25**

C	3.92143200	-0.25532400	-1.03772900
C	2.82144200	-1.19603100	-1.51371300

C	1.65483600	-0.86116400	-0.59385100
C	3.16869500	1.02728700	-0.70025400
H	4.38874700	-0.66942500	-0.13633600
H	4.70695200	-0.09731000	-1.78320200
H	3.10027500	-2.25176900	-1.46409700
H	2.53101100	-0.95901700	-2.54532500
H	0.69443800	-1.09485800	-1.08163300
H	3.18633300	1.74223000	-1.53782400
H	3.60984800	1.53720600	0.16902000
N	1.78779700	0.59215000	-0.43791400
C	1.68632900	-1.68006700	0.70926900
O	2.63663700	-2.33754000	1.07438300
O	0.55815500	-1.65022300	1.42083300
C	1.00529000	1.35832700	0.50579900
C	1.00929000	2.82823800	0.08682400
H	0.32304200	3.38890100	0.73311100
H	2.00527900	3.25780300	0.22655000
H	0.71474800	2.95949500	-0.96033100
N	1.53145700	1.28930900	1.88536700
H	2.30739900	0.63631000	1.94640500
H	0.83533700	0.97476700	2.55430200
N	-0.36222400	0.78894300	0.52280900
H	-0.01393700	-0.90581000	1.08494900
H	-0.86685600	1.22173300	1.29749400
C	-2.51539900	0.33060100	-0.49894900
C	-2.66407200	-1.05550800	-0.60150300
C	-3.62666100	1.10419600	-0.16111500
C	-3.89633300	-1.65521500	-0.36544400
H	-1.80630600	-1.67049200	-0.87408900
C	-4.86369200	0.50792900	0.07539000
H	-3.52070700	2.18651700	-0.08732300
C	-4.99935800	-0.87372300	-0.02446500
H	-3.99784400	-2.73457900	-0.44921300
H	-5.72160400	1.12335500	0.33590300
H	-5.96347300	-1.34230600	0.15831000
C	-1.17311900	0.97693800	-0.69249000
H	-1.31007800	2.04269100	-0.93303000
H	-0.63223000	0.52494700	-1.53383200

#### TS25-26

C	3.55213400	-0.23184600	-1.59580000
C	2.29156600	-1.05898300	-1.83953900
C	1.47124900	-0.82059900	-0.58123600
C	3.06688200	0.97246000	-0.77909900
H	4.27598600	-0.81931800	-1.01971800
H	4.04248400	0.07376000	-2.52515800
H	2.50054600	-2.11783700	-2.00837100
H	1.72941200	-0.66808500	-2.69686100
H	0.39765300	-0.97828300	-0.76058400
H	3.02479400	1.88832000	-1.38647500
H	3.75435700	1.17889200	0.06081800
N	1.72649000	0.59754600	-0.33198400
C	1.85147200	-1.79828400	0.54338900

O	2.65875500	-2.69246800	0.41471500
O	1.18195000	-1.65931000	1.69002000
C	1.03957000	1.39150300	0.65892900
C	1.09635500	2.86964600	0.26282300
H	0.47033900	3.45408200	0.94943200
H	2.11888700	3.25622300	0.33151100
H	0.73548400	3.03060100	-0.75936900
N	1.60255100	1.18999900	2.00683400
H	1.41650500	1.98933400	2.60850300
H	2.61184900	1.08347200	1.95778300
N	-0.32948400	0.87693600	0.76433200
H	0.68865200	-0.81052200	1.70390400
H	-0.73519900	1.20561200	1.63850600
C	-2.52248100	0.40306100	-0.24658100
C	-2.57767500	-0.88843500	0.28452900
C	-3.70087800	0.98035600	-0.72572400
C	-3.78081100	-1.58788000	0.32523200
H	-1.67117800	-1.34500000	0.67693000
C	-4.90480000	0.28215700	-0.68954500
H	-3.67331000	1.99217700	-1.12990800
C	-4.94834200	-1.00697900	-0.16412700
H	-3.80492800	-2.59217100	0.74217000
H	-5.81223400	0.74893400	-1.06628300
H	-5.88779500	-1.55370300	-0.13132500
C	-1.22599800	1.16421800	-0.34887500
H	-1.45421900	2.24009300	-0.44864000
H	-0.70008600	0.88390100	-1.27528100

#### TS26-27

C	3.60364100	-0.66788500	-1.33973900
C	2.30741000	-1.38821200	-1.69339300
C	1.32803600	-0.90101000	-0.62621600
C	3.13607300	0.71843900	-0.90976200
H	4.08944200	-1.17139500	-0.49707500
H	4.31380700	-0.62071300	-2.17064100
H	2.39560400	-2.47850600	-1.68573100
H	1.95689000	-1.08265600	-2.68896800
H	0.29778600	-0.94145700	-0.98963200
H	3.14635400	1.43698100	-1.74200600
H	3.74943100	1.12742000	-0.09575900
N	1.75403400	0.50642600	-0.44954600
C	1.40957700	-1.77917400	0.65019000
O	0.66184100	-2.77148300	0.63180800
O	2.24254600	-1.43675600	1.53579900
C	1.10032700	1.40604000	0.28867600
C	1.48841600	2.85079700	0.13740800
H	0.95416300	3.45941900	0.87229900
H	2.56150300	3.02501300	0.24998300
H	1.19349100	3.18277700	-0.86790000
N	1.73186600	1.16834200	2.17842800
H	2.00946200	0.16446500	2.11547500
H	2.53806000	1.73430900	2.43104500
N	-0.25533300	1.09732700	0.53211100

H	1.02820200	1.27600300	2.90474500
H	-0.61268100	1.65269200	1.30375500
C	-2.46010400	0.49696700	-0.35339500
C	-2.46514700	-0.80461700	0.16004700
C	-3.67401000	1.12036000	-0.64368200
C	-3.67122500	-1.46590500	0.36907100
H	-1.52524300	-1.30381100	0.40060500
C	-4.88148400	0.45680400	-0.43452600
H	-3.67430500	2.13742000	-1.03566100
C	-4.88121900	-0.83878700	0.07340400
H	-3.66355600	-2.47868300	0.76472800
H	-5.82073900	0.95561900	-0.66278400
H	-5.82136500	-1.35925400	0.24134300
C	-1.16318900	1.21295400	-0.61910500
H	-1.36695600	2.26686900	-0.87651100
H	-0.66103600	0.77810600	-1.49299200

#### TS12-28

C	0.68016800	1.24484600	0.53584900
N	0.99311000	2.10227400	-0.60814600
H	1.89314000	2.56169800	-0.49078600
N	-0.74635700	1.00060300	0.49064700
H	-1.06269800	0.55671800	1.34892700
C	-2.71677600	-0.05475100	-0.45260100
C	-3.12635000	-1.38440500	-0.34580500
C	-3.67359800	0.95735300	-0.32680600
C	-4.46654300	-1.70112800	-0.12557100
H	-2.38740200	-2.17967300	-0.44443100
C	-5.01027900	0.64632900	-0.10540900
H	-3.35783000	1.99695500	-0.40408700
C	-5.41076300	-0.68633200	-0.00510200
H	-4.77091400	-2.74258400	-0.04996200
H	-5.74499600	1.44314400	-0.01373200
H	-6.45662900	-0.93070900	0.16569400
C	-1.27351800	0.29562800	-0.67918000
H	-1.18084500	0.95694900	-1.55143400
H	-0.70381000	-0.61919700	-0.91835000
H	0.29304300	2.83946900	-0.64932000
C	0.99988600	1.91178300	1.87376800
H	0.44580800	2.85230800	1.96051400
H	0.72754000	1.27678900	2.72585600
H	2.07111200	2.13435100	1.95109500
N	1.43664600	-0.00843100	0.33745600
C	2.33628700	-2.00915600	1.19333700
C	3.45155100	-0.97276500	1.16814800
C	2.89588300	0.06162900	0.19085300
C	1.09577000	-1.13144200	1.21778400
H	2.35817400	-2.61222200	0.27440800
H	2.38689800	-2.69183900	2.04665700
H	4.42678600	-1.35353400	0.85426000
H	3.55891000	-0.51223000	2.15998300
H	3.29522400	1.06207400	0.42153000
H	0.89851000	-0.79624000	2.25249200



H	0.19533500	-1.65277200	0.86454200
C	3.33957700	-0.23073600	-1.24797800
O	4.47856300	-0.53408000	-1.52673100
O	2.39993900	-0.10594200	-2.18046500
H	1.57506100	0.18847900	-1.73373000

**TS28-29**

C	0.64976300	1.26244200	0.36952600
N	0.87500900	2.03714400	-0.83777800
H	1.62235500	1.70473200	-1.43185700
N	-0.76329400	0.93457800	0.44261600
H	-1.00768100	0.50986700	1.33380800
C	-2.77492900	-0.10221300	-0.43000300
C	-3.22981000	-1.40478300	-0.22295600
C	-3.69688700	0.94854300	-0.38770400
C	-4.58030700	-1.65926000	0.01416200
H	-2.51682800	-2.22922500	-0.25371600
C	-5.04390500	0.69987500	-0.15128400
H	-3.34226800	1.96670600	-0.54159300
C	-5.48989800	-0.60694700	0.04989200
H	-4.92027800	-2.68065000	0.17038500
H	-5.75150600	1.52566300	-0.12637100
H	-6.54406300	-0.80227600	0.23292500
C	-1.31903400	0.17826700	-0.67149200
H	-1.18190900	0.78838200	-1.57391700
H	-0.79553800	-0.77994300	-0.85234900
H	0.99960200	3.02476100	-0.65269400
C	0.98911200	2.07663600	1.61726500
H	0.40278200	3.00171200	1.61526800
H	0.74495000	1.53601600	2.53892300
H	2.05290300	2.33821700	1.64215000
N	1.46146300	0.01551200	0.27117600
C	2.45598400	-1.80724500	1.40894400
C	3.50569900	-0.71039400	1.28528200
C	2.92511500	0.15246700	0.16325900
C	1.16266100	-1.01811100	1.28082200
H	2.55404800	-2.52489900	0.58231800
H	2.51322300	-2.36746400	2.34669300
H	4.51552700	-1.06356600	1.05780900
H	3.54772400	-0.12052300	2.21087300
H	3.25430700	1.19715500	0.24239500
H	0.91310900	-0.56687800	2.25643700
H	0.30710500	-1.63383600	0.97233400
C	3.41327300	-0.34480100	-1.20021900
O	4.57774700	-0.32678000	-1.52609400
O	2.44748000	-0.80072900	-1.99762000
H	1.61734300	-0.70139300	-1.46516800

**TS29-30**

C	0.69881700	-1.17686200	-0.10958400
N	0.87911300	-2.01544200	1.06256900
H	0.72504000	-1.49345000	1.92173500
N	-0.72080600	-0.94625100	-0.27315100

H	-0.91057100	-0.27716800	-1.01183100
C	-2.91833100	-0.23350000	0.44422300
C	-3.34733000	1.05702400	0.75587800
C	-3.75344700	-1.05933100	-0.31493000
C	-4.59197500	1.51538900	0.32641100
H	-2.70176500	1.70676800	1.34711800
C	-4.99441900	-0.60470200	-0.74737900
H	-3.41835300	-2.06572400	-0.56223100
C	-5.41693100	0.68533500	-0.42646000
H	-4.91561600	2.52217900	0.58056900
H	-5.63685900	-1.25801600	-1.33345200
H	-6.38829800	1.04068300	-0.76248400
C	-1.57111700	-0.72757100	0.89036100
H	-1.67661300	-1.68310100	1.42284300
H	-1.15751900	-0.00297400	1.61662100
H	1.82441600	-2.38629700	1.09339100
C	1.16781000	-1.97813300	-1.31775700
H	0.57661700	-2.89595200	-1.35287200
H	0.99920400	-1.41989300	-2.24630500
H	2.22830700	-2.25148300	-1.26085900
N	1.46589300	0.13187500	0.01781100
C	1.84491500	2.44494000	0.04515000
C	2.77037100	1.85521600	-1.00956500
C	2.72410600	0.34549400	-0.71352500
C	0.74050300	1.40704100	0.10561200
H	2.35525900	2.51668400	1.01550700
H	1.47337000	3.44093000	-0.21456700
H	3.79128600	2.24884200	-0.99386400
H	2.35936000	2.03471900	-2.01083200
H	2.79683200	-0.21638700	-1.65118300
H	0.04155500	1.55959000	-0.73736400
H	0.15580800	1.46948400	1.03177300
C	3.93377200	-0.06432700	0.12344800
O	5.04778800	-0.17525200	-0.33412200
O	3.66486200	-0.25619200	1.41721800
H	2.68748000	-0.12523200	1.48162200

### TS30-31

C	-0.84271100	1.41546100	0.21569600
N	-0.94644300	2.30666200	1.36024300
H	-0.05530400	2.61125800	1.72921600
N	0.55825900	1.19191800	-0.12085300
H	0.66786700	0.51256200	-0.86633900
C	2.79344900	0.36041000	0.29829200
C	3.11886900	-0.91823600	0.75351500
C	3.55123000	0.92500100	-0.73192500
C	4.18404300	-1.62143600	0.19330300
H	2.53774900	-1.36323000	1.56111600
C	4.61329600	0.22502900	-1.29511300
H	3.29924200	1.92335200	-1.08814800
C	4.93213900	-1.05126200	-0.83260700
H	4.42979600	-2.61507500	0.56089600
H	5.19709900	0.67713100	-2.09355200

H	5.76419000	-1.59761100	-1.27036300
C	1.62631200	1.11252300	0.87357100
H	1.95739300	2.13213300	1.13513900
H	1.31998400	0.63329600	1.81627300
H	-1.51375900	1.92312700	2.10443100
C	-1.48596000	2.10458100	-0.98944100
H	-1.00078200	3.07683200	-1.10384500
H	-1.35615700	1.55016900	-1.92625700
H	-2.55402200	2.27524900	-0.81710000
N	-1.61795200	0.17933500	0.53501800
C	-1.85136300	-1.98245600	1.41887800
C	-1.79498800	-2.13399800	-0.09459700
C	-1.99267700	-0.69162900	-0.59636500
C	-1.08933300	-0.68577900	1.60458300
H	-2.88800500	-1.87667700	1.76655800
H	-1.39671600	-2.82112100	1.95476400
H	-2.53093600	-2.82374400	-0.51843700
H	-0.79805100	-2.48276400	-0.39453100
H	-1.39106900	-0.52281900	-1.49923200
H	-0.01405100	-0.88468300	1.46182900
H	-1.22469400	-0.22857200	2.59185200
C	-3.44990700	-0.47840900	-0.99779500
O	-3.92234500	-0.93859900	-2.01174000
O	-4.17255700	0.21071700	-0.11509800
H	-3.52198700	0.50004400	0.56961200

### TS31-32

C	0.74331600	-1.17612700	0.20121800
N	0.93174800	-1.86313500	1.47247700
H	0.39412200	-2.72649000	1.49443200
N	-0.67742400	-0.95516700	-0.10214500
H	-0.78294500	-0.30486300	-0.87774600
C	-2.93320700	-0.20461000	0.36734300
C	-3.40178800	1.08933900	0.59841400
C	-3.68398600	-1.05934400	-0.44611600
C	-4.60020800	1.52420700	0.03409400
H	-2.82270600	1.76140400	1.23188600
C	-4.87856000	-0.62864300	-1.01221700
H	-3.32025100	-2.06907500	-0.63150700
C	-5.34030900	0.66596300	-0.77313500
H	-4.95422500	2.53447500	0.22630600
H	-5.45580100	-1.30443000	-1.63921200
H	-6.27610800	1.00193900	-1.21361100
C	-1.63403400	-0.67165500	0.96305100
H	-1.80653200	-1.59663100	1.53434700
H	-1.29298300	0.08556800	1.69098600
H	0.62728000	-1.29181600	2.25636300
C	1.27856700	-2.09425600	-0.89084100
H	0.77846900	-3.06202600	-0.79005700
H	1.04152200	-1.71003400	-1.88860400
H	2.35768000	-2.25730000	-0.80645000
N	1.52964500	0.07201100	0.28388700
C	1.96801400	2.33471500	0.68630800

C	2.40053800	2.03268600	-0.74290300
C	2.44484200	0.49801200	-0.77606500
C	0.93950200	1.24557400	0.93076100
H	2.81175800	2.22556100	1.38121300
H	1.55568800	3.34065300	0.80999600
H	3.35622800	2.47699200	-1.03545000
H	1.63602500	2.38585300	-1.44634500
H	2.16969100	0.13546300	-1.77532100
H	-0.02273200	1.53039800	0.46489000
H	0.75449400	1.06517300	1.99860100
C	3.86916300	-0.00207900	-0.52042200
O	4.77118100	0.17848400	-1.30735900
O	4.04973400	-0.63419700	0.63805100
H	3.16512600	-0.67376300	1.07328200

### TS31-32

C	0.74331600	-1.17612700	0.20121800
N	0.93174800	-1.86313500	1.47247700
H	0.39412200	-2.72649000	1.49443200
N	-0.67742400	-0.95516700	-0.10214500
H	-0.78294500	-0.30486300	-0.87774600
C	-2.93320700	-0.20461000	0.36734300
C	-3.40178800	1.08933900	0.59841400
C	-3.68398600	-1.05934400	-0.44611600
C	-4.60020800	1.52420700	0.03409400
H	-2.82270600	1.76140400	1.23188600
C	-4.87856000	-0.62864300	-1.01221700
H	-3.32025100	-2.06907500	-0.63150700
C	-5.34030900	0.66596300	-0.77313500
H	-4.95422500	2.53447500	0.22630600
H	-5.45580100	-1.30443000	-1.63921200
H	-6.27610800	1.00193900	-1.21361100
C	-1.63403400	-0.67165500	0.96305100
H	-1.80653200	-1.59663100	1.53434700
H	-1.29298300	0.08556800	1.69098600
H	0.62728000	-1.29181600	2.25636300
C	1.27856700	-2.09425600	-0.89084100
H	0.77846900	-3.06202600	-0.79005700
H	1.04152200	-1.71003400	-1.88860400
H	2.35768000	-2.25730000	-0.80645000
N	1.52964500	0.07201100	0.28388700
C	1.96801400	2.33471500	0.68630800
C	2.40053800	2.03268600	-0.74290300
C	2.44484200	0.49801200	-0.77606500
C	0.93950200	1.24557400	0.93076100
H	2.81175800	2.22556100	1.38121300
H	1.55568800	3.34065300	0.80999600
H	3.35622800	2.47699200	-1.03545000
H	1.63602500	2.38585300	-1.44634500
H	2.16969100	0.13546300	-1.77532100
H	-0.02273200	1.53039800	0.46489000
H	0.75449400	1.06517300	1.99860100
C	3.86916300	-0.00207900	-0.52042200

O	4.77118100	0.17848400	-1.30735900
O	4.04973400	-0.63419700	0.63805100
H	3.16512600	-0.67376300	1.07328200

**TS32-33**

C	-0.61579400	-0.55633100	0.34967900
N	-0.89186200	-1.68958800	-1.06932900
H	-0.65182600	-2.66742100	-0.91802500
N	0.72505700	-0.16719700	0.27625800
H	0.90423100	0.57080500	-0.39609700
C	3.12901400	-0.46589000	0.15361900
C	3.91540500	-0.68681500	-0.97648200
C	3.58642500	0.41434200	1.13890500
C	5.14397100	-0.04397700	-1.12209500
H	3.56601300	-1.37352900	-1.74691500
C	4.80999900	1.05863400	0.99548600
H	2.97335800	0.59024100	2.02183900
C	5.59210500	0.82986700	-0.13651700
H	5.74947200	-0.22797800	-2.00626500
H	5.15813600	1.73860200	1.76939000
H	6.55047200	1.33141900	-0.24729900
C	1.80062200	-1.15087700	0.31647600
H	1.77152400	-1.66685800	1.28522500
H	1.68894900	-1.92320800	-0.46547800
H	-0.40747300	-1.36644900	-1.90434600
C	-0.94434500	-1.49104400	1.48511200
H	-0.25976400	-2.34181400	1.51284000
H	-0.85759900	-0.94329600	2.42964700
H	-1.96164000	-1.87946400	1.39271400
N	-1.50311800	0.46677200	0.16012900
C	-2.61956000	2.20770600	-0.96662400
C	-3.28758000	1.93666200	0.37668500
C	-2.88954800	0.48902300	0.66144500
C	-1.25994700	1.53395500	-0.81487100
H	-3.18824400	1.72392100	-1.77005200
H	-2.52936600	3.27142300	-1.20598900
H	-4.37368300	2.05506500	0.36506800
H	-2.87177300	2.59804500	1.14885300
H	-2.90440300	0.28865600	1.74011500
H	-0.50829800	2.24331200	-0.43198600
H	-0.89203000	1.13262300	-1.77249600
C	-3.89278600	-0.49197400	-0.00651100
O	-5.01886500	-0.49832200	0.51382700
O	-3.49815000	-1.17029300	-1.00228900
H	-1.93836100	-1.57476900	-1.18828900

**TS18-34**

N	-0.35119300	-0.89097800	0.42857700
H	-0.89643200	-1.43322200	1.09791800
H	-0.08894200	0.90107600	0.67693500
C	-2.51483100	-0.21366000	-0.47661800
C	-3.51783000	-1.13175000	-0.15194700
C	-2.81744100	1.14937200	-0.46464400

C	-4.79649900	-0.69987500	0.18888200
H	-3.29314700	-2.19912900	-0.17652100
C	-4.09674400	1.58440100	-0.12753200
H	-2.04263300	1.87210900	-0.71386800
C	-5.08753200	0.66235000	0.20172900
H	-5.56736400	-1.42641600	0.43545200
H	-4.31998600	2.64867700	-0.12371900
H	-6.08632300	1.00400100	0.46314800
C	-1.13402000	-0.71034800	-0.80747200
H	-0.59291600	-0.00116500	-1.44544000
H	-1.23840500	-1.64552100	-1.38280900
C	3.96150700	0.34387200	-0.98195300
C	3.76136100	0.84818100	0.43918800
C	2.26028900	0.68239400	0.63863900
C	3.04536800	-0.86453500	-1.01390800
H	3.62159300	1.10134200	-1.70078900
H	5.00022600	0.09049900	-1.21664200
H	4.08808700	1.87827300	0.60250000
H	4.29311800	0.19522500	1.14556600
H	2.02608600	0.45816100	1.69010600
H	3.54581000	-1.72536700	-0.52977700
H	2.76604400	-1.17856500	-2.02311900
N	1.86271400	-0.42727200	-0.25700000
C	1.47551200	1.95009700	0.30392600
O	1.97733700	2.99382000	-0.05014700
O	0.15655000	1.84288100	0.46839700
C	0.99334800	-1.48285800	0.28839100
C	1.42782300	-1.97177300	1.67460300
H	1.31425700	-1.20724900	2.44857400
H	0.82264600	-2.83605900	1.97309400
H	2.47967300	-2.28330500	1.64832800
N	1.02923800	-2.60978200	-0.63601500
H	1.42737900	-3.43970200	-0.21314900
H	0.12296100	-2.84625400	-1.01843000

#### TS34-35

N	-0.40568700	-0.81822300	0.35447200
H	-0.88695400	-1.09049100	1.20702400
H	0.28678800	0.97817800	-0.60321900
C	-2.64477900	-0.27266900	-0.41379200
C	-3.74033300	-1.08712900	-0.12209600
C	-2.79234800	1.11464600	-0.31985400
C	-4.96281200	-0.53356800	0.25394500
H	-3.63432800	-2.16937400	-0.19801700
C	-4.01184800	1.67107500	0.05243300
H	-1.94623100	1.76412200	-0.54087600
C	-5.10015500	0.84865600	0.34120900
H	-5.80736900	-1.18230200	0.47492800
H	-4.11409000	2.75194500	0.11554100
H	-6.05286900	1.28602200	0.63072600
C	-1.32836800	-0.89680900	-0.78705400
H	-0.87686100	-0.38418500	-1.64953600
H	-1.50444700	-1.93078100	-1.12041600

C	4.10514500	0.14945000	-0.68546000
C	3.73229900	0.66813500	0.69665000
C	2.21080800	0.66996900	0.61598100
C	3.09508100	-0.96864600	-0.87733900
H	3.95523700	0.93764800	-1.43667500
H	5.13852600	-0.20112200	-0.76561000
H	4.13238200	1.65675100	0.93443900
H	4.06210500	-0.03987700	1.46924000
H	1.74239200	0.56879300	1.60541800
H	3.46379600	-1.86794400	-0.34565400
H	2.93345700	-1.23882600	-1.92639900
N	1.85463100	-0.45627200	-0.27106600
C	1.68683700	2.00466600	0.07809400
O	2.23443500	3.06650600	0.27013400
O	0.53598200	1.92498800	-0.58862900
C	0.90452800	-1.45863100	0.25144200
C	1.29549000	-1.97361500	1.64271500
H	1.20988700	-1.20694900	2.42162000
H	0.64799400	-2.81154600	1.92852100
H	2.32982000	-2.33793800	1.63193900
N	0.85823900	-2.54772900	-0.72334100
H	1.74432500	-3.04534500	-0.75129900
H	0.16555200	-3.22634900	-0.41543300

#### TS35-36

N	-0.31698000	1.17452400	-0.19653500
H	-0.82565700	1.86117700	-0.74217900
H	1.79208200	-0.12627700	1.79572200
C	-2.45545400	0.18545300	0.33845200
C	-3.56028600	1.03725000	0.30332100
C	-2.57735100	-1.10284700	-0.18857700
C	-4.76797200	0.61490600	-0.24940100
H	-3.47318600	2.03990600	0.72338900
C	-3.78202400	-1.52995100	-0.73784200
H	-1.72252700	-1.77884800	-0.15346400
C	-4.87990200	-0.67050700	-0.77157800
H	-5.62282200	1.28727500	-0.26563500
H	-3.86759100	-2.53851500	-1.13584600
H	-5.82235900	-1.00704500	-1.19745200
C	-1.14545700	0.66631200	0.89677100
H	-0.62693500	-0.16031000	1.39646600
H	-1.33553500	1.42270100	1.67779700
C	3.84270600	-0.75074100	-0.94004200
C	2.59028600	-1.52198900	-1.33963200
C	1.51652200	-0.90135800	-0.43865800
C	3.30493300	0.66362800	-0.79340200
H	4.22517200	-1.11501600	0.02394300
H	4.65202900	-0.82049100	-1.67343100
H	2.66241000	-2.60547200	-1.21154900
H	2.34233900	-1.31687800	-2.38882600
H	0.52843200	-0.91211100	-0.92157100
H	3.25315900	1.14554000	-1.78681400
H	3.93973700	1.29362100	-0.15275900

N	1.98210200	0.45603500	-0.20736400
C	1.36622900	-1.71469200	0.84931700
O	1.02795400	-2.87871100	0.83754600
O	1.61784400	-1.07606200	1.99265500
C	1.05722800	1.57723000	0.02865300
C	1.35058000	2.74228500	-0.91508000
H	1.19721500	2.45173600	-1.96181300
H	0.68038700	3.57689900	-0.67824000
H	2.37721900	3.10446200	-0.80265600
N	1.25729900	1.95029500	1.44438100
H	2.21474500	2.27500700	1.57033300
H	0.64814500	2.72497600	1.70579000

### TS36-37

N	-0.33957300	1.36474800	-0.17991500
H	-0.80498100	2.24025100	-0.39115900
H	1.74424200	0.87037600	1.84552800
C	-2.40739000	0.17027500	0.33373200
C	-3.48047500	1.06345700	0.29527800
C	-2.58975500	-1.13103800	-0.13713800
C	-4.71290700	0.67062800	-0.21958500
H	-3.35304300	2.07447500	0.68530600
C	-3.82201500	-1.52792100	-0.64923600
H	-1.76589600	-1.84279900	-0.08358900
C	-4.88388100	-0.62705000	-0.69587300
H	-5.54226800	1.37392100	-0.24044500
H	-3.95474800	-2.54634500	-1.00650200
H	-5.84689700	-0.93981600	-1.09262000
C	-1.07052700	0.61842000	0.85430900
H	-0.48180100	-0.24158500	1.17760600
H	-1.21793100	1.24840700	1.74824500
C	3.65121000	-0.98159800	-1.01403400
C	2.35499100	-1.72290000	-1.32681300
C	1.34603700	-0.99752500	-0.44026900
C	3.21213000	0.47683100	-0.88654100
H	4.06110000	-1.33690100	-0.06109600
H	4.42288700	-1.11106300	-1.77897500
H	2.39273800	-2.79167500	-1.10155200
H	2.08159700	-1.59575700	-2.38266400
H	0.32340200	-1.11265200	-0.82236000
H	3.38108600	1.03166900	-1.82077000
H	3.75907800	0.99367600	-0.08295700
N	1.77273900	0.39705600	-0.60291400
C	1.39887300	-1.55463400	1.00986900
O	0.95885100	-2.70921700	1.13356700
O	1.87011100	-0.80368800	1.91627500
C	1.05013500	1.49954700	-0.24082900
C	1.45367900	2.78512900	-0.92500700
H	1.17710000	2.72476600	-1.98368100
H	0.94003500	3.63748400	-0.46888300
H	2.52881100	2.96509800	-0.86399700
N	1.58960800	1.85179700	1.49456000
H	2.46367900	2.37088300	1.53980400



H	0.90007800	2.34588600	2.05674100
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**TS24-38**

N	0.69235500	-0.04060200	0.53326700
H	0.94945400	0.63934700	-0.17339900
C	3.05991100	-0.48519100	0.29975000
C	3.54655900	-0.74099600	-0.98362600
C	3.79226100	0.34381800	1.15255200
C	4.74953500	-0.18229700	-1.40871900
H	2.97813600	-1.39126000	-1.64907400
C	4.99392500	0.90454700	0.73066500
H	3.41288100	0.54610900	2.15378100
C	5.47446800	0.64154800	-0.55115500
H	5.12336800	-0.39432000	-2.40756800
H	5.55987800	1.54433400	1.40359900
H	6.41598300	1.07521400	-0.87953600
C	1.73858400	-1.05009700	0.73275800
H	1.77353700	-1.32294400	1.79571800
H	1.50658300	-1.95664600	0.15469600
C	-2.36328100	2.70968200	-0.19120700
C	-3.52550900	1.73283400	-0.24325500
C	-2.98616700	0.45714800	0.42719400
C	-1.16674300	1.81091900	-0.45173900
H	-2.44780500	3.52007600	-0.92099800
H	-2.27435200	3.15517900	0.80794100
H	-3.77485400	1.51067000	-1.29081000
H	-4.43778600	2.08301100	0.24493700
H	-3.23222000	0.45286200	1.49914900
H	-0.24147700	2.23718200	-0.04781800
H	-1.02971600	1.62656400	-1.53267100
N	-1.52829500	0.58056000	0.25196900
C	-3.72801000	-0.72898000	-0.20628000
O	-4.89716800	-0.86701300	0.12930100
O	-3.13489700	-1.45203600	-1.10335300
C	-0.63603900	-0.42002900	0.50429800
C	-1.03708700	-1.43304300	1.53780100
H	-2.05068700	-1.80213100	1.37489300
H	-0.37058400	-2.29571100	1.51742300
H	-0.98879900	-0.95946800	2.52523100
O	-0.74246200	-1.53793900	-0.94884200
H	-0.30565600	-1.08125000	-1.67999100

**TS38-39**

N	0.73240500	-0.10069400	0.20939300
H	0.94906500	0.13710700	-0.75957300
C	3.13486800	-0.45240200	0.29400000
C	3.90362100	-1.05695100	-0.70054800
C	3.61995200	0.70078500	0.91792300
C	5.14020800	-0.52461700	-1.06322600
H	3.52960100	-1.95439900	-1.19211900
C	4.85186600	1.23582600	0.55809100
H	3.01845600	1.17637500	1.69190700
C	5.61559800	0.62260300	-0.43528500

H	5.73092700	-1.00816100	-1.83782500
H	5.22087000	2.13078100	1.05405700
H	6.58032000	1.03858900	-0.71627600
C	1.79195800	-1.00773500	0.67456400
H	1.72735700	-1.08921800	1.76768000
H	1.67644000	-2.02169700	0.25454800
C	-2.39735200	2.72829900	-0.21913100
C	-3.52749700	1.72830300	-0.42530100
C	-2.97060200	0.45725400	0.20684200
C	-1.11851600	1.88525300	-0.27216200
H	-2.39741600	3.52368900	-0.96943900
H	-2.49380200	3.20605300	0.76279200
H	-3.71273800	1.54747700	-1.49289300
H	-4.47414100	2.02038200	0.03400900
H	-2.96011700	0.57719200	1.30295700
H	-0.46795800	2.03472000	0.59558100
H	-0.51982600	2.07266300	-1.16842600
N	-1.56214100	0.45983100	-0.28318700
C	-3.87680300	-0.74425700	-0.08281900
O	-5.04715800	-0.63219500	0.21853200
O	-3.39938100	-1.84137600	-0.63119800
C	-0.59598500	-0.66052200	0.22013400
C	-0.94724300	-1.21604200	1.58052000
H	-1.98463400	-1.55329000	1.63074700
H	-0.33019800	-2.09595600	1.78277400
H	-0.77063300	-0.47213600	2.36677400
O	-0.86322100	-1.49880200	-0.85613400
H	-1.39147500	-0.33651600	-1.21530500
H	-2.38831200	-1.84342200	-0.74662200

#### TS27-40

C	4.19736000	0.11231500	-0.21447400
C	3.49457300	-0.90137400	-1.11225100
C	2.05172100	-0.80050000	-0.62600800
C	3.18209400	1.24851500	-0.07231300
H	4.39934900	-0.33983500	0.76489500
H	5.15157500	0.46275900	-0.61787000
H	3.88374900	-1.91752600	-1.01992600
H	3.54290500	-0.59490900	-2.16430800
H	1.34889300	-1.18708800	-1.37253000
H	3.41926200	2.09289800	-0.73261600
H	3.13783300	1.62533600	0.96057000
N	1.90065200	0.64739400	-0.47624700
C	1.87651400	-1.62531700	0.66817400
O	2.17801500	-2.80913200	0.62855000
O	1.43439400	-1.02895400	1.73673300
C	0.72291900	1.31550100	-0.30753900
C	0.80005300	2.81569800	-0.40740500
H	-0.15240400	3.25767500	-0.10331300
H	1.58291400	3.23311100	0.22825400
H	1.01268300	3.09740700	-1.44515500
N	-0.42746400	0.81216100	-0.87824200
H	-1.14931200	1.52237400	-0.90665500

C	-2.49078500	-0.37210600	-0.31849700
C	-2.92174200	0.30427800	0.82828200
C	-3.43685900	-0.90793500	-1.19095800
C	-4.28005000	0.43904700	1.09347800
H	-2.17457700	0.71339500	1.50921900
C	-4.79875300	-0.77534000	-0.92438100
H	-3.10422400	-1.43713100	-2.08309200
C	-5.22143200	-0.10059200	0.21678000
H	-4.60733700	0.95937500	1.99077900
H	-5.52847600	-1.19882700	-1.61058000
H	-6.28349800	0.00242700	0.42691000
C	-1.01854500	-0.50777000	-0.59521700
H	-0.86454900	-1.18593400	-1.44464100
H	-0.53735900	-0.95147900	0.28281700
O	0.37104000	1.13115200	1.50014200
H	0.98118200	0.00266900	1.65686600
H	0.81907900	1.81537300	2.01237900

#### TS40-41

C	-4.08555700	1.15873200	0.57841300
C	-3.52212800	-0.01854300	1.36222700
C	-2.34246500	-0.46898200	0.50747600
C	-2.81648900	1.85295600	0.12196300
H	-4.65926100	0.80252500	-0.28815500
H	-4.73319600	1.81245700	1.17032600
H	-4.23270900	-0.83229000	1.52298800
H	-3.15559000	0.32301700	2.33901500
H	-1.49205600	-0.78570900	1.13358700
H	-2.37032500	2.41314000	0.95883300
H	-2.94946500	2.53487600	-0.72289600
N	-1.91147000	0.74318500	-0.24997800
C	-2.67309900	-1.64736100	-0.41162700
O	-3.66097900	-2.32980800	-0.26322400
O	-1.77981000	-1.93705000	-1.35626000
C	-0.29253800	0.94864300	-0.30799800
C	-0.01170000	2.42937000	-0.44033300
H	1.03619400	2.53315300	-0.74330800
H	-0.63608500	2.87700300	-1.21914800
H	-0.16197500	2.97386100	0.49988300
N	0.37616700	0.38313000	0.80483800
H	0.79659300	1.08271000	1.40545500
C	2.65194800	-0.51724700	0.37685800
C	3.02527500	-0.00062900	-0.86908000
C	3.63640100	-0.73448400	1.34122300
C	4.35864000	0.28922400	-1.13872300
H	2.25453900	0.16440200	-1.62215100
C	4.97345500	-0.44347000	1.07316200
H	3.35295500	-1.14119500	2.31202200
C	5.33677500	0.06915800	-0.16818500
H	4.63960300	0.68282400	-2.11322400
H	5.73004500	-0.61880400	1.83478100
H	6.37888900	0.29499100	-0.38256600
C	1.20568300	-0.81421400	0.68287300

H	1.13827400	-1.38257600	1.62085400
H	0.77765400	-1.44498400	-0.10289100
O	-0.19951800	0.26625900	-1.49709700
H	-1.04365000	-1.27273600	-1.41621600
H	-1.46606500	0.48500400	-1.38807000

**TS33-42**

C	-0.61021800	-0.49707700	0.53723600
N	0.71128500	-0.10688100	0.47273900
H	0.91123300	0.61984000	-0.20517300
C	3.10157800	-0.44487900	0.23456500
C	3.79379600	-0.83095000	-0.91334000
C	3.63568700	0.56265600	1.04395000
C	5.00369300	-0.22534800	-1.24827500
H	3.38451700	-1.61746000	-1.54633000
C	4.84046200	1.17159000	0.71009200
H	3.09746100	0.86442800	1.94203200
C	5.52772400	0.77711500	-0.43757100
H	5.53636900	-0.53801600	-2.14321100
H	5.24869700	1.95143300	1.34862800
H	6.47177300	1.25047500	-0.69659900
C	1.79190200	-1.08724000	0.59290100
H	1.82791300	-1.44776200	1.62981400
H	1.60281400	-1.95592700	-0.05515600
C	-0.95158900	-1.49252600	1.60726200
H	-0.90422600	-0.99872700	2.58481300
H	-1.95210700	-1.90292800	1.45853100
H	-0.25413800	-2.33037700	1.59078200
N	-1.51605400	0.49534000	0.30866300
C	-3.38765100	1.85881100	0.39652200
C	-2.94537900	0.41470700	0.62698100
C	-1.23693800	1.59775900	-0.61899400
H	-4.47084800	1.93136200	0.28037000
H	-3.08046000	2.47536400	1.25074200
H	-3.09119300	0.12102100	1.67408000
H	-0.53113500	2.30726700	-0.16141200
H	-0.79324400	1.22693400	-1.55634900
C	-3.79617900	-0.54559900	-0.23369500
O	-5.00966500	-0.49296600	-0.08322400
O	-3.20410000	-1.34478800	-1.06517000
O	-0.82706600	-1.66427400	-0.86884200
H	-2.07174900	-1.47761500	-1.01628400
H	-0.35719100	-1.30509500	-1.63249400
C	-2.60145900	2.24080600	-0.85231400
H	-3.07864500	1.80365200	-1.73919500
H	-2.52838000	3.32018400	-1.01142900

**TS42-43**

C	-0.63338500	-1.00286700	-0.12726200
N	0.74545000	-0.65856600	-0.26978100
H	1.10664500	-1.09089900	-1.11414400
C	3.03422600	-0.24726700	0.41483500
C	4.09270900	-1.14959300	0.31548800

C	3.25347800	1.09194100	0.07884200
C	5.35101200	-0.72495700	-0.10912500
H	3.92864400	-2.19529200	0.57377700
C	4.50662300	1.52041300	-0.34288400
H	2.42803200	1.79964900	0.15037300
C	5.56013000	0.61052500	-0.43775800
H	6.16704000	-1.44000500	-0.18306800
H	4.66599300	2.56594100	-0.59678500
H	6.54075000	0.94505900	-0.76793700
C	1.67177500	-0.70866800	0.85317100
H	1.29763000	-0.04470400	1.64718600
H	1.75911800	-1.71584600	1.29735000
C	-0.96077800	-1.81529100	1.10527200
H	-0.72254800	-1.28111400	2.03354300
H	-2.01237200	-2.11112900	1.12782600
H	-0.36485600	-2.73346700	1.07583200
N	-1.49866100	0.33383400	-0.23746100
C	-3.15353600	1.91790700	0.52172300
C	-2.81182600	0.41177500	0.46316300
C	-0.85393900	1.64612900	-0.04398900
H	-4.13631300	2.11469600	0.08687700
H	-3.19662700	2.24300800	1.56626400
H	-2.67652800	0.03842300	1.49013000
H	-0.44367500	1.69551100	0.97899600
H	-0.03597300	1.76803500	-0.75565500
C	-3.95929800	-0.43232700	-0.10379900
O	-5.09523500	-0.15466400	0.21617600
O	-3.69762300	-1.47839100	-0.86842200
O	-1.11858700	-1.50248900	-1.31839100
H	-2.72238000	-1.62766400	-1.07105000
H	-1.51753200	-0.26026100	-1.33374400
C	-2.00925600	2.61020300	-0.21749600
H	-1.78781000	3.60726800	0.17399100
H	-2.24082200	2.71271900	-1.28505900

#### TS37-44

N	-0.47893300	0.80420700	-0.60338000
H	-1.18423800	1.52927900	-0.53356100
H	1.25401300	0.14377200	1.73932600
C	-2.53838200	-0.37618700	-0.10737200
C	-3.19201000	0.28002300	0.93952500
C	-3.29210500	-0.90470100	-1.15555300
C	-4.57784100	0.40441500	0.93763800
H	-2.60413800	0.68489000	1.76372100
C	-4.67971800	-0.78413700	-1.15852900
H	-2.78544400	-1.41869400	-1.97147500
C	-5.32376700	-0.12800700	-0.11272800
H	-5.07818200	0.90980700	1.76041300
H	-5.25825300	-1.20513200	-1.97742500
H	-6.40726800	-0.03620300	-0.11244100
C	-1.03952100	-0.47095600	-0.10939900

H	-0.73006300	-1.30322200	-0.75144300
H	-0.68489000	-0.67122200	0.90936300
C	4.18677600	0.04331000	-0.47836900
C	3.37986100	-1.01104400	-1.22786100
C	1.99000000	-0.83866900	-0.62017800
C	3.21764400	1.21771700	-0.34412200
H	4.45985400	-0.33623400	0.51423400
H	5.11056600	0.32859100	-0.98937700
H	3.75324900	-2.02952200	-1.10052300
H	3.33631900	-0.78100300	-2.29961500
H	1.21874600	-1.24118100	-1.28513600
H	3.39421300	1.98393900	-1.11099100
H	3.29684600	1.69737900	0.64241300
N	1.88566200	0.61892900	-0.53887500
C	1.91029600	-1.59073700	0.72537600
O	2.10471500	-2.79814700	0.70284000
O	1.67248800	-0.91461800	1.80910900
C	0.75366500	1.32004800	-0.24809300
C	0.83360200	2.80776100	-0.46339800
H	0.89719500	3.01081100	-1.53865400
H	-0.05756900	3.29415100	-0.05865200
H	1.70809000	3.24736000	0.01951100
H	1.19172100	1.97431300	1.99829200
O	0.66669000	1.26816000	1.60257400

#### TS44-45

N	-0.45845400	0.94404400	-0.14393900
H	-0.99242700	1.48836600	-0.81260800
H	1.35347300	-0.06978500	2.06561000
C	-2.63341300	-0.02289900	0.32226900
C	-3.80357300	0.67446500	0.62226600
C	-2.70140600	-1.11407900	-0.54930200
C	-5.02307400	0.28867300	0.06750200
H	-3.75831000	1.52456900	1.30204800
C	-3.91510000	-1.50141800	-1.10619800
H	-1.79098100	-1.66503600	-0.78465600
C	-5.08026800	-0.79872600	-0.79840000
H	-5.92811700	0.83896000	0.31427700
H	-3.95546800	-2.35659200	-1.77694600
H	-6.03050100	-1.10375700	-1.23043500
C	-1.31802400	0.40092400	0.91217000
H	-0.82538300	-0.46606900	1.37400300
H	-1.48141700	1.13320500	1.71638200
C	3.69127500	-0.28014500	-1.61653100
C	2.58434600	-1.31389600	-1.46270700
C	1.80032900	-0.80933000	-0.25414400
C	2.94667100	1.00838300	-1.32478000
H	4.47584000	-0.44368200	-0.86503700
H	4.16028200	-0.28117800	-2.60493600
H	2.94198600	-2.33391900	-1.30558400
H	1.93759900	-1.30466700	-2.34915900
H	0.71591500	-0.93916900	-0.40326400
H	2.32663600	1.29358500	-2.18894500

H	3.58833800	1.85371100	-1.06007200
N	2.06597900	0.65875700	-0.18792500
C	2.15642000	-1.53590200	1.04722600
O	2.71897600	-2.60759300	1.04975800
O	1.75778600	-0.97279200	2.18480800
C	0.77218300	1.56251000	0.20063400
C	0.91958000	2.91683200	-0.45740300
H	0.73128200	2.88502200	-1.53739400
H	0.18948000	3.58696300	0.00865000
H	1.91518500	3.33205100	-0.27671800
H	2.17480200	1.10527000	0.96916000
O	1.10116700	1.56166000	1.53456700

#### EtOH-5a

C	0.81335300	2.53396800	0.17349300
C	1.88043700	1.48277300	-0.13986900
C	1.08867400	0.20911100	-0.51618200
C	-0.46864100	1.91645000	-0.34480500
H	0.73365500	2.69013000	1.25646200
H	1.01767500	3.50493300	-0.28655200
H	2.53197800	1.29574000	0.71856300
H	2.52740100	1.77580500	-0.97130800
H	1.09553900	0.11645400	-1.61832800
H	-0.57937900	2.08112200	-1.43224700
H	-1.35732200	2.30793300	0.15819800
N	-0.29293200	0.47881900	-0.05518600
C	1.82462500	-1.02658500	-0.01499000
O	3.03081700	-1.09747900	-0.15726300
O	1.16032900	-2.03007100	0.53610700
H	0.17186900	-1.90362300	0.51126300
C	-1.37365500	-0.39053900	-0.56798300
C	-2.73589100	0.27317900	-0.47337400
H	-2.84181400	1.08870700	-1.19338300
H	-3.49382500	-0.48526500	-0.69253300
H	-2.91941700	0.65389700	0.53623900
N	-1.14460900	-0.80546600	-1.91972600
H	-0.40684300	-1.50110100	-1.99263800
H	-1.98567800	-1.22522100	-2.30530200
O	-1.40520000	-1.56009800	0.28476300
H	-0.63582100	0.37615800	1.88663000
O	-1.24174300	0.05573700	2.58816500
H	-0.69338500	-0.16896900	3.34775600
H	-1.62887900	-1.25502300	1.18964700

#### EtOH-5b

C	0.37688200	2.65519400	0.39346600
C	1.57042300	1.81917700	-0.03198700
C	0.92650200	0.51848300	-0.49594500
C	-0.48044000	1.62150700	1.10309900
H	0.64697200	3.49635100	1.03947600
H	-0.14677000	3.05863500	-0.48414200
H	2.21980900	1.61360500	0.82797300
H	2.18504300	2.26890200	-0.81772300

H	0.64255800	0.60679200	-1.55669700
H	-1.54390100	1.86777000	1.14500800
H	-0.13458700	1.48089500	2.13675900
N	-0.28596900	0.34780500	0.35314300
C	1.87792200	-0.67229300	-0.38456700
O	2.89988500	-0.66393000	0.26774500
O	1.54000200	-1.75484300	-1.08662100
H	0.61200800	-1.66218000	-1.40133200
C	-1.48968700	-0.15191400	-0.35162700
O	-1.13924100	-1.42162800	-0.92703400
H	-0.06936800	-1.22335700	1.57416500
O	-0.40016700	-2.12478700	1.77073700
H	0.32738900	-2.61187800	2.17261100
H	-1.04572200	-2.04048900	-0.17641100
C	-1.97134800	0.71045000	-1.50508000
H	-2.88263800	0.27563800	-1.92882400
H	-2.20142400	1.72055300	-1.15289700
H	-1.23186800	0.77064200	-2.30836500
N	-2.53776700	-0.26305700	0.62040400
H	-3.39127700	-0.59466200	0.18173600
H	-2.28542500	-0.90255900	1.37106300

#### EtOH-IM1

C	0.97426100	2.02677300	1.12428400
C	1.41209700	1.85225500	-0.32455900
C	0.80712200	0.51475400	-0.73376400
C	-0.45225100	1.51867500	1.09096600
H	1.58295900	1.40103600	1.79285000
H	1.03422600	3.05864700	1.47961100
H	2.49585400	1.83697100	-0.46098600
H	0.99653100	2.65893600	-0.94043900
H	0.39245400	0.55083700	-1.74765000
H	-1.12456000	2.22228200	0.58774500
H	-0.86592900	1.23175700	2.06179100
N	-0.35292500	0.29729400	0.22674200
C	1.74875800	-0.71507700	-0.68459400
O	2.94886900	-0.52732800	-0.91680200
O	1.17030700	-1.82391900	-0.44387800
H	-0.51380900	-1.68607600	-0.89687800
C	-1.68320600	-0.15607600	-0.44974500
C	-2.65790700	-0.47145400	0.66626100
H	-2.97486200	0.42767700	1.20454000
H	-3.53917900	-0.93759600	0.21594200
H	-2.21559100	-1.17869100	1.37603900
N	-2.13392500	0.88854300	-1.29777400
H	-2.01603900	0.64906700	-2.27564100
H	-3.09025400	1.17041400	-1.12000500
O	-1.36594200	-1.27922200	-1.19893900
H	-0.08897900	-0.47416300	0.86892300
O	0.32801500	-1.73777300	2.16617900
H	0.91990000	-1.57820800	2.90975900
H	0.87197900	-2.12691400	1.45604400



**EtOH-6a**

C	1.21245700	1.91703400	0.76954600
C	1.76056300	1.43515000	-0.56779900
C	0.92092500	0.19774000	-0.84050100
C	-0.28971900	1.76924500	0.59102900
H	1.56250300	1.25817100	1.57598100
H	1.49555200	2.94264900	1.01975200
H	2.82319000	1.18717800	-0.54394000
H	1.58750700	2.19030000	-1.34528500
H	0.80304700	-0.00953200	-1.91438700
H	-0.72236500	2.65339700	0.10386900
H	-0.82868200	1.57068100	1.52256600
N	-0.40552800	0.60322200	-0.30973400
C	1.46973100	-1.10637900	-0.19411400
O	2.68912200	-1.17254100	0.02075200
O	0.60498400	-2.01512000	0.00088900
H	-0.47851800	-1.57983600	1.42785200
C	-1.56150700	0.06574300	-0.63997800
C	-2.83063000	0.70579500	-0.20823900
H	-2.82468300	1.78403700	-0.38686500
H	-3.68340200	0.26167200	-0.72462400
H	-2.95126800	0.53505300	0.86851200
N	-1.59924400	-1.05400600	-1.35908300
H	-0.80273000	-1.69056300	-1.24162800
H	-2.50119600	-1.45881200	-1.56720800
O	-1.09699500	-1.14814500	2.05246300
H	-1.11336200	-1.70841400	2.83462500

**EtOH-6b**

C	0.38250600	2.57807200	-0.33526200
C	1.50485500	1.58763100	-0.06023000
C	0.98676100	0.26363800	-0.63043600
C	-0.86557000	1.76044700	-0.04711300
H	0.43627800	3.47584300	0.28604400
H	0.39330400	2.88810500	-1.38764100
H	1.65065900	1.47982400	1.02439200
H	2.46321900	1.86465600	-0.50649100
H	1.23441500	0.17552100	-1.69710200
H	-1.74276500	2.09672900	-0.61129800
H	-1.10870400	1.73106300	1.02397700
N	-0.47868900	0.40720200	-0.48838100
C	1.61132500	-0.92000800	0.13840000
O	2.71146500	-1.30265400	-0.30775800
O	0.99966100	-1.34568400	1.15329100
H	-0.35818000	-0.62072500	1.99907100
C	-1.34855400	-0.54462700	-0.74209600
O	-1.13540100	-0.21598100	2.45119500
H	-1.11269700	-0.54702500	3.35401600
C	-0.92357900	-1.84251400	-1.32708100
H	-0.12392600	-1.70774100	-2.05976400
H	-0.54613100	-2.48675600	-0.52518700
H	-1.76719000	-2.33993800	-1.80978300
N	-2.64265900	-0.36092800	-0.49250200

H	-3.29465800	-1.11166500	-0.66857900
H	-2.96644600	0.39691400	0.09361800

#### EtOH-6c

C	-0.92650200	2.14047700	-0.32719100
C	-1.41763300	1.31172900	0.85496600
C	-0.68643500	-0.01114600	0.68427400
C	0.55069000	1.78693400	-0.39483400
H	-1.43265400	1.82197500	-1.24760300
H	-1.08934700	3.21439400	-0.20311700
H	-2.50133500	1.17739300	0.87615700
H	-1.10412900	1.77530400	1.79819200
H	-0.44692000	-0.49182300	1.64517700
H	1.13727100	2.40652900	0.30079400
H	0.97508300	1.90101300	-1.39803500
N	0.57397800	0.37984600	0.02867800
C	-1.46260300	-1.04206000	-0.14579100
O	-2.58690100	-0.84807500	-0.56823700
O	-0.83129700	-2.18421300	-0.35133600
C	1.68684100	-0.39277900	0.09604600
C	2.97711700	0.24204500	-0.31831800
H	3.15091400	1.17979000	0.22014600
H	3.81188700	-0.43544800	-0.12750900
H	2.96285600	0.47647500	-1.38880000
N	1.56554200	-1.62635300	0.49002700
H	0.11589700	-2.14744300	0.04496900
H	2.46057500	-2.10551100	0.51036500

#### EtOH-6c-no-Hbond

C	0.58172400	2.23279700	0.31230900
C	1.27250000	1.44091800	-0.79371000
C	0.68114200	0.03003800	-0.64882600
C	-0.83122100	1.67545100	0.28769900
H	1.05193600	2.03571900	1.28530000
H	0.60536700	3.31277200	0.14378100
H	2.36436100	1.44045400	-0.72991300
H	0.99306000	1.84131000	-1.77496800
H	0.55483700	-0.46781100	-1.61820700
H	-1.42475600	2.15068500	-0.50887400
H	-1.36355300	1.80213700	1.23580400
N	-0.61262900	0.24949800	-0.00596200
C	1.59434900	-0.87391000	0.16510100
O	2.64102800	-1.29944700	-0.27288900
O	1.20791800	-1.14882200	1.41241900
C	-1.63462700	-0.65950400	-0.21194900
C	-2.99210200	-0.22171600	0.25086100
H	-3.32654900	0.66937100	-0.29248000
H	-3.72242700	-1.01765200	0.09012200
H	-2.98178800	0.03033600	1.31728400
N	-1.34691100	-1.79923400	-0.73621300
H	0.33260000	-0.73746600	1.55399100
H	-2.18845300	-2.36999700	-0.79177900

**EtOH-6b**

C	0.38250600	2.57807200	-0.33526200
C	1.50485500	1.58763100	-0.06023000
C	0.98676100	0.26363800	-0.63043600
C	-0.86557000	1.76044700	-0.04711300
H	0.43627800	3.47584300	0.28604400
H	0.39330400	2.88810500	-1.38764100
H	1.65065900	1.47982400	1.02439200
H	2.46321900	1.86465600	-0.50649100
H	1.23441500	0.17552100	-1.69710200
H	-1.74276500	2.09672900	-0.61129800
H	-1.10870400	1.73106300	1.02397700
N	-0.47868900	0.40720200	-0.48838100
C	1.61132500	-0.92000800	0.13840000
O	2.71146500	-1.30265400	-0.30775800
O	0.99966100	-1.34568400	1.15329100
H	-0.35818000	-0.62072500	1.99907100
C	-1.34855400	-0.54462700	-0.74209600
O	-1.13540100	-0.21598100	2.45119500
H	-1.11269700	-0.54702500	3.35401600
C	-0.92357900	-1.84251400	-1.32708100
H	-0.12392600	-1.70774100	-2.05976400
H	-0.54613100	-2.48675600	-0.52518700
H	-1.76719000	-2.33993800	-1.80978300
N	-2.64265900	-0.36092800	-0.49250200
H	-3.29465800	-1.11166500	-0.66857900
H	-2.96644600	0.39691400	0.09361800

**EtOH-7**

N	0.30380500	-0.63970100	-0.19175500
H	-0.24454700	0.83633000	-0.25647800
H	0.52242700	-0.86618500	0.78010600
C	2.70094800	-0.26599600	-0.36897700
C	2.89813500	1.11382400	-0.47746300
C	3.61285100	-1.02603300	0.36492800
C	3.98852200	1.72217200	0.13694100
H	2.19090700	1.71091100	-1.05329400
C	4.70704600	-0.42012700	0.98052100
H	3.46543400	-2.10227600	0.45006800
C	4.89614100	0.95492200	0.86729900
H	4.13402100	2.79573300	0.04239700
H	5.41261200	-1.02361800	1.54671700
H	5.75006900	1.42972000	1.34474700
C	1.50288900	-0.91298800	-1.00277300
H	1.68268100	-1.99369400	-1.11747800
H	1.33898900	-0.49658500	-2.00499200
C	-3.43761000	-0.22188100	1.96925900
C	-3.88165300	0.62014500	0.75917200
C	-2.77027500	0.43602400	-0.30038300
C	-2.01662700	-0.65563700	1.62785100
H	-3.48309600	0.33565500	2.90997900
H	-4.07525500	-1.10622200	2.07493200
H	-4.00281000	1.67888500	1.00461100

H	-4.84022700	0.27082400	0.36495600
H	-3.20419300	0.23496300	-1.28926700
H	-1.74762800	-1.61835000	2.07522700
H	-1.28845200	0.09719500	1.98957500
N	-2.05907500	-0.74026500	0.17281300
C	-1.99906700	1.75675500	-0.48382900
O	-2.61449300	2.78019100	-0.73685700
O	-0.68207300	1.76361400	-0.40964300
C	-0.97164400	-1.35382400	-0.57051800
C	-0.88075900	-2.83670700	-0.23364000
H	-1.82396000	-3.32862700	-0.48850100
H	-0.07311500	-3.31674900	-0.79747200
H	-0.67872800	-2.99374200	0.83007700
N	-1.24507500	-1.22153400	-1.97958200
H	-1.07196100	-0.28261900	-2.32944000
H	-0.68159400	-1.86538700	-2.52512800

#### EtOH-8

C	3.63582800	-0.02906900	-1.70343700
C	2.87465900	-1.32455400	-1.40574900
C	1.68474700	-0.91510600	-0.52164600
C	3.22214400	0.87800300	-0.56071100
H	4.71850200	-0.18008300	-1.75751900
H	3.30626800	0.40733100	-2.65401200
H	3.50451200	-2.02500300	-0.84877300
H	2.53674800	-1.83263300	-2.31363900
H	0.72683000	-1.16013400	-1.00551200
H	3.34986100	1.94089900	-0.79145600
H	3.80057100	0.65965700	0.35642700
N	1.80798800	0.54933000	-0.40688700
C	1.68535700	-1.66773100	0.81986500
O	2.61774600	-2.31432400	1.25280700
O	0.54864000	-1.57687300	1.51228800
C	1.03037700	1.33273400	0.54421400
C	1.04936100	2.80416400	0.13143900
H	0.26125700	3.34804900	0.66651800
H	2.00702800	3.26744000	0.38646900
H	0.88587800	2.91558900	-0.94407900
N	1.56124600	1.26608500	1.90081700
H	1.30212300	0.41138500	2.38596400
H	1.24750700	2.05304000	2.46148900
N	-0.34645600	0.76936900	0.52747000
H	-0.02532500	-0.85244000	1.11100600
H	-0.85761400	1.21330300	1.29146200
C	-2.48564500	0.31886400	-0.52506600
C	-2.66057800	-1.06500600	-0.62169200
C	-3.58360300	1.11652000	-0.19795600
C	-3.90667400	-1.63971200	-0.39100800
H	-1.81227600	-1.69644100	-0.88659300
C	-4.83390500	0.54546700	0.03295000
H	-3.45579300	2.19640400	-0.12626700
C	-4.99666800	-0.83448900	-0.06121500
H	-4.02948700	-2.71722800	-0.47159000

H	-5.68115400	1.17884700	0.28525700
H	-5.97121800	-1.28300500	0.11679200
C	-1.12874700	0.93685800	-0.71047600
H	-1.24134600	1.99820000	-0.98023400
H	-0.58333100	0.45124900	-1.52932100

**EtOH-11**

C	-1.05519600	1.26621600	-0.65169500
N	-1.21160000	2.12177200	0.48500600
H	-1.95254800	2.79532200	0.31346500
N	0.50126200	0.86474700	-0.65116700
H	0.73339300	0.43749300	-1.55241000
H	1.04465600	1.74450300	-0.57108500
C	2.34865600	-0.47971900	0.24501200
C	2.63872500	-1.62506800	-0.50134400
C	3.39745100	0.28257800	0.76522000
C	3.95958600	-2.00074400	-0.72949200
H	1.82238100	-2.22880300	-0.89850000
C	4.71866600	-0.09323800	0.53961500
H	3.17342600	1.17263400	1.35237400
C	5.00067300	-1.23444500	-0.20936500
H	4.17663600	-2.89538100	-1.30782000
H	5.52892200	0.50285300	0.95197900
H	6.03261800	-1.52925600	-0.38341300
C	0.92406200	-0.05942600	0.44531200
H	0.77139300	0.47522300	1.38830000
H	0.23750300	-0.91266500	0.42028100
O	1.31054000	3.41274200	0.27509100
H	1.88338400	3.65225400	1.01126000
H	0.42223400	3.23102100	0.64870400
C	-1.22691000	2.06373900	-1.93539300
H	-0.63132600	2.98221300	-1.90361600
H	-0.93967900	1.49448000	-2.82411800
H	-2.28453200	2.33314300	-2.03568800
N	-1.78080500	0.05157500	-0.59344400
C	-2.75165600	-1.94765300	-1.29673500
C	-3.74238100	-1.22871400	-0.38901200
C	-2.88610900	-0.21406400	0.36110300
C	-1.88071800	-0.80107700	-1.77645600
H	-2.15226900	-2.65450100	-0.70932600
H	-3.22350400	-2.48883500	-2.12257600
H	-4.26343300	-1.89730600	0.30054800
H	-4.48785300	-0.70123100	-0.99982000
H	-3.44987300	0.71099500	0.55554600
H	-2.36554100	-0.28133300	-2.62136800
H	-0.88823200	-1.13646000	-2.11715800
C	-2.32122100	-0.72125100	1.71607500
O	-2.42338100	-1.93695600	1.98814800
O	-1.76926200	0.16260000	2.43544300
H	-1.43469500	1.57709200	1.33514500

**EtOH-12**

C	-0.77516600	0.94850100	-0.76197100
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N	-1.00320200	1.98135700	0.26688500
H	-1.72815300	2.62562900	-0.04461600
N	0.63668900	0.56975500	-0.69172200
H	0.87663400	0.00315200	-1.50399300
H	1.61938300	2.21168200	-0.70818000
C	2.51335400	-0.48483500	0.43926000
C	2.90087200	-1.66826300	-0.19531600
C	3.50093500	0.36228600	0.94761100
C	4.24853800	-1.99455300	-0.32794300
H	2.13763900	-2.34411900	-0.58242700
C	4.84956100	0.03903100	0.81981000
H	3.20492100	1.27899700	1.45802000
C	5.22577500	-1.13996000	0.17882400
H	4.53595400	-2.91998500	-0.82163600
H	5.60710200	0.70586200	1.22504900
H	6.27813000	-1.39571100	0.08080800
C	1.06044200	-0.11784400	0.53944400
H	0.90945300	0.56847100	1.38287000
H	0.44593200	-1.01005100	0.73715600
O	1.79405600	3.15568200	-0.49652400
H	2.72392500	3.21162900	-0.25345500
H	-0.15875500	2.54843800	0.36085300
C	-1.03932300	1.51075300	-2.15740200
H	-0.44989200	2.42080700	-2.31354500
H	-0.77676100	0.79708900	-2.94565200
H	-2.10230100	1.75981200	-2.26922500
N	-1.63014600	-0.19153200	-0.42215300
C	-2.84591000	-2.12479400	-0.96490800
C	-3.84145600	-0.98838400	-0.77174600
C	-3.02403800	0.04715000	-0.01013000
C	-1.57217700	-1.36566900	-1.29621800
H	-2.72338800	-2.68581600	-0.02855200
H	-3.13159500	-2.82971600	-1.75097300
H	-4.75199200	-1.27279600	-0.23884600
H	-4.12367300	-0.57007600	-1.74722500
H	-3.36474500	1.06596800	-0.25726000
H	-1.57204500	-1.09063900	-2.36629300
H	-0.66481500	-1.95467400	-1.10361200
C	-3.13744900	-0.10063400	1.51269000
O	-3.95467900	-0.81596200	2.06178300
O	-2.27790900	0.61759700	2.22200900
H	-1.68983100	1.16374300	1.60949300

#### EtOH-18

N	-0.31886000	-0.88998700	0.34805200
H	-0.78932900	-1.38162400	1.10672100
H	-0.15217100	0.83270900	0.47468600
C	-2.55229200	-0.30952800	-0.45938000
C	-3.48320000	-1.11499900	0.20431800
C	-2.89476300	1.01114200	-0.75687100
C	-4.72544200	-0.60818600	0.57571300
H	-3.23295700	-2.15343100	0.42455800
C	-4.13905600	1.52055100	-0.39141200

H	-2.17652700	1.64502800	-1.27452600
C	-5.05565000	0.71326400	0.27822400
H	-5.43936400	-1.24679800	1.09067900
H	-4.39278200	2.55052100	-0.63158100
H	-6.02680900	1.11031200	0.56415200
C	-1.20638500	-0.87090800	-0.82807300
H	-0.73312800	-0.25104500	-1.60180600
H	-1.33924200	-1.87959800	-1.25008100
C	4.07679400	0.44876200	-0.71597400
C	3.68057400	0.89823500	0.68268800
C	2.17225600	0.69221100	0.68502500
C	3.20257400	-0.77665500	-0.89989500
H	3.81797500	1.22152400	-1.45248200
H	5.14223200	0.22157200	-0.81891300
H	3.95742200	1.92798700	0.92250400
H	4.13393100	0.23286300	1.42957400
H	1.81433200	0.41307500	1.68724300
H	3.65086400	-1.63932900	-0.37639800
H	3.07420500	-1.06115700	-1.94918700
N	1.91279800	-0.38706300	-0.29898300
C	1.39347400	1.94740700	0.29941000
O	1.90242700	3.02076700	0.03924500
O	0.07515600	1.79652000	0.28982300
C	1.03999500	-1.48141900	0.14524100
C	1.45790300	-2.11389900	1.47313000
H	1.27218000	-1.45008700	2.32343700
H	0.89450200	-3.03823800	1.64700300
H	2.52271000	-2.36744100	1.45041000
N	1.12090300	-2.51131300	-0.86649300
H	0.50428800	-3.28710500	-0.64361600
H	0.87242000	-2.15535700	-1.78580500

#### EtOH-19

N	-0.65324000	-0.18286600	0.26105600
H	1.69683200	1.37905800	-1.13198000
H	-0.75705900	-0.88388500	-0.46979700
C	-3.06925400	-0.02790600	0.43008700
C	-3.40819100	1.26778900	0.02851300
C	-3.92038500	-1.08176700	0.09645600
C	-4.57616600	1.50528400	-0.68865300
H	-2.74284400	2.09245100	0.28411900
C	-5.09065300	-0.84980000	-0.62634800
H	-3.66340500	-2.09412200	0.40758500
C	-5.42067700	0.44430400	-1.01930300
H	-4.83129000	2.51879500	-0.99009400
H	-5.74432000	-1.68124900	-0.88015100
H	-6.33395200	0.62894300	-1.58021700
C	-1.78940900	-0.28366000	1.17628900
H	-1.85683400	-1.26415000	1.67950300
H	-1.66007300	0.47496800	1.96159500
C	2.98645900	-2.14490800	-1.04820600
C	3.83841500	-0.88987100	-0.94130000
C	3.01930100	-0.02241300	0.02553700

C	1.57956100	-1.56740900	-1.11147900
H	3.23276700	-2.76586400	-1.91498100
H	3.10528000	-2.75866400	-0.14439800
H	3.91050300	-0.39820300	-1.92268200
H	4.85392900	-1.05664300	-0.57166300
H	3.30112600	-0.24168500	1.06557400
H	0.82361500	-2.27624600	-0.75456900
H	1.31305800	-1.30124200	-2.14447400
N	1.62229400	-0.34484000	-0.27516000
C	3.30663200	1.44304200	-0.22351800
O	4.29860300	2.01252700	0.18396200
O	2.41668000	2.04846300	-1.00933300
C	0.68317000	-0.26207200	0.86817400
C	0.86339900	-1.43209400	1.83797800
H	1.89215600	-1.46934500	2.21342700
H	0.20107000	-1.33282400	2.70496300
H	0.63380500	-2.38777900	1.35530400
N	0.98555700	0.96584200	1.57516200
H	0.50687200	1.74883300	1.13551500
H	0.70101200	0.92287000	2.54763200

#### EtOH-20

N	-0.65059400	-0.25095300	0.21924900
H	1.64989600	1.42462800	-1.05379600
H	-0.68805000	-0.80926900	-0.62918800
C	-3.07650100	-0.14720000	0.37469900
C	-3.36574200	1.20820800	0.18513200
C	-3.98093500	-1.09975100	-0.09474400
C	-4.53525000	1.60159800	-0.45605800
H	-2.65980600	1.95474400	0.54897500
C	-5.15494300	-0.71080100	-0.74104400
H	-3.76384300	-2.15793800	0.04959300
C	-5.43420600	0.64062600	-0.92258600
H	-4.75039800	2.65928600	-0.59174300
H	-5.85008900	-1.46524300	-1.10272300
H	-6.34891400	0.94719000	-1.42476700
C	-1.80411100	-0.55935800	1.06171700
H	-1.86854800	-1.62825200	1.33113700
H	-1.68315500	0.00474600	1.99606800
C	3.06762200	-2.04961800	-1.07916900
C	3.89885000	-0.79222400	-0.88351600
C	3.01600500	0.04347200	0.05992900
C	1.66439500	-1.47643500	-1.19983500
H	3.36744200	-2.63522400	-1.95368600
H	3.13920500	-2.69555900	-0.19307100
H	4.02211600	-0.27048100	-1.84374700
H	4.89332000	-0.95833800	-0.46086700
H	3.28172100	-0.18105000	1.10452800
H	0.88647400	-2.20469000	-0.94755500
H	1.47072100	-1.13768100	-2.22794300
N	1.63635800	-0.31208000	-0.28007000
C	3.27534600	1.51953600	-0.17884800
O	4.26456500	2.09932800	0.21889200



O	2.34935800	2.11812200	-0.92477500
C	0.66306600	-0.35941500	0.85256900
C	0.86383600	-1.61514300	1.70590800
H	1.88033300	-1.65066200	2.11638600
H	0.16895800	-1.61964200	2.55104900
H	0.69849300	-2.52884800	1.12545000
N	0.77950000	0.78405700	1.72270600
H	1.61369900	0.78552600	2.29916000
H	0.68760900	1.65900800	1.21568300

**EtOH-21**

N	-0.48614200	-0.35398600	0.06680200
H	3.53879100	-0.38315200	1.08481300
H	-0.27174700	-0.04286000	-0.87757800
C	-2.92149800	-0.54787500	-0.13752400
C	-3.23675100	0.53440000	0.69098800
C	-3.85219600	-0.95393900	-1.09430200
C	-4.45640200	1.19140000	0.56789500
H	-2.50733700	0.85911200	1.43293200
C	-5.07740800	-0.29859400	-1.22123000
H	-3.61399100	-1.79299600	-1.74763600
C	-5.38241300	0.77592100	-0.39074900
H	-4.68888900	2.03046900	1.22021700
H	-5.79101100	-0.62712100	-1.97371700
H	-6.33562900	1.29030600	-0.48957300
C	-1.61587800	-1.27846200	0.03494000
H	-1.52273900	-2.04836400	-0.75093800
H	-1.62281400	-1.80797100	0.99675400
C	1.53186400	2.52174500	-0.10670900
C	2.71097300	1.90806400	-0.84266900
C	2.43392000	0.40097200	-0.70973200
C	1.37413600	1.59143400	1.08596200
H	1.70128600	3.56336600	0.18316100
H	0.63176400	2.48516700	-0.73566800
H	3.64934900	2.16272200	-0.32869700
H	2.80795500	2.20951300	-1.88925600
H	1.82811400	0.06020500	-1.56393900
H	0.34645700	1.57884600	1.46260700
H	2.03784800	1.89087800	1.90950600
N	1.76928000	0.24739800	0.59073900
C	3.75529900	-0.34335100	-0.75261800
O	4.35034800	-0.59423900	-1.77958000
O	4.25299900	-0.63589300	0.44748400
C	0.73819900	-0.81418600	0.72477400
C	1.27938500	-2.12615300	0.16087600
H	2.19711200	-2.43389800	0.67568400
H	0.53338200	-2.91196000	0.31017300
H	1.48415000	-2.06000400	-0.91352100
N	0.40491300	-1.04195100	2.11631600
H	1.23569200	-1.31351500	2.63531400
H	0.03174600	-0.19618100	2.53970500

**EtOH-22**

N	-0.47043500	-0.39701800	0.11125000
H	3.53479900	-0.46777900	0.97568800
H	-0.29132900	-0.04285700	-0.82657000
C	-2.90026800	-0.54190200	-0.12727400
C	-3.20109100	0.55935000	0.68131000
C	-3.82473600	-0.93908900	-1.09350700
C	-4.40280700	1.24292300	0.53023900
H	-2.47564400	0.87798800	1.42961800
C	-5.03131200	-0.25600800	-1.24889900
H	-3.59642000	-1.79234800	-1.73166000
C	-5.32342400	0.83629500	-0.43720700
H	-4.62532200	2.09599900	1.16762800
H	-5.74067700	-0.57742800	-2.00834100
H	-6.26259900	1.37144400	-0.55737700
C	-1.61371100	-1.29978900	0.07408100
H	-1.52929100	-2.08575200	-0.69730500
H	-1.66161300	-1.81883800	1.04236300
C	1.44656800	2.49628000	0.13057600
C	2.59410600	1.98583500	-0.72563200
C	2.37589900	0.46233600	-0.69744700
C	1.39984000	1.47015000	1.25082300
H	1.60044900	3.51822200	0.49090700
H	0.50765500	2.47089200	-0.43977100
H	3.55532300	2.23495100	-0.25281500
H	2.61321500	2.37056200	-1.74884500
H	1.74594500	0.16321000	-1.54945800
H	0.40665400	1.39911600	1.70384300
H	2.12126800	1.71614800	2.04293400
N	1.78210700	0.18477800	0.61389700
C	3.71923600	-0.23029700	-0.84708800
O	4.29677800	-0.35166700	-1.90748300
O	4.24835400	-0.63371000	0.30515600
C	0.77973800	-0.89436300	0.71081900
C	1.30660300	-2.15935800	0.03926900
H	2.24112200	-2.49311500	0.50295100
H	0.57168600	-2.96484600	0.14467600
H	1.47129000	-2.01291100	-1.03352900
N	0.59368200	-1.18821800	2.12086600
H	-0.06956200	-0.54238100	2.54264400
H	0.23666500	-2.12823300	2.25856300

#### EtOH-23

N	-0.71459900	-0.22262400	-0.17230500
H	2.49584500	-1.03437700	1.41704100
H	-0.77562900	0.25793500	-1.06837500
C	-3.13095600	-0.48553100	-0.01714500
C	-3.45070300	0.38468600	1.03029700
C	-4.06554700	-0.68974300	-1.03203000
C	-4.68112800	1.03190400	1.06359600
H	-2.72122100	0.54955300	1.82298500
C	-5.30106000	-0.04191300	-1.00381400
H	-3.82372300	-1.36424200	-1.85286300
C	-5.61115400	0.81954500	0.04422800

H	-4.91954800	1.70132200	1.88716200
H	-6.02014200	-0.21133500	-1.80207900
H	-6.57381900	1.32490600	0.07027800
C	-1.80031600	-1.18814000	-0.04253600
H	-1.81296000	-1.94565200	-0.84580100
H	-1.66277300	-1.73070800	0.90406000
C	2.22862500	2.61006000	-0.27692800
C	3.38472800	1.76174600	-0.82014400
C	2.89063400	0.28800800	-0.73668900
C	1.41683100	1.61566700	0.53415200
H	2.57697700	3.46173800	0.31569800
H	1.61203300	2.99541500	-1.09722000
H	4.28637000	1.88922900	-0.21166200
H	3.65463200	2.02757100	-1.84589500
H	2.93739600	-0.18928900	-1.72484100
H	0.37152800	1.90350100	0.67595500
H	1.87187200	1.47185600	1.53447600
N	1.51029400	0.41731700	-0.29629300
C	3.88865900	-0.49953500	0.12261100
O	5.04147300	-0.61428700	-0.25958300
O	3.50492100	-1.02571000	1.27226500
C	0.65492100	-0.71794100	-0.01582300
C	0.98743700	-1.87543300	-0.95082600
H	2.00004700	-2.26274600	-0.79562000
H	0.29411800	-2.70573400	-0.78298400
H	0.88834000	-1.55121500	-1.99238700
N	0.86157100	-1.17612300	1.37538300
H	0.36944300	-0.55843700	2.01962500
H	0.51337800	-2.11958700	1.52980100

#### EtOH-24

N	-0.55145700	-0.26788200	0.59226700
H	0.84572600	2.52139100	-0.95967200
H	-0.80955600	-1.00114200	-0.05805500
C	-2.93580300	0.17075700	0.44269700
C	-3.13764700	0.49797500	-0.90202500
C	-3.93278800	-0.51688800	1.13479300
C	-4.31742900	0.13763400	-1.54500700
H	-2.36084500	1.04107400	-1.44009800
C	-5.11819300	-0.87303700	0.49435000
H	-3.77944300	-0.77282600	2.18208700
C	-5.31064100	-0.54823300	-0.84610800
H	-4.46634600	0.39725500	-2.59031900
H	-5.89098000	-1.40611200	1.04280700
H	-6.23467300	-0.82654500	-1.34712700
C	-1.65126000	0.55300500	1.11861500
H	-1.73361900	0.41093000	2.20386100
H	-1.41305500	1.60618200	0.91174700
C	2.68795900	-2.74194000	-0.53329600
C	3.69847900	-1.60490700	-0.58742600
C	3.10821600	-0.51639000	0.32014400
C	1.36090300	-2.00454300	-0.51146900
H	2.76363900	-3.43021200	-1.37920800

H	2.80383100	-3.32004700	0.39183200
H	3.76985600	-1.22066500	-1.61469600
H	4.70299100	-1.89136400	-0.26617600
H	3.49929100	-0.60480100	1.34211900
H	0.55086700	-2.59069900	-0.06312900
H	1.05711900	-1.68105900	-1.51913100
N	1.66271400	-0.82924600	0.31656600
C	3.45209500	0.87811400	-0.25270000
O	4.59014900	1.29230200	0.06368000
O	2.60637700	1.41765100	-1.00547100
C	0.73741300	-0.05113000	0.84657800
C	1.08888000	1.05367600	1.77521700
H	2.15276200	1.07512800	2.00725800
H	0.79364400	2.00770900	1.32245300
H	0.53055000	0.93407300	2.70954600
N	-0.02447100	3.01820100	-0.75193200
H	-0.57072800	3.03665700	-1.60878200
H	0.22816400	3.98338900	-0.55747100

#### EtOH-25

C	3.92144200	-0.36292300	-0.99712800
C	2.79004200	-1.25743300	-1.48881800
C	1.63326900	-0.88362800	-0.57414300
C	3.21465100	0.93976000	-0.63064600
H	4.38043500	-0.80755900	-0.10596200
H	4.70947700	-0.21648700	-1.74195200
H	3.02648000	-2.32390600	-1.44883500
H	2.51391200	-1.00123900	-2.51912200
H	0.66780500	-1.09713500	-1.06013100
H	3.29548800	1.68629800	-1.43556900
H	3.65685500	1.38642800	0.27396200
N	1.81037100	0.56445900	-0.42608300
C	1.63477100	-1.69045800	0.73291900
O	2.50518800	-2.47192600	1.06099000
O	0.57155300	-1.49652400	1.51358100
C	1.01103400	1.40319600	0.46059400
C	1.04360600	2.84074000	-0.05354400
H	0.33130500	3.45113900	0.51246600
H	2.03893400	3.28015300	0.07362900
H	0.79393600	2.88481400	-1.11781200
N	1.41690400	1.44790800	1.86688600
H	2.27478400	1.97849800	1.98119000
H	1.57153600	0.51837000	2.24896000
N	-0.35167200	0.83467100	0.49209300
H	0.00992500	-0.74855200	1.13772200
H	-0.83616800	1.30337000	1.25809900
C	-2.50117000	0.31595600	-0.50953600
C	-2.65073800	-1.07226200	-0.58228500
C	-3.60985500	1.09716300	-0.17905400
C	-3.88265500	-1.66679100	-0.32708800
H	-1.79525800	-1.69326600	-0.84812100
C	-4.84589700	0.50623500	0.07715200
H	-3.50175000	2.18013200	-0.12484100

C	-4.98359200	-0.87766700	0.00484000
H	-3.98580700	-2.74749600	-0.39039300
H	-5.70151100	1.12733900	0.33168700
H	-5.94719300	-1.34173600	0.20157800
C	-1.16140100	0.95981100	-0.73056300
H	-1.30372200	2.01388700	-1.01416900
H	-0.62366000	0.47509700	-1.55542600

#### EtOH-26

C	-3.54835000	0.51491600	-1.45518100
C	-2.25246100	1.25097800	-1.77133100
C	-1.35804800	0.84919600	-0.59404900
C	-3.06506800	-0.82960500	-0.91666500
H	-4.09886900	1.05590400	-0.67277300
H	-4.21464200	0.41006100	-2.31632600
H	-2.36285700	2.33456200	-1.86067200
H	-1.80786800	0.86808900	-2.69831400
H	-0.29873200	0.96426700	-0.86423800
H	-3.04281700	-1.59741300	-1.70588700
H	-3.73390100	-1.19981000	-0.12328900
N	-1.71065700	-0.55188500	-0.42684900
C	-1.56215200	1.83241200	0.56819100
O	-1.34174400	3.02080300	0.38936300
O	-1.97823600	1.39406000	1.73908200
C	-1.11007700	-1.41777200	0.55765500
C	-1.23864200	-2.87789300	0.12433100
H	-0.70555900	-3.51708600	0.83829400
H	-2.28524400	-3.20036200	0.09931700
H	-0.81480800	-3.03298800	-0.87376000
N	-1.77538300	-1.21559300	1.87798700
H	-1.24632600	-1.64502300	2.63554800
H	-2.68284400	-1.67741100	1.87907600
N	0.26566700	-0.98448600	0.75780600
H	-1.95214600	0.37241800	1.83746200
H	0.63339900	-1.39006400	1.61556500
C	2.47523600	-0.49477000	-0.20898700
C	2.53034200	0.75841500	0.40716400
C	3.64856000	-1.02827200	-0.74952300
C	3.72984300	1.46403500	0.47388400
H	1.62364100	1.17455600	0.84262200
C	4.84795800	-0.32360400	-0.68832000
H	3.61954300	-2.01021800	-1.22146600
C	4.89263100	0.92731600	-0.07508800
H	3.75556600	2.43788700	0.95802800
H	5.75152800	-0.75548300	-1.11306300
H	5.82894800	1.47797200	-0.02162800
C	1.18368500	-1.26121300	-0.33954300
H	1.41627700	-2.33533900	-0.44503600
H	0.67942500	-0.97450500	-1.27486000

#### EtOH-27

C	3.57333800	-1.47559100	-0.15454300
C	2.36520300	-1.98913100	-0.92866700

C	1.24908400	-1.07926100	-0.43685000
C	3.37111500	0.03611300	-0.10814400
H	3.56562400	-1.88601300	0.86235900
H	4.52878800	-1.74189800	-0.61456300
H	2.13655700	-3.03992100	-0.73562100
H	2.50779100	-1.85554000	-2.00874300
H	0.40283600	-1.07245900	-1.12534800
H	3.94384000	0.55509300	-0.88684400
H	3.64882100	0.45494900	0.86436700
N	1.92509300	0.23266700	-0.37067600
C	0.71580400	-1.49970900	0.96596600
O	0.16901500	-2.62804700	0.97837200
O	0.88339200	-0.70188700	1.91538400
C	1.34091000	1.40223100	-0.15288900
C	2.13082900	2.49628600	0.48658500
H	1.54956300	3.41843700	0.54094600
H	2.42845200	2.19969900	1.49846100
H	3.04359000	2.69768600	-0.08332400
N	-1.22848700	4.17729100	0.24086700
H	-1.19556400	4.38180200	1.23627300
H	-0.92682800	5.02030300	-0.24046400
N	0.09183200	1.70863700	-0.47892200
H	-2.20932700	4.04438700	0.00647500
H	-0.24452300	2.64185300	-0.17685500
C	-1.85564000	0.14546500	-0.69768600
C	-2.29731200	0.40616500	0.60003000
C	-2.42595800	-0.91142300	-1.41048700
C	-3.29158100	-0.37991000	1.17693500
H	-1.85093700	1.21978000	1.16994200
C	-3.42113000	-1.69752600	-0.83581500
H	-2.08236000	-1.12402600	-2.42301300
C	-3.85688200	-1.43298900	0.46122200
H	-3.62211700	-0.17070200	2.19170000
H	-3.85154100	-2.52220700	-1.39899500
H	-4.62995800	-2.04884800	0.91434000
C	-0.83630500	1.03056700	-1.37152500
H	-1.36476000	1.83943300	-1.89634800
H	-0.28511800	0.48977600	-2.14847200

#### **EtOH-28**

C	-0.66907100	-0.98431200	0.86837200
N	-0.93009300	-2.14047300	0.01228600
H	-1.80639500	-2.58870300	0.26967200
N	0.74652400	-0.69239400	0.76732700
H	1.02992200	-0.03166200	1.48702200
C	2.73358200	-0.00615500	-0.43439200
C	3.20609500	1.30447200	-0.35151500
C	3.65024900	-1.06022900	-0.37913300
C	4.57054500	1.56204500	-0.22182800
H	2.49545900	2.13049900	-0.39319100
C	5.01257700	-0.80860700	-0.25183200
H	3.28424000	-2.08503700	-0.43809200
C	5.47600300	0.50528400	-0.17305900

H	4.92531900	2.58843100	-0.16178400
H	5.71646400	-1.63706500	-0.21635800
H	6.54104700	0.70285500	-0.07605800
C	1.26043200	-0.28150500	-0.53849600
H	1.07252100	-1.09539100	-1.25029900
H	0.75470200	0.61674200	-0.93565900
H	-0.19965100	-2.82502800	0.19606400
C	-0.98177600	-1.26983200	2.33719100
H	-0.42941800	-2.15856300	2.65935500
H	-0.69787900	-0.43941700	2.99392400
H	-2.05250300	-1.46080100	2.47781500
N	-1.48015100	0.13801600	0.33129900
C	-2.53885800	2.22193400	0.60664000
C	-3.60564900	1.14544900	0.75837700
C	-2.92200100	-0.08805300	0.15349200
C	-1.27496700	1.45623100	0.95615200
H	-2.49516600	2.58141100	-0.43078700
H	-2.69949000	3.08663600	1.25651700
H	-4.55994700	1.37396900	0.27481700
H	-3.79952700	0.95785200	1.82245400
H	-3.28415100	-1.00409200	0.64041200
H	-1.17811500	1.37915200	2.05215700
H	-0.36170300	1.92950500	0.57281800
C	-3.26497700	-0.22922200	-1.32837300
O	-4.38552800	-0.47846700	-1.72560100
O	-2.24611400	-0.02959100	-2.15420900
H	-1.46965200	0.10211800	-1.54828200

#### EtOH-29

C	0.66381200	1.23067700	0.51767500
N	0.93795000	2.18776400	-0.53470700
H	0.96286600	1.75820400	-1.45539700
N	-0.75678200	0.92775000	0.51832900
H	-1.00437400	0.37961100	1.33905200
C	-2.75524900	-0.02760000	-0.46298600
C	-3.17192400	-1.35123700	-0.31545800
C	-3.70445900	0.99481400	-0.36830600
C	-4.51407200	-1.65182900	-0.08177700
H	-2.43729300	-2.15338800	-0.38847200
C	-5.04335200	0.70012400	-0.13508000
H	-3.38058700	2.02917600	-0.47840200
C	-5.45171800	-0.62678200	0.00873600
H	-4.82527200	-2.68813200	0.02872400
H	-5.77263700	1.50419700	-0.06684500
H	-6.49858900	-0.85897400	0.19023200
C	-1.30751500	0.30925200	-0.68425700
H	-1.22079400	1.02888900	-1.51063600
H	-0.76458200	-0.60439400	-0.98810200
H	1.81973400	2.66826700	-0.38895300
C	0.99874300	1.87768500	1.85645500
H	0.44662000	2.81694900	1.95283200
H	0.72017700	1.22924100	2.69357400
H	2.06985900	2.09411600	1.94146400

N	1.44573700	-0.03161900	0.29227700
C	2.39022600	-2.01180100	1.17484700
C	3.47750000	-0.94515800	1.17173100
C	2.90951700	0.09541500	0.19979400
C	1.12522200	-1.17015700	1.17677800
H	2.44459700	-2.62036100	0.26151700
H	2.44462100	-2.68835800	2.03235600
H	4.46755900	-1.30114100	0.87181400
H	3.56510900	-0.49145200	2.16763900
H	3.26978200	1.10265400	0.44761500
H	0.90531900	-0.83443100	2.20393000
H	0.24559600	-1.71314700	0.80700700
C	3.37834600	-0.18066500	-1.22685700
O	4.53379800	-0.07021400	-1.58066400
O	2.41463100	-0.57268700	-2.05544400
H	1.59605500	-0.55802100	-1.49114900

### EtOH-30

C	-0.79207400	1.40591300	0.15463300
N	-0.71598200	2.35946400	1.23782300
H	-0.41697700	1.93147200	2.10993200
N	0.56317600	0.93932700	-0.16221200
H	0.54034900	0.00998500	-0.57384600
C	2.84859200	0.31044900	0.28632700
C	3.06770400	-1.02701900	0.62392800
C	3.73652500	0.94200900	-0.58804600
C	4.15768600	-1.72191600	0.10348000
H	2.37764400	-1.52427400	1.30689300
C	4.82875400	0.25319400	-1.10796000
H	3.56462700	1.98383100	-0.85706600
C	5.04136900	-1.08139100	-0.76260900
H	4.31975000	-2.76194800	0.37722300
H	5.51756000	0.75773700	-1.78167500
H	5.89585700	-1.61942000	-1.16634600
C	1.64487400	1.03487800	0.81872700
H	1.87981200	2.09469400	0.97823800
H	1.39389900	0.60986400	1.80752000
H	-1.63604800	2.76049600	1.39901000
C	-1.35183200	2.14062900	-1.05930800
H	-0.70958800	3.00159700	-1.26238000
H	-1.35548000	1.51081800	-1.95449500
H	-2.37286100	2.49719500	-0.87582400
N	-1.72343500	0.28344500	0.49698100
C	-2.09024700	-1.80722400	1.53792200
C	-1.82535000	-2.07843600	0.06333600
C	-2.02646900	-0.69416100	-0.56747600
C	-1.40406900	-0.46694100	1.72946200
H	-3.16856400	-1.72013600	1.72995100
H	-1.69170100	-2.58016600	2.20110200
H	-2.46939600	-2.83942400	-0.38718800
H	-0.78225700	-2.39097500	-0.07996300
H	-1.39729400	-0.57863400	-1.45983300
H	-0.31771900	-0.62923600	1.82680800



H	-1.75265200	0.07478300	2.61547500
C	-3.46935000	-0.52687800	-1.04119600
O	-3.93853900	-1.15225100	-1.96964500
O	-4.18060800	0.34395300	-0.33472000
H	-3.52876900	0.70384400	0.32592100

**EtOH-31**

C	-0.80990800	1.40795400	0.12598800
N	-0.86204300	2.36680300	1.21005000
H	-0.34201000	3.20138200	0.95177600
N	0.57097300	0.98843000	-0.18696400
H	0.58725500	0.12326300	-0.72190800
C	2.82698300	0.27614500	0.29632600
C	2.98194100	-1.09589900	0.51008700
C	3.78592300	0.95647300	-0.45734700
C	4.07915500	-1.77650000	-0.01318700
H	2.23499800	-1.63208500	1.09720000
C	4.88617900	0.28116800	-0.97938700
H	3.66537800	2.02556100	-0.63014200
C	5.03503000	-1.08740300	-0.75716200
H	4.19098800	-2.84371100	0.16403700
H	5.63093700	0.82332500	-1.55754900
H	5.89569500	-1.61491800	-1.16163600
C	1.61866400	0.98931700	0.83409200
H	1.88235600	2.02885500	1.07470800
H	1.32632800	0.50945400	1.78389000
H	-0.44322000	2.00791500	2.06402400
C	-1.36550500	2.09689600	-1.11602200
H	-0.77606300	2.99849700	-1.31018500
H	-1.28369500	1.46392100	-2.00566300
H	-2.41201400	2.38490500	-0.97195000
N	-1.70475300	0.28483600	0.49790900
C	-2.12530200	-1.75166000	1.60386600
C	-1.85324900	-2.08067400	0.14167400
C	-2.00456500	-0.71367700	-0.54170200
C	-1.39662700	-0.42948700	1.75216400
H	-3.20166100	-1.62329700	1.78193500
H	-1.75609400	-2.51377300	2.29584900
H	-2.51396500	-2.83792500	-0.29045700
H	-0.81755800	-2.42595900	0.02284800
H	-1.35347600	-0.64772800	-1.42373400
H	-0.31742400	-0.62893000	1.84826100
H	-1.72225400	0.15589900	2.61915100
C	-3.43472800	-0.52863500	-1.04746000
O	-3.89295000	-1.15092300	-1.98354900
O	-4.14993900	0.34975800	-0.35427200
H	-3.50456100	0.71008100	0.31357300

**EtOH-32**

C	-0.66432200	-1.00298300	0.18663900
N	-1.00261700	-1.65004200	-1.09501900
H	-0.68797000	-2.61771000	-1.11714900
N	0.78131700	-0.77581000	0.30985900

H	0.93584100	-0.06490500	1.02168500
C	2.98981900	-0.12769800	-0.42559900
C	3.39713600	1.20745400	-0.44038500
C	3.87718000	-1.10090400	0.04266900
C	4.66939800	1.56745500	0.00235700
H	2.71105800	1.97064300	-0.80792000
C	5.14811100	-0.74666900	0.48364100
H	3.56227100	-2.14386500	0.05692600
C	5.54689600	0.59052000	0.46508100
H	4.97435800	2.61121400	-0.01651300
H	5.83207500	-1.51340000	0.84052500
H	6.54106300	0.86775100	0.80781300
C	1.60494700	-0.51088200	-0.86835600
H	1.66029000	-1.42648000	-1.47426700
H	1.21448500	0.28770200	-1.52443000
H	-0.57451900	-1.17909600	-1.88875200
C	-1.06992400	-1.95935500	1.30145000
H	-0.46722700	-2.86872200	1.22162100
H	-0.86642100	-1.50006200	2.27461400
H	-2.12792400	-2.23941600	1.25518100
N	-1.38897100	0.24834100	0.31878600
C	-2.25856500	2.33475800	-0.39948300
C	-2.91511300	1.87989700	0.90020200
C	-2.74723900	0.36109300	0.82303000
C	-1.08781100	1.36391400	-0.58452500
H	-2.97187700	2.22638000	-1.22793700
H	-1.93814100	3.38032200	-0.38075800
H	-3.96039600	2.18331600	0.99638000
H	-2.35996800	2.24716700	1.77098900
H	-2.84059400	-0.09243200	1.81963000
H	-0.12683700	1.82418000	-0.30962600
H	-1.01005600	1.05114700	-1.63959000
C	-3.89067900	-0.24068300	-0.01316900
O	-5.05108800	0.00260200	0.26993900
O	-3.59993500	-1.02538200	-1.03719800
H	-2.61841200	-1.27443100	-1.11704700

### EtOH-33

C	-0.69037000	-0.00680100	0.93863300
N	0.04090100	-2.32966600	-1.18193100
H	0.05691300	-3.18912600	-1.72436000
N	0.59882600	0.22105300	0.68715500
H	0.85143400	0.93058700	0.00898400
C	2.98290800	-0.20053100	0.53800900
C	3.43415000	-0.96482300	-0.54012000
C	3.71277700	0.92195800	0.93615400
C	4.60317900	-0.61344700	-1.21051000
H	2.86122200	-1.83990500	-0.84519900
C	4.87963600	1.27698500	0.26454800
H	3.36572800	1.51552700	1.78150600
C	5.32607600	0.50839800	-0.80924800
H	4.95042800	-1.21654200	-2.04593100
H	5.44429300	2.15020200	0.58213200

H	6.23930000	0.78233700	-1.33209100
C	1.70841600	-0.56515000	1.24228500
H	1.79279500	-0.36750400	2.31933400
H	1.48948900	-1.62901100	1.09210400
H	0.51720900	-1.62986200	-1.74623300
C	-1.02991500	-1.05248900	1.93677400
H	-0.47334700	-0.88861000	2.86449700
H	-2.09358800	-1.08640200	2.16330300
H	-0.73131700	-2.02555900	1.52821100
N	-1.61764000	0.68480800	0.30620800
C	-2.66423400	1.98557300	-1.36280900
C	-3.60821300	1.80019300	-0.18072800
C	-3.07365600	0.53857400	0.49466200
C	-1.30258100	1.62406500	-0.78369900
H	-2.92328900	1.28938600	-2.16930700
H	-2.67545900	2.99833600	-1.77351800
H	-4.65590500	1.68296200	-0.46785500
H	-3.53266300	2.65242000	0.50654000
H	-3.31387600	0.53093700	1.56332600
H	-0.78638000	2.50255000	-0.37105400
H	-0.64567700	1.13983900	-1.51871000
C	-3.64328400	-0.75509800	-0.14743700
O	-4.86171000	-0.93575200	0.07481900
O	-2.85851500	-1.47441300	-0.80977400
H	-0.93945000	-2.03904600	-1.11516900

#### EtOH-34

N	-0.34262900	-0.88866000	0.40124100
H	-0.85214700	-1.39171400	1.12657200
H	-0.10209200	0.82682600	0.59948000
C	-2.53455600	-0.26382300	-0.47520000
C	-3.50991200	-1.12274300	0.04101600
C	-2.85131000	1.08487600	-0.65241800
C	-4.77243100	-0.64484200	0.38234200
H	-3.27758700	-2.18083500	0.16717500
C	-4.11544500	1.56629200	-0.31738400
H	-2.09818400	1.76161800	-1.05344800
C	-5.07776900	0.70332100	0.20242500
H	-5.52042100	-1.32649300	0.78078100
H	-4.34937000	2.61819500	-0.46490600
H	-6.06465300	1.07876400	0.46277100
C	-1.17392600	-0.80441500	-0.81702800
H	-0.65678900	-0.14905400	-1.52886900
H	-1.27925100	-1.78444400	-1.30200900
C	3.98368300	0.39139100	-0.95143800
C	3.75939900	0.87104000	0.47512100
C	2.25932200	0.67824000	0.66072200
C	3.08531600	-0.82856200	-1.00310000
H	3.63787900	1.14901300	-1.66785900
H	5.02780800	0.15521700	-1.17729500
H	4.06939700	1.90260400	0.65916400
H	4.29572900	0.21709600	1.17566400
H	2.02318500	0.41860100	1.70342300

H	3.59833300	-1.67409000	-0.50309500
H	2.83181000	-1.14157800	-2.02097500
N	1.88090900	-0.40759800	-0.27285800
C	1.45124100	1.93888400	0.35965500
O	1.94100500	3.01991700	0.09411700
O	0.13474500	1.79239200	0.44327800
C	1.00422300	-1.46781000	0.24188000
C	1.43871600	-2.00848100	1.61030000
H	1.28669100	-1.29089300	2.42398800
H	0.86410800	-2.90968600	1.85388600
H	2.50047700	-2.28282000	1.58380900
N	0.97710600	-2.53341200	-0.75931700
H	1.87328100	-3.01541100	-0.78089300
H	0.29878500	-3.23191000	-0.46134600

### EtOH-35

N	-0.21965100	-1.14211400	0.56578900
H	-0.61080500	-1.64273700	1.35875200
H	0.94319600	0.66193700	-1.50420200
C	-2.43989300	-0.49458500	-0.23867100
C	-3.65127600	-1.08489400	-0.60491500
C	-2.46794900	0.74825500	0.40381300
C	-4.86501100	-0.44881900	-0.34877900
H	-3.64275000	-2.05733300	-1.09664900
C	-3.67758300	1.38613500	0.66228100
H	-1.53189400	1.21557200	0.70619400
C	-4.88137100	0.79044100	0.28615900
H	-5.79798900	-0.92603600	-0.64050900
H	-3.68135800	2.35324300	1.16044900
H	-5.82618500	1.28887000	0.49068600
C	-1.13883600	-1.18100800	-0.56450500
H	-0.65661100	-0.67719500	-1.41315200
H	-1.35282200	-2.20478700	-0.91333600
C	3.90543000	0.74988400	-0.65450100
C	3.30596800	1.32361400	0.62357800
C	1.84401100	0.86929700	0.53308700
C	3.24441500	-0.61629900	-0.72547000
H	3.62193600	1.36098100	-1.52255800
H	4.99692900	0.68481700	-0.63328000
H	3.40470600	2.40854500	0.72682600
H	3.77013000	0.85454400	1.50116600
H	1.39262400	0.73409600	1.52291200
H	3.78097500	-1.31486600	-0.06045500
H	3.23841800	-1.04544100	-1.73322700
N	1.86463800	-0.37366700	-0.25582800
C	0.99553300	1.92392500	-0.16853100
O	0.71086200	2.99220800	0.33454100
O	0.60700200	1.59161800	-1.39554300
C	1.15927800	-1.52990900	0.34700300
C	1.75055000	-1.91987300	1.70543100
H	1.62502000	-1.13015200	2.45502000
H	1.25455600	-2.82356300	2.07862000
H	2.81867600	-2.14413200	1.61592600

N	1.25724600	-2.62458800	-0.62361000
H	2.20925100	-2.98341300	-0.66366700
H	0.68586000	-3.39795600	-0.28782300

#### EtOH-36

N	-0.42357100	1.14477000	-0.22821600
H	-0.96946800	1.92907800	-0.57202300
H	1.62996100	0.15886500	1.81270000
C	-2.51400800	0.05749500	0.32797300
C	-3.60113900	0.92798700	0.42638400
C	-2.69377800	-1.18368700	-0.28768000
C	-4.84713200	0.56835000	-0.08439300
H	-3.46925100	1.89426600	0.91391600
C	-3.93760000	-1.54974400	-0.79396400
H	-1.85152000	-1.87186600	-0.36081200
C	-5.01672000	-0.67196400	-0.69554700
H	-5.68646100	1.25472800	0.00040200
H	-4.06714500	-2.52252700	-1.26286700
H	-5.98930700	-0.95788400	-1.08921200
C	-1.16209700	0.46924100	0.84134700
H	-0.61307400	-0.42271100	1.16378300
H	-1.29363600	1.09794600	1.73924400
C	3.87019900	-0.64528200	-0.96781200
C	2.66421900	-1.48341800	-1.38468300
C	1.56325300	-0.90435300	-0.49268600
C	3.28366500	0.74673200	-0.70134000
H	4.30279800	-1.05616100	-0.04541000
H	4.66483700	-0.62653500	-1.71923700
H	2.80413500	-2.55788600	-1.24205500
H	2.39906200	-1.29741100	-2.43176800
H	0.56218200	-1.12158900	-0.89106200
H	3.49174000	1.43756500	-1.53088200
H	3.72727500	1.18788100	0.20826700
N	1.84228300	0.51325300	-0.58089800
C	1.63288300	-1.58272800	0.88767100
O	1.56251800	-2.79683200	0.97866400
O	1.77607500	-0.83560200	1.97104000
C	0.96484000	1.54098500	-0.05046200
C	1.18399300	2.84022600	-0.81728100
H	0.94292900	2.70112300	-1.87699600
H	0.54510800	3.62722800	-0.40077600
H	2.22117500	3.18004600	-0.74039800
N	1.27819600	1.72808800	1.39923000
H	2.15008500	2.24702600	1.49392400
H	0.56799200	2.29646200	1.85765200

#### EtOH-37

N	0.01030600	1.61045900	-1.02637800
H	0.05568800	2.54462000	-1.41070500
H	-3.47742600	0.09627100	-1.16008600
C	2.20428700	0.44270900	-0.69575300
C	2.53738800	1.27370100	0.37317300
C	3.02002400	-0.65541100	-0.98504600

C	3.66974000	1.00992200	1.14309500
H	1.90913500	2.12852500	0.61631000
C	4.15216200	-0.91595700	-0.22012300
H	2.75700600	-1.31556900	-1.81133600
C	4.47988300	-0.08310700	0.84926300
H	3.91616900	1.66230100	1.97748600
H	4.77478800	-1.77614200	-0.45421400
H	5.36042600	-0.28983200	1.45252100
C	0.99821500	0.68448400	-1.57059200
H	0.51840700	-0.26118400	-1.84190200
H	1.31725600	1.12829000	-2.52044400
C	-2.39041700	-1.13482900	1.96011800
C	-0.98843500	-1.67899700	1.72754500
C	-0.55585200	-0.96017000	0.45223800
C	-2.23878200	0.34295300	1.64659800
H	-3.10010100	-1.59509700	1.26002600
H	-2.76017900	-1.29742500	2.97597900
H	-0.94439700	-2.76365700	1.60303100
H	-0.32845900	-1.39991600	2.55922000
H	0.53414300	-0.86970500	0.40413200
H	-1.90192300	0.90883300	2.52566100
H	-3.15310300	0.79521700	1.25185900
N	-1.16814900	0.37772200	0.61573800
C	-1.04633900	-1.70382700	-0.81745400
O	-0.45633500	-2.78847700	-1.02548300
O	-1.94618900	-1.16650900	-1.50663800
C	-0.91830300	1.47320500	-0.07274800
C	-1.73587500	2.68859900	0.21268100
H	-1.70309700	2.93555100	1.27804500
H	-1.38215800	3.55125500	-0.35425000
H	-2.77867700	2.47777900	-0.06237700
N	-4.25690300	0.73502100	-0.96821600
H	-4.99071400	0.18329100	-0.53116900
H	-4.62554900	1.03441900	-1.86680000

#### **EtOH-38**

N	0.70599000	-0.13155400	0.21089800
H	0.88590900	0.20130200	-0.73544900
C	3.10824500	-0.45934200	0.24559900
C	3.90115900	-1.06176700	-0.73136300
C	3.56411500	0.71128000	0.86065300
C	5.13183800	-0.50965900	-1.08692300
H	3.55265900	-1.97336400	-1.21556500
C	4.78945400	1.26640700	0.50744800
H	2.94649400	1.18423100	1.62338400
C	5.57730100	0.65556400	-0.46926300
H	5.74089300	-0.99128000	-1.84841600
H	5.13443300	2.17487200	0.99599900
H	6.53646100	1.08749600	-0.74513000
C	1.77594500	-1.04114600	0.62806100
H	1.73136400	-1.15324900	1.71924100
H	1.67076300	-2.04791500	0.19073500
C	-2.25061300	2.67167500	-0.54107500

C	-3.48128300	1.76699200	-0.42017900
C	-2.94192700	0.46206300	0.19675700
C	-1.10718200	1.83891300	0.01954100
H	-2.05836300	2.92184900	-1.58979200
H	-2.36176100	3.61308500	0.00543900
H	-3.92080700	1.56189800	-1.40288100
H	-4.27341300	2.18280000	0.20756500
H	-3.01766500	0.55117000	1.29793400
H	-0.98154800	2.02031600	1.10332900
H	-0.15373700	2.06063100	-0.46138300
N	-1.52913900	0.44437600	-0.22497400
C	-3.88927900	-0.66852400	-0.17284400
O	-5.06842500	-0.55830800	0.10834900
O	-3.45176000	-1.74258700	-0.80868300
C	-0.64545200	-0.59799900	0.31598500
C	-0.97201200	-1.03923300	1.73028100
H	-1.97931500	-1.46072200	1.79087100
H	-0.28264200	-1.81846500	2.06326100
H	-0.90193500	-0.18726300	2.41481100
O	-0.84789700	-1.78669200	-0.50168300
H	-0.46441600	-1.59854600	-1.37206000
H	-2.45852300	-1.78923500	-0.82329200

#### EtOH-40

C	2.20982600	2.27679600	0.82738800
C	1.97211700	1.98636800	-0.64938400
C	2.05939500	0.46653000	-0.71212400
C	1.42363500	1.16685500	1.50477400
H	3.27929400	2.18484800	1.06111500
H	1.87886400	3.27274200	1.13584200
H	2.68744400	2.46790700	-1.32030100
H	0.96160700	2.30478500	-0.93725300
H	1.43424600	0.05201100	-1.51636100
H	0.35360800	1.43078100	1.57320400
H	1.78201800	0.95329100	2.51959100
N	1.62583800	0.01335200	0.62297200
C	3.48753400	-0.01931900	-0.98660400
O	4.39878100	0.70326800	-1.33636400
O	3.69211200	-1.32716400	-0.83414300
C	0.74194700	-1.12022100	0.80114300
C	0.98560600	-1.77127400	2.15403400
H	0.37137200	-2.67361200	2.26167400
H	2.04057500	-2.04892100	2.23592700
H	0.72750000	-1.08988700	2.96947400
N	-0.65667800	-0.78169300	0.71053500
H	-1.24092300	-1.54641600	1.04058400
C	-2.64048200	0.00436700	-0.44134600
C	-3.55617900	-0.84330900	-1.06592800
C	-3.12003300	1.07807400	0.31563900
C	-4.92783200	-0.62350700	-0.94069700
H	-3.19005500	-1.68141600	-1.65821900
C	-4.48688100	1.30196100	0.44258000
H	-2.40758200	1.74204000	0.80530600

C	-5.39526700	0.44927700	-0.18641500
H	-5.63058600	-1.29090300	-1.43426900
H	-4.84617500	2.14413700	1.02966800
H	-6.46426700	0.62423400	-0.08980700
C	-1.16219100	-0.24349600	-0.54867400
H	-0.65191300	0.71028400	-0.74269200
H	-0.95657600	-0.90575500	-1.40664700
O	1.15378500	-2.03395700	-0.24003600
H	2.85414100	-1.77372800	-0.56499200
H	0.72869000	-2.88982400	-0.09836800

#### EtOH-42

C	-0.61823900	-0.67789600	0.25836900
N	0.73463100	-0.19256200	0.28306300
H	0.90384800	0.49643500	-0.44646700
C	3.13879400	-0.48504700	0.13003800
C	3.87128000	-0.60483200	-1.05128200
C	3.64268500	0.31316900	1.16183500
C	5.09075100	0.05532700	-1.20094800
H	3.48511500	-1.22580500	-1.85893700
C	4.85745600	0.97482100	1.01590900
H	3.07248700	0.40915300	2.08522600
C	5.58520700	0.84664100	-0.16777300
H	5.65286700	-0.04942800	-2.12603100
H	5.24088400	1.58935600	1.82720700
H	6.53654500	1.36110700	-0.28154000
C	1.81715100	-1.18185800	0.29261200
H	1.79881900	-1.70556100	1.25732800
H	1.70115200	-1.94534100	-0.49400900
C	-0.91690000	-1.56138200	1.45171300
H	-0.79516800	-0.99177100	2.37738500
H	-1.93584700	-1.95619300	1.40211800
H	-0.24320600	-2.42063500	1.46208900
N	-1.50812700	0.44349500	0.21284200
C	-3.20788600	1.92180400	0.42224300
C	-2.87742200	0.45534800	0.67964100
C	-1.34206200	1.49341300	-0.79173900
H	-4.27508900	2.12683000	0.32265000
H	-2.77216300	2.55179400	1.21085200
H	-2.95350100	0.22159500	1.74957000
H	-0.53312000	2.18505000	-0.50049100
H	-1.14086600	1.10415700	-1.80333300
C	-3.91258300	-0.41985900	-0.04201700
O	-5.08524500	-0.34691100	0.26610700
O	-3.51352700	-1.23163000	-1.01010200
O	-0.85010400	-1.55496800	-0.90744400
H	-2.52628400	-1.29868600	-1.09133300
H	-0.35580900	-1.21996900	-1.66897100
O	-2.57807400	2.16269500	-0.82934600

#### EtOH-44

N	-0.41608900	1.09004100	-0.31020800
H	-0.97429900	1.91478300	-0.51284100



H	1.69981700	0.07968400	1.78612200
C	-2.53471500	0.01593600	0.21857700
C	-3.62885300	0.38759800	0.99989400
C	-2.76296700	-0.63078400	-1.00071500
C	-4.92993800	0.11322900	0.57870600
H	-3.46004100	0.89394800	1.94955900
C	-4.05882300	-0.90581500	-1.42464800
H	-1.91135900	-0.91748700	-1.61668400
C	-5.14720300	-0.53427900	-0.63408100
H	-5.77336500	0.40812300	1.19886100
H	-4.22243200	-1.41262900	-2.37312000
H	-6.16060000	-0.74965000	-0.96484100
C	-1.13134400	0.28885100	0.68588100
H	-0.61592500	-0.67105600	0.82262200
H	-1.15705700	0.77160700	1.67462900
C	3.97032900	-0.54455500	-0.81960300
C	2.83103800	-1.41560200	-1.34206800
C	1.64714600	-0.91229000	-0.51062600
C	3.31172700	0.81537800	-0.56971700
H	4.35406400	-0.95996600	0.12191800
H	4.81366200	-0.47612600	-1.51240000
H	3.00455000	-2.48839000	-1.22555600
H	2.62723100	-1.20498400	-2.39817600
H	0.68698300	-1.15958400	-0.98375100
H	3.52274800	1.51903400	-1.38713200
H	3.68326400	1.27172400	0.36306000
N	1.87631800	0.51564400	-0.51413900
C	1.66764800	-1.62351200	0.85160900
O	1.58759000	-2.83396500	0.92835000
O	1.80510100	-0.89057400	1.95424500
C	0.94248900	1.49989600	-0.04842700
C	1.19267900	2.84071000	-0.71746200
H	1.05687900	2.74838400	-1.79930900
H	0.49122300	3.58408300	-0.32519000
H	2.20800200	3.20182300	-0.52832700
H	1.76671100	2.36065200	1.57409400
O	1.09769000	1.68424700	1.40527600

#### EtOH-Product

N	-1.59510300	-0.62256200	-0.55284700
H	-1.63706900	-0.63419400	-1.56311300
C	0.82221100	-0.51790900	0.01384400
C	2.02923900	-1.21734400	-0.05182100
C	0.85169900	0.87767200	0.04705900
C	3.24476300	-0.53723200	-0.07618400
H	2.01491200	-2.30628900	-0.08710000
C	2.06530900	1.56071900	0.01892200
H	-0.08252100	1.43533600	0.09183900
C	3.26590100	0.85537700	-0.04092000
H	4.17607800	-1.09649200	-0.13051000
H	2.07314300	2.64800700	0.04422200
H	4.21320300	1.38889000	-0.06494800
C	-0.47791900	-1.27972300	0.09433300

H	-0.76387200	-1.41888400	1.14413300
H	-0.35029800	-2.27879400	-0.33930700
C	-2.55446300	0.05142200	0.12905100
C	-3.63570200	0.68205200	-0.70360200
H	-3.54944900	0.46931700	-1.77243900
H	-4.60690600	0.32871800	-0.34478100
H	-3.60693700	1.76585400	-0.55375800
O	-2.54759900	0.15078200	1.35769900

**EtOH-TS3-IM1**

C	1.45141800	2.10510800	0.95940000
C	2.06476200	1.38167200	-0.23655300
C	1.08155100	0.25050600	-0.55753100
C	-0.03330700	1.92585500	0.72010800
H	1.73968900	1.61992200	1.90085300
H	1.73956100	3.15808300	1.02066900
H	3.06231200	0.98254400	-0.03763700
H	2.13621800	2.05925000	-1.09432900
H	0.74789100	0.32109500	-1.60332500
H	-0.38131600	2.56086800	-0.10564500
H	-0.66846700	2.08572300	1.59440400
N	-0.15029100	0.51359500	0.26646900
C	1.62158900	-1.16841000	-0.37128500
O	2.80439500	-1.38416600	-0.17163300
O	0.74295700	-2.13055700	-0.50686500
H	-0.24559600	-1.76961500	-0.65151100
C	-1.60181900	0.08210700	-0.56511500
C	-2.69494000	0.64485100	0.32277000
H	-2.72151100	1.73922300	0.32432200
H	-3.64741700	0.27889600	-0.07522000
H	-2.59303500	0.28497600	1.35140400
N	-1.49809400	0.74559900	-1.81427600
H	-1.51832600	0.08668200	-2.58325900
H	-2.15967600	1.49882800	-1.95683900
O	-1.54721300	-1.23405300	-0.62384900
H	-0.17882400	-0.10279400	1.09464200
O	-1.12898600	-1.60118500	2.11084700
H	-0.61135500	-2.37744200	2.35088200
H	-1.46619900	-1.77105000	1.20647000

**EtOH-TS3-5b-H<sub>2</sub>O**

C	0.52988400	2.66207400	0.17383700
C	1.68614600	1.70019700	-0.03016200
C	0.98903700	0.42121700	-0.45710100
C	-0.49123300	1.80081900	0.89132200
H	0.80058600	3.54354800	0.76088500
H	0.13744200	3.00962900	-0.79076900
H	2.22361100	1.52503500	0.91009100
H	2.41471200	2.02361800	-0.77847500
H	0.71148100	0.48421500	-1.51724300
H	-1.53339100	2.08520300	0.74325500
H	-0.30123700	1.75567200	1.96857100
N	-0.29295700	0.40315200	0.34896500

C	1.86773800	-0.82610100	-0.29694900
O	2.96025600	-0.77683300	0.22267900
O	1.42105100	-1.94586900	-0.84839300
H	0.45687800	-1.86597800	-1.06285600
C	-1.53714500	-0.21816500	-0.36570800
O	-1.18538400	-1.54624200	-0.58831200
H	-0.19896800	-0.32763500	1.15992900
O	-0.56482200	-1.69036200	1.80088700
H	0.14076200	-2.24743200	2.14137800
H	-0.97066000	-1.89225200	0.38466300
C	-1.84678100	0.47475400	-1.66849000
H	-2.78906600	0.07238700	-2.05323600
H	-1.96656600	1.55356500	-1.52885500
H	-1.08268300	0.28490000	-2.42582600
N	-2.60757700	-0.04506500	0.56843200
H	-3.49447100	-0.25931600	0.12402400
H	-2.47938200	-0.66609400	1.36729600

#### EtOH-TSIM1-5a

C	0.89808800	2.62258900	0.08389800
C	1.86589300	1.43671200	0.11110400
C	1.05393900	0.27200900	-0.44627500
C	-0.48598800	2.00360100	-0.12145400
H	0.94561100	3.19485500	1.01451000
H	1.12752700	3.31238800	-0.73348000
H	2.17370500	1.19926100	1.13744100
H	2.77489800	1.59764200	-0.47155300
H	0.97339400	0.36401600	-1.54253100
H	-0.84129700	2.14365000	-1.15031400
H	-1.24064700	2.38938000	0.56806900
N	-0.31285800	0.54045800	0.10667400
C	1.74717900	-1.06894100	-0.20201400
O	2.96209900	-1.10382500	-0.26591000
O	1.04633900	-2.16679500	-0.01770700
H	0.04152400	-2.00302400	0.07433300
C	-1.47890000	-0.33829500	-0.42144500
C	-2.80106700	0.33837000	-0.10804300
H	-2.97414800	1.23109300	-0.71537200
H	-3.59062500	-0.38922300	-0.31974800
H	-2.86209600	0.60021300	0.95256900
N	-1.32506200	-0.50855300	-1.83351200
H	-0.76685900	-1.32878500	-2.05486600
H	-2.22654000	-0.62053100	-2.28565000
O	-1.37565200	-1.52653700	0.29772900
H	-0.36622400	0.25623700	1.28350400
O	-0.78697700	-0.42468200	2.32416500
H	-0.07785900	-0.81486100	2.84775200
H	-1.18626000	-1.17719600	1.40235400

#### EtOH-TS5a-6a

C	-1.36492400	1.94130300	-0.59493000
C	-1.80274000	1.29484900	0.71472400
C	-0.90523900	0.05974400	0.77623800

C	0.14858800	1.73400600	-0.61642800
H	-1.82935700	1.41577900	-1.44000700
H	-1.63862100	2.99694100	-0.67152000
H	-2.86198300	1.03127400	0.74702600
H	-1.57456800	1.94623900	1.56666000
H	-0.80783200	-0.30229100	1.80868500
H	0.69015300	2.61681000	-0.25152900
H	0.51089500	1.50946000	-1.62970600
N	0.36518800	0.60066800	0.29722500
C	-1.50714000	-1.08987900	-0.05815600
O	-2.65149300	-1.44935000	0.20914100
O	-0.79429100	-1.63087700	-0.99485700
H	0.33449300	-1.35789500	-1.11069000
C	1.55064600	-0.08073900	0.32663300
C	2.79496600	0.72593600	0.08539900
H	2.91938000	1.43684300	0.90914500
H	3.66522700	0.06596700	0.05084900
H	2.74989400	1.28583800	-0.85095800
N	1.68277200	-1.00645600	1.34822900
H	0.90456400	-1.64262600	1.47509700
H	2.54963700	-1.52752600	1.28967900
O	1.54592300	-1.11288700	-1.12618700
H	1.76634600	-0.60071000	-1.91655800

#### EtOH-TS6a-6c

C	-0.94823600	2.13720200	-0.35893700
C	-1.47660500	1.30352300	0.80317100
C	-0.71226800	-0.00581500	0.68183800
C	0.53862100	1.82379100	-0.34879700
H	-1.39635800	1.79579400	-1.30098000
H	-1.14473100	3.20738400	-0.25351500
H	-2.55502900	1.13571900	0.76129200
H	-1.23169400	1.78657400	1.75724700
H	-0.48223300	-0.44982500	1.66232900
H	1.06988700	2.44447100	0.38782800
H	1.01765100	1.95277800	-1.32442000
N	0.56955900	0.41178300	0.06434600
C	-1.42625000	-1.10063500	-0.14295100
O	-2.55540900	-0.90999200	-0.59164500
O	-0.75695000	-2.19719800	-0.27028500
C	1.66663400	-0.35425500	0.07893700
C	2.97596500	0.26416900	-0.27577500
H	3.13814500	1.19637200	0.27381400
H	3.79409800	-0.42578100	-0.06096200
H	3.00125400	0.50095100	-1.34551600
N	1.53931800	-1.62272300	0.38924300
H	0.42247600	-2.05607300	0.15134100
H	2.39610300	-2.16213800	0.38695300

#### EtOH-TSIM2

C	0.73494400	2.14813900	0.40201800
C	1.28280900	1.41003000	-0.81394600
C	0.67279700	0.01729000	-0.65724000

C	-0.70570800	1.66569200	0.46322300
H	1.27599300	1.84053800	1.30790700
H	0.80589600	3.23598100	0.32075200
H	2.37346200	1.37608300	-0.86711300
H	0.90526500	1.86492700	-1.73741900
H	0.50739800	-0.48608600	-1.62034000
H	-1.34396300	2.25895200	-0.20935000
H	-1.13151000	1.71361400	1.47114000
N	-0.61140800	0.27577200	-0.00810400
C	1.59159700	-0.90962500	0.13498800
O	2.77639300	-1.00289400	-0.10245100
O	1.04086400	-1.64107600	1.10537400
C	-1.69381500	-0.54450900	-0.22076400
C	-3.01892500	-0.00725000	0.23155500
H	-3.26127400	0.92985300	-0.28214600
H	-3.81039000	-0.73155800	0.02813600
H	-3.01041900	0.20350100	1.30683600
N	-1.49277700	-1.70776900	-0.74461400
H	0.07702900	-1.50588800	1.11570600
H	-2.37844500	-2.20278200	-0.82746700

#### EtOH-TS6c-6d

C	0.85688200	2.01559800	0.69123200
C	1.21265800	1.44799900	-0.67728700
C	0.57603700	0.05380300	-0.63616000
C	-0.57560200	1.54371800	0.86136500
H	1.50309500	1.58965700	1.47123300
H	0.94330400	3.10467200	0.74274300
H	2.28483000	1.40804800	-0.89024800
H	0.72653900	2.03620700	-1.46515400
H	0.24431500	-0.26863800	-1.63148600
H	-1.25703100	2.17451000	0.27182500
H	-0.92028400	1.52741300	1.90088100
N	-0.55978700	0.16459900	0.30869300
C	1.56551100	-0.99438900	-0.13651100
O	2.56575300	-1.30285300	-0.75031300
O	1.25224500	-1.54134000	1.03356800
C	-1.82776400	-0.27011500	-0.23108200
C	-2.38006400	-1.48715000	0.43277300
H	-2.48158300	-1.30633300	1.50974800
H	-3.34857000	-1.77987900	0.01920700
H	-1.67634800	-2.32207500	0.31903100
N	-2.34045700	0.38708900	-1.18903000
H	0.40251000	-1.09880700	1.29449800
H	-3.22899600	-0.02983400	-1.47192600

#### EtOH-TS6d-6b

C	1.35900400	1.92223100	0.39668400
C	1.93975300	1.07650700	-0.73202200
C	0.95525700	-0.08929500	-0.80793500
C	-0.14801400	1.83349500	0.18350600
H	1.62559900	1.48461500	1.36769000
H	1.71311900	2.95641100	0.38947200

H	2.96245000	0.73675800	-0.55023500
H	1.92076000	1.62845200	-1.67973300
H	0.96972100	-0.57265600	-1.79088700
H	-0.53054300	2.64231700	-0.45327900
H	-0.70343900	1.85777300	1.12290200
N	-0.32600000	0.56061700	-0.54832600
C	1.29418800	-1.17270300	0.24053500
O	2.32108700	-1.82396900	0.03443400
O	0.52318600	-1.33961500	1.25537100
C	-1.51843000	-0.00089600	-0.79569800
C	-1.61687500	-1.03850300	-1.86545500
H	-2.66426800	-1.22210800	-2.11468100
H	-1.07731300	-0.74520300	-2.77054900
H	-1.19101800	-1.98448400	-1.50800700
N	-2.53325700	0.34555800	-0.03338000
H	-0.51036100	-0.73836600	1.65823400
H	-3.40396300	-0.09543200	-0.31370800
O	-1.49661200	-0.32399500	2.08506600
H	-2.11966200	0.14632300	1.17471600
H	-1.34686700	0.27799400	2.82335000

#### EtOH-TS6a-7

N	-0.40066700	0.81315500	0.05865700
H	-0.12106800	-0.18566400	0.13270500
H	-0.63779700	1.16963700	0.98443500
C	-2.78108100	0.27812100	-0.32270400
C	-2.83753000	-1.11903000	-0.28227900
C	-3.86486200	1.01753600	0.15249400
C	-3.95950500	-1.76365700	0.22800100
H	-1.99062100	-1.69929500	-0.64988800
C	-4.99179500	0.37281600	0.66077500
H	-3.82713000	2.10572200	0.12087200
C	-5.04026200	-1.01804100	0.70011500
H	-3.99466900	-2.85017700	0.25379500
H	-5.83223400	0.95912100	1.02479500
H	-5.91872400	-1.52201900	1.09607700
C	-1.54926400	0.96285300	-0.84932300
H	-1.74393000	2.03145500	-1.00661600
H	-1.25574600	0.52817000	-1.81322700
C	3.14647800	-0.43992500	1.98961200
C	3.88802300	-0.76905300	0.69934200
C	2.83577100	-0.48252800	-0.37375800
C	2.36702200	0.82002100	1.63045900
H	2.45151300	-1.25225100	2.23800900
H	3.80742300	-0.28698500	2.84734700
H	4.25234100	-1.79811600	0.64730300
H	4.74207000	-0.09219000	0.56816300
H	3.31377700	-0.22448300	-1.32864100
H	2.93880900	1.72929700	1.86782200
H	1.40895700	0.87639400	2.16538800
N	2.17134900	0.70290800	0.18033500
C	1.94305700	-1.72416400	-0.62855900
O	2.53185800	-2.68677100	-1.16489100

O	0.72493900	-1.67698400	-0.29389200
C	1.27851800	1.48363100	-0.49703700
C	1.14786200	2.91280900	-0.04245500
H	2.07810200	3.44000800	-0.28131400
H	0.32263000	3.41157700	-0.55973800
H	0.97540500	2.98931500	1.03331700
N	1.30449700	1.34439400	-1.87359600
H	1.26648900	0.39968200	-2.23801600
H	0.68918000	1.96930700	-2.37819000

**EtOH-TS6a-8**

C	-2.56871200	0.13206300	2.48970300
C	-2.82936200	-1.07965300	1.60457800
C	-1.81143200	-0.88974700	0.50228100
C	-2.28565800	1.26156900	1.49958900
H	-3.39950200	0.37695100	3.15758600
H	-1.68442400	-0.05035600	3.11414400
H	-3.83670700	-1.05787900	1.16999700
H	-2.70050200	-2.03441900	2.12374000
H	-0.80522300	-1.09930500	0.91484700
H	-1.49377300	1.92866900	1.86473200
H	-3.17985500	1.87299800	1.31941400
N	-1.90761300	0.56944100	0.24955000
C	-1.93618400	-1.78999900	-0.74141500
O	-2.98716900	-2.43450000	-0.90971800
O	-0.91433800	-1.78136100	-1.49473500
C	-1.48769000	1.25059100	-0.86029800
C	-1.46939900	2.74937600	-0.75086900
H	-1.03154700	3.18295200	-1.65395600
H	-2.49581700	3.12028300	-0.65933500
H	-0.89706700	3.09707600	0.11127300
N	-1.89635300	0.81404900	-2.11037700
H	-1.73922900	-0.17396700	-2.30206800
H	-1.56397500	1.39647200	-2.86983800
N	0.39595200	0.84258200	-0.92639200
H	0.31335900	-0.16349300	-1.14249000
H	0.82709700	1.29639800	-1.73263300
C	2.51818100	0.38089900	0.27248800
C	2.57561600	-1.01670200	0.28149400
C	3.70658700	1.10965900	0.22426700
C	3.80101500	-1.67312800	0.24130200
H	1.65205700	-1.59654200	0.31863300
C	4.93679100	0.45388900	0.18858400
H	3.66827500	2.19807700	0.21710900
C	4.98531400	-0.93731600	0.19618100
H	3.83407800	-2.75981200	0.24984800
H	5.85676400	1.03266600	0.15416300
H	5.94404700	-1.44954700	0.16774000
C	1.18309800	1.07440700	0.29549600
H	1.31210200	2.15550700	0.42202500
H	0.57900800	0.71621800	1.14093800

**EtOH-TS6a-11**

C	-1.43322000	1.25365100	-0.78019900
N	-1.65706800	2.12978800	0.27712100
H	-2.25011400	2.91517900	0.03409600
N	0.45689000	1.01981200	-0.74427000
H	0.77912100	0.67002300	-1.64780600
H	0.86116700	1.95404900	-0.60316700
C	2.32124700	-0.31316800	0.17619400
C	2.61989500	-1.56652300	-0.36242600
C	3.36781200	0.54552100	0.52501800
C	3.94359200	-1.95878600	-0.55011100
H	1.80569000	-2.24077600	-0.62964500
C	4.69071600	0.15588800	0.33953800
H	3.13922500	1.52438200	0.94707200
C	4.98070100	-1.09804100	-0.19850000
H	4.16415800	-2.93877600	-0.96666300
H	5.49826100	0.82847600	0.61874500
H	6.01451300	-1.40387100	-0.34017700
C	0.89179200	0.11718800	0.33638200
H	0.72372900	0.64286200	1.28446000
H	0.22775900	-0.75673700	0.32843200
O	0.85268500	3.60569900	0.49383200
H	1.28994200	3.76254900	1.33781900
H	-0.04331200	3.28094800	0.70597600
C	-1.52195200	1.91014300	-2.13305900
H	-0.96381600	2.85193900	-2.13576400
H	-1.14167800	1.27523400	-2.93599000
H	-2.57688300	2.12533800	-2.34346600
N	-1.91916900	-0.01652000	-0.65220600
C	-2.29971900	-2.28339800	-1.09763300
C	-3.38179200	-1.77767800	-0.15055300
C	-2.79112400	-0.50650900	0.44779000
C	-1.79108400	-1.00013100	-1.73165100
H	-1.49783900	-2.76454900	-0.52359800
H	-2.66824300	-2.99488500	-1.84240200
H	-3.64097400	-2.49833400	0.62890100
H	-4.28977500	-1.53060200	-0.71687900
H	-3.56692900	0.24838300	0.63803500
H	-2.40833200	-0.71221500	-2.59709500
H	-0.74884000	-1.07712100	-2.07377400
C	-2.00308500	-0.71391500	1.77079400
O	-1.64521100	-1.87041600	2.07507700
O	-1.77690900	0.34540800	2.42386600
H	-1.87860900	1.67595900	1.17667100

#### EtOH-TS11-12

C	-0.93052900	0.98987500	-0.90931000
N	-1.19221300	2.04331600	0.06112500
H	-1.96804800	2.61463400	-0.27030300
N	0.58524400	0.70078800	-0.76345500
H	0.92646000	0.22378200	-1.60154500
H	1.03913000	1.69151500	-0.68466800
C	2.44880800	-0.41335700	0.36885800
C	2.85056700	-1.59951800	-0.25132100



C	3.41815100	0.45743700	0.87183200
C	4.20279300	-1.90898200	-0.37108900
H	2.09752000	-2.28771500	-0.63603300
C	4.77042200	0.14891700	0.75430800
H	3.10844700	1.37922800	1.36257700
C	5.16382300	-1.03397400	0.13118900
H	4.50604000	-2.83595200	-0.85145800
H	5.51747500	0.83131200	1.15209200
H	6.21994200	-1.27644600	0.04188600
C	0.99292800	-0.06605900	0.45476300
H	0.77532600	0.57444800	1.31595000
H	0.35173000	-0.95091300	0.52316900
O	1.01461800	3.17535700	-0.23054200
H	1.53090900	3.40724800	0.54759500
H	-0.22629600	2.72283900	0.06513300
C	-1.12402500	1.48474900	-2.33574100
H	-0.57842500	2.42116600	-2.49284200
H	-0.78753300	0.75730900	-3.08155000
H	-2.19226500	1.66869900	-2.50213900
N	-1.64553000	-0.20583400	-0.57631400
C	-2.59605300	-2.30844500	-0.83909700
C	-3.69283500	-1.37107600	-0.34712500
C	-2.93128700	-0.14695100	0.15286800
C	-1.64212200	-1.33481800	-1.50505000
H	-2.09917000	-2.80098400	0.00845300
H	-2.95794400	-3.08147400	-1.52312100
H	-4.32175700	-1.79726700	0.43763100
H	-4.33523700	-1.08235100	-1.18879700
H	-3.49144600	0.77281200	-0.08669600
H	-2.02127000	-1.05996200	-2.50546200
H	-0.62864200	-1.74441400	-1.63131300
C	-2.67935300	-0.14113700	1.67453100
O	-3.19587900	-0.97556400	2.41353700
O	-1.90198700	0.80944600	2.09955600
H	-1.53918900	1.47073100	1.19384100

#### **EtOH-TS6b-18**

N	0.43077900	-0.77152500	-0.74913100
H	0.94672500	-1.10946200	-1.56254100
H	0.19013400	0.23000500	-0.86358800
C	2.59102200	-0.27546300	0.33884500
C	3.75352000	-1.04608600	0.31670900
C	2.68884100	1.11516200	0.21207000
C	5.00077300	-0.43955600	0.17141300
H	3.68191200	-2.12854100	0.41566100
C	3.93226800	1.72060700	0.06445700
H	1.77894600	1.71720100	0.22427200
C	5.09127600	0.94405700	0.04414700
H	5.90087700	-1.04974300	0.15711600
H	4.00007900	2.80169900	-0.03206800
H	6.06323400	1.41826700	-0.07045200
C	1.23637400	-0.91622900	0.47190400
H	0.66953800	-0.43351700	1.27889800

H	1.33573300	-1.98254900	0.71233400
C	-2.77347800	0.38453100	2.10945400
C	-3.64865600	0.80362200	0.93531900
C	-2.75514600	0.51852200	-0.27687800
C	-2.14966600	-0.90687500	1.60777600
H	-1.98978100	1.13442100	2.28201700
H	-3.32605300	0.24444600	3.04270400
H	-3.96523800	1.84925200	0.96398400
H	-4.54649300	0.17305800	0.89375100
H	-3.36906400	0.27806000	-1.15468700
H	-2.81392600	-1.76635100	1.79190800
H	-1.18347300	-1.11588000	2.08447100
N	-2.01207200	-0.67268200	0.16445900
C	-1.91510700	1.76789400	-0.64625800
O	-2.58802400	2.72060200	-1.09603500
O	-0.66530500	1.74329600	-0.46928000
C	-1.32223600	-1.50738800	-0.65996000
C	-1.63662300	-1.43293000	-2.12991000
H	-1.51689000	-0.42201700	-2.52748100
H	-0.98325300	-2.10627000	-2.69196400
H	-2.67256500	-1.75257600	-2.28613200
N	-1.16164700	-2.80573100	-0.20022900
H	-0.57249700	-3.39076500	-0.78002800
H	-0.95970500	-2.92955600	0.78411700

#### EtOH-TS7-19

N	-0.43140700	-0.64684200	0.11691600
H	0.65805900	1.16890000	-0.37801400
H	-0.43496400	-1.01171500	-0.83564600
C	-2.85361400	-0.36861000	0.23355100
C	-2.91528400	1.02883700	0.26063700
C	-3.92140700	-1.07897400	-0.31456100
C	-4.02194300	1.69986900	-0.24761500
H	-2.08011900	1.58720600	0.68401900
C	-5.03399900	-0.40998200	-0.82625300
H	-3.88088300	-2.16742600	-0.34153500
C	-5.08621200	0.98040100	-0.79432600
H	-4.05834100	2.78652500	-0.21750200
H	-5.85777000	-0.97773800	-1.25302600
H	-5.95147900	1.50428000	-1.19386100
C	-1.65295300	-1.07926900	0.79633600
H	-1.81184600	-2.16973800	0.74233100
H	-1.54757800	-0.82764300	1.86179900
C	3.68507400	-1.02906000	-1.61604600
C	3.78146800	0.41222900	-1.13852800
C	2.87648800	0.41899600	0.10527900
C	2.21187100	-1.34559700	-1.40033600
H	4.00726300	-1.16406600	-2.65310000
H	4.30033300	-1.67713000	-0.97728200
H	3.36802900	1.08691400	-1.90277700
H	4.79549900	0.74803900	-0.90406400
H	3.45815900	0.18249500	1.01032300
H	2.04073400	-2.41807000	-1.25290400

H	1.61397900	-1.03560900	-2.27598300
N	1.86915800	-0.56872400	-0.20924800
C	2.32222300	1.81732000	0.29910100
O	2.98427000	2.72587600	0.76046600
O	1.07397400	2.02861000	-0.12555900
C	0.85842800	-1.00275000	0.75622000
C	0.98458300	-2.48737100	1.09461500
H	1.99391400	-2.70155600	1.46563100
H	0.26241900	-2.76583200	1.87031600
H	0.78806500	-3.12128100	0.22489600
N	1.02121900	-0.23959200	1.97811900
H	0.42076300	0.58037900	1.99365900
H	0.82868400	-0.79295200	2.80451500

#### EtOH-TS19-20

N	-0.66623600	-0.17043800	0.23536000
H	1.72036200	1.49700800	-0.99438700
H	-0.69782300	-0.63109700	-0.67038200
C	-3.09674900	-0.15589800	0.35320700
C	-3.39972300	1.20426900	0.23220200
C	-3.98987000	-1.09359100	-0.16474300
C	-4.57302100	1.61645300	-0.38974500
H	-2.70264100	1.94059700	0.63217300
C	-5.16790200	-0.68512800	-0.79113800
H	-3.76127300	-2.15518200	-0.07487200
C	-5.46149900	0.67057200	-0.90431700
H	-4.79927300	2.67717700	-0.47239500
H	-5.85498400	-1.42792100	-1.19016100
H	-6.37943600	0.99238300	-1.39073300
C	-1.82381400	-0.59204000	1.02536300
H	-1.85944500	-1.68167500	1.19701900
H	-1.75577700	-0.12114700	2.01732200
C	2.96073500	-2.06724400	-1.04429900
C	3.89087200	-0.89770400	-0.77055400
C	3.02849000	0.03524100	0.10413900
C	1.62531700	-1.36470000	-1.22680200
H	3.25527400	-2.65281200	-1.92064600
H	2.92473900	-2.74250900	-0.17936800
H	4.14817500	-0.39518500	-1.71368500
H	4.82557900	-1.16308600	-0.26994100
H	3.23649100	-0.14576700	1.16870800
H	0.76833500	-2.02642600	-1.06923100
H	1.54077600	-0.95814200	-2.24469300
N	1.62818600	-0.24191500	-0.25398700
C	3.39760300	1.47617400	-0.21166600
O	4.45618800	1.97593100	0.10670300
O	2.48024900	2.13259000	-0.91699000
C	0.65415000	-0.34026000	0.85595900
C	0.80377600	-1.65374000	1.63012400
H	1.82157000	-1.74033300	2.02711900
H	0.12577900	-1.66515200	2.48912200
H	0.58761500	-2.53254200	1.01130600
N	0.85415100	0.75888000	1.81676800

H	1.56402400	1.41608200	1.51137900
H	-0.00245100	1.30743300	1.84528300

#### EtOH-TS20-21

N	0.66737600	-0.40994400	0.07288600
H	-2.84673100	-0.67076700	-1.51603800
H	0.74589000	0.41202000	0.67020700
C	3.08871800	-0.51345500	0.08854600
C	3.46357200	-0.15998200	-1.21195900
C	3.90334300	-0.12485100	1.15239300
C	4.62857700	0.56363900	-1.44342000
H	2.82910100	-0.45937600	-2.04570300
C	5.07258700	0.60201700	0.92593400
H	3.61944400	-0.39653700	2.16883600
C	5.43716400	0.94736300	-0.37230800
H	4.91033700	0.82718200	-2.46050400
H	5.69780700	0.89689400	1.76572300
H	6.34904800	1.51205500	-0.55233300
C	1.81691700	-1.27917200	0.32900400
H	1.83230700	-1.68778800	1.35519100
H	1.75241600	-2.13339200	-0.35341200
C	-1.53552900	2.32765900	0.33556600
C	-2.88699400	1.82982700	0.84643800
C	-2.88521600	0.31621400	0.49814300
C	-1.23386500	1.34475300	-0.78633100
H	-1.56673500	3.36989500	0.00102000
H	-0.77003600	2.25110600	1.12074600
H	-3.71040700	2.33710600	0.32924500
H	-3.02982600	1.99237300	1.91854500
H	-2.95581000	-0.28473800	1.40900900
H	-0.19775200	1.31477400	-1.12287500
H	-1.85785500	1.58668800	-1.66291300
N	-1.65876500	0.03659200	-0.25393000
C	-4.11290300	-0.06505500	-0.32199600
O	-5.25157100	0.13695900	0.04732100
O	-3.83880000	-0.65398600	-1.48250800
C	-0.66335800	-0.98769600	0.23384500
C	-0.93637100	-1.40657600	1.67738900
H	-1.87788100	-1.95604500	1.78915200
H	-0.13980200	-2.08054400	2.00480700
H	-0.95050400	-0.53564800	2.34424100
N	-0.70219400	-2.18885400	-0.58298100
H	-1.59807400	-2.65785500	-0.47771000
H	-0.59674300	-1.93385400	-1.56302000

#### EtOH-TS22-23

N	-0.63463800	-0.30723600	-0.00208100
H	3.02600900	-0.65419600	1.32804700
H	-0.58831200	0.14990000	-0.91269700
C	-3.06760900	-0.50761300	-0.05695500
C	-3.34614000	0.55410600	0.81013600
C	-4.03680500	-0.89084000	-0.98446700
C	-4.56919000	1.21437600	0.75230000

H	-2.58693600	0.85932600	1.52934000
C	-5.26491900	-0.23200000	-1.04554800
H	-3.82685700	-1.71359400	-1.66729000
C	-5.53357800	0.82242900	-0.17774500
H	-4.77365400	2.03707900	1.43404900
H	-6.00926100	-0.54187500	-1.77567900
H	-6.48902600	1.33992900	-0.22508400
C	-1.75315900	-1.23822500	0.02993100
H	-1.71629500	-2.00397200	-0.76576900
H	-1.71190800	-1.77962900	0.98670800
C	1.78745600	2.57108100	-0.27216300
C	3.06493600	1.89981600	-0.75789900
C	2.71713200	0.39268200	-0.72896500
C	1.30826100	1.60319700	0.79749200
H	1.95705900	3.58585900	0.10158700
H	1.04687800	2.61865000	-1.08271300
H	3.88069500	2.10664100	-0.05060500
H	3.39912600	2.21641700	-1.74952400
H	2.45592100	0.04297600	-1.73930600
H	0.23649400	1.67298100	1.00667300
H	1.85463100	1.76883000	1.74350600
N	1.62938700	0.29516000	0.22014100
C	3.95375300	-0.37777300	-0.28879800
O	4.92420500	-0.53764000	-1.00089800
O	3.92825100	-0.82802900	0.96607300
C	0.70506000	-0.82286200	0.32687300
C	1.11358600	-1.97513500	-0.58547800
H	2.12627200	-2.33734400	-0.38036500
H	0.43482800	-2.81935000	-0.42514000
H	1.03843200	-1.68721900	-1.63930100
N	0.76948300	-1.30280200	1.70949100
H	0.32493500	-0.62571800	2.32806500
H	0.27899300	-2.18561300	1.82895100

#### **EtOH-TS23-24**

N	-0.67330400	-0.17201500	-0.36969400
H	1.68522300	-1.01496500	1.82467200
H	-0.81877500	0.68055500	-0.89500100
C	-3.08638400	-0.45252600	-0.18587300
C	-3.24229800	0.44587100	0.87407700
C	-4.18636600	-0.74236700	-0.99361900
C	-4.47564400	1.04070500	1.12096000
H	-2.38562400	0.68165800	1.50449100
C	-5.42456300	-0.15218800	-0.74541600
H	-4.07162400	-1.43531100	-1.82620100
C	-5.57169000	0.74165800	0.31190600
H	-4.58322000	1.73892900	1.94783700
H	-6.27286500	-0.38728400	-1.38397900
H	-6.53565600	1.20696200	0.50379400
C	-1.76296400	-1.12741500	-0.43368000
H	-1.79919900	-1.66669500	-1.39427000
H	-1.59566100	-1.88599300	0.34522700
C	2.33512900	2.61872100	-0.56790600

C	3.54948200	1.69995400	-0.53161400
C	2.97756400	0.27236100	-0.64132900
C	1.29177200	1.80889100	0.17857100
H	2.52104500	3.59326700	-0.10705600
H	2.00010300	2.78406900	-1.59986700
H	4.06071000	1.81188300	0.43446100
H	4.28072300	1.90066300	-1.31928000
H	3.05942400	-0.10171500	-1.67093900
H	0.26867100	2.13566800	-0.02257100
H	1.45312800	1.85910500	1.26895800
N	1.55155100	0.44905600	-0.30576300
C	3.80958300	-0.64610100	0.27779200
O	4.83415100	-1.12837400	-0.25336200
O	3.44152200	-0.77769200	1.47754500
C	0.65217600	-0.56498700	-0.24204900
C	1.06938000	-1.86402600	-0.87604800
H	2.02964500	-2.22507600	-0.50001300
H	0.32423900	-2.64236100	-0.70207300
H	1.14982600	-1.70658900	-1.95875000
N	0.68068900	-1.13224400	1.60509600
H	0.11713800	-0.48247900	2.14938800
H	0.38374500	-2.08065800	1.82559900

#### EtOH-TS8-25

C	3.92900200	-0.30986200	-0.99077600
C	2.81952700	-1.23278400	-1.47803700
C	1.64640700	-0.87144400	-0.57704300
C	3.19387100	0.99104000	-0.69186000
H	4.36704000	-0.71578900	-0.07034300
H	4.73454700	-0.17912000	-1.71958200
H	3.07480400	-2.29406600	-1.42334100
H	2.54874000	-0.99371300	-2.51415400
H	0.69048500	-1.08903500	-1.08024500
H	3.22428200	1.67937900	-1.55106400
H	3.63961300	1.52029400	0.16297800
N	1.80833200	0.57786000	-0.42018800
C	1.62982500	-1.69342500	0.72284100
O	2.52771700	-2.43191200	1.07757200
O	0.51792900	-1.58377300	1.44600500
C	1.01917000	1.38650900	0.48185300
C	1.03278800	2.83710900	0.00177800
H	0.34754900	3.42810400	0.62119200
H	2.03256100	3.26448600	0.12183000
H	0.74054300	2.92612300	-1.05029600
N	1.53404700	1.37347400	1.87031500
H	2.31762000	0.73251900	1.95653700
H	0.83445600	1.07101400	2.54183500
N	-0.35015800	0.82337000	0.51619000
H	-0.02230200	-0.80875500	1.10316200
H	-0.85170200	1.28507200	1.27642800
C	-2.50049700	0.33471200	-0.50284400
C	-2.65156100	-1.04961700	-0.62783100
C	-3.60739400	1.10392700	-0.13921300

C	-3.88262500	-1.65266800	-0.38923600
H	-1.79835000	-1.66045800	-0.92279900
C	-4.84257200	0.50432800	0.10022700
H	-3.49904700	2.18428100	-0.04621400
C	-4.98138700	-0.87593600	-0.02294200
H	-3.98701600	-2.73009500	-0.49311400
H	-5.69696500	1.11608400	0.38024000
H	-5.94455100	-1.34631500	0.16046700
C	-1.16140700	0.98534000	-0.70499300
H	-1.30251700	2.04657800	-0.95851900
H	-0.61939500	0.52258900	-1.53938100

**EtOH-TS25-26**

C	3.50973800	-0.39199000	-1.56734200
C	2.20343600	-1.13278700	-1.82627700
C	1.39420700	-0.84020700	-0.56957000
C	3.04082100	0.90312800	-0.91627800
H	4.12993900	-0.96622700	-0.86617300
H	4.09919900	-0.21656700	-2.47214900
H	2.32887300	-2.20328200	-2.00354700
H	1.68159600	-0.69220000	-2.68588400
H	0.31356000	-0.89275000	-0.77543700
H	2.85559800	1.68148400	-1.67621500
H	3.79047600	1.30328900	-0.21599200
N	1.80376500	0.52101700	-0.24145300
C	1.63470200	-1.87658300	0.53500600
O	2.23756300	-2.91906500	0.37382500
O	1.08059200	-1.60994000	1.71813400
C	1.12857500	1.41029400	0.67218300
C	1.23484200	2.85873100	0.19047400
H	0.64527500	3.50316700	0.85416000
H	2.27283500	3.20670600	0.21994700
H	0.86144100	2.98000300	-0.83296200
N	1.68890600	1.26578100	2.03144800
H	1.49605100	2.09287200	2.59435100
H	2.70020800	1.18138500	1.96971700
N	-0.25709000	0.95004800	0.81027800
H	0.69554300	-0.70346800	1.72994600
H	-0.64116800	1.33747700	1.67037800
C	-2.44611400	0.47074600	-0.22361400
C	-2.55245500	-0.74123500	0.46243500
C	-3.57504800	0.97081700	-0.88012000
C	-3.75870100	-1.43953300	0.48707800
H	-1.68348800	-1.13421000	0.98633300
C	-4.77902400	0.27286100	-0.86218000
H	-3.50687000	1.92127100	-1.40919400
C	-4.87547500	-0.93719400	-0.17632100
H	-3.82427100	-2.38052700	1.02896100
H	-5.64648500	0.67843000	-1.37821900

**EtOH-TS26-27**

C	3.61843800	-0.66947300	-1.32557400
C	2.32712100	-1.40003300	-1.67350200

C	1.34162900	-0.90669900	-0.61119900
C	3.14034900	0.71959700	-0.92248900
H	4.10702600	-1.15695200	-0.47416100
H	4.33064700	-0.63246300	-2.15451600
H	2.42245500	-2.48994700	-1.66278600
H	1.97459800	-1.09996200	-2.66902500
H	0.31494800	-0.94301500	-0.98600200
H	3.12161900	1.41340700	-1.77403800
H	3.75994300	1.16166100	-0.13215800
N	1.76919100	0.49522400	-0.43181900
C	1.40128300	-1.79075700	0.65477500
O	0.66514300	-2.80161200	0.61086300
O	2.19688000	-1.46567300	1.57645800
C	1.09855200	1.40882300	0.27079100
C	1.46597000	2.85226700	0.08697100
H	0.92649600	3.46953200	0.80997600
H	2.53650400	3.04382200	0.19036900
H	1.16203700	3.15501300	-0.92475000
N	1.75362400	1.24105900	2.18749000
H	2.00276900	0.23898900	2.18521500
H	2.58215200	1.79941700	2.37770800
N	-0.25025800	1.08115100	0.53530500
H	1.07625100	1.42775600	2.92302900
H	-0.60005100	1.65907800	1.29486900
C	-2.46029500	0.49527500	-0.35491300
C	-2.47325600	-0.81237800	0.14296300
C	-3.67307200	1.12773600	-0.63089100
C	-3.68099400	-1.47141600	0.35238100
H	-1.53234400	-1.31472200	0.37151900
C	-4.88338300	0.46773700	-0.42232700
H	-3.66997200	2.14952600	-1.00894400
C	-4.88957800	-0.83396900	0.07081000
H	-3.67953400	-2.48856900	0.73777900
H	-5.82076700	0.97509900	-0.63879000
H	-5.83194200	-1.35025700	0.23888300
C	-1.16032300	1.20685400	-0.61734900
H	-1.35825400	2.26215800	-0.86626600
H	-0.66331900	0.77530600	-1.49600000

#### EtOH-TS12-28

C	-0.67152900	-1.05353800	0.81070500
N	-0.93904700	-2.14571900	-0.12878400
H	-1.81115000	-2.61794700	0.09984600
N	0.74936000	-0.77519400	0.72832100
H	1.03288200	-0.14542200	1.47538400
C	2.72564700	0.01131200	-0.43586700
C	3.17156900	1.33315900	-0.39819100
C	3.66264500	-1.02101600	-0.32660700
C	4.52945000	1.62217000	-0.26187400
H	2.44633300	2.14277900	-0.48252900
C	5.01776000	-0.73813400	-0.19079900
H	3.31774300	-2.05445500	-0.35044400
C	5.45465600	0.58689200	-0.15882500



H	4.86301000	2.65713800	-0.23845300
H	5.73703600	-1.55027200	-0.11208000
H	6.51414300	0.80959500	-0.05554700
C	1.26248700	-0.30485800	-0.55974000
H	1.11231700	-1.10327700	-1.29832400
H	0.72208300	0.58146500	-0.93514400
H	-0.20424600	-2.84103800	-0.01625300
C	-0.99452500	-1.43038200	2.25528500
H	-0.42458900	-2.32037000	2.54182900
H	-0.74306100	-0.62428600	2.95482900
H	-2.06185200	-1.65428500	2.37053100
N	-1.46145100	0.10282400	0.33693000
C	-2.44508100	2.20718400	0.71765900
C	-3.53164800	1.15308100	0.88073700
C	-2.91231500	-0.05327400	0.17598800
C	-1.18765700	1.39591500	0.97824400
H	-2.44150200	2.59642900	-0.31058300
H	-2.54951700	3.05493200	1.40063600
H	-4.50335800	1.42673900	0.46157800
H	-3.66733900	0.91688900	1.94443900
H	-3.28942600	-0.99095900	0.61512800
H	-1.03512500	1.28847600	2.06695900
H	-0.28324400	1.85894500	0.56108600
C	-3.31043700	-0.11094200	-1.30185300
O	-4.44215600	0.09884600	-1.69014600
O	-2.34161700	-0.43387600	-2.15176400
H	-1.52911400	-0.60964000	-1.62205000

#### EtOH-TS28-29

C	0.63729800	1.14483100	0.60425100
N	0.82983600	2.14802900	-0.43252500
H	1.60679700	1.96427300	-1.05346300
N	-0.76949600	0.77632700	0.62247300
H	-0.98544200	0.18712000	1.42363000
C	-2.78293400	-0.06429700	-0.43366000
C	-3.25703100	-1.36352900	-0.24649800
C	-3.69613600	0.99489200	-0.42743200
C	-4.61823500	-1.60501300	-0.06064300
H	-2.55040300	-2.19402300	-0.24925000
C	-5.05462100	0.75957700	-0.24443800
H	-3.32779100	2.01075900	-0.56799700
C	-5.51935600	-0.54359700	-0.06027800
H	-4.97407900	-2.62285500	0.08259000
H	-5.75496000	1.59186400	-0.24766400
H	-6.58160000	-0.72909700	0.08158900
C	-1.31437500	0.20306200	-0.60350800
H	-1.14466900	0.93374200	-1.40468000
H	-0.81000000	-0.73236700	-0.90780400
H	0.94673500	3.07617100	-0.04139800
C	0.97481400	1.71031100	1.98293300
H	0.37910700	2.61171100	2.16232800
H	0.74915800	1.00018200	2.78624000
H	2.03489300	1.97869900	2.04863100

N	1.47434000	-0.04065600	0.26032400
C	2.52917600	-2.01443500	1.04399600
C	3.54658200	-0.88415200	1.11988000
C	2.93381000	0.15161500	0.17423800
C	1.21225600	-1.25649100	1.06180000
H	2.64244500	-2.56925500	0.10211900
H	2.60800900	-2.73168500	1.86567000
H	4.56369600	-1.16370600	0.83071300
H	3.58079900	-0.46885700	2.13546200
H	3.23869900	1.17341100	0.43822100
H	0.94999400	-1.00050000	2.10131900
H	0.37899300	-1.83221900	0.63932300
C	3.40914300	-0.08353700	-1.26050200
O	4.57002700	0.00914900	-1.59989300
O	2.44104600	-0.40299000	-2.11505800
H	1.61592700	-0.41396300	-1.55871300

#### **EtOH-TS29-30**

C	0.69660800	-1.18909700	-0.12279400
N	0.86918800	-2.04220200	1.04275000
H	0.72763600	-1.52085500	1.90520400
N	-0.72414900	-0.95119400	-0.28883000
H	-0.89891300	-0.26781800	-1.01901300
C	-2.91780800	-0.22435900	0.44011100
C	-3.32786200	1.07921300	0.72418600
C	-3.77617800	-1.06147200	-0.28042400
C	-4.57554000	1.53936300	0.30417000
H	-2.66512800	1.73799600	1.28523300
C	-5.02062700	-0.60554800	-0.70347400
H	-3.45951200	-2.07943100	-0.50448100
C	-5.42343600	0.69803200	-0.41097500
H	-4.88343300	2.55636600	0.53622200
H	-5.68053900	-1.26788600	-1.25920500
H	-6.39687800	1.05479700	-0.73946500
C	-1.56858500	-0.71943400	0.87965400
H	-1.67677600	-1.67064300	1.41900800
H	-1.14720900	0.00552200	1.59842000
H	1.81440600	-2.41479600	1.06783900
C	1.16348800	-1.97882500	-1.33956700
H	0.56930900	-2.89429000	-1.38964000
H	1.00104200	-1.40799700	-2.26126200
H	2.22128100	-2.26089400	-1.28211500
N	1.47193700	0.11123800	0.02212600
C	1.85680700	2.42920000	0.03635500
C	2.75597100	1.83173200	-1.03556600
C	2.72686300	0.32788800	-0.71282500
C	0.75377500	1.39245000	0.13156300
H	2.39053900	2.51052000	0.99314400
H	1.47687000	3.42163900	-0.22334300
H	3.77343300	2.23433100	-1.05388200
H	2.31458400	1.98880800	-2.02724000
H	2.80913700	-0.25162600	-1.63839500
H	0.03371500	1.54510700	-0.69168900

H	0.19950700	1.45670900	1.07544200
C	3.93542400	-0.04775300	0.13849300
O	5.06255800	-0.13449100	-0.30293900
O	3.66305900	-0.24024300	1.42752600
H	2.67976800	-0.13093400	1.48675300

**EtOH-TS30-31**

C	-0.83841300	1.40056600	0.23037800
N	-0.94283300	2.26790700	1.39672400
H	-0.04559700	2.54371700	1.77677700
N	0.56479200	1.18495800	-0.11918500
H	0.65724500	0.47251200	-0.83745300
C	2.80232200	0.35368900	0.30295200
C	3.12558700	-0.93562900	0.73007300
C	3.57168700	0.94571300	-0.70368100
C	4.19822900	-1.62338200	0.16389900
H	2.53671700	-1.40219800	1.51933800
C	4.64144300	0.26147200	-1.27283100
H	3.32488600	1.95341600	-1.03659400
C	4.95676500	-1.02658200	-0.83974700
H	4.44084700	-2.62591000	0.50871300
H	5.23362300	0.73458000	-2.05278700
H	5.79394000	-1.56089900	-1.28272200
C	1.62625700	1.08623700	0.88587400
H	1.94752700	2.10134800	1.17177800
H	1.31541300	0.58334600	1.81415100
H	-1.49122000	1.84473700	2.13548200
C	-1.48506800	2.11527500	-0.95784900
H	-1.00094900	3.09029000	-1.05528400
H	-1.35537400	1.57994300	-1.90556600
H	-2.55321900	2.28251200	-0.77976400
N	-1.60905000	0.15712100	0.52302800
C	-1.85392700	-2.01979000	1.36163700
C	-1.83149600	-2.13758600	-0.15569600
C	-2.01322600	-0.67970900	-0.62215700
C	-1.06977200	-0.73970000	1.56306800
H	-2.88092100	-1.90737600	1.73450400
H	-1.39949000	-2.87706500	1.86647400
H	-2.58849500	-2.80668600	-0.57604400
H	-0.84836500	-2.49490600	-0.48700700
H	-1.42795400	-0.49998800	-1.53346600
H	-0.00125800	-0.94880800	1.39313300
H	-1.18091000	-0.30244800	2.56153200
C	-3.47396000	-0.43187300	-0.97864500
O	-3.98455400	-0.83306400	-2.00370900
O	-4.16699700	0.21929600	-0.04848700
H	-3.49298200	0.46792000	0.63475400

**EtOH-TS31-32**

C	0.70375100	-1.11054100	0.07797100
N	0.90945500	-1.86392600	1.31237100
H	0.35723200	-2.71941400	1.30719800
N	-0.71803100	-0.83414100	-0.17003900

H	-0.81717000	-0.14587700	-0.91351900
C	-2.96936300	-0.14622900	0.38544800
C	-3.35792700	1.19469200	0.37226600
C	-3.83328800	-1.10504100	-0.15173100
C	-4.58753400	1.57393100	-0.16509500
H	-2.69238100	1.94769600	0.79412100
C	-5.06281600	-0.73198800	-0.68558200
H	-3.53369100	-2.15263600	-0.14436300
C	-5.44244600	0.61083100	-0.69414400
H	-4.87775800	2.62210200	-0.16667500
H	-5.72965200	-1.48849500	-1.09312400
H	-6.40397600	0.90352500	-1.10946900
C	-1.63017900	-0.55137000	0.93602900
H	-1.74484500	-1.46542400	1.53522100
H	-1.27881700	0.23691200	1.62433600
H	0.61970000	-1.32389300	2.12466500
C	1.17653900	-1.98815200	-1.07409500
H	0.63895700	-2.93921600	-1.01739400
H	0.94079600	-1.53239000	-2.04167900
H	2.24973300	-2.19962600	-1.02405400
N	1.52757900	0.10593100	0.19360000
C	2.10295200	2.31873300	0.69211500
C	2.60540600	2.01138600	-0.71282700
C	2.55840900	0.47796700	-0.76829200
C	0.99493600	1.29456600	0.86187200
H	2.89540600	2.14880200	1.43404000
H	1.74731600	3.34663800	0.80776600
H	3.60177400	2.40415200	-0.93511500
H	1.90805000	2.41470000	-1.45699100
H	2.35270100	0.14384900	-1.79399000
H	0.06870200	1.65427200	0.37819000
H	0.76548900	1.09409200	1.91723000
C	3.91592400	-0.12054200	-0.39538700
O	4.91185000	0.03591600	-1.07267100
O	3.94240900	-0.82794900	0.73085400
H	3.01915200	-0.83800400	1.08532900

#### **EtOH-TS32-33**

C	-0.61269800	-0.56871200	0.31423200
N	-0.88713400	-1.68254500	-1.12756500
H	-0.63391600	-2.66003300	-0.99363000
N	0.72433100	-0.17554300	0.24144600
H	0.90311500	0.54212300	-0.45377900
C	3.12953000	-0.47511200	0.15032400
C	3.89808400	-0.63300300	-1.00279800
C	3.60382100	0.34780300	1.17655000
C	5.12577900	0.01623300	-1.13063100
H	3.53415500	-1.27314700	-1.80556800
C	4.82655700	0.99870500	1.05134900
H	3.00545900	0.47201800	2.07839600
C	5.59095300	0.83350000	-0.10421400
H	5.71685300	-0.11716200	-2.03353800
H	5.18740400	1.63337500	1.85734900

H	6.54832000	1.33997300	-0.20145000
C	1.80045800	-1.16302600	0.29200900
H	1.75799000	-1.68014700	1.25867000
H	1.69639500	-1.92881200	-0.49509600
H	-0.39962000	-1.34041900	-1.95402200
C	-0.93629600	-1.52133500	1.43518600
H	-0.25880400	-2.37729300	1.44003900
H	-0.83682600	-0.99300800	2.38950100
H	-1.95585900	-1.90411600	1.34609100
N	-1.50619400	0.45384200	0.13459500
C	-2.61001600	2.23485500	-0.93615800
C	-3.26964800	1.94031600	0.40588400
C	-2.87428400	0.48435800	0.66759100
C	-1.25571600	1.54853600	-0.80905200
H	-3.18749900	1.77690700	-1.74846700
H	-2.51345500	3.30320000	-1.14920700
H	-4.35479100	2.07244000	0.40517400
H	-2.84368800	2.58320700	1.18718400
H	-2.86789900	0.27522000	1.74493700
H	-0.49977800	2.24059700	-0.40576900
H	-0.89088000	1.17306900	-1.77690800
C	-3.89977000	-0.47910700	0.02018100
O	-5.00008800	-0.53406800	0.61101900
O	-3.57593100	-1.10403700	-1.02957600
H	-1.91607800	-1.58750100	-1.26350600

#### **EtOH-TS18-34**

N	-0.32674700	-0.93680900	0.39801400
H	-0.83610800	-1.49241100	1.08449300
H	-0.12832100	0.80963900	0.65232300
C	-2.51176300	-0.26279700	-0.47122200
C	-3.47951200	-1.13039900	0.04472100
C	-2.83905800	1.08256500	-0.65069500
C	-4.74547100	-0.66279100	0.38657400
H	-3.24026800	-2.18716100	0.16953200
C	-4.10727300	1.55317300	-0.31534800
H	-2.09214200	1.76532000	-1.05219600
C	-5.06177400	0.68279200	0.20592100
H	-5.48766600	-1.35044000	0.78534500
H	-4.35000000	2.60285900	-0.46395800
H	-6.05149300	1.05026900	0.46671700
C	-1.14793100	-0.79525300	-0.81796800
H	-0.62113300	-0.11980600	-1.50348200
H	-1.28541700	-1.75333900	-1.34534100
C	3.96832900	0.45250300	-0.93621000
C	3.72426300	0.91509500	0.49219100
C	2.22612800	0.69491300	0.66104300
C	3.08908600	-0.78035800	-1.01392700
H	3.62021900	1.21524600	-1.64648400
H	5.01841900	0.23494700	-1.15459800
H	4.01650100	1.94953300	0.69061400
H	4.26309500	0.26225600	1.19208900
H	1.98495100	0.42632100	1.69990000

H	3.60021500	-1.63512300	-0.53237600
H	2.84615600	-1.08076400	-2.03665500
N	1.87297100	-0.39235200	-0.28136600
C	1.39766200	1.94068600	0.36333000
O	1.86113200	3.02490200	0.06727400
O	0.08441800	1.77557700	0.48636900
C	1.03218000	-1.49506800	0.22766100
C	1.48848700	-2.02298300	1.59053900
H	1.35802700	-1.29203000	2.39364700
H	0.90835300	-2.91342900	1.85846700
H	2.54777100	-2.30419200	1.54614900
N	1.09568100	-2.58281100	-0.73961200
H	1.47472600	-3.42825200	-0.32864200
H	0.19626800	-2.81193800	-1.14361200

#### EtOH-TS34-35

N	-0.37551200	-0.91867100	0.31827200
H	-0.82591200	-1.26676700	1.16059900
H	0.22954800	0.94485900	-0.57152200
C	-2.61233200	-0.34693100	-0.43450800
C	-3.57463500	-1.08325000	0.26234800
C	-2.87807200	0.99026900	-0.73813200
C	-4.77436600	-0.49585600	0.65587400
H	-3.38021300	-2.13133500	0.49240200
C	-4.07877500	1.58090200	-0.35071000
H	-2.13969600	1.57414700	-1.28653300
C	-5.02876900	0.83974400	0.34943100
H	-5.51410000	-1.08233900	1.19593100
H	-4.27413700	2.62165400	-0.59888400
H	-5.96687400	1.29996200	0.65067800
C	-1.31086000	-0.99839300	-0.81322600
H	-0.86381900	-0.49696500	-1.68323900
H	-1.50616200	-2.03567000	-1.12755900
C	4.06888800	0.35394200	-0.66660400
C	3.66843100	0.76237300	0.74448900
C	2.14888100	0.67910300	0.66435300
C	3.12525700	-0.80692500	-0.92731600
H	3.87372400	1.17591300	-1.37024100
H	5.12025000	0.06817500	-0.76395500
H	4.01516900	1.75321600	1.04809100
H	4.03819900	0.02675500	1.47094200
H	1.69394800	0.48280300	1.64561300
H	3.54487900	-1.71198700	-0.44946600
H	2.98086000	-1.02470500	-1.99090700
N	1.85470300	-0.40175800	-0.29725900
C	1.53752000	2.00835400	0.22187200
O	1.99525500	3.09450700	0.51194800
O	0.41215500	1.90489400	-0.48046000
C	0.96379200	-1.48912900	0.16587200
C	1.39509500	-2.07088000	1.51671800
H	1.28265000	-1.35941700	2.34287700
H	0.78918100	-2.95316100	1.75386800
H	2.44434500	-2.38588200	1.47506000

N	0.96529700	-2.51169400	-0.87957000
H	1.87462300	-2.96519700	-0.93025200
H	0.31252400	-3.24433600	-0.60828100

#### EtOH-TS35-36

N	-0.31364300	1.19478800	-0.22401900
H	-0.81142300	1.92953100	-0.71659300
H	1.82720200	-0.09404600	1.77947500
C	-2.45015900	0.19731600	0.32300200
C	-3.57622800	1.02149600	0.34102900
C	-2.55299200	-1.07556300	-0.24598000
C	-4.78590000	0.58548100	-0.19836100
H	-3.50336100	2.01323600	0.78765300
C	-3.75882600	-1.51680900	-0.78218100
H	-1.67852900	-1.72751600	-0.25668000
C	-4.87896500	-0.68500600	-0.76067900
H	-5.65652100	1.23697200	-0.17550700
H	-3.82847600	-2.51281200	-1.21374300
H	-5.82236300	-1.03088600	-1.17678600
C	-1.13919300	0.68671200	0.87242300
H	-0.61662000	-0.13817200	1.37092100
H	-1.32824100	1.44377700	1.65184600
C	3.82076700	-0.78810400	-0.95178300
C	2.55724300	-1.55462400	-1.32393100
C	1.49945500	-0.91009000	-0.41913300
C	3.29716400	0.63203200	-0.81811100
H	4.21552300	-1.14229100	0.01103900
H	4.61730600	-0.87468000	-1.69678600
H	2.62441100	-2.63702600	-1.18304000
H	2.29603900	-1.36148300	-2.37170500
H	0.50416500	-0.92502400	-0.88889000
H	3.23276200	1.09935500	-1.81650600
H	3.94277700	1.26570500	-0.19401900
N	1.97847600	0.44408100	-0.20957200
C	1.36133900	-1.69570300	0.88548000
O	1.00670900	-2.85847200	0.91236100
O	1.64079600	-1.03788800	2.00835300
C	1.06718100	1.58090900	0.01422200
C	1.38095200	2.73722600	-0.93214200
H	1.22721800	2.44600900	-1.97832800
H	0.72053600	3.58037200	-0.69949100
H	2.41123600	3.08611900	-0.81499200
N	1.26478600	1.95965300	1.42923800
H	2.22334500	2.28553400	1.54849300
H	0.66460800	2.74690700	1.67526600

#### EtOH-TS36-37

N	-0.34756800	1.34063900	-0.22517500
H	-0.81197300	2.22249000	-0.41681700
H	1.70145200	0.96902000	1.90171700
C	-2.41466900	0.16075800	0.31933900
C	-3.50069900	1.03846200	0.35106700
C	-2.59132600	-1.11909100	-0.21090900

C	-4.74107100	0.64950800	-0.14971500
H	-3.37434700	2.03334900	0.77906500
C	-3.83054900	-1.51246700	-0.70942600
H	-1.75354100	-1.81679500	-0.21983400
C	-4.90683200	-0.62690800	-0.68308300
H	-5.57989100	1.34084800	-0.11751900
H	-3.95796700	-2.51355100	-1.11477100
H	-5.87527500	-0.93489100	-1.07010800
C	-1.06914800	0.60404200	0.82227900
H	-0.48216900	-0.25995300	1.13775000
H	-1.19932000	1.23835500	1.71385400
C	3.68904200	-0.95227000	-0.98319800
C	2.40596500	-1.70978100	-1.30787800
C	1.37577700	-1.00014700	-0.42879700
C	3.22861900	0.49845500	-0.85917900
H	4.10049700	-1.30393100	-0.02926500
H	4.46587800	-1.07031400	-1.74410600
H	2.45981500	-2.78040000	-1.09359100
H	2.13854900	-1.57961000	-2.36435900
H	0.36050500	-1.12624400	-0.82778800
H	3.38486600	1.04942200	-1.79657800
H	3.76535900	1.03029000	-0.06022100
N	1.78954800	0.39609100	-0.57114600
C	1.41058300	-1.56890400	1.01315200
O	0.94864600	-2.72549100	1.13008800
O	1.88858600	-0.84749400	1.93322800
C	1.03905000	1.49457100	-0.26611600
C	1.44463300	2.77451200	-0.95454000
H	1.20206500	2.69542800	-2.02030600
H	0.90268800	3.62251100	-0.52614800
H	2.51337800	2.97402900	-0.86043100
N	1.53920500	1.91183900	1.50118600
H	2.40393100	2.44718300	1.54308900
H	0.83309600	2.42222400	2.02780200

#### EtOH-TS24-38

N	0.69608700	-0.08341000	0.42040700
H	0.93137800	0.57305400	-0.31663800
C	3.07623100	-0.49852200	0.24750500
C	3.59628500	-0.65103700	-1.03934300
C	3.78983100	0.25124700	1.18558300
C	4.81360600	-0.06757600	-1.38445500
H	3.04236700	-1.23692300	-1.77285400
C	5.00658600	0.83534800	0.84456900
H	3.38433300	0.37345100	2.18952300
C	5.52050000	0.67593900	-0.44181700
H	5.21263000	-0.19745800	-2.38768100
H	5.55663200	1.41291500	1.58373500
H	6.47269400	1.12875100	-0.70780600
C	1.74427200	-1.09470700	0.60111700
H	1.74775800	-1.41911800	1.64918700
H	1.54793200	-1.97749300	-0.02606900
C	-2.34011000	2.70948400	-0.15753600



C	-3.52805800	1.76278600	-0.14768400
C	-2.97665200	0.45924200	0.46361300
C	-1.18549800	1.78558400	-0.50093700
H	-2.45131400	3.52812100	-0.87392000
H	-2.18033100	3.14147700	0.83836200
H	-3.85212500	1.56974100	-1.18033600
H	-4.39403500	2.12918900	0.40885700
H	-3.17979100	0.42684500	1.54431500
H	-0.22720200	2.18885700	-0.15757200
H	-1.12422300	1.60394200	-1.58839700
N	-1.53002900	0.56165800	0.22600900
C	-3.75880000	-0.69512900	-0.17027500
O	-4.92929900	-0.82511700	0.18204900
O	-3.20461300	-1.42532900	-1.08584400
C	-0.63923900	-0.46416700	0.42982400
C	-1.00635800	-1.44591800	1.50938500
H	-2.03513800	-1.79640800	1.41036000
H	-0.36030400	-2.32385000	1.47669300
H	-0.89733800	-0.95294400	2.48167300
O	-0.81755200	-1.54118700	-0.96150600
H	-0.36953000	-1.11071200	-1.70361500
H	-2.05065700	-1.45155400	-1.10761900

#### EtOH-TS38-39

N	0.72966400	-0.10535200	0.20073700
H	0.94185400	0.14436700	-0.76588400
C	3.13288000	-0.45351300	0.28820500
C	3.90790000	-1.05931400	-0.70123200
C	3.61379800	0.70153300	0.91293000
C	5.14600600	-0.52603600	-1.05908900
H	3.53851500	-1.95853100	-1.19304800
C	4.84686600	1.23821000	0.55734200
H	3.00986600	1.17728400	1.68490300
C	5.61665000	0.62401000	-0.43148600
H	5.74110700	-1.01043500	-1.82981100
H	5.21171000	2.13494800	1.05308800
H	6.58177700	1.04130800	-0.70911600
C	1.78969000	-1.01139700	0.66521400
H	1.72386600	-1.09545100	1.75770800
H	1.67918000	-2.02583400	0.24481200
C	-2.39603400	2.72937100	-0.22645200
C	-3.52663200	1.72903000	-0.42866200
C	-2.97105100	0.45894000	0.20844400
C	-1.11706300	1.88655200	-0.25627200
H	-2.38973600	3.51112000	-0.99035800
H	-2.49949900	3.22104700	0.74716800
H	-3.71227700	1.54540600	-1.49530100
H	-4.47006200	2.02757200	0.03319400
H	-2.96617500	0.57962300	1.30440800
H	-0.48981100	2.03508800	0.62830500
H	-0.50057900	2.07470300	-1.13928500
N	-1.56135800	0.46048200	-0.27827000
C	-3.87009100	-0.74334500	-0.08416600

O	-5.04972500	-0.63992000	0.19828200
O	-3.38612300	-1.84630100	-0.61248000
C	-0.60122900	-0.65104600	0.22528800
C	-0.94395900	-1.21053400	1.58511700
H	-1.98193000	-1.54394000	1.64379900
H	-0.32628600	-2.09031500	1.78577000
H	-0.76285600	-0.46616200	2.36923700
O	-0.87879200	-1.49862000	-0.85677400
H	-1.38859100	-0.34692200	-1.21867700
H	-2.36748200	-1.83682800	-0.73149700

**EtOH-TS27-40**

C	4.20676100	0.10748600	-0.23669400
C	3.49191000	-0.91644500	-1.11278600
C	2.05303500	-0.80725700	-0.61282200
C	3.19362300	1.24463600	-0.08994600
H	4.42656600	-0.33308700	0.74447100
H	5.15357100	0.45368400	-0.65978000
H	3.88627700	-1.93054000	-1.01749900
H	3.52526300	-0.62216900	-2.16833600
H	1.34350600	-1.20349600	-1.34868500
H	3.42204600	2.08371700	-0.75891400
H	3.16662900	1.62981700	0.94004900
N	1.90661800	0.63923500	-0.47551400
C	1.88416200	-1.61532300	0.68952500
O	2.17084100	-2.80906900	0.67021500
O	1.45794800	-1.00588700	1.75447500
C	0.72220800	1.30844000	-0.28631100
C	0.80426100	2.80774800	-0.41379700
H	-0.14509900	3.25856400	-0.11246400
H	1.59389000	3.23387200	0.20776400
H	1.01026100	3.06884600	-1.45745200
N	-0.42243100	0.80261100	-0.88430900
H	-1.13478400	1.51987200	-0.95384100
C	-2.50084100	-0.36407500	-0.31372300
C	-2.94179100	0.37953800	0.78694500
C	-3.44152500	-0.97037600	-1.14593500
C	-4.30174500	0.50990300	1.04828200
H	-2.20324700	0.84970200	1.43690200
C	-4.80526200	-0.84257700	-0.88390400
H	-3.10368500	-1.54773700	-2.00550700
C	-5.23713000	-0.10172100	0.21251800
H	-4.63449900	1.08595000	1.90875400
H	-5.52927000	-1.31930100	-1.54056000
H	-6.30022500	-0.00018900	0.41782300
C	-1.02728000	-0.50469900	-0.58584800
H	-0.87632300	-1.19915200	-1.42288100
H	-0.55124800	-0.94307400	0.29856800
O	0.38886300	1.13017400	1.45972800
H	0.99473200	0.04786800	1.65110100
H	0.82278400	1.84052800	1.95088100

**EtOH-TS40-41**

C	-4.10096800	1.13641800	0.58232100
C	-3.53813800	-0.04983500	1.35270100
C	-2.34477600	-0.47845800	0.50469900
C	-2.83202300	1.84553100	0.15122600
H	-4.66395600	0.79387200	-0.29690400
H	-4.75623100	1.77665900	1.17987500
H	-4.24499200	-0.86956600	1.49793700
H	-3.18342700	0.27868400	2.33754100
H	-1.49671600	-0.79203000	1.13657400
H	-2.39479200	2.38810400	1.00322400
H	-2.96175300	2.54279600	-0.68078600
N	-1.92135200	0.74426900	-0.23817400
C	-2.64339500	-1.65251900	-0.42562500
O	-3.61265300	-2.36930200	-0.29117600
O	-1.74449000	-1.91290000	-1.37290700
C	-0.31182800	0.96237900	-0.29534100
C	-0.03810900	2.44568300	-0.40174200
H	1.00905500	2.56163300	-0.70250400
H	-0.66804900	2.90665500	-1.16815300
H	-0.18824700	2.96885000	0.54974200
N	0.36954800	0.37604700	0.79576800
H	0.76126100	1.06076000	1.43175000
C	2.65287200	-0.51086000	0.36628500
C	3.03383100	0.04424400	-0.86095100
C	3.63473200	-0.76757700	1.32428300
C	4.37011400	0.33225900	-1.12051000
H	2.26721900	0.24288800	-1.60995700
C	4.97496400	-0.47901600	1.06727000
H	3.34608800	-1.20028900	2.28191200
C	5.34533700	0.07139400	-0.15638600
H	4.65545000	0.75801400	-2.08015100
H	5.72844200	-0.68362200	1.82462600
H	6.38946200	0.29666200	-0.36134900
C	1.20412200	-0.81341900	0.65969100
H	1.13469900	-1.39733200	1.58752200
H	0.78462800	-1.43621800	-0.13705900
O	-0.21779800	0.30256200	-1.50682200
H	-1.02275400	-1.22750200	-1.42675200
H	-1.47363700	0.50854300	-1.39053400

#### EtOH-TS33-42

C	-0.61322600	-0.51126500	0.51090700
N	0.70580800	-0.12491600	0.37966100
H	0.89805400	0.53389800	-0.36793500
C	3.10573900	-0.44694400	0.22219200
C	3.80842800	-0.82797200	-0.92124000
C	3.63189300	0.55575600	1.04272400
C	5.02268900	-0.22162600	-1.24033700
H	3.40292300	-1.60795500	-1.56432100
C	4.84118000	1.16519300	0.72499100
H	3.08492200	0.85374700	1.93671000
C	5.53996800	0.77564400	-0.41802600
H	5.56373400	-0.52893800	-2.13210300

H	5.24322300	1.94128800	1.37193200
H	6.48722200	1.24937400	-0.66455800
C	1.79261000	-1.09128700	0.56486000
H	1.80158100	-1.40989000	1.61478400
H	1.63750600	-1.98695300	-0.05518600
C	-0.91990000	-1.42083900	1.66583200
H	-0.79619400	-0.86310200	2.60054700
H	-1.94250100	-1.79923300	1.61026200
H	-0.25427100	-2.28431900	1.66844400
N	-1.52259300	0.49188200	0.28701700
C	-3.29886200	1.89672600	0.30438100
C	-2.94364400	0.44845700	0.60924100
C	-1.28802800	1.56332700	-0.68631900
H	-4.35528400	2.04846200	0.08046200
H	-2.98535900	2.55512800	1.12753400
H	-3.10525900	0.22347100	1.67034700
H	-0.55342700	2.28253300	-0.28627400
H	-0.94293900	1.18170500	-1.66028200
C	-3.82751200	-0.50449200	-0.22021400
O	-5.04292400	-0.40318400	-0.07176800
O	-3.26708400	-1.35002500	-1.01905200
O	-0.90733800	-1.69996000	-0.79247300
H	-2.10516300	-1.50577400	-0.96286800
H	-0.41412400	-1.42010100	-1.57614100
O	-2.53954800	2.16364900	-0.87071300

#### EtOH-TS42-43

C	-0.63118700	-1.05520100	-0.04056400
N	0.73720200	-0.69629300	-0.21725900
H	1.09567500	-1.14935000	-1.05229200
C	3.02798400	-0.23419400	0.42451700
C	4.05534900	-1.14731800	0.18433700
C	3.26114000	1.12441600	0.19115200
C	5.29690800	-0.71425700	-0.27994800
H	3.87997800	-2.20723700	0.36618600
C	4.49834800	1.56120300	-0.27065500
H	2.46583200	1.84501300	0.38004600
C	5.52012800	0.64090300	-0.50777000
H	6.08929400	-1.43690000	-0.46051500
H	4.66950600	2.62144100	-0.44240500
H	6.48812000	0.98255500	-0.86685700
C	1.68219300	-0.70966400	0.89673700
H	1.30804700	-0.03889000	1.68306400
H	1.79024100	-1.70921500	1.35045200
C	-0.95081000	-1.77787500	1.24465300
H	-0.71068900	-1.18176700	2.13278300
H	-2.00228700	-2.07363800	1.28646500
H	-0.35324400	-2.69492100	1.27487100
N	-1.50752300	0.27253600	-0.24537200
C	-2.98785500	1.95215900	0.52703700
C	-2.80157900	0.42275200	0.45701900
C	-0.87837200	1.60277900	-0.15086500
H	-3.95126400	2.27835700	0.13062800

H	-2.88226600	2.30472800	1.56145900
H	-2.71560100	0.02382100	1.47840200
H	-0.38391100	1.70042000	0.83357400
H	-0.15925400	1.76437700	-0.95407300
C	-3.98151900	-0.31791600	-0.16804300
O	-5.11152300	0.09094200	-0.00112900
O	-3.75184200	-1.44984100	-0.81336800
O	-1.13575700	-1.63572600	-1.18853700
H	-2.78072200	-1.67900700	-0.94118000
H	-1.53089700	-0.39953800	-1.29304000
O	-1.94946400	2.48579200	-0.28131400

#### EtOH-TS37-44

N	-0.47759900	0.80605400	-0.59656300
H	-1.17936900	1.53634500	-0.53977500
H	1.26545000	0.16993100	1.72976900
C	-2.54337100	-0.36951500	-0.10078000
C	-3.20419400	0.30055600	0.93302700
C	-3.29077100	-0.91618200	-1.14464800
C	-4.59069300	0.42022500	0.92413900
H	-2.62237600	0.72542400	1.75151500
C	-4.67933900	-0.79985300	-1.15542700
H	-2.77911000	-1.43915100	-1.95165500
C	-5.33050700	-0.13090200	-0.12156900
H	-5.09582800	0.93827200	1.73595100
H	-5.25257000	-1.23331800	-1.97151200
H	-6.41416100	-0.04163000	-0.12804400
C	-1.04393100	-0.46137000	-0.09474500
H	-0.73321500	-1.30102700	-0.72710300
H	-0.69628400	-0.65614500	0.92831000
C	4.19055800	0.03554300	-0.49301100
C	3.37483500	-1.01904700	-1.23197200
C	1.98787700	-0.84013200	-0.61584400
C	3.22600000	1.21236900	-0.35291200
H	4.47464300	-0.34099200	0.49806300
H	5.10904300	0.31674900	-1.01495600
H	3.75146700	-2.03721800	-1.10992100
H	3.32039700	-0.79104900	-2.30309300
H	1.21296500	-1.24502100	-1.27588900
H	3.39752600	1.97587900	-1.12255600
H	3.31767800	1.69464200	0.63085400
N	1.88947700	0.61498000	-0.53628200
C	1.90883600	-1.58683200	0.72929800
O	2.08601800	-2.80237100	0.72046100
O	1.68336600	-0.90927500	1.81286900
C	0.75751400	1.32076500	-0.21926700
C	0.84034300	2.80595400	-0.45753000
H	0.88980800	2.99089400	-1.53604800
H	-0.04417500	3.30190400	-0.04968800
H	1.72331100	3.25018100	0.00511800
H	1.21089600	1.98417300	1.94699100
O	0.68584200	1.26470200	1.57179900

**EtOH-TS44-45**

N	-0.44956200	0.96264900	-0.08912700
H	-0.96732800	1.54600600	-0.73842900
H	1.35021000	-0.16438200	2.03843100
C	-2.62857900	-0.00712400	0.34813500
C	-3.74053600	0.83604700	0.38393800
C	-2.73946700	-1.24771400	-0.28595200
C	-4.94612000	0.44691400	-0.19771800
H	-3.65984200	1.80344600	0.87921800
C	-3.94143800	-1.64112000	-0.86669600
H	-1.87594800	-1.91226100	-0.31438700
C	-5.04827800	-0.79305900	-0.82337700
H	-5.80659600	1.11077400	-0.15824200
H	-4.01828700	-2.61269100	-1.34949300
H	-5.98909000	-1.10212400	-1.27280800
C	-1.32670000	0.42917400	0.95784700
H	-0.84054600	-0.42982800	1.43780500
H	-1.51102100	1.17404900	1.74699400
C	3.66974800	-0.20847900	-1.65776500
C	2.56378200	-1.24831700	-1.54551700
C	1.78382200	-0.80112800	-0.31137800
C	2.92855400	1.06431400	-1.30058300
H	4.46109900	-0.40497700	-0.92142800
H	4.12866300	-0.16140300	-2.64932200
H	2.92199500	-2.27475700	-1.44094500
H	1.91204600	-1.19873500	-2.42616700
H	0.69767500	-0.91553400	-0.46452100
H	2.29736100	1.38736500	-2.14215500
H	3.57290500	1.89586400	-1.00334000
N	2.06167400	0.66006600	-0.16877700
C	2.12428700	-1.59500100	0.94991300
O	2.66439100	-2.68080300	0.90920300
O	1.73564000	-1.08402200	2.11492500
C	0.79508300	1.54703400	0.27277600
C	0.94849200	2.93791900	-0.29999000
H	0.76471800	2.96861500	-1.38009300
H	0.21416700	3.57953400	0.19852500
H	1.94455300	3.33971400	-0.09314300
H	2.19133000	1.04548000	1.01871600
O	1.13387400	1.47108500	1.61316300

**H<sub>2</sub>O-5a**

C	-0.75702400	2.58933000	-0.26771600
C	-1.76490300	1.43661800	-0.16241500
C	-0.93343200	0.25682800	0.36503500
C	0.59983400	1.95076400	0.02742800
H	-0.77230100	3.02803600	-1.27029500
H	-0.97168700	3.39330600	0.44275800
H	-2.17301900	1.18395600	-1.14897800
H	-2.60916900	1.64510400	0.50004100
H	-0.90441700	0.31142700	1.46896400
H	0.88591700	2.13281300	1.08136200
H	1.39726200	2.34533300	-0.60770700

N	0.38795500	0.51642800	-0.21623900
C	-1.65867400	-1.03409800	0.04615700
O	-2.73944400	-1.25086400	0.56411400
O	-1.16170300	-1.88229600	-0.84131800
H	-0.20327600	-1.70783100	-1.02920600
C	1.47990300	-0.39836300	0.07868700
C	2.83977800	0.27514700	-0.01776000
H	2.97042100	1.02645500	0.76730700
H	3.60893100	-0.49302900	0.10902400
H	2.98780800	0.75797700	-0.99121100
N	1.25211100	-1.09262400	1.32760900
H	2.01690000	-1.74038600	1.50202400
H	1.24111100	-0.42612500	2.09706400
O	1.45614000	-1.46425900	-0.89552000
H	1.77221100	-1.10166900	-1.73543900

### H<sub>2</sub>O-5b

C	-0.78568600	2.56861000	-0.27193100
C	-1.78483300	1.42307300	-0.07465700
C	-0.91699400	0.22309500	0.35124700
C	0.57277000	1.94927400	0.02624900
H	-0.82037600	2.93590500	-1.30286800
H	-0.98575700	3.41986700	0.38567200
H	-2.30727400	1.19037200	-1.00968200
H	-2.54770500	1.62716600	0.68085900
H	-0.83835100	0.23319800	1.45590500
H	0.84572000	2.09534200	1.08798900
H	1.37321300	2.37709000	-0.57940300
N	0.38719800	0.51513400	-0.26711800
C	-1.67230500	-1.05325900	0.01910100
O	-2.79003000	-1.20964200	0.47606800
O	-1.14226100	-1.96828500	-0.77497300
H	-0.17399600	-1.80709100	-0.93530800
C	1.52593700	-0.34743000	0.06044800
O	1.43979900	-1.51602700	-0.80386400
H	1.69123000	-1.23106400	-1.69516900
N	2.74010100	0.37302600	-0.17260300
H	3.53611200	-0.24308600	-0.03774200
H	2.78422700	0.75128900	-1.11610400
C	1.53542900	-0.90721900	1.47078100
H	1.47389100	-0.09393900	2.20095800
H	0.70552300	-1.60055300	1.63730100
H	2.46647500	-1.45684100	1.64036300

### H<sub>2</sub>O-IM1

C	0.97144100	2.02673800	1.12971000
C	1.41955000	1.84836000	-0.31546000
C	0.81323200	0.51201000	-0.72778300
C	-0.45556200	1.52101000	1.08746600
H	1.57404800	1.40193600	1.80453100
H	1.03023300	3.05944500	1.48266600
H	2.50423500	1.83019100	-0.44380800
H	1.01121900	2.65521800	-0.93582700

H	0.40335600	0.55062400	-1.74359100
H	-1.12337500	2.22477400	0.57850600
H	-0.87600400	1.23663900	2.05602100
N	-0.35233300	0.29753700	0.22606200
C	1.75239200	-0.71888100	-0.67811300
O	2.95104200	-0.53411600	-0.92313300
O	1.17632300	-1.82634400	-0.42700800
H	-0.50997600	-1.68987200	-0.88694100
C	-1.67874800	-0.15366300	-0.45852200
C	-2.66552600	-0.45625000	0.65028700
H	-2.98369200	0.44848100	1.17825700
H	-3.54461700	-0.92148500	0.19479400
H	-2.23325400	-1.15982000	1.36987800
N	-2.11634200	0.88611800	-1.31876700
H	-1.99299300	0.63858600	-2.29391800
H	-3.07165100	1.17687200	-1.14999100
O	-1.35979200	-1.28494100	-1.19634400
H	-0.09478100	-0.47363500	0.87137400
O	0.29667600	-1.73738100	2.17578300
H	0.87222400	-1.55486700	2.92706500
H	0.86109200	-2.12234400	1.48001800

#### H<sub>2</sub>O-6a

C	-1.01693800	2.09882400	-0.27927200
C	-1.46496600	1.23950100	0.89699700
C	-0.71112100	-0.06556400	0.69805700
C	0.46983600	1.80159600	-0.36730900
H	-1.52280200	1.77159800	-1.19521000
H	-1.20929100	3.16578400	-0.13941800
H	-2.54360000	1.06991100	0.92103000
H	-1.15869200	1.70382700	1.84315300
H	-0.44539200	-0.54726400	1.64959600
H	1.04481800	2.42825200	0.32851400
H	0.88451700	1.92324700	-1.37255300
N	0.55605900	0.38975000	0.06127300
C	-1.43402300	-1.13165300	-0.17618900
O	-2.49626100	-0.81568700	-0.74123300
O	-0.85245900	-2.25514300	-0.21294200
C	1.68276700	-0.30229000	0.05690500
C	2.95235000	0.35197600	-0.35925500
H	3.08833500	1.31313800	0.14418900
H	3.80748800	-0.28906600	-0.13905300
H	2.93526600	0.53961100	-1.43862700
N	1.68657100	-1.57449800	0.42668400
H	0.78544800	-2.08870000	0.39386900
H	2.55782600	-2.08480300	0.40260600

#### H<sub>2</sub>O-6c

C	1.21300200	1.92604800	0.79341900
C	1.72470300	1.47778300	-0.56962700
C	0.88506500	0.24334900	-0.85370500
C	-0.29152100	1.77172500	0.65325000
H	1.58930600	1.25334500	1.57596200



H	1.49536400	2.94873400	1.05600700
H	2.78898200	1.23591200	-0.57995500
H	1.52691900	2.25046800	-1.32339100
H	0.72699200	0.07403600	-1.92901400
H	-0.74094900	2.65863400	0.18635900
H	-0.80627000	1.56873900	1.59746900
N	-0.42607900	0.61547900	-0.25779000
C	1.45777400	-1.08070900	-0.27403200
O	2.66023100	-1.11800000	0.02664700
O	0.62296000	-2.03594300	-0.20721600
H	-0.39446500	-1.72797900	1.30325500
C	-1.59374400	0.09662800	-0.58338500
C	-2.84801200	0.73383200	-0.10403800
H	-2.85501700	1.80768400	-0.30966100
H	-3.71964900	0.27488600	-0.57325600
H	-2.92753900	0.59608700	0.98041100
N	-1.65979000	-0.99078600	-1.34364600
H	-0.85114400	-1.62141500	-1.31518500
H	-2.56771800	-1.38117900	-1.55266100
O	-0.92272600	-1.38241900	2.05141800
H	-0.83106000	-2.03184300	2.75562100

#### H<sub>2</sub>O-6c-no-Hbond

C	0.57452100	2.23771300	0.31218000
C	1.27496400	1.44557100	-0.78767000
C	0.68227900	0.03398300	-0.64957500
C	-0.83703900	1.67750600	0.27913900
H	1.03824400	2.04418700	1.28892300
H	0.59704000	3.31727300	0.14105700
H	2.36627000	1.44573500	-0.71394900
H	1.00465800	1.84598500	-1.77137700
H	0.56016400	-0.45955700	-1.62174100
H	-1.42666300	2.14973000	-0.52199100
H	-1.37536600	1.80391400	1.22376700
N	-0.61301200	0.25160900	-0.01060100
C	1.59120100	-0.87336100	0.16451800
O	2.63090500	-1.31345400	-0.27683200
O	1.21136300	-1.13494800	1.41653900
C	-1.62966900	-0.66372800	-0.21060100
C	-2.98979200	-0.23017400	0.24769400
H	-3.32613300	0.65821400	-0.29881200
H	-3.71660300	-1.02942400	0.08768000
H	-2.98249200	0.02499500	1.31335500
N	-1.33568400	-1.80607900	-0.72679200
H	0.33969100	-0.71689900	1.56192000
H	-2.17487500	-2.38069900	-0.77885400

#### H<sub>2</sub>O-6d

C	1.14178900	2.03969300	0.51825500
C	1.82007400	1.30077600	-0.62963800
C	0.95792600	0.03925000	-0.77107100
C	-0.33942200	1.81487100	0.25132600
H	1.42529100	1.58941400	1.47959400

H	1.40071600	3.10091200	0.55934800
H	2.87293700	1.06385200	-0.45420100
H	1.74756100	1.88086200	-1.55694800
H	1.00433000	-0.35802800	-1.79180200
H	-0.76455400	2.57421900	-0.42108700
H	-0.94461400	1.80712000	1.16310200
N	-0.37258500	0.50718100	-0.42133500
C	1.49362300	-1.06727100	0.13697400
O	2.54349500	-1.62028000	-0.12538600
O	0.80931000	-1.39859700	1.22253000
C	-1.54682900	-0.06074600	-0.82518500
C	-1.44663400	-1.24420300	-1.74303000
H	-2.44289000	-1.63217100	-1.96461500
H	-0.96166200	-0.97454900	-2.68784800
H	-0.86240800	-2.05512600	-1.29154500
N	-2.65596200	0.42943700	-0.36710100
H	-0.04572700	-0.91705300	1.36632700
H	-3.44214000	-0.08456600	-0.76020600
O	-1.64822100	-0.62957200	2.12674500
H	-2.21343700	-0.13795200	1.49532600
H	-1.69341700	-0.15989800	2.96670800

#### H<sub>2</sub>O-6b

C	0.29869500	2.58869500	-0.33305000
C	1.44868000	1.62898400	-0.06489900
C	0.96470700	0.29325700	-0.63738000
C	-0.92687200	1.73730500	-0.04568300
H	0.32992500	3.48547100	0.29116800
H	0.29883600	2.90261600	-1.38421200
H	1.60105000	1.52084900	1.01874400
H	2.39717500	1.93430600	-0.51400900
H	1.19973500	0.22003900	-1.70815000
H	-1.80805000	2.05050600	-0.61687700
H	-1.17636900	1.70539700	1.02398800
N	-0.50245800	0.39201600	-0.47656000
C	1.64183500	-0.87178400	0.11332800
O	2.72964000	-1.24072800	-0.37399900
O	1.08419300	-1.29755000	1.15923100
H	-0.29420100	-0.61811000	2.01067000
C	-1.34701700	-0.58430700	-0.72722300
O	-1.08162000	-0.25352400	2.47846700
H	-1.02637400	-0.58915600	3.37831000
C	-0.87646500	-1.88024700	-1.28123700
H	-0.14010700	-1.72466700	-2.07463800
H	-0.39607100	-2.45388400	-0.48105100
H	-1.71084100	-2.45877000	-1.68098600
N	-2.64734400	-0.43249500	-0.49822700
H	-3.28406100	-1.19172200	-0.69229900
H	-3.02111500	0.36348200	0.00011800

#### H<sub>2</sub>O-7

N	-0.28629300	0.73119200	-0.14922900
H	0.21766000	-0.77216200	-0.23477000

H	-0.46031100	0.89466000	0.84406300
C	-2.68058600	0.35875200	-0.33077400
C	-2.85758600	-0.99119000	-0.64928200
C	-3.58709500	0.97597500	0.53263300
C	-3.92140000	-1.71041200	-0.11448400
H	-2.15214200	-1.47557100	-1.32458800
C	-4.65504000	0.25868800	1.06992400
H	-3.45490100	2.02831000	0.78249600
C	-4.82328500	-1.08571100	0.74772800
H	-4.05120100	-2.75908400	-0.37177100
H	-5.35638500	0.75147100	1.73920300
H	-5.65642200	-1.64643000	1.16480400
C	-1.50476900	1.11376500	-0.88216900
H	-1.69680800	2.19707400	-0.82512200
H	-1.36084100	0.85793200	-1.93940500
C	3.14104600	-0.37249100	1.96344800
C	3.85895200	-0.65410300	0.64758100
C	2.73687600	-0.44737900	-0.37166100
C	2.19694700	0.78328200	1.62395500
H	2.56085900	-1.25651100	2.26275000
H	3.81895500	-0.13118100	2.78713700
H	4.30033300	-1.65193100	0.58827600
H	4.64334300	0.08953900	0.46437600
H	3.14144800	-0.23924500	-1.37250500
H	2.61425600	1.75229800	1.93623100
H	1.23227700	0.66382400	2.14450500
N	2.07450800	0.72679900	0.16449600
C	1.92835200	-1.74968400	-0.51793700
O	2.50041000	-2.79339300	-0.79188100
O	0.61931200	-1.71850100	-0.36088900
C	1.00793200	1.42509600	-0.51518100
C	0.97764300	2.88441100	-0.08239400
H	1.94036700	3.35573400	-0.30357200
H	0.19114200	3.43086000	-0.61408700
H	0.78030400	2.97653900	0.99027800
N	1.23844200	1.36892400	-1.93867400
H	1.02788800	0.45516800	-2.33310900
H	0.66787400	2.05147200	-2.42750500

## H<sub>2</sub>O-8

C	3.63087300	-0.03943500	-1.70846500
C	2.87505800	-1.33418500	-1.39598000
C	1.68318400	-0.91869800	-0.51731100
C	3.22225600	0.87337800	-0.56867300
H	4.71350700	-0.18822600	-1.76915800
H	3.29333700	0.38993200	-2.65945100
H	3.50811400	-2.02417200	-0.82947700
H	2.54020900	-1.85583600	-2.29723600
H	0.72642900	-1.16400500	-1.00323000
H	3.34991400	1.93514000	-0.80437200
H	3.80452000	0.65796000	0.34691800
N	1.80867800	0.54611200	-0.40806000
C	1.67748800	-1.66559900	0.82716500

O	2.60741100	-2.31228900	1.26648600
O	0.53902500	-1.57003100	1.51512200
C	1.03341800	1.33449800	0.54081500
C	1.05581800	2.80448400	0.12367700
H	0.26873500	3.35137400	0.65697900
H	2.01438200	3.26651800	0.37763200
H	0.89286600	2.91323700	-0.95219000
N	1.56412100	1.27042200	1.89821700
H	1.29481700	0.42138800	2.38778100
H	1.25522100	2.06278200	2.45413700
N	-0.34470100	0.77428700	0.52659200
H	-0.03103600	-0.84266000	1.11096100
H	-0.85441600	1.22268400	1.28903300
C	-2.48329000	0.32085300	-0.52595300
C	-2.65857400	-1.06241400	-0.63060900
C	-3.58018500	1.11665200	-0.19057300
C	-3.90418500	-1.63847400	-0.40010000
H	-1.81103600	-1.69222000	-0.90172500
C	-4.82990000	0.54424800	0.04022600
H	-3.45162300	2.19593600	-0.11180900
C	-4.99318900	-0.83515900	-0.06237900
H	-4.02743500	-2.71544100	-0.48727700
H	-5.67636500	1.17610000	0.29892100
H	-5.96738300	-1.28460400	0.11527100
C	-1.12701100	0.94010400	-0.71181000
H	-1.24028800	2.00121500	-0.98182700
H	-0.58121900	0.45420900	-1.53017300

## H<sub>2</sub>O-11

C	-1.04865300	1.26048300	-0.63187600
N	-1.16650500	2.09587900	0.52476800
H	-1.89526600	2.78894900	0.38090600
N	0.49829100	0.84071600	-0.67572800
H	0.70671400	0.43137200	-1.59113200
H	1.05281500	1.71374700	-0.58930700
C	2.36324500	-0.49792500	0.20728700
C	2.70018500	-1.51026500	-0.69601700
C	3.37712400	0.15747000	0.90939700
C	4.03215400	-1.85606900	-0.90204100
H	1.91041300	-2.03557200	-1.23354200
C	4.71031300	-0.19035900	0.70746400
H	3.11908100	0.93811200	1.62382100
C	5.03902700	-1.19514400	-0.19992300
H	4.28416300	-2.64703000	-1.60395300
H	5.49314500	0.32219100	1.26098400
H	6.07985900	-1.46771200	-0.35644500
C	0.92782300	-0.10908900	0.39588700
H	0.75988900	0.39420800	1.35358000
H	0.25118600	-0.96929500	0.33929200
O	1.36326400	3.37312300	0.25459100
H	1.97932800	3.53344800	0.97750700
H	0.48901200	3.19117700	0.65930300
C	-1.24534900	2.08531000	-1.89429500

H	-0.64403100	2.99982800	-1.85717900
H	-0.98137800	1.53363400	-2.80094000
H	-2.30344100	2.36237600	-1.96376600
N	-1.78912800	0.05171200	-0.57410000
C	-2.85369700	-1.89219900	-1.30470800
C	-3.80091500	-1.15210900	-0.36851100
C	-2.89333200	-0.18918900	0.38855800
C	-1.94311200	-0.77196000	-1.77337900
H	-2.27656700	-2.63718800	-0.74306300
H	-3.35880600	-2.39419100	-2.13566500
H	-4.34452100	-1.81119100	0.31274300
H	-4.52985700	-0.58007400	-0.95889800
H	-3.41811100	0.75243600	0.60939200
H	-2.42112300	-0.21626200	-2.59870300
H	-0.97152900	-1.14103700	-2.13755800
C	-2.32468200	-0.74457500	1.72174500
O	-2.44817700	-1.96556500	1.96265300
O	-1.74433700	0.10657400	2.45809500
H	-1.38636800	1.54057200	1.36780800

## H<sub>2</sub>O-12

C	-0.77774400	0.92837800	-0.78010900
N	-0.99534300	1.98145500	0.23083500
H	-1.71570000	2.62607500	-0.09070500
N	0.63184700	0.54289300	-0.70862900
H	0.86710100	-0.03395000	-1.51491700
H	1.62557500	2.16991100	-0.76043400
C	2.51398200	-0.48262500	0.44221500
C	2.92254300	-1.61314700	-0.27159300
C	3.48444000	0.32177800	1.04359100
C	4.27406600	-1.92573800	-0.39344100
H	2.17277400	-2.25971500	-0.72907300
C	4.83759200	0.01032200	0.92835800
H	3.17370000	1.19301100	1.62009100
C	5.23496900	-1.11255500	0.20564700
H	4.57733100	-2.80907700	-0.95069500
H	5.58156300	0.64354000	1.40608500
H	6.29041100	-1.35830000	0.11555600
C	1.05690100	-0.12856400	0.53060800
H	0.89549700	0.56384500	1.36695900
H	0.45014300	-1.02495600	0.73397700
O	1.82681200	3.11694400	-0.58787900
H	2.73595400	3.14263800	-0.27158700
H	-0.14585500	2.54321300	0.31126700
C	-1.04418100	1.46739700	-2.18415000
H	-0.44879900	2.37009900	-2.35964100
H	-0.79068000	0.73740100	-2.96024700
H	-2.10575700	1.72226300	-2.29562400
N	-1.63777000	-0.20058300	-0.41659300
C	-2.86630400	-2.13618000	-0.91879600
C	-3.85491800	-0.99094200	-0.74342800
C	-3.02895100	0.05423900	-0.00462600
C	-1.59055400	-1.39012000	-1.27078500

H	-2.74179800	-2.67912900	0.02803100
H	-3.15937200	-2.85494500	-1.68941200
H	-4.76542400	-1.26006400	-0.20257400
H	-4.13823200	-0.58940700	-1.72553400
H	-3.36497700	1.07005200	-0.26961100
H	-1.59524900	-1.13327700	-2.34516400
H	-0.68512700	-1.98047000	-1.07355700
C	-3.13594100	-0.06437500	1.52092000
O	-3.95102200	-0.76897700	2.08774200
O	-2.27263500	0.66564100	2.21308600
H	-1.68484800	1.19881200	1.58745600

## H<sub>2</sub>O-18

N	-0.31767200	-0.89084000	0.34789800
H	-0.78653400	-1.38268700	1.10750300
H	-0.15309500	0.82500100	0.47532300
C	-2.55172300	-0.31220200	-0.45941800
C	-3.48150900	-1.11417200	0.21015300
C	-2.89475700	1.00691100	-0.76334800
C	-4.72302900	-0.60514800	0.58107800
H	-3.23091800	-2.15136100	0.43554300
C	-4.13838900	1.51850600	-0.39846000
H	-2.17729400	1.63768600	-1.28595400
C	-5.05376800	0.71479600	0.27727200
H	-5.43599000	-1.24090800	1.10086400
H	-4.39271300	2.54711400	-0.64388100
H	-6.02441000	1.11336100	0.56285500
C	-1.20643400	-0.87546200	-0.82754500
H	-0.73392200	-0.25818300	-1.60377800
H	-1.33989000	-1.88544700	-1.24581100
C	4.07577600	0.45358400	-0.71783100
C	3.68003300	0.90247300	0.68116000
C	2.17219100	0.69294100	0.68553700
C	3.20391700	-0.77368700	-0.90026700
H	3.81438400	1.22534600	-1.45457900
H	5.14155700	0.22863100	-0.82183700
H	3.95500800	1.93273900	0.92097600
H	4.13566200	0.23826700	1.42758200
H	1.81683800	0.41200400	1.68810600
H	3.65419300	-1.63453700	-0.37552100
H	3.07572400	-1.05966500	-1.94916000
N	1.91356800	-0.38570500	-0.29948300
C	1.38919400	1.94594700	0.30232500
O	1.89446900	3.02186400	0.04337800
O	0.07172100	1.79111900	0.29239900
C	1.04186700	-1.48138800	0.14456600
C	1.46046100	-2.11382600	1.47211700
H	1.27384100	-1.45068100	2.32271900
H	0.89766700	-3.03861700	1.64521700
H	2.52560200	-2.36608200	1.44961400
N	1.12301400	-2.51068300	-0.86767000
H	0.50620700	-3.28634300	-0.64464500
H	0.87320600	-2.15454900	-1.78660300

**H<sub>2</sub>O-19**

N	-0.65347000	-0.18561100	0.25963100
H	1.69741000	1.37220100	-1.14078900
H	-0.75556100	-0.89345000	-0.46499200
C	-3.06937500	-0.02917100	0.43029000
C	-3.41398700	1.26760700	0.03698900
C	-3.91495100	-1.08491300	0.08823500
C	-4.58198500	1.50440800	-0.68058300
H	-2.75354100	2.09400100	0.29984800
C	-5.08521300	-0.85360400	-0.63485300
H	-3.65339400	-2.09806800	0.39281000
C	-5.42087300	0.44160300	-1.01970400
H	-4.84158300	2.51873500	-0.97542000
H	-5.73450100	-1.68646200	-0.89520500
H	-6.33422900	0.62561800	-1.58070000
C	-1.78922500	-0.28394700	1.17625400
H	-1.85607800	-1.26350200	1.68107000
H	-1.65924700	0.47633500	1.95967300
C	2.98989200	-2.14788500	-1.03687900
C	3.84068800	-0.89162000	-0.93527200
C	3.01918700	-0.02032200	0.02623500
C	1.58269600	-1.57194600	-1.10543500
H	3.23805100	-2.77292800	-1.90012900
H	3.10776200	-2.75674900	-0.12969600
H	3.91355800	-0.40493000	-1.91905900
H	4.85572200	-1.05581600	-0.56313800
H	3.29995700	-0.23464700	1.06760900
H	0.82680700	-2.27959400	-0.74639000
H	1.31778300	-1.31069100	-2.14001000
N	1.62287300	-0.34499500	-0.27486900
C	3.30472300	1.44398700	-0.22962800
O	4.29461100	2.01815600	0.17761100
O	2.41604200	2.04389800	-1.02053800
C	0.68297000	-0.25892600	0.86783200
C	0.86520500	-1.42385100	1.84315600
H	1.89389800	-1.45736200	2.21910800
H	0.20237500	-1.32153800	2.70937000
H	0.63764100	-2.38221000	1.36492100
N	0.98183500	0.97355400	1.56904800
H	0.49839500	1.75210200	1.12655200
H	0.69637600	0.93337200	2.54148800

**H<sub>2</sub>O-20**

N	-0.65091500	-0.25090500	0.21789400
H	1.65007800	1.41965000	-1.05849700
H	-0.68643500	-0.81268300	-0.62842900
C	-3.07697300	-0.14908100	0.37422100
C	-3.37150300	1.20666200	0.19520900
C	-3.97641800	-1.10149700	-0.10513400
C	-4.54111000	1.60065700	-0.44563000
H	-2.66973300	1.95321800	0.56718800
C	-5.15053400	-0.71196700	-0.75097900

H	-3.75515700	-2.15990600	0.03076200
C	-5.43500400	0.63983300	-0.92213000
H	-4.76035200	2.65853900	-0.57294700
H	-5.84179600	-1.46625300	-1.12032700
H	-6.34985300	0.94670000	-1.42386400
C	-1.80420300	-0.56153300	1.06032400
H	-1.86734600	-1.63086000	1.32775100
H	-1.68390900	0.00133400	1.99546900
C	3.06911700	-2.05214500	-1.06910800
C	3.90096100	-0.79475700	-0.87619200
C	3.01615600	0.04564400	0.06151000
C	1.66677700	-1.47834200	-1.19569600
H	3.37066500	-2.64102100	-1.94079000
H	3.13782700	-2.69480200	-0.18047200
H	4.02751600	-0.27727900	-1.83830500
H	4.89391200	-0.96038100	-0.44977600
H	3.28001000	-0.17359600	1.10760000
H	0.88763300	-2.20528100	-0.94373700
H	1.47645500	-1.14210700	-2.22517400
N	1.63676300	-0.31103800	-0.27919000
C	3.27529700	1.52028100	-0.18479300
O	4.26488600	2.10287000	0.20895300
O	2.34887500	2.11506700	-0.93284100
C	0.66254400	-0.35682900	0.85281600
C	0.86352500	-1.61035900	1.70902600
H	1.87973400	-1.64422900	2.12029100
H	0.16794400	-1.61363700	2.55360200
H	0.69906200	-2.52527200	1.13030100
N	0.77734700	0.78920500	1.72020800
H	1.61095000	0.79160300	2.29761600
H	0.68854400	1.66253800	1.20977900

#### H<sub>2</sub>O-21

N	-0.48608800	-0.35372700	0.06259000
H	3.53586500	-0.38326300	1.08811500
H	-0.26972800	-0.04505400	-0.88218400
C	-2.92193100	-0.54793900	-0.13937100
C	-3.23801500	0.53029100	0.69422100
C	-3.85228100	-0.95020000	-1.09816200
C	-4.45805100	1.18724700	0.57392300
H	-2.50906900	0.85191700	1.43801700
C	-5.07790400	-0.29492900	-1.22226000
H	-3.61345200	-1.78598500	-1.75542300
C	-5.38366500	0.77565900	-0.38690200
H	-4.69108900	2.02316800	1.23007400
H	-5.79114900	-0.62031000	-1.97645400
H	-6.33710600	1.29003800	-0.48361000
C	-1.61577900	-1.27842100	0.02983300
H	-1.52303100	-2.04637100	-0.75785600
H	-1.62203300	-1.81012900	0.99042100
C	1.53191600	2.52089000	-0.10931000
C	2.71170400	1.90722100	-0.84417300
C	2.43545200	0.39994300	-0.70971700



C	1.37442000	1.59170800	1.08419000
H	1.70081600	3.56283600	0.17961700
H	0.63227100	2.48303800	-0.73882000
H	3.64958200	2.16316100	-0.32997900
H	2.80853300	2.20762700	-1.89107400
H	1.83156800	0.05757200	-1.56455900
H	0.34712000	1.57970400	1.46175700
H	2.03873700	1.89144200	1.90703700
N	1.76891300	0.24713200	0.58976100
C	3.75745400	-0.34303100	-0.74867100
O	4.35641900	-0.59327900	-1.77399400
O	4.25191900	-0.63584100	0.45230800
C	0.73716300	-0.81377800	0.72297600
C	1.27883800	-2.12638000	0.16100200
H	2.19519000	-2.43396200	0.67837700
H	0.53220800	-2.91184300	0.30899700
H	1.48576200	-2.06109700	-0.91303100
N	0.40215400	-1.04009800	2.11450500
H	1.23328800	-1.30870900	2.63461100
H	0.02823700	-0.19364800	2.53598900

## H<sub>2</sub>O-22

N	-0.46918600	-0.40471700	0.11831800
H	3.53793800	-0.47793500	0.95639700
H	-0.29451300	-0.04622000	-0.81873600
C	-2.89786100	-0.54274300	-0.12426000
C	-3.19924700	0.55720700	0.68608500
C	-3.81812700	-0.93320000	-1.09729500
C	-4.39714000	1.24636000	0.52958500
H	-2.47756900	0.87020200	1.44042600
C	-5.02098800	-0.24465700	-1.25795600
H	-3.58935200	-1.78535400	-1.73672500
C	-5.31349000	0.84656300	-0.44486100
H	-4.62006700	2.09839100	1.16823400
H	-5.72696700	-0.56082100	-2.02274800
H	-6.24962300	1.38607500	-0.56922400
C	-1.61460200	-1.30510800	0.08094000
H	-1.53119800	-2.09190100	-0.68961300
H	-1.66567400	-1.82260600	1.04980800
C	1.43242600	2.48857800	0.16855600
C	2.57274500	1.99645600	-0.70796800
C	2.36611500	0.47091600	-0.69444300
C	1.40706600	1.44872300	1.27648900
H	1.58417600	3.50702500	0.53948700
H	0.48673400	2.46354200	-0.39037100
H	3.53792900	2.24764000	-0.24444800
H	2.57569000	2.39275400	-1.72691800
H	1.73149000	0.17641800	-1.54435600
H	0.42161200	1.36763100	1.74423900
H	2.13976000	1.68858500	2.06006500
N	1.78540500	0.17263600	0.61858300
C	3.71314000	-0.21004200	-0.86212100
O	4.28711100	-0.30927000	-1.92717600

O	4.24986900	-0.63030700	0.28015200
C	0.78322000	-0.90818700	0.70724700
C	1.30890400	-2.16468800	0.01890100
H	2.24403500	-2.50449300	0.47705700
H	0.57418600	-2.97147000	0.11502100
H	1.47214900	-2.00433300	-1.05213300
N	0.60287300	-1.21828500	2.11455600
H	-0.06213600	-0.58004700	2.54515900
H	0.24895400	-2.16098100	2.24199200

## H<sub>2</sub>O-23

N	-0.71464400	-0.22131500	-0.17525500
H	2.48751100	-1.04090600	1.41397800
H	-0.77655300	0.25673900	-1.07267300
C	-3.13079600	-0.48524900	-0.01683400
C	-3.45367000	0.37762700	1.03578300
C	-4.06256600	-0.68259500	-1.03578500
C	-4.68426600	1.02463500	1.07003900
H	-2.72679900	0.53660000	1.83210000
C	-5.29827500	-0.03507200	-1.00655300
H	-3.81824800	-1.35139100	-1.86052000
C	-5.61145000	0.81916000	0.04657800
H	-4.92521100	1.68805800	1.89771200
H	-6.01521900	-0.19928300	-1.80782400
H	-6.57432900	1.32407800	0.07350900
C	-1.80000800	-1.18745900	-0.04343100
H	-1.81308000	-1.94513600	-0.84637200
H	-1.66129800	-1.72916200	0.90333500
C	2.23156700	2.61050000	-0.27374200
C	3.38708700	1.76193800	-0.81799800
C	2.89202500	0.28847500	-0.73555600
C	1.41755400	1.61539200	0.53424600
H	2.58054000	3.46022100	0.32128700
H	1.61643100	2.99875500	-1.09373600
H	4.28900400	1.88859300	-0.20977000
H	3.65632500	2.02844800	-1.84376400
H	2.94092700	-0.18896400	-1.72356700
H	0.37249600	1.90427300	0.67515800
H	1.87086700	1.46903700	1.53492800
N	1.51075000	0.41849100	-0.29850500
C	3.88695000	-0.50003600	0.12643400
O	5.04213000	-0.61265700	-0.25118400
O	3.49922500	-1.03023400	1.27210500
C	0.65484900	-0.71719000	-0.02047400
C	0.98672200	-1.87240700	-0.95847300
H	1.99909100	-2.26071900	-0.80419800
H	0.29294800	-2.70270000	-0.79288000
H	0.88791200	-1.54518800	-1.99911000
N	0.86210800	-1.17865900	1.36966100
H	0.37124600	-0.56210500	2.01604200

H 0.51276400 -2.12205800 1.52227800

**H<sub>2</sub>O-24**

N	-0.55313500	-0.26918100	0.59037000
H	0.85003400	2.52163000	-0.95988000
H	-0.81145600	-1.00320500	-0.05905900
C	-2.93820900	0.16871800	0.44461900
C	-3.13991600	0.50158300	-0.89873700
C	-3.93587600	-0.52052100	1.13416200
C	-4.32025800	0.14530300	-1.54300900
H	-2.36249800	1.04533400	-1.43526300
C	-5.12185100	-0.87265700	0.49245700
H	-3.78240900	-0.78124600	2.18021600
C	-5.31421600	-0.54217000	-0.84666900
H	-4.46886400	0.40908200	-2.58732200
H	-5.89501500	-1.40731200	1.03883700
H	-6.23858100	-0.81753500	-1.34871000
C	-1.65345200	0.54712400	1.12244600
H	-1.73530700	0.39813200	2.20671300
H	-1.41644000	1.60191500	0.92275300
C	2.68671700	-2.74123400	-0.53772800
C	3.69783100	-1.60476700	-0.58968700
C	3.10692800	-0.51752000	0.31921100
C	1.35980800	-2.00361800	-0.51741300
H	2.76342200	-3.42882900	-1.38403500
H	2.80126400	-3.31982900	0.38716600
H	3.77013800	-1.21929500	-1.61651600
H	4.70187000	-1.89224800	-0.26772400
H	3.49458700	-0.61075900	1.34209000
H	0.54976400	-2.58944800	-0.06885500
H	1.05607300	-1.68141900	-1.52540700
N	1.66112300	-0.82722400	0.30994100
C	3.45799700	0.87690500	-0.24722200
O	4.59629200	1.28737900	0.07583600
O	2.61991700	1.42368200	-1.00343200
C	0.73542500	-0.05243800	0.84465200
C	1.08707100	1.05044400	1.77549700
H	2.15064100	1.06983300	2.00920400
H	0.79322000	2.00554900	1.32395100
H	0.52788700	0.92999500	2.70911300
N	-0.02015900	3.01900300	-0.75463500
H	-0.57104200	3.02482700	-1.60869200
H	0.23023900	3.98724300	-0.57300900

**H<sub>2</sub>O-25**

C	3.92314700	-0.36936800	-0.98794500
C	2.79217700	-1.26283100	-1.48229900
C	1.63264600	-0.88508100	-0.57277200
C	3.21712200	0.93615400	-0.63126900
H	4.37595200	-0.81091400	-0.09195200
H	4.71577000	-0.22785000	-1.72880700
H	3.02594900	-2.32977200	-1.43949400
H	2.52071800	-1.00800000	-2.51416000
H	0.66879000	-1.09742100	-1.06248000

H	3.29934900	1.67665900	-1.44161900
H	3.65837200	1.38914500	0.27047700
N	1.81235900	0.56275300	-0.42550200
C	1.62581400	-1.69149100	0.73451700
O	2.48885200	-2.48124000	1.06359100
O	0.56353300	-1.48884600	1.51351100
C	1.01338100	1.40536900	0.45749900
C	1.04716600	2.84115500	-0.06107500
H	0.33578500	3.45400500	0.50342700
H	2.04307600	3.27977900	0.06383800
H	0.79645300	2.88203200	-1.12521300
N	1.41901800	1.45360400	1.86406100
H	2.27636700	1.98559300	1.97654700
H	1.57672300	0.52476700	2.24672600
N	-0.35027500	0.83857400	0.49032800
H	0.00722800	-0.73618200	1.13566400
H	-0.83436700	1.31117800	1.25423800
C	-2.49919400	0.31717600	-0.51086300
C	-2.64972100	-1.07069900	-0.58850300
C	-3.60649000	1.09788800	-0.17433100
C	-3.88137700	-1.66551000	-0.33216400
H	-1.79534400	-1.69107300	-0.85927700
C	-4.84220000	0.50668500	0.08296300
H	-3.49724700	2.18052900	-0.11597500
C	-4.98096100	-0.87695000	0.00568900
H	-3.98545900	-2.74589300	-0.39952800
H	-5.69680400	1.12732800	0.34198000
H	-5.94437000	-1.34114900	0.20308400
C	-1.15978100	0.96134000	-0.73305800
H	-1.30226500	2.01495200	-1.01782600
H	-0.62185900	0.47542600	-1.55701500

## H<sub>2</sub>O-26

C	-3.54642700	0.51584800	-1.45824600
C	-2.25052700	1.25296500	-1.77176300
C	-1.35701000	0.84973500	-0.59420900
C	-3.06322400	-0.82914500	-0.92114100
H	-4.09836300	1.05531700	-0.67575400
H	-4.21143400	0.41192600	-2.32046600
H	-2.36154600	2.33661600	-1.85989200
H	-1.80479200	0.87166000	-2.69881500
H	-0.29743200	0.96509700	-0.86372400
H	-3.03898000	-1.59565100	-1.71146500
H	-3.73300500	-1.20104000	-0.12956100
N	-1.70949000	-0.55135100	-0.42866500
C	-1.56094500	1.83097300	0.56962300
O	-1.33991500	3.02023500	0.39223100
O	-1.97542100	1.39146700	1.73970900
C	-1.11143500	-1.41651900	0.55792900
C	-1.24190700	-2.87710400	0.12761800
H	-0.71150800	-3.51570400	0.84397200
H	-2.28900400	-3.19770100	0.10127700
H	-0.81627600	-3.03476400	-0.86928000

N	-1.77834700	-1.21030000	1.87717000
H	-1.25168500	-1.64011900	2.63629400
H	-2.68691800	-1.67007500	1.87771500
N	0.26484200	-0.98485700	0.75963300
H	-1.95030300	0.36630700	1.83838100
H	0.63123600	-1.39457500	1.61609400
C	2.47437500	-0.49580300	-0.20832900
C	2.53034600	0.75715900	0.40829700
C	3.64721900	-1.02900800	-0.75036200
C	3.72994900	1.46283900	0.47414100
H	1.62407800	1.17285800	0.84514500
C	4.84672000	-0.32433900	-0.69012000
H	3.61775400	-2.01081700	-1.22248600
C	4.89219800	0.92636400	-0.07635700
H	3.75641900	2.43634300	0.95901100
H	5.74981900	-0.75616200	-1.11590600
H	5.82863700	1.47686500	-0.02348300
C	1.18281700	-1.26247700	-0.33776300
H	1.41539000	-2.33660000	-0.44203500
H	0.67867900	-0.97675500	-1.27341200

#### H<sub>2</sub>O-27

C	4.39002700	0.19337300	0.09296400
C	3.77857300	-0.64202100	-1.02332400
C	2.30101400	-0.66264600	-0.64564700
C	3.36973400	1.30470500	0.29781600
H	4.48659600	-0.40680100	1.00590600
H	5.37713500	0.59400700	-0.15234200
H	4.18601100	-1.65345600	-1.09408300
H	3.91105200	-0.14533100	-1.99308700
H	1.67001300	-0.85088600	-1.51943100
H	3.60316500	2.18083500	-0.32060200
H	3.29578400	1.62596900	1.34191200
N	2.08777500	0.71247800	-0.15581700
C	2.00012500	-1.73741500	0.43343200
O	2.13941800	-2.91706000	0.03000000
O	1.64220000	-1.34272600	1.56718200
C	0.94197700	1.36296700	-0.03790000
C	0.98146500	2.76280300	0.48811600
H	-0.00826000	3.21993500	0.44433000
H	1.31511300	2.76147600	1.53116800
H	1.67981300	3.37918400	-0.08512300
N	-2.56122600	2.73136900	-0.07134300
H	-2.82393600	2.82558500	0.90662000
H	-2.55783300	3.66861300	-0.46527800
N	-0.26727200	0.90767800	-0.34528200
H	-3.31955300	2.22665300	-0.52565200
H	-1.02949900	1.60564300	-0.25510900
C	-2.17393500	-0.57776300	-0.37879700
C	-2.49962300	-0.65110500	0.97866700
C	-3.19151400	-0.63184300	-1.32963100
C	-3.82639700	-0.76087800	1.37965500
H	-1.70222700	-0.61009100	1.72112200

C	-4.52329700	-0.74833900	-0.93070100
H	-2.94111600	-0.57527300	-2.38806700
C	-4.84214000	-0.80659500	0.42333400
H	-4.07129800	-0.81285400	2.43782400
H	-5.31048700	-0.78902400	-1.67973500
H	-5.88031400	-0.89114800	0.73532300
C	-0.73528300	-0.41115000	-0.78622400
H	-0.63615400	-0.50775400	-1.87513800
H	-0.13625400	-1.19224000	-0.31148500

### H<sub>2</sub>O-28

C	-0.67119600	-0.94608000	0.91015700
N	-0.93235900	-2.13697600	0.10232700
H	-1.80333200	-2.57888800	0.38735500
N	0.74482100	-0.65815900	0.79911600
H	1.02445200	0.03500700	1.48927100
C	2.73388300	-0.02446600	-0.43018600
C	3.20308000	1.28875900	-0.37050700
C	3.65388600	-1.07490900	-0.36462200
C	4.56745800	1.55224300	-0.25350900
H	2.48963100	2.11188400	-0.42097700
C	5.01654500	-0.81735600	-0.25040800
H	3.29117600	-2.10177900	-0.40637000
C	5.47650600	0.49884700	-0.19481000
H	4.91941600	2.58049200	-0.21179100
H	5.72317800	-1.64311300	-0.20737700
H	6.54159600	0.70102100	-0.10851700
C	1.26065000	-0.30335200	-0.52257300
H	1.07334800	-1.14642600	-1.19948300
H	0.75656400	0.57785800	-0.95777100
H	-0.19702300	-2.80973900	0.30904900
C	-0.98534400	-1.17244500	2.38870300
H	-0.43889000	-2.05180300	2.74478200
H	-0.69602300	-0.31907000	3.01268800
H	-2.05740400	-1.35061300	2.53533300
N	-1.48169300	0.15360600	0.32659900
C	-2.54362000	2.24593600	0.51588700
C	-3.61050000	1.17521400	0.70290500
C	-2.92274900	-0.08152500	0.15258300
C	-1.28112900	1.49554500	0.90125600
H	-2.49462500	2.56689000	-0.53383000
H	-2.70878300	3.13418600	1.13204000
H	-4.56197700	1.38426000	0.20501500
H	-3.81090400	1.02947600	1.77225200
H	-3.28657800	-0.97615700	0.67670100
H	-1.19062700	1.46135000	1.99980600
H	-0.36638200	1.95479400	0.50497400
C	-3.25821000	-0.28643800	-1.32320400
O	-4.37652700	-0.55384600	-1.71596700
O	-2.23540100	-0.12195600	-2.15177700
H	-1.46233200	0.03765900	-1.54751800

### H<sub>2</sub>O-29

C	0.66290400	1.22302200	0.53035200
N	0.93397900	2.19115500	-0.51298600
H	0.96375300	1.76950600	-1.43723300
N	-0.75752300	0.91722600	0.52953200
H	-1.00139700	0.35896400	1.34468100
C	-2.75640600	-0.02696200	-0.46191400
C	-3.17554300	-1.34972600	-0.31305500
C	-3.70454000	0.99698500	-0.37262900
C	-4.51892900	-1.64777600	-0.08309200
H	-2.44187600	-2.15311200	-0.38168600
C	-5.04471400	0.70490300	-0.14309500
H	-3.37909100	2.03074200	-0.48437800
C	-5.45544800	-0.62114000	0.00229600
H	-4.83199900	-2.68337500	0.02869100
H	-5.77302200	1.51020700	-0.07904800
H	-6.50321800	-0.85145500	0.18096400
C	-1.30727400	0.30722800	-0.67830600
H	-1.21704900	1.03154400	-1.50014100
H	-0.76592100	-0.60578700	-0.98628500
H	1.81334100	2.67426200	-0.36091700
C	0.99789900	1.85725500	1.87528100
H	0.44766200	2.79671600	1.98047100
H	0.71791700	1.20163300	2.70624500
H	2.06929800	2.07096600	1.96291800
N	1.44710600	-0.03491700	0.29158800
C	2.39845400	-2.02008500	1.15551900
C	3.48256500	-0.95028900	1.16087200
C	2.91053500	0.09703000	0.19851000
C	1.13096900	-1.18243900	1.16669700
H	2.45351400	-2.61992100	0.23647900
H	2.45597100	-2.70430000	2.00667500
H	4.47333600	-1.30099100	0.85706900
H	3.56980100	-0.50476100	2.16042300
H	3.26823000	1.10321800	0.45429500
H	0.91121600	-0.85631500	2.19692800
H	0.25273600	-1.72477800	0.79299100
C	3.37748000	-0.16645900	-1.23091100
O	4.53223200	-0.05046900	-1.58650600
O	2.41382500	-0.55451600	-2.06097400
H	1.59568700	-0.54662700	-1.49538900

### H<sub>2</sub>O-30

C	-0.79052400	1.40653700	0.14767800
N	-0.71431100	2.36536200	1.22636000
H	-0.41296600	1.94147000	2.09976000
N	0.56512500	0.93848800	-0.16681000
H	0.54035600	0.00959800	-0.57970700
C	2.84821200	0.30459300	0.28776600
C	3.05633700	-1.03964500	0.60522200
C	3.74911400	0.94588200	-0.56597700
C	4.14836700	-1.73155200	0.08512000
H	2.35589400	-1.54463200	1.27179000
C	4.84358500	0.25996100	-1.08538000



H	3.58621800	1.99315100	-0.81913100
C	5.04522800	-1.08135500	-0.76019300
H	4.30187100	-2.77690700	0.34304500
H	5.54255500	0.77219000	-1.74263300
H	5.90138200	-1.61719600	-1.16331700
C	1.64279000	1.02624600	0.81989500
H	1.87831600	2.08466900	0.98737100
H	1.38699500	0.59485500	1.80443500
H	-1.63576400	2.76318600	1.38825900
C	-1.34871700	2.13568000	-1.07038900
H	-0.70453100	2.99387500	-1.27902500
H	-1.35491500	1.50049000	-1.96182200
H	-2.36839200	2.49655400	-0.88810200
N	-1.72359500	0.28710700	0.49473300
C	-2.09824600	-1.79598700	1.54780900
C	-1.83015100	-2.07700000	0.07558300
C	-2.02654600	-0.69602800	-0.56427600
C	-1.40916600	-0.45640000	1.73292200
H	-3.17681800	-1.70516000	1.73662600
H	-1.70295300	-2.56571100	2.21659800
H	-2.47481700	-2.83943200	-0.37166700
H	-0.78736400	-2.39232900	-0.06320200
H	-1.39558500	-0.58776700	-1.45631500
H	-0.32380000	-0.62126700	1.83412200
H	-1.75870300	0.09194600	2.61437300
C	-3.46808400	-0.52797600	-1.04104500
O	-3.93767400	-1.15600800	-1.96803800
O	-4.17899100	0.34666300	-0.33953000
H	-3.52739700	0.70874400	0.32069800

### H<sub>2</sub>O-31

C	-0.80672400	1.40554100	0.11982000
N	-0.85637800	2.37026500	1.19880200
H	-0.32939200	3.19986900	0.93839700
N	0.57295000	0.97817100	-0.18907600
H	0.58474100	0.10805900	-0.71628300
C	2.82969300	0.26998800	0.29714700
C	2.97730700	-1.10588400	0.49156600
C	3.79881600	0.95796400	-0.43621400
C	4.07699900	-1.78271000	-0.03144700
H	2.22229400	-1.64791600	1.06282600
C	4.90180100	0.28637400	-0.95770200
H	3.68461700	2.03019600	-0.59320500
C	5.04301200	-1.08608300	-0.75526300
H	4.18286000	-2.85297900	0.13027300
H	5.65457000	0.83434400	-1.51981000
H	5.90559200	-1.61080600	-1.15931600
C	1.61888300	0.97949600	0.83426600
H	1.88011300	2.01910200	1.07641400
H	1.32566800	0.49769700	1.78273100
H	-0.44277300	2.01272700	2.05593600
C	-1.35688300	2.09042100	-1.12690900
H	-0.76419800	2.98937100	-1.32355200

H	-1.27478900	1.45302200	-2.01339600
H	-2.40285200	2.38261100	-0.98703900
N	-1.70760700	0.28862200	0.49611500
C	-2.13931900	-1.73988600	1.61276700
C	-1.86510900	-2.07852000	0.15317800
C	-2.00910500	-0.71468600	-0.53843900
C	-1.40558700	-0.41999000	1.75547800
H	-3.21557700	-1.60622600	1.78759000
H	-1.77454600	-2.49948300	2.30978200
H	-2.52816200	-2.83548000	-0.27592500
H	-0.83065900	-2.42871200	0.03861500
H	-1.35607900	-0.65618500	-1.41952500
H	-0.32762900	-0.62315700	1.85524500
H	-1.73098900	0.17181900	2.61812400
C	-3.43750000	-0.52597900	-1.04713800
O	-3.89819800	-1.15073100	-1.98081100
O	-4.14943600	0.35912300	-0.35953300
H	-3.50218600	0.71930900	0.30732100

### H<sub>2</sub>O-32

C	-0.66355100	-0.99786400	0.18864300
N	-1.00134600	-1.64704700	-1.09210100
H	-0.68720000	-2.61493600	-1.11270100
N	0.78173300	-0.76657800	0.31163200
H	0.93322200	-0.04688000	1.01523900
C	2.99220000	-0.12948200	-0.42601200
C	3.39632600	1.20676700	-0.43532100
C	3.88239500	-1.10264500	0.03694000
C	4.66809000	1.56785000	0.00798700
H	2.70807000	1.96987800	-0.79889400
C	5.15297500	-0.74733400	0.47845000
H	3.57041000	-2.14657900	0.04628400
C	5.54844600	0.59091900	0.46563300
H	4.97056400	2.61240300	-0.00663000
H	5.83916100	-1.51405900	0.83106400
H	6.54225100	0.86906600	0.80868300
C	1.60725700	-0.51333800	-0.86797700
H	1.66140700	-1.43394000	-1.46612800
H	1.21960100	0.28065500	-1.53113400
H	-0.57318500	-1.17781800	-1.88684900
C	-1.06688700	-1.95378300	1.30469300
H	-0.46226400	-2.86193400	1.22539000
H	-0.86408000	-1.49280600	2.27720200
H	-2.12423100	-2.23649800	1.25929100
N	-1.39024700	0.25237900	0.31956800
C	-2.26684300	2.33363800	-0.40573800
C	-2.92268600	1.88027400	0.89480600
C	-2.74906200	0.36178800	0.82263800
C	-1.09231700	1.36670700	-0.58691000
H	-2.97899300	2.22030100	-1.23455300
H	-1.95028300	3.38039700	-0.38965400
H	-3.96909200	2.18044900	0.98933800
H	-2.36965800	2.25226000	1.76489900

H	-2.84146500	-0.08894800	1.82062400
H	-0.13361500	1.83168100	-0.31227800
H	-1.01226100	1.05122400	-1.64086500
C	-3.88946300	-0.24710500	-0.01217300
O	-5.05152000	-0.00972600	0.27151700
O	-3.59580700	-1.03105600	-1.03530700
H	-2.61198900	-1.27729200	-1.11564800

### H<sub>2</sub>O-33

C	-0.68865500	-0.00770400	0.93499400
N	0.03182100	-2.33928600	-1.18349600
H	0.04003900	-3.19230700	-1.73621900
N	0.59990500	0.21792500	0.68047700
H	0.85234200	0.92753800	0.00224600
C	2.98574800	-0.19799300	0.53958900
C	3.43937100	-0.96855800	-0.53308200
C	3.71357900	0.92801100	0.93154500
C	4.60900200	-0.62017200	-1.20401900
H	2.86786400	-1.84598900	-0.83417400
C	4.88106000	1.28003100	0.25938900
H	3.36406000	1.52700100	1.77198100
C	5.33013000	0.50498700	-0.80869500
H	4.95799200	-1.22800200	-2.03527200
H	5.44399800	2.15615500	0.57197000
H	6.24377200	0.77667300	-1.33199300
C	1.71090300	-0.55951300	1.24486700
H	1.79276200	-0.35145000	2.32007200
H	1.49607500	-1.62566700	1.10554400
H	0.52061200	-1.63916300	-1.73651600
C	-1.02780700	-1.04913200	1.93783400
H	-0.47341400	-0.87875500	2.86569200
H	-2.09174000	-1.08365900	2.16304800
H	-0.72625500	-2.02390200	1.53567000
N	-1.61658200	0.68160900	0.30044500
C	-2.66425300	1.98533800	-1.36516600
C	-3.60583700	1.80214400	-0.18093100
C	-3.07200000	0.53970600	0.49415600
C	-1.30217500	1.62285600	-0.78824700
H	-2.92573200	1.28908700	-2.17094100
H	-2.67502400	2.99781600	-1.77643900
H	-4.65460500	1.68761600	-0.46534000
H	-3.52637000	2.65411300	0.50603500
H	-3.30875900	0.53458000	1.56361000
H	-0.78619200	2.50063300	-0.37406600
H	-0.64559100	1.14088700	-1.52480900
C	-3.64804400	-0.75231700	-0.14330700
O	-4.86644200	-0.93079000	0.08463000
O	-2.87019400	-1.47595800	-0.80939200
H	-0.94489400	-2.03706600	-1.11755200

### H<sub>2</sub>O-34

N	-0.33630700	-0.90070200	0.38975500
H	-0.83588500	-1.40839000	1.11857800

H	-0.11196400	0.81209300	0.59177500
C	-2.53533500	-0.27595000	-0.47296000
C	-3.49329300	-1.11630500	0.10347500
C	-2.86721000	1.05999200	-0.70868400
C	-4.75204700	-0.63115700	0.44794700
H	-3.25108100	-2.16584200	0.27458500
C	-4.12784900	1.54848300	-0.37054700
H	-2.12879400	1.72175800	-1.15877500
C	-5.07201000	0.70493300	0.21050300
H	-5.48655000	-1.29837000	0.89307400
H	-4.37330000	2.59030800	-0.56395500
H	-6.05622000	1.08537600	0.47362900
C	-1.17822700	-0.82162500	-0.82135000
H	-0.66707300	-0.17053800	-1.54131500
H	-1.28900400	-1.80430200	-1.29986000
C	3.99188800	0.42043800	-0.92306900
C	3.74683100	0.88557400	0.50492300
C	2.24590000	0.68139700	0.67040700
C	3.10164700	-0.80422500	-0.99678400
H	3.65059300	1.18249600	-1.63704200
H	5.04009500	0.19238700	-1.13787600
H	4.04800700	1.91725500	0.70269600
H	4.27845400	0.22863000	1.20609400
H	1.99829600	0.40993200	1.70736700
H	3.61283300	-1.65095600	-0.49748500
H	2.86346500	-1.10967000	-2.02070200
N	1.88480500	-0.39734800	-0.27872600
C	1.43221900	1.93811400	0.36982800
O	1.91619800	3.02445900	0.11370200
O	0.11643300	1.78123400	0.43995200
C	1.01348700	-1.47070600	0.21942900
C	1.45343400	-2.03071000	1.57793300
H	1.30087600	-1.32582100	2.40255300
H	0.88298800	-2.93770600	1.80919700
H	2.51610900	-2.30031500	1.54428600
N	0.99120200	-2.51923600	-0.79967800
H	1.89147700	-2.99305600	-0.83167300
H	0.32110500	-3.22933300	-0.51014200

## H<sub>2</sub>O-35

N	-0.20239900	-1.14988400	0.60401900
H	-0.57395200	-1.64873900	1.40757100
H	0.89371000	0.64515300	-1.49427000
C	-2.43568100	-0.51795300	-0.20202900
C	-3.62350800	-1.00788500	-0.75209800
C	-2.49199900	0.62828800	0.59659000
C	-4.83754000	-0.36410900	-0.52546700
H	-3.59474400	-1.90859400	-1.36499500
C	-3.70489900	1.27322600	0.82804300
H	-1.57655300	1.01037800	1.04482000
C	-4.88207800	0.78116500	0.26699600
H	-5.75135300	-0.76265800	-0.96072900
H	-3.73003100	2.16404400	1.45215200

H	-5.82889600	1.28372200	0.45107000
C	-1.13460900	-1.21342200	-0.51177500
H	-0.66107400	-0.73430200	-1.37987100
H	-1.35338700	-2.24501900	-0.83460900
C	3.88034500	0.77255100	-0.71185800
C	3.30390400	1.34796800	0.57602000
C	1.84331700	0.88567400	0.51468800
C	3.22799200	-0.59876100	-0.76232600
H	3.57388300	1.37747600	-1.57652900
H	4.97241900	0.71503600	-0.71400100
H	3.39869200	2.43380000	0.67275500
H	3.78788400	0.88467800	1.44580900
H	1.40798500	0.75781300	1.51277400
H	3.78486100	-1.29001800	-0.10678800
H	3.20218800	-1.03282500	-1.76762800
N	1.85693200	-0.36501900	-0.26231300
C	0.97924800	1.93013400	-0.18362500
O	0.71367200	3.01022500	0.30503600
O	0.55472400	1.57495900	-1.39167200
C	1.17769800	-1.52233500	0.36751900
C	1.79705200	-1.88761700	1.72017300
H	1.67304100	-1.09141100	2.46307500
H	1.32083000	-2.79404400	2.11201700
H	2.86660900	-2.09774500	1.61450100
N	1.27387900	-2.62905600	-0.58993800
H	2.22920500	-2.97803300	-0.63804500
H	0.71717700	-3.40401600	-0.23348000

## H<sub>2</sub>O-36

N	-0.42500900	1.14666600	-0.22873800
H	-0.96988000	1.93768000	-0.55900900
H	1.62987200	0.16476600	1.81189600
C	-2.51414100	0.05537600	0.32686600
C	-3.60000500	0.92737200	0.42721800
C	-2.69642200	-1.18516600	-0.28948000
C	-4.84702300	0.56974200	-0.08250500
H	-3.46630700	1.89316600	0.91509200
C	-3.94137300	-1.54922500	-0.79475000
H	-1.85521600	-1.87453100	-0.36415800
C	-5.01912000	-0.66994200	-0.69448400
H	-5.68522500	1.25731300	0.00365800
H	-4.07278400	-2.52144900	-1.26431100
H	-5.99254400	-0.95408500	-1.08736100
C	-1.16103800	0.46475500	0.83905300
H	-0.61128800	-0.42902500	1.15501500
H	-1.29022000	1.08870600	1.74042100
C	3.86986600	-0.64447300	-0.97054300
C	2.66441500	-1.48474500	-1.38438000
C	1.56363400	-0.90517300	-0.49230700
C	3.28205600	0.74715300	-0.70537100
H	4.30449000	-1.05337900	-0.04821100
H	4.66323000	-0.62593100	-1.72326500
H	2.80581300	-2.55884600	-1.24032000

H	2.39784300	-1.30108600	-2.43151000
H	0.56274900	-1.12606400	-0.88923400
H	3.48914700	1.43743900	-1.53545200
H	3.72511200	1.18959100	0.20367500
N	1.84032200	0.51274900	-0.58463000
C	1.63548500	-1.58026900	0.88957400
O	1.56624900	-2.79487400	0.98287600
O	1.77862300	-0.83165400	1.97092900
C	0.96459300	1.54028700	-0.05041800
C	1.18469500	2.84126900	-0.81379400
H	0.94342100	2.70514400	-1.87383800
H	0.54612800	3.62737200	-0.39532600
H	2.22193800	3.18045300	-0.73583100
N	1.27942100	1.72340900	1.39960700
H	2.14964000	2.24507300	1.49510100
H	0.56823000	2.28837700	1.86078100

### H<sub>2</sub>O-37

N	0.00950900	1.61080100	-1.02551700
H	0.05923300	2.54655600	-1.40575300
H	-3.47648100	0.09613400	-1.16322900
C	2.20388900	0.44324000	-0.69586700
C	2.53582700	1.27283400	0.37452400
C	3.02154300	-0.65291500	-0.98750800
C	3.66856400	1.00916200	1.14396100
H	1.90670100	2.12656500	0.61893200
C	4.15407500	-0.91338300	-0.22299800
H	2.76060400	-1.31087200	-1.81629800
C	4.48032500	-0.08220500	0.84821800
H	3.91401200	1.66047300	1.97945300
H	4.77852000	-1.77171400	-0.45914600
H	5.36121200	-0.28865500	1.45106800
C	0.99727400	0.68499700	-1.57004900
H	0.51769400	-0.26092600	-1.84113300
H	1.31592300	1.12891100	-2.51992600
C	-2.39264400	-1.13418300	1.96096800
C	-0.98943300	-1.67614900	1.73079400
C	-0.55681700	-0.95898000	0.45419000
C	-2.24316500	0.34311600	1.64454500
H	-3.10127300	-1.59733700	1.26165200
H	-2.76254600	-1.29514000	2.97697700
H	-0.94323700	-2.76116100	1.60967700
H	-0.33074000	-1.39335100	2.56209700
H	0.53310200	-0.86587100	0.40777700
H	-1.90755400	0.91121600	2.52246400
H	-3.15800600	0.79367900	1.24919100
N	-1.17230000	0.37743500	0.61383700
C	-1.04311400	-1.70698700	-0.81336500
O	-0.44831400	-2.78992800	-1.02076800
O	-1.94621200	-1.17708000	-1.50413900
C	-0.91920900	1.47404000	-0.07221100
C	-1.73437800	2.69039500	0.21515700
H	-1.70239000	2.93426800	1.28120700

H	-1.37753700	3.55353400	-0.34892000
H	-2.77712600	2.48315200	-0.06233700
N	-4.25637000	0.73685400	-0.98134700
H	-4.98837700	0.19316000	-0.53141400

### H<sub>2</sub>O-38

N	0.70626000	-0.13046100	0.21376400
H	0.88669000	0.19816200	-0.73404400
C	3.10796600	-0.45965200	0.24825400
C	3.89124700	-1.05647300	-0.73994300
C	3.57230400	0.70425400	0.86961600
C	5.12092000	-0.50527100	-1.10044000
H	3.53568800	-1.96260200	-1.22920800
C	4.79670600	1.25854600	0.51154900
H	2.96210700	1.17266700	1.64112000
C	5.57489800	0.65336100	-0.47642700
H	5.72240500	-0.98236800	-1.87075400
H	5.14839400	2.16181200	1.00492900
H	6.53325200	1.08458500	-0.75621700
C	1.77583700	-1.03922500	0.63448700
H	1.73196200	-1.14672200	1.72609100
H	1.66955400	-2.04740200	0.20079800
C	-2.25063000	2.67144200	-0.54214400
C	-3.48157300	1.76752200	-0.41893100
C	-2.94190100	0.46185400	0.19671900
C	-1.10729400	1.83952100	0.01958500
H	-2.05873400	2.91922200	-1.59148300
H	-2.36131300	3.61396000	0.00248500
H	-3.92351600	1.56337200	-1.40074200
H	-4.27168700	2.18393500	0.21100600
H	-3.01923600	0.54919200	1.29788400
H	-0.98209500	2.02208700	1.10318200
H	-0.15394200	2.06074600	-0.46168900
N	-1.52889000	0.44456500	-0.22373500
C	-3.88746900	-0.66873400	-0.17619800
O	-5.06788000	-0.56026400	0.10212100
O	-3.44797800	-1.74175700	-0.81194100
C	-0.64514900	-0.59680300	0.31948100
C	-0.97226900	-1.03536800	1.73445500
H	-1.97905500	-1.45813700	1.79505500
H	-0.28200900	-1.81283500	2.06971300
H	-0.90414000	-0.18200200	2.41742800
O	-0.84732100	-1.78728400	-0.49602800
H	-0.45782600	-1.60402600	-1.36485500
H	-2.45421300	-1.78778400	-0.82451500

### H<sub>2</sub>O-40

C	2.17322400	2.28801000	0.83329800
C	1.94103400	2.00191300	-0.64533500
C	2.04798900	0.48377300	-0.71664200
C	1.40336900	1.16289500	1.50484700
H	3.24374800	2.21114000	1.06781500
H	1.82688400	3.27719200	1.14650400

H	2.65114700	2.49592300	-1.31274900
H	0.92730800	2.30906400	-0.93344200
H	1.42620300	0.06552300	-1.52156700
H	0.32991900	1.41170700	1.57576500
H	1.76529000	0.94960900	2.51847200
N	1.62287500	0.01788800	0.61651100
C	3.48223100	0.01843700	-0.99470900
O	4.38625900	0.75641800	-1.33225800
O	3.70312400	-1.28825300	-0.85790700
C	0.76429200	-1.13606800	0.79235600
C	1.03870000	-1.79869800	2.13356500
H	0.43986300	-2.71129000	2.24057700
H	2.09885500	-2.06155500	2.19587400
H	0.78369900	-1.13011300	2.96053200
N	-0.64092200	-0.82477700	0.72178100
H	-1.20655600	-1.60840800	1.03941200
C	-2.64452400	-0.02514800	-0.40755400
C	-3.53848300	-0.62250700	-1.29661200
C	-3.14662100	0.81636600	0.59120000
C	-4.90917900	-0.38368700	-1.19629600
H	-3.15702700	-1.28187500	-2.07547500
C	-4.51268400	1.05561800	0.69601100
H	-2.45230800	1.28338700	1.28902800
C	-5.39925800	0.45535700	-0.19954300
H	-5.59348300	-0.85620100	-1.89733700
H	-4.88910800	1.71511500	1.47487500
H	-6.46743600	0.64280200	-0.11867300
C	-1.16462000	-0.26878400	-0.51984000
H	-0.66026600	0.69157800	-0.70136900
H	-0.96123200	-0.90848500	-1.39510700
O	1.18126900	-2.02922100	-0.26529200
H	2.86970500	-1.74892200	-0.59626100
H	0.77309000	-2.89439300	-0.12973700

## H<sub>2</sub>O-42

C	-0.61765000	-0.67435400	0.26173000
N	0.73428100	-0.18559400	0.27033200
H	0.89871100	0.48356600	-0.47875500
C	3.14031900	-0.47906800	0.13198000
C	3.88645500	-0.62736300	-1.03748600
C	3.63335600	0.34253000	1.15073800
C	5.10850600	0.02802500	-1.18821100
H	3.50880300	-1.26653600	-1.83482300
C	4.85039100	0.99982200	1.00351400
H	3.05320900	0.46015800	2.06540200
C	5.59178700	0.84317500	-0.16833400
H	5.68132300	-0.09931200	-2.10386200
H	5.22503800	1.63300400	1.80452700
H	6.54498200	1.35398700	-0.28316800
C	1.81780700	-1.17370000	0.29752100
H	1.79539300	-1.68380900	1.26928300
H	1.70543900	-1.94783400	-0.47904200
C	-0.90825500	-1.53891500	1.47088200



H	-0.78350900	-0.95426100	2.38674300
H	-1.92673600	-1.93612000	1.43251700
H	-0.23301900	-2.39672200	1.49196100
N	-1.51043800	0.44461400	0.20415200
C	-3.20949700	1.92370300	0.40897800
C	-2.87782500	0.45953500	0.67595900
C	-1.35123200	1.48177900	-0.81484300
H	-4.27713800	2.12836700	0.31312000
H	-2.76989900	2.55965100	1.19048800
H	-2.95007000	0.23386600	1.74785200
H	-0.53731800	2.17400800	-0.54003100
H	-1.16216400	1.08034400	-1.82400400
C	-3.91409700	-0.42203300	-0.03617300
O	-5.08756300	-0.34373300	0.26892200
O	-3.51548200	-1.24650600	-0.99342900
O	-0.85489500	-1.57009500	-0.88844000
H	-2.52782500	-1.31624000	-1.07376900
H	-0.35953800	-1.25184600	-1.65652200
O	-2.58618200	2.15455700	-0.84790800

#### H<sub>2</sub>O-44

N	-0.41632100	1.09120500	-0.31295300
H	-0.97352400	1.91707100	-0.51414700
H	1.70409700	0.08678600	1.78516800
C	-2.53443000	0.01679800	0.21845000
C	-3.62905600	0.40209300	0.99251800
C	-2.76223900	-0.64531100	-0.99271400
C	-4.93020200	0.12616400	0.57226400
H	-3.46061900	0.92059400	1.93565100
C	-4.05811300	-0.92205400	-1.41566600
H	-1.91054400	-0.94310400	-1.60340600
C	-5.14700700	-0.53687600	-0.63221300
H	-5.77394400	0.43174800	1.18678200
H	-4.22142200	-1.44080600	-2.35769900
H	-6.16037400	-0.75364100	-0.96212900
C	-1.13119800	0.29185800	0.68496900
H	-0.61522000	-0.66741200	0.82382900
H	-1.15728300	0.77707400	1.67249900
C	3.96979300	-0.54788900	-0.81867900
C	2.83052700	-1.42108000	-1.33747300
C	1.64643300	-0.91404400	-0.50832700
C	3.31137600	0.81314300	-0.57517800
H	4.35336400	-0.95902800	0.12478900
H	4.81317200	-0.48278300	-1.51168800
H	3.00411200	-2.49343400	-1.21679700
H	2.62673800	-1.21488600	-2.39443400
H	0.68638700	-1.16384800	-0.98045500
H	3.52206800	1.51280400	-1.39599500
H	3.68252500	1.27412500	0.35525400
N	1.87559700	0.51377300	-0.51791000
C	1.66631500	-1.61972900	0.85662900
O	1.58218400	-2.82996600	0.93853200
O	1.80732800	-0.88361600	1.95625800

C	0.94326000	1.49986200	-0.05255200
C	1.19460400	2.83931900	-0.72368000
H	1.05779900	2.74570700	-1.80528800
H	0.49430800	3.58404500	-0.33198600
H	2.21046200	3.19945500	-0.53578800
H	1.76705300	2.36435700	1.56839000
O	1.09993000	1.68568300	1.40063600

### H<sub>2</sub>O-Product

N	-1.60337700	-0.61622800	-0.57064100
H	-1.66746100	-0.61299700	-1.57978900
C	0.81841100	-0.51931600	-0.01133400
C	2.02910400	-1.21581100	-0.03974300
C	0.84338600	0.87626200	0.00767900
C	3.24274800	-0.53261100	-0.04090300
H	2.01870900	-2.30510600	-0.06453400
C	2.05596600	1.56268300	0.00276400
H	-0.09258400	1.43241700	0.02106600
C	3.25946900	0.86069700	-0.01958400
H	4.17650400	-1.08985600	-0.06638800
H	2.05984700	2.65021200	0.01599400
H	4.20560000	1.39677500	-0.02562300
C	-0.47831900	-1.28992000	0.04376000
H	-0.75621800	-1.47460000	1.08887600
H	-0.34739300	-2.26984100	-0.43041500
C	-2.54518900	0.04962900	0.14172600
C	-3.64106800	0.69801900	-0.65698700
H	-3.57583700	0.50507800	-1.73100300
H	-4.60602100	0.33962700	-0.28639700
H	-3.60684400	1.77877700	-0.48765300
O	-2.51146300	0.12816700	1.37201000

### H<sub>2</sub>O-TS3-IM1

C	1.45822800	2.10458500	0.96018800
C	2.07179200	1.37576500	-0.23243800
C	1.08435200	0.24790600	-0.55366900
C	-0.02653700	1.92760400	0.71950700
H	1.74420700	1.62239200	1.90380900
H	1.74838400	3.15720400	1.01772100
H	3.06733700	0.97351300	-0.02976800
H	2.14841800	2.05085500	-1.09165100
H	0.75159000	0.32014600	-1.59985900
H	-0.37197200	2.56157300	-0.10816000
H	-0.66235700	2.09151800	1.59251400
N	-0.14668000	0.51475100	0.26904000
C	1.62025500	-1.17219200	-0.36981000
O	2.80255300	-1.39360100	-0.17322000
O	0.73915700	-2.13320700	-0.50461600
H	-0.24510500	-1.77153700	-0.64974700
C	-1.60463500	0.08581300	-0.56837400
C	-2.69385200	0.65664700	0.31854400
H	-2.71393400	1.75103600	0.31813400
H	-3.64872700	0.29610800	-0.07878300

H	-2.59366700	0.29782600	1.34769400
N	-1.49369200	0.74652300	-1.81660200
H	-1.51140300	0.08929100	-2.58695400
H	-2.14654400	1.50667200	-1.96221900
O	-1.55371300	-1.22985900	-0.62311500
H	-0.17837500	-0.10015500	1.09784300
O	-1.14517900	-1.60402400	2.11002600
H	-0.62844300	-2.38262600	2.34443700
H	-1.47697500	-1.76397300	1.20163800

**H<sub>2</sub>O-TS3-5b-H<sub>2</sub>O**

C	1.45822800	2.10458500	0.96018800
C	2.07179200	1.37576500	-0.23243800
C	1.08435200	0.24790600	-0.55366900
C	-0.02653700	1.92760400	0.71950700
H	1.74420700	1.62239200	1.90380900
H	1.74838400	3.15720400	1.01772100
H	3.06733700	0.97351300	-0.02976800
H	2.14841800	2.05085500	-1.09165100
H	0.75159000	0.32014600	-1.59985900
H	-0.37197200	2.56157300	-0.10816000
H	-0.66235700	2.09151800	1.59251400
N	-0.14668000	0.51475100	0.26904000
C	1.62025500	-1.17219200	-0.36981000
O	2.80255300	-1.39360100	-0.17322000
O	0.73915700	-2.13320700	-0.50461600
H	-0.24510500	-1.77153700	-0.64974700
C	-1.60463500	0.08581300	-0.56837400
C	-2.69385200	0.65664700	0.31854400
H	-2.71393400	1.75103600	0.31813400
H	-3.64872700	0.29610800	-0.07878300
H	-2.59366700	0.29782600	1.34769400
N	-1.49369200	0.74652300	-1.81660200
H	-1.51140300	0.08929100	-2.58695400
H	-2.14654400	1.50667200	-1.96221900
O	-1.55371300	-1.22985900	-0.62311500
H	-0.17837500	-0.10015500	1.09784300
O	-1.14517900	-1.60402400	2.11002600
H	-0.62844300	-2.38262600	2.34443700
H	-1.47697500	-1.76397300	1.20163800

**H<sub>2</sub>O-TS-IM1-5a**

C	0.89741400	2.62225100	0.08688000
C	1.86695200	1.43737300	0.10695400
C	1.05390400	0.27150800	-0.44695800
C	-0.48556400	2.00333400	-0.12378500
H	0.94320200	3.18706800	1.02212100
H	1.12633500	3.31881800	-0.72478000
H	2.18152400	1.19988400	1.13109600
H	2.77183400	1.60042600	-0.48157300
H	0.97257100	0.36112200	-1.54334400
H	-0.83681400	2.14256400	-1.15415500
H	-1.24283500	2.38968700	0.56244100

N	-0.31277700	0.54031500	0.10610100
C	1.74675600	-1.06894400	-0.20086800
O	2.96188900	-1.10526000	-0.26595200
O	1.04602100	-2.16627100	-0.01358500
H	0.04078000	-2.00221600	0.07782200
C	-1.47836000	-0.33846900	-0.42202200
C	-2.80076900	0.33829200	-0.11034700
H	-2.97318400	1.23016700	-0.71902000
H	-3.59028600	-0.38930000	-0.32217000
H	-2.86269000	0.60193800	0.94976000
N	-1.32415100	-0.51135100	-1.83340200
H	-0.76583100	-1.33158200	-2.05429000
H	-2.22533300	-0.62276300	-2.28628700
O	-1.37547000	-1.52641400	0.29944700
H	-0.36755700	0.25792100	1.28375000
O	-0.78888100	-0.42129200	2.32526900
H	-0.07678200	-0.80891600	2.84685200
H	-1.18691900	-1.17574300	1.40233500

#### H<sub>2</sub>O-TS-5a-6a

C	1.36480000	1.93222500	0.61748900
C	1.81722800	1.29353100	-0.69106600
C	0.91297900	0.06654400	-0.77577700
C	-0.15133700	1.74232800	0.60942700
H	1.80735100	1.39049700	1.46363900
H	1.64947800	2.98384300	0.71164700
H	2.87258200	1.01418800	-0.70786500
H	1.61090300	1.95683700	-1.54006900
H	0.82030600	-0.28108500	-1.81333500
H	-0.67666800	2.63162700	0.23451200
H	-0.53770000	1.51818700	1.61424800
N	-0.36299700	0.61191600	-0.30609300
C	1.50044100	-1.09869900	0.05377600
O	2.64226600	-1.44843300	-0.21445600
O	0.77087300	-1.64694600	0.97383300
H	-0.34275500	-1.36946200	1.11000500
C	-1.54254600	-0.06028000	-0.35320300
C	-2.79541300	0.73208700	-0.12218100
H	-2.93174800	1.42710400	-0.95838600
H	-3.65658300	0.06151500	-0.07143500
H	-2.75425200	1.30813200	0.80432900
N	-1.65796200	-1.02035900	-1.33690300
H	-0.86779200	-1.64684200	-1.43436100
H	-2.51620600	-1.55211300	-1.25900300
O	-1.56411000	-1.10779300	1.16004800
H	-1.75935400	-0.60436300	1.96086700

#### H<sub>2</sub>O-TS-6a-6c

C	-0.94351100	2.13977600	-0.35981600
C	-1.47253100	1.30750500	0.80303000
C	-0.71100400	-0.00352700	0.68087200
C	0.54252000	1.82247700	-0.35118800
H	-1.39348400	1.79967400	-1.30155200

H	-1.13725900	3.21038500	-0.25401100
H	-2.55167000	1.14351200	0.76427200
H	-1.22396100	1.78954000	1.75655100
H	-0.48151400	-0.44809200	1.66130100
H	1.07591700	2.44174200	0.38501700
H	1.02079300	1.95080100	-1.32723700
N	0.56997400	0.41020400	0.06103700
C	-1.42841500	-1.09603700	-0.14143800
O	-2.55964300	-0.90970300	-0.58536700
O	-0.75939700	-2.19431700	-0.27506800
C	1.66646400	-0.35886600	0.07943400
C	2.97691100	0.25891500	-0.27280700
H	3.14064700	1.18788900	0.28187800
H	3.79368400	-0.43374200	-0.06171500
H	3.00254700	0.50177200	-1.34115200
N	1.53442600	-1.62597800	0.39017100
H	0.40077200	-2.05845200	0.14149700
H	2.39244500	-2.16391300	0.39166900

#### H<sub>2</sub>O-TS-IM2

C	0.73460000	2.14905100	0.40490100
C	1.28540000	1.41209100	-0.81040800
C	0.67376600	0.01944300	-0.65759000
C	-0.70640800	1.66731300	0.46194200
H	1.27299800	1.84037300	1.31198300
H	0.80624600	3.23688300	0.32461300
H	2.37619100	1.37784000	-0.86069100
H	0.91059300	1.86822600	-1.73431300
H	0.51083500	-0.48134500	-1.62254200
H	-1.34311800	2.26165000	-0.21097800
H	-1.13424300	1.71322900	1.46900900
N	-0.61153300	0.27809500	-0.01157800
C	1.58956100	-0.91044700	0.13431000
O	2.77501500	-1.00515800	-0.10106900
O	1.03700800	-1.64442500	1.10148700
C	-1.69233200	-0.54422800	-0.22066300
C	-3.01831800	-0.00692100	0.22837500
H	-3.26116300	0.92771600	-0.28953800
H	-3.80870400	-0.73312600	0.02760200
H	-3.01056300	0.20850600	1.30268900
N	-1.48989000	-1.71010500	-0.73932600
H	0.07266200	-1.51151500	1.10996700
H	-2.37557000	-2.20550400	-0.82001700

#### H<sub>2</sub>O-TS-6c-6d

C	0.85738800	2.01518500	0.69042400
C	1.21130400	1.44798700	-0.67872100
C	0.57532100	0.05347700	-0.63660400
C	-0.57459600	1.54268900	0.86303900
H	1.50504300	1.58940100	1.46926600
H	0.94340800	3.10426400	0.74191500
H	2.28320300	1.40890100	-0.89329300

H	0.72375300	2.03600100	-1.46586000
H	0.24334900	-0.27023700	-1.63146200
H	-1.25745500	2.17399300	0.27574300
H	-0.91706600	1.52501700	1.90318900
N	-0.55973500	0.16405700	0.30881600
C	1.56549100	-0.99367200	-0.13666900
O	2.56615500	-1.30222200	-0.75053700
O	1.25349900	-1.54017300	1.03354000
C	-1.82820200	-0.27005400	-0.23040500
C	-2.37918100	-1.48885100	0.43093000
H	-2.47935300	-1.31060500	1.50842300
H	-3.34795400	-1.78086900	0.01759300
H	-1.67510200	-2.32304300	0.31416700
N	-2.34254700	0.38913300	-1.18624500
H	0.40302500	-1.09867300	1.29486600
H	-3.23125900	-0.02787300	-1.46853300

### H<sub>2</sub>O-TS-6a-7

N	-0.40800800	0.84337800	0.04752900
H	-0.16756100	-0.16505000	0.03652100
H	-0.56851000	1.14521800	1.00860200
C	-2.80441000	0.34519300	-0.27256500
C	-2.85895000	-1.04581100	-0.41161800
C	-3.85917600	1.00878900	0.35486900
C	-3.95097300	-1.75945800	0.07142200
H	-2.03407000	-1.56734300	-0.89877300
C	-4.95627700	0.29543400	0.83615600
H	-3.82242600	2.09196700	0.46371400
C	-5.00304800	-1.08917000	0.69624200
H	-3.98522400	-2.84036800	-0.04265200
H	-5.77421000	0.82300500	1.32124400
H	-5.85829600	-1.64665100	1.07064900
C	-1.60290200	1.09977100	-0.77278700
H	-1.80199800	2.17798900	-0.78453300
H	-1.36345200	0.78973600	-1.79826300
C	3.14014000	-0.34289600	2.01492400
C	3.88897900	-0.74159600	0.74943800
C	2.84152200	-0.51668400	-0.33927000
C	2.39267000	0.91091300	1.58344000
H	2.42305300	-1.12993300	2.28725100
H	3.78967600	-0.16416700	2.87634900
H	4.24856400	-1.77278400	0.74984200
H	4.74402900	-0.07187200	0.58989300
H	3.31894300	-0.29024100	-1.30405800
H	3.00409600	1.81362300	1.73353000
H	1.45493700	1.04513200	2.13871800
N	2.15198800	0.68499200	0.15324300
C	1.95433800	-1.76562100	-0.57985500
O	2.57183800	-2.83110700	-0.78739000
O	0.69880600	-1.60837200	-0.60234200
C	1.27131300	1.44039100	-0.56872200
C	1.18481700	2.90131200	-0.22064000

H	2.12877700	3.38317800	-0.49868200
H	0.37184400	3.38528000	-0.76987000
H	1.01872200	3.05804600	0.84739400
N	1.26696400	1.18443400	-1.92972900
H	1.12012600	0.21062200	-2.17911100
H	0.68297800	1.80742500	-2.47342700

**H<sub>2</sub>O-TS-6a-8**

C	-2.55151500	0.13548100	2.49569400
C	-2.81882300	-1.07790000	1.61480700
C	-1.81027700	-0.88907000	0.50358100
C	-2.27950900	1.26334900	1.50103400
H	-3.37655000	0.38010400	3.17068300
H	-1.66124600	-0.04462600	3.11217900
H	-3.83000900	-1.05661100	1.18906000
H	-2.68496100	-2.03184400	2.13436400
H	-0.80088600	-1.09912400	0.90715700
H	-1.48657000	1.93345800	1.85757800
H	-3.17659800	1.87196400	1.32598100
N	-1.90928500	0.56922900	0.24918200
C	-1.94859800	-1.78748300	-0.73943600
O	-3.01272400	-2.41052300	-0.91231500
O	-0.92597400	-1.79882200	-1.49094200
C	-1.48817700	1.24854000	-0.86140300
C	-1.47383500	2.74739200	-0.75493400
H	-1.04092700	3.18152600	-1.66001500
H	-2.50127600	3.11471700	-0.65999900
H	-0.90010800	3.09822800	0.10494900
N	-1.89339300	0.80767600	-2.11155800
H	-1.73024700	-0.17955500	-2.30185100
H	-1.56104900	1.39018400	-2.87114100
N	0.39739300	0.84259000	-0.92516800
H	0.31976700	-0.16298000	-1.14211300
H	0.82827400	1.29771700	-1.73084000
C	2.52017800	0.38058700	0.27163900
C	2.57701300	-1.01706900	0.28318900
C	3.70893000	1.10854500	0.21873400
C	3.80192800	-1.67442100	0.24076400
H	1.65324400	-1.59628100	0.32468500
C	4.93864400	0.45193100	0.18077800
H	3.67112400	2.19690300	0.20934400
C	4.98653900	-0.93934700	0.19081600
H	3.83449400	-2.76112600	0.25162700
H	5.85881200	1.03015400	0.14257600
H	5.94492900	-1.45213000	0.16059500
C	1.18555900	1.07503900	0.29637700
H	1.31530300	2.15609200	0.42106900
H	0.58272600	0.71808200	1.14313800

**H<sub>2</sub>O-TS-6a-11**

C	-1.43024200	1.25573700	-0.77841900
N	-1.64676600	2.13247800	0.27958500
H	-2.23563200	2.92160200	0.03825800

N	0.46117900	1.01416000	-0.74812500
H	0.78010400	0.66258100	-1.65212500
H	0.86944400	1.94687200	-0.60877600
C	2.32448700	-0.31928900	0.17430300
C	2.62506400	-1.56561700	-0.37976000
C	3.36993000	0.53380200	0.53991200
C	3.94946800	-1.95612000	-0.56620500
H	1.81198900	-2.23534800	-0.66142500
C	4.69359100	0.14584000	0.35563400
H	3.14014200	1.50728900	0.97347200
C	4.98548400	-1.10085000	-0.19793000
H	4.17147100	-2.93029800	-0.99543700
H	5.50009600	0.81429800	0.64748400
H	6.01978300	-1.40525100	-0.33912600
C	0.89454200	0.11096000	0.33210400
H	0.72552800	0.63645300	1.28019500
H	0.22998400	-0.76271300	0.32202800
O	0.86913900	3.60255000	0.48834800
H	1.30753100	3.75371200	1.33284900
H	-0.02792500	3.28071900	0.70028200
C	-1.51983000	1.91231300	-2.13090800
H	-0.95834300	2.85205100	-2.13503100
H	-1.14386800	1.27605900	-2.93473100
H	-2.57455400	2.13129100	-2.33832000
N	-1.91963100	-0.01290000	-0.64848500
C	-2.32016900	-2.27503100	-1.09873000
C	-3.39714400	-1.76224500	-0.14968900
C	-2.79458600	-0.49768700	0.45100700
C	-1.80380900	-0.99456100	-1.73151600
H	-1.52003600	-2.76221900	-0.52718200
H	-2.69489900	-2.98282000	-1.84386200
H	-3.66414400	-2.48220800	0.62783400
H	-4.30255800	-1.50494600	-0.71542700
H	-3.56371000	0.26324100	0.64426000
H	-2.42272900	-0.69911900	-2.59307100
H	-0.76387200	-1.07872000	-2.07808000
C	-2.00753600	-0.71464600	1.77237100
O	-1.65959800	-1.87502700	2.07613800
O	-1.77120200	0.34061300	2.42839800
H	-1.86949800	1.68059000	1.17897100

#### H<sub>2</sub>O-TS-11-12

C	-0.92793000	0.97391500	-0.92081300
N	-1.18553100	2.04003100	0.03838700
H	-1.95827600	2.61172400	-0.29970700
N	0.58689000	0.68309500	-0.77493900
H	0.92600200	0.19944000	-1.61020600
H	1.04386000	1.67176100	-0.70496800
C	2.45354400	-0.41426000	0.37016000
C	2.86388500	-1.59841500	-0.24833400
C	3.41621900	0.46050000	0.87911700
C	4.21808000	-1.90168800	-0.36103400
H	2.11613700	-2.28961100	-0.63781500



C	4.77056200	0.15800800	0.76881400
H	3.09986000	1.38051100	1.36893600
C	5.17254200	-1.02269200	0.14700000
H	4.52801700	-2.82689700	-0.84050300
H	5.51243800	0.84345800	1.17103700
H	6.23019600	-1.26037200	0.06309900
C	0.99536000	-0.07456500	0.44914800
H	0.77126600	0.56982100	1.30577400
H	0.35961800	-0.96292900	0.52055800
O	1.02775900	3.16318300	-0.25666100
H	1.54403700	3.39067000	0.52290400
H	-0.21914700	2.71390400	0.03959900
C	-1.12489700	1.45407400	-2.35149500
H	-0.57863600	2.38795600	-2.52108100
H	-0.79117200	0.71806400	-3.08982400
H	-2.19330200	1.63753600	-2.51696000
N	-1.64583700	-0.21524000	-0.57073900
C	-2.60701500	-2.31561600	-0.81147100
C	-3.70080500	-1.36683000	-0.33524900
C	-2.93502700	-0.14008300	0.15176800
C	-1.64733400	-1.35480500	-1.48738300
H	-2.11407400	-2.79912900	0.04364200
H	-2.97030200	-3.09587400	-1.48642000
H	-4.33531900	-1.77948100	0.45226900
H	-4.33842700	-1.08552700	-1.18300000
H	-3.49020300	0.77858500	-0.10305400
H	-2.02461400	-1.08885500	-2.49075500
H	-0.63628200	-1.77127300	-1.60836900
C	-2.68980200	-0.11272700	1.67436400
O	-3.21896700	-0.93140600	2.42374900
O	-1.90651800	0.83611900	2.08829900
H	-1.53283000	1.48924600	1.16523900

#### H<sub>2</sub>O-TS-6b-18

N	0.43340200	-0.77397400	-0.74970200
H	0.95093900	-1.12171000	-1.55795600
H	0.19779300	0.22647600	-0.87419300
C	2.58974400	-0.27282100	0.34219500
C	3.75036200	-1.04626700	0.31664100
C	2.69094300	1.11763400	0.21610100
C	4.99870800	-0.44257700	0.16874900
H	3.67613300	-2.12858700	0.41449400
C	3.93543300	1.72040800	0.06584500
H	1.78237000	1.72161000	0.23075400
C	5.09248200	0.94097300	0.04219100
H	5.89727000	-1.05494500	0.15185900
H	4.00579900	2.80142900	-0.03005100
H	6.06533500	1.41286000	-0.07440900
C	1.23379400	-0.91065200	0.47583400
H	0.66435400	-0.42133000	1.27689300
H	1.33038600	-1.97525100	0.72404900
C	-2.77587000	0.38184100	2.10902200
C	-3.64942000	0.80156100	0.93391900

C	-2.75396600	0.51799900	-0.27750800
C	-2.15035500	-0.90836000	1.60683500
H	-1.99302800	1.13209600	2.28430300
H	-3.33007700	0.24013100	3.04100700
H	-3.96732600	1.84679800	0.96367500
H	-4.54651500	0.17020700	0.89024300
H	-3.36682000	0.27702300	-1.15599400
H	-2.81474500	-1.76827400	1.78796900
H	-1.18531300	-1.11802800	2.08532600
N	-2.00938300	-0.67150700	0.16407200
C	-1.91581900	1.76832100	-0.64589700
O	-2.58953500	2.72091700	-1.09721000
O	-0.66642500	1.74723600	-0.46774400
C	-1.32088300	-1.50748700	-0.66077000
C	-1.63453800	-1.43219900	-2.13081400
H	-1.51473600	-0.42102800	-2.52771700
H	-0.98069400	-2.10485000	-2.69304300
H	-2.67033700	-1.75201600	-2.28770300
N	-1.16176700	-2.80553000	-0.20104300
H	-0.57286500	-3.39125700	-0.78047300
H	-0.95970200	-2.92974500	0.78325300

#### H<sub>2</sub>O-TS-8-25

C	3.92942200	-0.31749700	-0.98438100
C	2.81921500	-1.23904500	-1.47238700
C	1.64485400	-0.87327200	-0.57485100
C	3.19616700	0.98593500	-0.69275600
H	4.36300600	-0.72079600	-0.06057000
H	4.73792200	-0.19118900	-1.71065800
H	3.07158800	-2.30088500	-1.41527000
H	2.55147100	-1.00129700	-2.50956200
H	0.68979900	-1.08963400	-1.08016600
H	3.22823600	1.66959100	-1.55562600
H	3.64213700	1.51896600	0.15954700
N	1.80997400	0.57580400	-0.41971200
C	1.62186800	-1.69392300	0.72567600
O	2.51349300	-2.44036700	1.08084900
O	0.51130700	-1.57510300	1.44874300
C	1.02131600	1.38941900	0.47833900
C	1.03678700	2.83782600	-0.00799300
H	0.35203600	3.43215700	0.60869900
H	2.03720400	3.26441800	0.10975100
H	0.74455200	2.92256000	-1.06040400
N	1.53540200	1.38167500	1.86749900
H	2.32108300	0.74341100	1.95519200
H	0.83628100	1.07793900	2.53900200
N	-0.34868000	0.82822400	0.51501600
H	-0.02462400	-0.79651400	1.10418800
H	-0.84952600	1.29407300	1.27325900
C	-2.49833000	0.33567700	-0.50368300
C	-2.65008100	-1.04814900	-0.63354500
C	-3.60403000	1.10399300	-0.13434900
C	-3.88090700	-1.65170800	-0.39441700

H	-1.79773100	-1.65803500	-0.93291600
C	-4.83887200	0.50389900	0.10568100
H	-3.49451200	2.18384300	-0.03698900
C	-4.97855300	-0.87591700	-0.02265600
H	-3.98606300	-2.72866700	-0.50244500
H	-5.69238900	1.11487100	0.39004200
H	-5.94154200	-1.34658900	0.16095500
C	-1.15975200	0.98695300	-0.70698700
H	-1.30137600	2.04761800	-0.96217500
H	-0.61743900	0.52285500	-1.54037100

**S-IM1**

C	0.85091000	2.28367400	1.09722500
C	1.36792100	1.97868500	-0.30900000
C	0.82602500	0.58613900	-0.64221000
C	-0.47353400	1.54867100	1.12784100
H	1.52574900	1.87362000	1.86007200
H	0.73745600	3.35335200	1.29330300
H	2.45856400	1.98095900	-0.38083600
H	0.97890300	2.71172700	-1.02438000
H	0.22468300	0.60881500	-1.56105000
H	-1.22185100	2.05043900	0.50185400
H	-0.89106800	1.35175000	2.12032400
N	-0.14991800	0.25598500	0.46616800
C	1.87309900	-0.53309600	-0.80552500
O	3.05325700	-0.24304800	-0.93632900
O	1.38590000	-1.72930600	-0.82867400
H	0.20910500	-1.78836800	-0.66590400
C	-1.41588700	-0.60131200	-0.00094300
N	-2.09019200	0.12531700	-1.02488400
H	-2.06650900	-0.43258200	-1.87257200
O	-0.95764100	-1.80431800	-0.35455100
H	0.29247600	-0.36325000	1.16971600
O	0.10486400	-1.95370600	2.24737000
H	0.88280100	-2.47169800	2.47904000
H	-0.27527500	-2.37817500	1.45524100
H	-2.02219000	-0.60793300	0.92819400
C	-3.43781600	0.58717900	-0.71674400
H	-3.41347700	1.31428700	0.10259600
H	-3.85141900	1.09752500	-1.59032900
H	-4.12252300	-0.22618500	-0.43064800

**S-5a**

C	-2.13600800	-1.57931900	0.17670100
C	-2.05539400	-0.70386500	-1.07403800
C	-0.82832100	0.16395700	-0.78396500
C	-0.67216900	-1.81405000	0.57198400
H	-2.65808700	-1.03581900	0.97532800
H	-2.67990600	-2.51371300	0.01125400
H	-2.95374800	-0.10808500	-1.25303100
H	-1.84959700	-1.30914200	-1.96414200
H	-0.39944700	0.56842600	-1.71136000
H	-0.31197500	-2.81690300	0.29443400

H	-0.54099800	-1.70685700	1.66238700
N	0.06354500	-0.80063200	-0.17868700
C	-1.24000600	1.37211300	0.07234100
O	-2.11168800	2.12788900	-0.29711400
O	-0.61739100	1.56851700	1.23412700
H	0.12491200	0.93936800	1.39910000
C	1.43557400	-0.59759500	0.09571500
N	2.06761100	0.22739600	-0.86994200
H	1.68302400	1.16904600	-0.84616500
O	1.62767300	-0.00140000	1.43179800
H	1.68200800	-0.69096400	2.10486000
H	1.94376500	-1.57563700	0.12085200
C	3.51899000	0.27538500	-0.75386900
H	3.92445000	-0.73288500	-0.89748000
H	3.91981800	0.90838600	-1.54988400
H	3.87293400	0.65762700	0.21456300

### S-6a

C	-2.56955800	-0.79029000	0.72890800
C	-2.45717500	-0.33242400	-0.72257000
C	-0.97920700	-0.01896400	-0.89189300
C	-1.32676600	-1.64469600	0.91626600
H	-2.53247600	0.08231200	1.39090500
H	-3.48549200	-1.34919400	0.93981700
H	-3.06350700	0.55101900	-0.93512800
H	-2.75292200	-1.14069700	-1.40461200
H	-0.60444600	-0.23184000	-1.90332100
H	-1.48680900	-2.67303000	0.56281800
H	-0.95796400	-1.67405700	1.94598300
N	-0.33677000	-0.98106200	0.04287200
C	-0.55798700	1.43161500	-0.51274200
O	-1.39187700	2.17079800	0.01482000
O	0.66308500	1.68493400	-0.77318600
H	1.49241600	1.67765600	0.87046200
C	0.94156800	-1.28403200	0.07715200
N	1.87001500	-0.69866600	-0.64434900
H	1.59266700	0.23466800	-1.02002000
O	1.88368000	1.35033700	1.70654400
H	1.69093500	2.03053500	2.35814000
H	1.23785500	-2.09505700	0.74502100
C	3.27832700	-1.02330400	-0.51105700
H	3.39402300	-1.96188800	0.03774600
H	3.73004400	-1.13994800	-1.49955700
H	3.79863900	-0.22835900	0.03226800

### S-6b

C	1.54137800	2.24732200	0.11835200
C	2.21346700	0.87974200	0.14935200
C	1.30844600	-0.01049600	-0.70621600
C	0.06434800	1.89540000	0.21059900
H	1.85802400	2.90421400	0.93329600
H	1.74642900	2.75794600	-0.83163000
H	2.22641200	0.49337300	1.17866900

H	3.24168600	0.87681400	-0.21856300
H	1.61311200	0.00488100	-1.76111300
H	-0.60119700	2.64923000	-0.22774600
H	-0.24530500	1.68607600	1.24657100
N	-0.00869300	0.64837100	-0.56546800
C	1.32341700	-1.47819900	-0.19624900
O	2.38772100	-2.06935200	-0.42509100
O	0.29216600	-1.88717600	0.40507100
H	-0.62278500	-0.97011400	1.61128500
C	-1.11867500	0.01206600	-0.83429700
O	-1.15959600	-0.36129000	2.17118400
H	-1.12020400	-0.72324300	3.06065700
N	-2.32313800	0.42569900	-0.47620100
H	-1.05357600	-0.90241500	-1.41930900
H	-2.37031500	1.12152200	0.26099100
C	-3.51139900	-0.39059300	-0.67020400
H	-4.35485300	0.24008100	-0.95982700
H	-3.32630500	-1.11301900	-1.46788800
H	-3.75651700	-0.93273300	0.24896400

#### S-6c

C	2.23989700	-1.29289000	-0.31467500
C	2.02863100	-0.40518400	0.90907100
C	0.64945700	0.19785900	0.67660500
C	0.86622600	-1.91239200	-0.52379700
H	2.51286500	-0.67629400	-1.18043200
H	3.01991100	-2.04640700	-0.17396800
H	2.79216100	0.36762100	1.02312400
H	2.00665300	-1.01530800	1.82083300
H	0.09167300	0.36370800	1.61195100
H	0.72858000	-2.79841100	0.11580500
H	0.67178200	-2.20096100	-1.56276100
N	-0.03935900	-0.83657300	-0.10785800
C	0.68579500	1.53615600	-0.07400000
O	1.71449800	2.09268900	-0.38846800
O	-0.50321100	2.06150800	-0.33999700
C	-1.38630000	-0.93625100	-0.16729900
N	-2.17094000	0.00888300	0.20744300
H	-1.24497800	1.45250800	-0.04518400
H	-1.75325800	-1.89017100	-0.57812900
C	-3.59676900	-0.21929800	0.12389700
H	-3.84743200	-1.21602100	-0.27234000
H	-4.05494900	-0.12187200	1.11520200
H	-4.06283500	0.53386200	-0.52228700

#### S-6c-no-Hbond

C	-1.93622100	-1.64489800	0.18065800
C	-1.81154800	-0.67504900	-0.99159700
C	-0.58644100	0.17019400	-0.61944300
C	-0.48608700	-1.99205500	0.47691800
H	-2.39132900	-1.14480300	1.04678600
H	-2.53915600	-2.52747500	-0.05040400
H	-2.69804900	-0.05829100	-1.16272200

H	-1.59969700	-1.22654100	-1.91563500
H	-0.00402600	0.48154700	-1.49643900
H	-0.12133200	-2.77225400	-0.21011000
H	-0.31614800	-2.33331100	1.50435100
N	0.20874000	-0.71908400	0.22998900
C	-0.99397500	1.45654100	0.09231600
O	-1.63165100	2.31999800	-0.46126000
O	-0.63015100	1.56368300	1.37355300
C	1.58625300	-0.67086500	0.17887800
N	2.22219600	0.30606300	-0.32699100
H	-0.12643800	0.75992900	1.60422800
C	3.66478100	0.25627600	-0.27841200
H	4.05898600	-0.66618200	0.18127500
H	4.07440400	0.33805100	-1.29205200
H	4.04787000	1.11433300	0.28682500
H	2.07219500	-1.54416900	0.64866100

**S-6d**

C	1.41466300	1.65717900	1.11323200
C	1.95937200	1.47521800	-0.30200900
C	1.10702200	0.31886700	-0.83294700
C	-0.08863200	1.44069500	0.95544300
H	1.83851400	0.89349500	1.77954700
H	1.64969000	2.63500600	1.54265900
H	3.02914600	1.25527500	-0.34590400
H	1.76287200	2.36822200	-0.90781700
H	1.02873900	0.33030500	-1.92826100
H	-0.63390800	2.37199500	0.74365900
H	-0.54819500	0.98080500	1.83773800
N	-0.18238600	0.55803100	-0.21269100
C	1.74234300	-1.02552100	-0.46549600
O	2.80275700	-1.34803600	-0.95397100
O	1.11599100	-1.80926300	0.40306700
C	-1.36461100	0.22918100	-0.79498200
N	-2.49156300	0.36776300	-0.20240800
H	0.25074200	-1.47230400	0.73856000
O	-1.34872300	-1.53042400	1.61899900
H	-1.97441400	-0.84819500	1.30544900
H	-1.52569200	-1.69303500	2.54985900
H	-1.26436900	-0.19424500	-1.80955000
C	-3.67476100	0.01125800	-0.95632400
H	-4.34480900	0.87542500	-1.03826200
H	-3.45123400	-0.34677400	-1.97487600
H	-4.23201700	-0.77602000	-0.43336600

**S-7**

N	-0.36426300	0.48860500	0.16162900
H	0.06047100	-1.22590700	-0.39018600
H	-0.49888700	0.05759700	1.07848600
C	-2.79556000	0.49463000	-0.01850100
C	-3.02300900	-0.57645800	-0.88801100
C	-3.74034200	0.77631100	0.96822500
C	-4.17230000	-1.34977600	-0.77188800

H	-2.28909600	-0.80277800	-1.66130800
C	-4.89619500	0.00589400	1.08482300
H	-3.56947700	1.60830600	1.65070400
C	-5.11307300	-1.05885500	0.21591800
H	-4.33656000	-2.18088600	-1.45346600
H	-5.62539400	0.23703000	1.85780900
H	-6.01266700	-1.66290800	0.30614200
C	-1.54075500	1.31248600	-0.13772100
H	-1.60069800	2.18881100	0.53274200
H	-1.44211500	1.70014500	-1.16092000
C	4.17626500	-0.21166600	1.05339300
C	3.90680200	-0.65891800	-0.37851100
C	2.38296200	-0.67673400	-0.46053200
C	3.09784000	0.83496900	1.24490500
H	4.02544100	-1.04691900	1.75015400
H	5.18541000	0.18438900	1.20331700
H	4.34025800	-1.62985300	-0.63073300
H	4.29320700	0.09202800	-1.07986800
H	2.04882200	-0.31653000	-1.44700300
H	3.38955500	1.76998300	0.72948100
H	2.88377500	1.07147500	2.29492900
N	1.91648600	0.23431600	0.61208500
C	1.78640500	-2.07131300	-0.27253900
O	2.44461800	-3.07427700	-0.10859400
O	0.45460200	-2.13381900	-0.34025500
C	0.91056200	1.21069900	0.22815200
N	1.20160700	1.92182600	-0.99667900
H	0.76031300	1.48988000	-1.80220500
C	1.02434800	3.36384300	-0.98510700
H	1.67076200	3.80708800	-0.21856300
H	1.33930800	3.77402700	-1.94936300
H	-0.00888900	3.69981800	-0.79171300
H	0.89220100	1.96607800	1.03747400

**S-8**

C	3.49231900	-0.75059100	-1.94393400
C	2.97260700	-1.79716700	-0.95234200
C	1.79100900	-1.13432500	-0.22465000
C	3.06772100	0.55558300	-1.29942800
H	4.57358700	-0.82201100	-2.09814100
H	3.00025100	-0.85529700	-2.91883900
H	3.74185400	-2.04129600	-0.21246700
H	2.67175500	-2.72988600	-1.43868200
H	0.84143200	-1.65328200	-0.43826500
H	2.99674900	1.39931800	-1.99832600
H	3.76050000	0.84894200	-0.48947100
N	1.74356100	0.22055100	-0.79559300
C	1.96530500	-1.16816200	1.30287900
O	2.98179000	-1.49433500	1.87313300
O	0.88261900	-0.79985500	1.99725100
C	0.95878100	1.29322100	-0.24754700
N	1.59065800	2.00187800	0.84073900
H	1.69676200	1.41943700	1.66707600

N	-0.36257400	0.75126900	0.12135400
H	0.20261500	-0.40404400	1.38186000
H	-0.86484300	1.47122000	0.64016400
C	-2.56669300	-0.03131800	-0.59505100
C	-2.76643600	-1.18206800	0.17391900
C	-3.66882000	0.75495000	-0.93142600
C	-4.04213300	-1.53951600	0.59537600
H	-1.91084500	-1.80365000	0.43950400
C	-4.94999500	0.39876900	-0.51337900
H	-3.52168500	1.65169100	-1.53255600
C	-5.13823100	-0.74848200	0.25116600
H	-4.18416100	-2.43867200	1.19017900
H	-5.80088500	1.01856300	-0.78651000
H	-6.13675700	-1.02921800	0.57757500
C	-1.18420100	0.35614400	-1.03289400
H	-1.23688000	1.17246500	-1.77451200
H	-0.68675800	-0.48617800	-1.53089500
C	1.01405700	3.29285800	1.16768900
H	1.64675300	3.80069200	1.90142800
H	0.98944000	3.91635200	0.26520200
H	-0.00938000	3.25868900	1.58264700
H	0.84196900	2.04442400	-1.05781200

#### S-11

C	-1.18200600	0.98468600	-0.93237400
N	-1.56108300	2.03416500	-0.04315100
N	0.41677100	0.80462800	-0.79327700
H	0.75412500	0.33768100	-1.63927800
H	0.83196100	1.75551100	-0.77469400
C	2.36164400	-0.26874300	0.22883000
C	2.76423800	-1.50139300	-0.28932200
C	3.32750900	0.69072500	0.54307200
C	4.11493600	-1.77215600	-0.49239200
H	2.01081300	-2.25646300	-0.51606000
C	4.67727900	0.42183400	0.34105500
H	3.01311100	1.65013900	0.95362900
C	5.07181700	-0.81016300	-0.17779900
H	4.42131600	-2.73778600	-0.88706700
H	5.42356200	1.17103500	0.59353000
H	6.12708800	-1.02278700	-0.33075100
C	0.90495400	0.03389900	0.39665300
H	0.68260900	0.63527800	1.28413200
H	0.30530100	-0.88054700	0.46585900
O	0.81180000	3.52613700	-0.21593800
H	1.23636200	3.98922200	0.51273500
H	-0.09678800	3.28537000	0.07330100
N	-1.81823300	-0.23904600	-0.77034400
C	-2.25619100	-2.51271700	-1.07897000
C	-3.31397200	-1.92384000	-0.15039300
C	-2.69911800	-0.62506900	0.35916500
C	-1.68732100	-1.28437900	-1.77640500
H	-1.47520100	-2.99428700	-0.47797600
H	-2.65462300	-3.24774900	-1.78536700



H	-3.56358700	-2.59100200	0.67860500
H	-4.23085300	-1.70260100	-0.71425100
H	-3.46950100	0.14713800	0.50713100
H	-2.25065200	-1.02659600	-2.69129800
H	-0.63529500	-1.43692100	-2.07217300
C	-1.87492000	-0.73905100	1.67077700
O	-1.49932600	-1.87024800	2.02919300
O	-1.60459500	0.37379600	2.21109300
H	-1.69611300	1.62881700	0.90386700
C	-2.75000200	2.74888300	-0.50586900
H	-3.04330200	3.47510600	0.25613300
H	-2.52195400	3.29806600	-1.42761500
H	-3.60908500	2.08836900	-0.69929700
H	-1.23757600	1.34420300	-1.97663900

### S-12

C	-0.74786400	0.67307900	-0.86260400
N	-1.07079600	1.87999400	-0.09340700
N	0.68086400	0.39670500	-0.77444500
H	0.96402200	-0.22701100	-1.52742800
H	1.55474800	2.13759100	-0.93769500
C	2.61576000	-0.43462200	0.44223700
C	3.05842600	-1.65456700	-0.07529300
C	3.56233200	0.50596700	0.85434000
C	4.41891300	-1.92595600	-0.19171200
H	2.32755100	-2.40505900	-0.37893000
C	4.92400800	0.23673600	0.74492900
H	3.22256900	1.45199600	1.27538300
C	5.35475300	-0.97900400	0.21843600
H	4.74968400	-2.88144300	-0.59219500
H	5.65065000	0.97392000	1.07878100
H	6.41792800	-1.19184500	0.13635200
C	1.14613800	-0.13774000	0.51931500
H	0.95711400	0.61878400	1.29307100
H	0.58291200	-1.03612900	0.81349300
O	1.62931400	3.09173600	-0.72826600
H	2.56608800	3.30766900	-0.75468400
H	-0.19770800	2.27517700	0.25450400
N	-1.54443200	-0.45016300	-0.39847900
C	-2.60465500	-2.49185100	-0.85453200
C	-3.68954300	-1.42325500	-0.82598300
C	-2.99192000	-0.23098100	-0.17730100
C	-1.37388900	-1.66997900	-1.18721600
H	-2.49302700	-2.95059500	0.13674800
H	-2.79232700	-3.28756700	-1.58167400
H	-4.58640000	-1.71432200	-0.27371200
H	-3.98132800	-1.16189800	-1.85145400
H	-3.33337100	0.71081900	-0.63692500
H	-1.34476400	-1.43993300	-2.27333100
H	-0.43562200	-2.18002200	-0.92953400
C	-3.25594800	-0.12208300	1.32847100
O	-4.01902000	-0.84835900	1.92851000
O	-2.58699900	0.84555700	1.94339800

H	-1.99435200	1.31819200	1.28571000
H	-0.94810500	0.86707300	-1.94087000
C	-1.72188800	2.93293600	-0.87712500
H	-1.83559300	3.82197500	-0.25149700
H	-1.14279000	3.20858500	-1.77070300
H	-2.72143500	2.61473800	-1.19399100

**S-18**

N	0.29666900	0.62450600	0.53862700
H	0.83310300	1.04310400	1.29686200
H	0.00743000	-1.14033100	0.57247000
C	2.48446100	0.08578000	-0.40668100
C	3.50268500	0.96531600	-0.02885600
C	2.76608100	-1.28038900	-0.48434700
C	4.77688400	0.49235400	0.27412800
H	3.29475400	2.03524600	0.01632200
C	4.04009900	-1.75575900	-0.18483500
H	1.98039800	-1.97403300	-0.77991400
C	5.04716700	-0.87169600	0.19630800
H	5.56027700	1.18948100	0.56251500
H	4.24702100	-2.82122700	-0.25201000
H	6.04236900	-1.24469500	0.42665900
C	1.10900900	0.61990100	-0.69231200
H	0.58959600	-0.00154800	-1.43364500
H	1.20465100	1.63028300	-1.12256300
C	-4.19076700	-0.19248300	-0.63599100
C	-3.82845500	-0.86700300	0.67909800
C	-2.30683300	-0.77151800	0.70042800
C	-3.22262700	0.97269600	-0.65089400
H	-3.99262100	-0.87020300	-1.47683400
H	-5.23564000	0.12844300	-0.69000700
H	-4.17139900	-1.90123600	0.76093700
H	-4.24275900	-0.29325500	1.51844700
H	-1.93040200	-0.59509400	1.72345900
H	-3.57068600	1.76701700	0.03399700
H	-3.09150200	1.42359400	-1.63992000
N	-1.95986600	0.37921100	-0.17338200
C	-1.63188300	-2.04548700	0.18929400
O	-2.23185200	-3.00483300	-0.24192800
O	-0.30313600	-2.03845400	0.26757400
C	-1.01753600	1.30207700	0.42543400
N	-1.03223400	2.54808700	-0.29006900
H	-1.30335100	1.54207200	1.47468400
H	-0.82369000	2.41319800	-1.27573400
C	-0.22510100	3.59314200	0.30689300
H	-0.31965900	4.50942600	-0.28232200
H	-0.59943400	3.80765600	1.31556200
H	0.85034800	3.35418000	0.39362500

**S-19**

N	-0.39185500	0.47365000	0.07343900
H	1.43556000	-1.34266700	1.51553300
H	-0.50083100	-0.21021100	0.82001300

C	-2.83393300	0.48597500	0.00852400
C	-3.02223600	-0.49276300	-0.97253400
C	-3.82487900	0.67363300	0.97209300
C	-4.17914600	-1.26363500	-0.98903700
H	-2.24636800	-0.65107800	-1.71987700
C	-4.98761700	-0.09516800	0.95624900
H	-3.68403700	1.42993300	1.74380800
C	-5.16659600	-1.06613600	-0.02408500
H	-4.31188300	-2.02294400	-1.75636900
H	-5.75096800	0.06249300	1.71485600
H	-6.07056300	-1.67057800	-0.03626000
C	-1.58273200	1.31852200	0.01982100
H	-1.62211700	2.03164300	0.86613500
H	-1.53626200	1.92564300	-0.89661800
C	4.22604000	-0.13271000	0.64772800
C	3.73534800	-0.61313600	-0.71409200
C	2.22006900	-0.72627600	-0.50414000
C	3.14611300	0.86532700	1.02478400
H	4.25479300	-0.96458100	1.36551500
H	5.22277800	0.31738900	0.61638000
H	4.17768800	-1.55452700	-1.05338500
H	3.93334200	0.15315300	-1.47385400
H	1.66690500	-0.50726600	-1.42521500
H	3.31052300	1.80919000	0.47760000
H	3.09596400	1.08902100	2.09740300
N	1.89454600	0.22834100	0.57561600
C	1.83580100	-2.14601900	-0.09748700
O	1.93441700	-3.09250700	-0.84442500
O	1.40895700	-2.26573900	1.16091800
C	0.84559300	1.20198400	0.25936800
N	1.14865700	2.01737800	-0.89832700
H	0.64733200	1.68078000	-1.71428600
C	1.04590100	3.45798500	-0.74370900
H	1.77208400	3.80798700	-0.00011600
H	1.29790200	3.94077400	-1.69265200
H	0.04935400	3.81752500	-0.43271600
H	0.80601400	1.88320600	1.13615800

**S-20**

N	0.69875700	0.09637300	-0.02169500
H	-2.13565600	-0.14415200	1.71967400
H	0.86987200	-0.89837200	-0.14998200
C	3.12647900	0.29977500	-0.17770100
C	3.44528500	0.25123300	1.18315700
C	4.05857200	-0.16623500	-1.10511900
C	4.67153300	-0.25079000	1.60442300
H	2.71816900	0.60959600	1.91020500
C	5.29030700	-0.66745800	-0.68646700
H	3.81720500	-0.13466000	-2.16719500
C	5.59851300	-0.71177400	0.66949800
H	4.90820200	-0.28087800	2.66560100
H	6.00677400	-1.02684000	-1.42165500
H	6.55764500	-1.10360400	0.99998100

C	1.79952900	0.84327500	-0.62696200
H	1.75200600	0.83265000	-1.73331500
H	1.70689700	1.89600100	-0.32137500
C	-2.73301700	-2.53139200	-0.39630300
C	-3.62417100	-1.42210600	-0.94086600
C	-2.98295700	-0.14666000	-0.37346600
C	-1.35773800	-1.89426700	-0.48101000
H	-2.98066600	-2.75283100	0.65091700
H	-2.80200600	-3.46505600	-0.96246200
H	-4.67985200	-1.50946900	-0.66708700
H	-3.56508700	-1.40048500	-2.03629900
H	-3.04347700	0.68011600	-1.09350200
H	-0.98369600	-1.92356100	-1.52376500
H	-0.62110800	-2.38915700	0.16284300
N	-1.58796000	-0.50568000	-0.05479800
C	-3.70866000	0.33492800	0.87874500
O	-4.83696600	0.77301700	0.85075900
O	-3.01680600	0.20113400	2.00799700
C	-0.60580400	0.46841000	-0.53775300
N	-0.98023800	1.79097100	-0.11952600
H	-0.53343400	2.02584900	0.76141600
C	-0.92233900	2.85812100	-1.10045600
H	-1.64013200	2.66505500	-1.90724100
H	-1.22090800	3.79582000	-0.62332800
H	0.06921400	3.00881500	-1.56132900
H	-0.61688900	0.45995800	-1.65834200

### S-21

N	0.75670000	-0.01871400	-0.10753200
H	-2.62895900	1.35882300	0.61628900
H	0.87585800	-0.53561600	0.76063200
C	3.16892600	0.31518100	-0.18892000
C	4.12948300	0.78570200	0.70628100
C	3.48548100	-0.77015700	-1.01175900
C	5.38759400	0.18901200	0.77924200
H	3.89009200	1.62972800	1.35277000
C	4.73904000	-1.36761400	-0.94189000
H	2.73309300	-1.14471300	-1.70378500
C	5.69431500	-0.88904700	-0.04492300
H	6.12560000	0.56641200	1.48343300
H	4.97425600	-2.20997800	-1.58854000
H	6.67411200	-1.35765300	0.01104600
C	1.81463000	0.96436700	-0.27843700
H	1.68236600	1.41786500	-1.27481700
H	1.76948900	1.79554100	0.44988800
C	-2.88413000	-2.04083900	1.26839600
C	-3.25406800	-2.11390000	-0.21258200
C	-2.76269800	-0.75722400	-0.72456000
C	-1.54528200	-1.29497000	1.27937700
H	-3.64265500	-1.45851600	1.80809900
H	-2.82133700	-3.02231200	1.74730300
H	-4.32050400	-2.26973700	-0.39352100
H	-2.68965500	-2.90640200	-0.71779900

H	-2.59895500	-0.76855900	-1.81238800
H	-0.69919900	-1.99299800	1.38092300
H	-1.49305700	-0.58340500	2.12159500
N	-1.50641100	-0.62405700	-0.01845500
C	-3.85863000	0.29283000	-0.47086800
O	-4.94069000	0.18540800	-1.01037700
O	-3.60228500	1.28874100	0.36780700
C	-0.60032100	0.45365800	-0.26208000
N	-0.94929500	1.65563200	0.55538700
H	-0.43277400	1.65381900	1.43214800
C	-0.83569300	2.94717400	-0.11916400
H	-1.51894000	2.96257800	-0.97698600
H	-1.15394300	3.74100800	0.56305800
H	0.17482100	3.18422300	-0.48245400
H	-0.73474400	0.77162900	-1.31081400

### S-22

N	-0.54717700	0.02154400	-0.70309800
H	-0.61405600	-0.72289200	-1.38870700
C	-2.94108700	0.35187600	-0.20814700
C	-4.04961400	0.35221500	-1.05390300
C	-3.05082000	-0.23387500	1.05622700
C	-5.25362300	-0.21858200	-0.64468800
H	-3.97071300	0.80826300	-2.04014500
C	-4.24930700	-0.80620900	1.46667700
H	-2.19104200	-0.23431900	1.72654600
C	-5.35454800	-0.79941000	0.61530600
H	-6.11174500	-0.20977100	-1.31234000
H	-4.32610800	-1.25378700	2.45474700
H	-6.29258200	-1.24456400	0.93799500
C	-1.64879900	0.98528600	-0.64640200
H	-1.32718600	1.78840000	0.02773200
H	-1.76003000	1.43955200	-1.63786500
C	3.18254000	-2.14351200	-0.83109600
C	3.54249500	-1.76329200	0.60294400
C	2.76596300	-0.47196500	0.80327100
C	1.69718800	-1.80359200	-0.93587700
H	3.75362500	-1.52034300	-1.53053000
H	3.38109400	-3.19136900	-1.07156300
H	4.61101500	-1.59505900	0.75268300
H	3.20091400	-2.53359900	1.30706300
H	2.53731200	-0.26781700	1.85679300
H	1.05182500	-2.65872600	-0.69215800
H	1.42270600	-1.42311200	-1.92864900
N	1.51314400	-0.75142000	0.07529500
C	3.49117100	0.79094200	0.22411700
O	4.67706300	0.90199500	0.56476600
O	2.78527300	1.55195900	-0.48916800
C	0.51421600	0.09086400	0.08450600
H	0.53786100	0.91340100	0.79968400
O	0.67105100	3.08884900	0.23874600
H	1.51771300	2.69495300	-0.07154100
H	0.87588400	3.99302900	0.49250600

**S-23**

C	3.22431500	0.50488000	1.98800400
C	2.15340800	1.54931700	1.68881400
C	1.40310500	0.98985900	0.47880600
C	2.50167000	-0.79051400	1.67008200
H	4.07453900	0.62744600	1.30328000
H	3.59774100	0.55043600	3.01564300
H	2.55654700	2.54532000	1.48821700
H	1.45805500	1.62276600	2.53540200
H	0.31863600	1.16327600	0.59045300
H	1.84569900	-1.09944500	2.51019400
H	3.18650200	-1.62228000	1.45995100
N	1.73515100	-0.43644500	0.48608700
C	1.81063200	1.62421700	-0.84970100
O	2.73597700	2.39136300	-0.98927700
O	1.03986000	1.27852600	-1.88506500
C	0.98347100	-1.43944300	-0.21323200
N	1.60030100	-1.79625600	-1.48688700
H	1.12782800	-2.61596100	-1.86226000
N	-0.35744800	-0.95557400	-0.52124900
H	0.41423100	0.56910400	-1.61074200
H	-0.75241900	-1.49859700	-1.28708400
C	-2.60642900	-0.40289100	0.32628800
C	-2.73315000	0.76014100	-0.43899900
C	-3.76056400	-0.99722700	0.84044800
C	-3.98578100	1.31623100	-0.67986100
H	-1.84376500	1.23261100	-0.85226700
C	-5.01512200	-0.43974900	0.60594000
H	-3.67434800	-1.90864500	1.43145100
C	-5.13100000	0.71943200	-0.15633300
H	-4.06669300	2.22026200	-1.27895000
H	-5.90351900	-0.91638300	1.01397800
H	-6.10948600	1.15489300	-0.34458700
C	-1.25728400	-0.99486400	0.62968300
H	-1.38245300	-2.02334300	1.01382500
H	-0.77681900	-0.43086700	1.44575200
C	3.02914700	-2.05704400	-1.41631800
H	3.30338100	-2.85574700	-0.70291900
H	3.38749400	-2.34536300	-2.40829700
H	3.55277400	-1.14048400	-1.12240000
H	0.93485800	-2.32427000	0.46871200

**S-24**

C	-2.44081900	-1.43040500	2.04238900
C	-1.64342900	-2.09015700	0.92058200
C	-1.56537500	-0.98924300	-0.13237400
C	-1.87972900	-0.01661500	2.05891800
H	-3.50739400	-1.41143200	1.77983400
H	-2.33908900	-1.93567100	3.00761900
H	-2.10392900	-2.99918300	0.52641000
H	-0.63199300	-2.33821800	1.26968800
H	-0.62989900	-1.03570900	-0.71491000

H	-0.95790600	0.02567200	2.66906100
H	-2.58386700	0.71965400	2.47267700
N	-1.61387200	0.25255500	0.64746100
C	-2.69809100	-1.07873100	-1.16188500
O	-3.35352700	-2.08431900	-1.33968500
O	-2.89721700	0.00567600	-1.90330900
C	-0.83205300	1.39473600	0.26621400
N	-1.51332200	2.10531600	-0.82101200
H	-0.86618300	2.70270100	-1.32910900
N	0.49616100	1.04298100	-0.20057700
H	-2.31281000	0.76945100	-1.62451100
H	0.95763300	1.84826000	-0.61826300
C	2.70707100	0.12250200	0.29564700
C	2.81735700	-0.70068700	-0.82961500
C	3.87083500	0.58209600	0.91180300
C	4.06666300	-1.06018000	-1.32245700
H	1.91053700	-1.05410000	-1.31863200
C	5.12530300	0.22194300	0.42134300
H	3.79426200	1.22694600	1.78685700
C	5.22547400	-0.59997800	-0.69679800
H	4.13817600	-1.70324300	-2.19671400
H	6.02402600	0.58767000	0.91277800
H	6.20240300	-0.88250700	-1.08207900
C	1.35246100	0.48301600	0.83850100
H	1.46576000	1.16397500	1.70416900
H	0.86136000	-0.42251900	1.22406600
C	-2.65656200	2.88022700	-0.34575400
H	-2.37747500	3.64312600	0.39793700
H	-3.14656700	3.36973100	-1.19157500
H	-3.37843600	2.19631600	0.11465000
H	-0.79006000	2.04111500	1.17380800

#### S-25

C	4.16389400	-0.10833400	0.21412600
C	3.58182600	-1.51321500	0.09707600
C	2.10504700	-1.25477000	-0.19172900
C	3.46582700	0.63557100	-0.91175600
H	3.89556300	0.33270600	1.18130400
H	5.25235700	-0.07925600	0.11134600
H	3.69452500	-2.11754500	1.00079100
H	4.04901100	-2.05374400	-0.73705500
H	1.66017100	-2.07672600	-0.76348900
H	3.98437000	0.49449100	-1.86932700
H	3.34932700	1.71040700	-0.73202200
N	2.13575300	-0.01085600	-0.98875500
C	1.28381500	-1.05496100	1.12962900
O	1.06796000	-2.12139200	1.73366100
O	0.93441700	0.11538200	1.41257900
C	1.08396800	0.71227100	-1.29356700
N	-0.55646400	2.65007200	0.40154700
H	-1.46446500	2.98122900	0.71599200
N	-0.18222300	0.37099800	-1.44398700
H	-0.35804900	1.78847000	0.91610400

H	-0.78488300	1.19523300	-1.41892500
C	-2.20591300	-0.69018300	-0.60726500
C	-2.26720900	-0.50902500	0.77863000
C	-3.37831000	-0.64016300	-1.36186800
C	-3.49381500	-0.28053400	1.39378400
H	-1.34968100	-0.54493800	1.36886500
C	-4.60592300	-0.41158600	-0.74354600
H	-3.32977900	-0.78936900	-2.44037000
C	-4.66315400	-0.23106800	0.63568600
H	-3.53767000	-0.14932900	2.47232900
H	-5.51569500	-0.37967400	-1.33842700
H	-5.62055500	-0.05761300	1.12183600
C	-0.87944200	-0.91263200	-1.28088000
H	-1.02314100	-1.35643000	-2.27469300
H	-0.27061300	-1.60259800	-0.69352800
C	0.47482800	3.63110800	0.72779400
H	0.33458700	4.54173600	0.13444600
H	0.51447400	3.91789200	1.78937800
H	1.45931800	3.21676900	0.47363600
H	1.26971600	1.76999600	-1.48642900

**S-26**

C	-0.70710700	-0.62243400	-0.94781000
N	-0.70123600	2.14643300	1.01277800
N	0.58775600	-0.42232500	-0.73661600
H	1.10790900	-0.13471300	-1.55715400
C	2.81340800	-0.33908500	0.22405800
C	3.46348800	-1.47093600	-0.27681500
C	3.54282600	0.83342200	0.42295200
C	4.82098800	-1.43030800	-0.57495100
H	2.89705000	-2.38971700	-0.42890800
C	4.90412000	0.87551700	0.12857300
H	3.03867200	1.71648800	0.81376000
C	5.54356200	-0.25510400	-0.37126400
H	5.31858300	-2.31665500	-0.96103200
H	5.46411600	1.79321500	0.29054500
H	6.60574200	-0.22324700	-0.60107100
C	1.34320700	-0.38504800	0.52655600
H	1.02099400	0.49595000	1.10087900
H	1.10554500	-1.28844800	1.10069600
H	-1.11847000	2.66571300	1.78015400
N	-1.64274800	-0.99067400	-0.11252600
C	-3.02345400	-0.89685600	1.78955000
C	-3.80945600	-1.49516700	0.62852900
C	-3.04965800	-0.97669900	-0.58065500
C	-1.57195800	-1.07439500	1.36363000
H	-3.25365200	0.17337700	1.88271600
H	-3.22618500	-1.37235900	2.75339300
H	-4.85223600	-1.17368000	0.58894300
H	-3.77879200	-2.59246900	0.66880000
H	-3.14866600	-1.63218100	-1.45500200
H	-1.18807600	-2.06313100	1.64824900
H	-0.91745900	-0.28768500	1.74840200



C	-3.48552700	0.46599000	-1.02124200
O	-4.71090100	0.59879500	-1.17031800
O	-2.55686700	1.29297000	-1.20076500
H	-1.46104600	1.91403100	0.36469800
H	-1.01950400	-0.51384700	-1.98319000
C	0.25557900	2.99370800	0.30989500
H	0.68304700	2.43501400	-0.53387000
H	-0.16605700	3.92404300	-0.10033600
H	1.08410800	3.26650400	0.97650600

**S-27**

N	-0.28350600	0.73779500	-0.53682500
H	-0.80261200	1.13579300	-1.31427900
H	1.34018300	-0.79118100	1.48263500
C	-2.46288800	0.15242700	0.33886500
C	-3.54090100	1.00299700	0.09137300
C	-2.64672600	-1.22826000	0.23092500
C	-4.78783000	0.48630100	-0.25644800
H	-3.40026500	2.08131900	0.17784300
C	-3.89073200	-1.74769500	-0.11174000
H	-1.80485400	-1.89365200	0.42172500
C	-4.96381100	-0.89103000	-0.35670100
H	-5.62142600	1.15925900	-0.44410600
H	-4.02468500	-2.82429100	-0.18690000
H	-5.93629000	-1.29875500	-0.62289900
C	-1.11162600	0.71797100	0.66700500
H	-0.62268300	0.08995900	1.42379600
H	-1.24176500	1.71957300	1.11662800
C	4.20692100	-0.36812500	0.19846000
C	3.52457500	-1.13282100	-0.92791000
C	2.03425200	-0.88366700	-0.65564800
C	3.34847900	0.87997000	0.28647100
H	4.16093100	-0.93510500	1.13899200
H	5.25824400	-0.14142300	-0.00337700
H	3.76263500	-2.19986700	-0.97115100
H	3.79402600	-0.68939800	-1.89487600
H	1.45718200	-0.81184900	-1.58600900
H	3.59786500	1.57660600	-0.53363600
H	3.45300200	1.42885400	1.22663700
N	1.96996600	0.37252900	0.12208400
C	1.42085900	-2.03941400	0.12576000
O	1.25153600	-3.13931700	-0.34816900
O	1.11154700	-1.74880200	1.39135000
C	1.03277700	1.34976300	-0.42981100
N	1.14256400	2.56927300	0.33613500
H	1.32848500	1.60781000	-1.46978800
H	0.92636500	2.39678600	1.31527800
C	0.36328600	3.66841900	-0.20206200
H	0.48365200	4.54856000	0.43561100
H	0.74211500	3.92742700	-1.19865700
H	-0.71775000	3.46033700	-0.29991800

**S-28**

N	-0.64840300	0.40426400	-0.89482900
H	-1.27274700	0.99516900	-1.43733500
H	3.44201600	0.59826500	-0.90096500
C	-2.64232500	-0.06425200	0.39464900
C	-3.56384200	0.90957400	0.77942400
C	-3.11067800	-1.28620400	-0.09636900
C	-4.93344600	0.66757600	0.68200300
H	-3.20275500	1.86466600	1.16174900
C	-4.47542400	-1.53230500	-0.19345300
H	-2.38892000	-2.04188100	-0.40708700
C	-5.39041100	-0.55403400	0.19677900
H	-5.64247000	1.43336800	0.98804000
H	-4.82979200	-2.48813700	-0.57272600
H	-6.45819000	-0.74651700	0.12333000
C	-1.16653900	0.20525500	0.45211600
H	-0.65308400	-0.66130900	0.89789200
H	-0.98153100	1.06749400	1.12141700
C	2.40794500	-2.42513500	-0.70392400
C	2.22272700	-1.98408800	0.74455000
C	2.15113000	-0.45187400	0.63587700
C	1.48555500	-1.46915400	-1.43756500
H	3.44906200	-2.27838500	-1.02247800
H	2.14951300	-3.47510600	-0.86974200
H	3.01301200	-2.30983100	1.42709400
H	1.26806900	-2.36452500	1.13103500
H	1.49019500	-0.04599100	1.41465000
H	0.43451300	-1.79366100	-1.35639200
H	1.71732200	-1.35460200	-2.50447100
N	1.69676500	-0.19525300	-0.73780600
C	3.53150100	0.15988500	0.88826700
O	4.05252600	0.14897800	1.98144900
O	4.12324900	0.66492500	-0.18841500
C	0.73329000	0.85646100	-1.02872600
N	1.12029100	2.05773200	-0.31365200
H	0.83616400	1.09180900	-2.10201700
H	1.09564200	1.92244600	0.69348100
C	0.33737500	3.22669900	-0.67395300
H	0.72469800	4.10179200	-0.14470300
H	0.44264600	3.41584600	-1.74935000
H	-0.74127500	3.14024400	-0.44972900

**S-29**

N	-0.48883100	0.99823100	-0.95362200
H	-0.91736900	1.31982600	-1.81320700
H	3.49156000	0.10544200	-0.04884000
C	-2.61988000	0.53114800	0.16949600
C	-3.80017000	1.12317500	0.62223000
C	-2.65970100	-0.79423500	-0.27041800
C	-4.99349400	0.40538600	0.64785200
H	-3.78405700	2.16028000	0.95694800
C	-3.84998200	-1.51451800	-0.24690700
H	-1.74372400	-1.24929600	-0.64462000
C	-5.02186500	-0.91745700	0.21410300

H	-5.90449400	0.88316600	1.00143000
H	-3.86402000	-2.54623100	-0.59149000
H	-5.95302300	-1.47895800	0.22928500
C	-1.32591300	1.30462000	0.19751700
H	-0.76969300	1.05540900	1.11029500
H	-1.56683300	2.38052000	0.28737400
C	1.99456800	-2.26629500	-1.32490500
C	1.27511200	-2.21638600	0.01895200
C	1.49223500	-0.76321100	0.47428100
C	1.64302100	-0.91110000	-1.90875100
H	3.08022400	-2.35690300	-1.18166800
H	1.67034100	-3.09736400	-1.95850800
H	1.63506700	-2.94019300	0.75659900
H	0.20138500	-2.39264500	-0.12453000
H	0.62984500	-0.39775800	1.04172600
H	0.61085700	-0.92925400	-2.30033700
H	2.31245700	-0.58323300	-2.71379000
N	1.73797700	0.00697600	-0.76045800
C	2.69450000	-0.68741100	1.40960900
O	2.67265500	-1.09986200	2.54669400
O	3.79298800	-0.17958100	0.84904900
C	0.94339800	1.23132000	-0.94562100
N	1.33210400	2.21128400	0.04338200
H	1.21009200	1.56177400	-1.97092100
H	0.61231800	2.92526200	0.09269600
C	2.61947100	2.84657400	-0.19973100
H	2.71696200	3.71632800	0.45574400
H	3.44629500	2.17307600	0.04342300
H	2.74411100	3.18120300	-1.24490400

**S-30**

N	-0.29698100	1.12590400	-1.17371000
H	-0.61076500	1.50898400	-2.05608300
H	1.89640000	1.18043900	1.38372000
C	-2.44133900	0.65827300	-0.01925300
C	-3.50621400	1.10187300	0.77048500
C	-2.57025300	-0.54997700	-0.70371900
C	-4.66951300	0.34884700	0.88459600
H	-3.41881400	2.04963100	1.30257800
C	-3.73716700	-1.30515900	-0.59410800
H	-1.74571200	-0.88887700	-1.32842000
C	-4.78880800	-0.86099200	0.20151400
H	-5.48765700	0.70742700	1.50526300
H	-3.82303700	-2.24523200	-1.13488900
H	-5.69905500	-1.44983900	0.28641000
C	-1.17741700	1.48603400	-0.07507200
H	-0.63344800	1.36106900	0.87108600
H	-1.46296900	2.55371400	-0.09744900
C	2.17700000	-2.37034900	-1.20817400
C	1.13847100	-2.34333000	-0.09394400
C	1.19365900	-0.90104900	0.40519500
C	1.95068200	-1.01947600	-1.85663400
H	3.18968400	-2.42379600	-0.78597900

H	2.04929700	-3.20546300	-1.90375000
H	1.32289600	-3.05848200	0.71130300
H	0.14183400	-2.53959500	-0.51174300
H	0.17796300	-0.55867000	0.65820700
H	1.04375900	-1.05496500	-2.49241700
H	2.78943200	-0.67526800	-2.47616800
N	1.76432900	-0.12079200	-0.71482000
C	2.03752000	-0.72981700	1.67030600
O	2.47028400	-1.65641700	2.32055900
O	2.24106800	0.52849100	2.05663600
C	1.14564500	1.14936900	-1.05001700
N	1.60831000	2.14543300	-0.07689400
H	1.53315800	1.39582000	-2.05584000
H	0.99535600	2.95657400	-0.10422700
C	2.99037600	2.56354600	-0.31765500
H	3.29821400	3.27864300	0.45038900
H	3.64259300	1.68708500	-0.25340600
H	3.12460200	3.02363300	-1.30929100

**S-31**

N	-0.10893400	-1.97401100	0.01703600
H	-0.04355100	-2.97883300	0.09902200
H	2.83939700	-1.23069300	-0.92829100
C	-2.29319000	-0.83222800	-0.41572400
C	-2.98312900	0.09586300	-1.20001700
C	-2.78990600	-1.15930500	0.84580600
C	-4.15675400	0.67909000	-0.73427700
H	-2.58336700	0.37755300	-2.17387200
C	-3.96280000	-0.57075100	1.31501700
H	-2.25288700	-1.87027800	1.47181100
C	-4.65076200	0.34650700	0.52576800
H	-4.67884000	1.40584100	-1.35168600
H	-4.33811100	-0.82999500	2.30235000
H	-5.56402800	0.80740500	0.89406500
C	-1.04503700	-1.46059300	-0.98215700
H	-0.50920900	-0.76591900	-1.63899400
H	-1.31246200	-2.32092200	-1.60666500
C	2.20198200	1.89365500	1.45503300
C	0.81137800	2.30235400	0.98018100
C	0.37682000	1.09841900	0.15385400
C	2.01247600	0.43637000	1.84354300
H	2.91772300	1.97816200	0.62673400
H	2.57506500	2.49313300	2.29010600
H	0.79678400	3.20765100	0.36924000
H	0.13939400	2.44526400	1.83723900
H	-0.71464700	1.01004000	0.10078200
H	1.65974400	0.34049100	2.87886700
H	2.89762500	-0.19428000	1.70036700
N	0.93651600	-0.03056800	0.93197400
C	0.93954700	1.15004100	-1.30545200
O	0.57392800	2.15495900	-1.93883900
O	1.64650000	0.18116200	-1.67482700
C	0.75463300	-1.31284700	0.78283900

N	3.50399100	-1.71886100	-0.31990700
H	1.39192000	-1.94842800	1.39521900
H	3.67403100	-2.63436500	-0.72653400
C	4.74792400	-0.95384900	-0.29881800
H	5.26522400	-0.89465600	-1.26890900
H	4.52994900	0.07675200	0.00736500
H	5.44673100	-1.37516700	0.43381400

**S-32**

N	-0.70022200	-0.13732000	-0.01622600
H	-0.81085100	0.31346600	0.88876300
C	-3.12478300	-0.41558900	-0.20282500
C	-4.17535200	-1.05614400	0.45518700
C	-3.35566500	0.83380300	-0.78676700
C	-5.43667400	-0.46793200	0.52601900
H	-4.00337200	-2.02777400	0.91765200
C	-4.61269300	1.42532100	-0.71416900
H	-2.53717200	1.33947500	-1.29588700
C	-5.65762200	0.77583600	-0.05829900
H	-6.24464200	-0.97998400	1.04362300
H	-4.77916500	2.39751800	-1.17298400
H	-6.63941900	1.24006700	-0.00124000
C	-1.77670900	-1.07647500	-0.30154700
H	-1.61223500	-1.44805800	-1.32538000
H	-1.76029400	-1.96788400	0.34826600
C	2.99975600	1.79888200	1.24537500
C	3.34900300	1.84520700	-0.24062800
C	2.83115300	0.49031100	-0.72680200
C	1.63091400	1.11598600	1.27485100
H	3.73816100	1.18401100	1.77801700
H	2.98676900	2.78389900	1.72033600
H	4.41448800	1.97894400	-0.44093900
H	2.78969900	2.64106900	-0.74664800
H	2.63020000	0.49538400	-1.80872600
H	0.81553000	1.85653400	1.30141800
H	1.52568700	0.46712100	2.16075300
N	1.59999400	0.36015300	0.02542400
C	3.91101900	-0.58188300	-0.50251900
O	5.02819200	-0.43290900	-0.94736300
O	3.59374000	-1.67026200	0.19330000
C	0.61978700	-0.61599000	-0.24680000
H	0.71105500	-0.93118300	-1.29664800
O	0.88826900	-1.87264700	0.47316000
H	2.63218500	-1.73285500	0.41003400
H	0.55056500	-1.79103000	1.37595700

**S-34**

C	-0.76932600	-1.78535600	1.82962400
C	-0.36742500	-1.94216900	0.36577800
C	-1.02896400	-0.73754200	-0.29889100
C	-0.64789900	-0.28492300	2.05044900
H	-1.81177900	-2.10484100	1.96923300
H	-0.14409900	-2.36334300	2.51698000

H	-0.69294700	-2.88258200	-0.08513600
H	0.72190700	-1.85924200	0.25982300
H	-0.44929000	-0.38269200	-1.16607300
H	0.39317000	-0.01226400	2.30343900
H	-1.29891700	0.07812800	2.85795700
N	-1.03356800	0.27275900	0.75556800
C	-2.41672400	-1.07588300	-0.84953900
O	-2.70062800	-2.17673100	-1.26891200
O	-3.30530600	-0.08265400	-0.91442100
C	-0.98792300	1.67158900	0.52221700
N	-0.27673700	2.05684700	-0.67003600
H	-2.96681800	0.75645100	-0.52925800
H	-0.71140800	2.89619900	-1.04034000
C	1.96058800	1.00418600	-0.39311300
C	2.05602200	0.14983100	-1.49608700
C	2.65240400	0.67631100	0.77247100
C	2.81690200	-1.01205400	-1.42904600
H	1.52483100	0.40537400	-2.41315600
C	3.41901800	-0.48664700	0.84491600
H	2.59159400	1.34265300	1.63375900
C	3.50152100	-1.33353900	-0.25604600
H	2.88077300	-1.66787600	-2.29433400
H	3.95335000	-0.72816000	1.76102200
H	4.09936700	-2.24048100	-0.20548000
C	1.15614100	2.27404700	-0.48137300
H	1.50004900	2.85511200	-1.34640700
H	1.35984400	2.88736800	0.41688200
H	-0.55744700	2.13559100	1.43430000
O	-2.30697800	2.22215900	0.31861000
H	-2.78275500	2.16808300	1.15770200

**S-34**

C	-0.64191800	-0.59784400	0.58453400
N	0.64010100	-0.31541200	0.05790800
H	0.65624800	-0.34432400	-0.95946900
C	3.07974800	-0.38287200	0.23781900
C	4.16448200	-1.20664300	-0.06427200
C	3.24009100	1.00336700	0.15210000
C	5.39179400	-0.66140600	-0.43571000
H	4.04598000	-2.28844500	-0.00897600
C	4.46356000	1.55060700	-0.22126000
H	2.39274900	1.64943400	0.37746900
C	5.54401400	0.71988500	-0.51512300
H	6.22697400	-1.31744700	-0.66995100
H	4.57566400	2.63077300	-0.28315300
H	6.49904700	1.14887000	-0.80921200
C	1.77180600	-0.98308300	0.67967000
H	1.65441500	-0.86334000	1.76796700
H	1.79221400	-2.07139800	0.49587200
H	-0.62721700	-2.31659000	-0.35560800
N	-1.63012100	0.22886300	-0.06036500
C	-2.63454200	2.35156300	-0.20300500
C	-3.45609300	1.53947300	0.78846900

C	-2.98955500	0.11117700	0.52890600
C	-1.28716700	1.66330900	-0.12057900
H	-3.05463100	2.25275200	-1.21246700
H	-2.57869400	3.41601700	0.04391500
H	-4.53651500	1.64363900	0.66251900
H	-3.19504300	1.82709500	1.81531700
H	-2.95154300	-0.47556100	1.46252100
H	-0.75123500	1.97361700	0.79623500
H	-0.63248200	1.87070600	-0.97296700
C	-3.90113000	-0.63891100	-0.44331900
O	-4.85898600	-0.14721800	-0.99299800
O	-3.57301400	-1.91723300	-0.64875900
H	-2.74387900	-2.12562000	-0.16485500
H	-0.61544900	-0.43658200	1.68282200
O	-1.03012600	-1.98298400	0.45923700

### S-38

N	0.10226700	2.14763200	-0.44621200
H	0.09146500	3.14118900	-0.63463300
C	-1.94088900	0.84533000	0.18517600
C	-2.41000700	-0.10495100	1.09254400
C	-2.49675500	0.88900100	-1.09587500
C	-3.41481000	-0.99940800	0.72973100
H	-1.96326800	-0.16647900	2.08551900
C	-3.50215900	-0.00112100	-1.46047000
H	-2.11532300	1.61245200	-1.81446700
C	-3.96443400	-0.94887200	-0.54788600
H	-3.75566500	-1.74650500	1.44253300
H	-3.92367800	0.04044100	-2.46260100
H	-4.74346200	-1.65069700	-0.83633300
C	-0.86895200	1.82082000	0.60536400
H	-0.37028100	1.44996700	1.51027900
H	-1.35211800	2.75683000	0.91748600
C	3.03424200	-1.52681000	-1.08511000
C	1.54993400	-1.81001300	-1.31450400
C	0.88070500	-0.76423600	-0.42015100
C	3.10630300	-0.00572300	-0.90215200
H	3.36836700	-2.03114200	-0.16871900
H	3.67126200	-1.88043600	-1.90094300
H	1.25249600	-2.82978600	-1.05771500
H	1.26743100	-1.61004000	-2.35434800
H	-0.15604500	-0.56997300	-0.72893100
H	3.48443100	0.51305300	-1.79744400
H	3.77707900	0.25505800	-0.06506000
N	1.72169900	0.38997100	-0.65592400
C	0.81791600	-1.28996200	1.02244600
O	0.31203700	-2.35874200	1.28221600
O	1.35025900	-0.53858600	1.99042300
C	1.46117000	1.73617000	-0.30277100
H	2.07415600	2.37024400	-0.96167100
O	1.91180700	2.01427500	1.07392500
H	1.67776500	0.33316000	1.66761600
H	2.84122500	2.27251600	1.06382800

**S-Product**

N	1.91719700	-0.64715800	0.61358300
H	1.74140300	-1.03131200	1.53290400
C	-0.38352900	-0.41231000	-0.24188200
C	-0.57348600	0.96989100	-0.14697200
C	-1.48707000	-1.25659800	-0.12687400
C	-1.84418200	1.49394000	0.06095200
H	0.28493800	1.63444100	-0.24191300
C	-2.76313500	-0.73393100	0.08006100
H	-1.34698500	-2.33472800	-0.20060700
C	-2.94345800	0.64221900	0.17547200
H	-1.98033300	2.57084000	0.12909100
H	-3.61515300	-1.40405300	0.16821500
H	-3.93697200	1.05400500	0.33664800
C	0.99606300	-0.97289100	-0.46514500
H	1.44030300	-0.56187200	-1.37891400
H	0.94748700	-2.06258000	-0.58282900
C	2.94119000	0.22787300	0.47971100
H	3.50696200	0.35516100	1.42273500
O	3.23545200	0.82013100	-0.54654400

**S-TS3-IM1**

C	0.82324800	2.31327500	1.08114900
C	1.33983500	1.99523500	-0.32219000
C	0.81486200	0.58979300	-0.63106600
C	-0.48963700	1.55809000	1.12493200
H	1.50666600	1.92442300	1.84741600
H	0.69497500	3.38421200	1.26115800
H	2.42992700	2.01448500	-0.39862300
H	0.93599100	2.71045400	-1.04728200
H	0.21137500	0.59090300	-1.54963800
H	-1.24550100	2.04126200	0.49300200
H	-0.90365800	1.37190700	2.12072700
N	-0.15209200	0.26194300	0.48071800
C	1.88369000	-0.50449700	-0.78816600
O	3.06085200	-0.20868800	-0.89377700
O	1.42345000	-1.72059800	-0.84088500
H	0.32565400	-1.78662600	-0.69918500
C	-1.42484800	-0.63205100	0.00202300
N	-2.10261400	0.10292100	-1.01386300
H	-2.08418800	-0.45287600	-1.86313500
O	-0.94421200	-1.81021600	-0.35785400
H	0.29104700	-0.35076400	1.18855300
O	0.13570300	-2.00102900	2.20521700
H	0.91327300	-2.53939600	2.38499900
H	-0.26626000	-2.36764400	1.39238500
H	-2.02154600	-0.63379400	0.93961600
C	-3.44681400	0.56865700	-0.69772300
H	-3.41710400	1.28914000	0.12727600
H	-3.86201000	1.08724400	-1.56584100
H	-4.13405300	-0.24375400	-0.41478300



**S-TSIM1-5a**

C	0.39271200	2.66141800	0.28154800
C	1.55585900	1.82015500	-0.21756300
C	0.88498400	0.49167500	-0.51820100
C	-0.38263100	1.68454900	1.15302000
H	0.70450500	3.55102900	0.83599900
H	-0.22798500	2.98810600	-0.56266300
H	2.31659600	1.68103600	0.56168900
H	2.05916300	2.22559400	-1.09918400
H	0.31089000	0.58604500	-1.45484500
H	-1.46198100	1.86822000	1.14976900
H	-0.03664500	1.69612800	2.19326000
N	-0.10791900	0.32130900	0.59265500
C	1.86724800	-0.66345400	-0.71123800
O	3.05700400	-0.46036100	-0.80861300
O	1.35826300	-1.87787000	-0.86047200
H	0.38120700	-1.91312600	-0.64673100
C	-1.39792400	-0.44428500	0.20543600
N	-1.97470400	0.08906800	-0.98574900
H	-1.67751600	-0.48473000	-1.77187400
O	-1.07049200	-1.76827300	0.14346200
H	0.26356100	-0.44957500	1.44964900
O	0.16570300	-1.54985900	2.15407900
H	0.97610400	-2.05501700	2.27727400
H	-0.49880000	-1.91704100	1.18948900
H	-2.07016000	-0.22232200	1.05428400
C	-3.43402200	0.15679700	-0.95754100
H	-3.79560600	0.51954700	-1.92328100
H	-3.91142100	-0.81246300	-0.74618100
H	-3.75473300	0.87568900	-0.19542100

**S-TS5a-6a**

C	-2.22562000	-1.41919600	0.33132200
C	-2.20717500	-0.56053700	-0.93096100
C	-0.87474300	0.17696800	-0.80658500
C	-0.77558100	-1.87775800	0.48055800
H	-2.51727300	-0.80498900	1.19311600
H	-2.92300200	-2.25939700	0.27299100
H	-3.04502900	0.13592100	-1.00599200
H	-2.19071400	-1.19130200	-1.82838800
H	-0.51503500	0.50745000	-1.79112800
H	-0.60618600	-2.87415900	0.04901300
H	-0.45743700	-1.90288200	1.53219800
N	-0.01109800	-0.87668600	-0.27538700
C	-1.02990200	1.44016600	0.07157000
O	-1.84881200	2.27016800	-0.30073000
O	-0.30351700	1.56409900	1.13752200
H	0.54671700	0.82545400	1.37606800
C	1.32188800	-0.75457800	-0.08805800
N	2.04554600	0.03822200	-0.92590000
H	1.59316700	0.89986900	-1.20938500
O	1.53074600	0.06427400	1.54074500
H	1.37679100	-0.54278100	2.27530800

H	1.82973100	-1.67385400	0.20829800
C	3.47400900	0.16393100	-0.68680200
H	3.90582200	-0.83459200	-0.56379900
H	3.94279800	0.62904300	-1.55683100
H	3.69393200	0.75316800	0.21097800

**S-TS6a-6c**

C	-2.40588500	-0.99498800	0.56361100
C	-2.28367600	-0.48757400	-0.87116900
C	-0.82580800	-0.06838700	-0.97552200
C	-1.10982100	-1.76460800	0.77082800
H	-2.45178500	-0.14402600	1.25497700
H	-3.28848500	-1.61861300	0.73075300
H	-2.94686800	0.35329600	-1.08649500
H	-2.49099300	-1.29701800	-1.58298900
H	-0.40596300	-0.21557500	-1.98250700
H	-1.19095500	-2.79805200	0.40375900
H	-0.77341500	-1.78035400	1.81273500
N	-0.15252900	-1.01661500	-0.05924800
C	-0.54840300	1.39891500	-0.57053000
O	-1.47222700	2.15495500	-0.30082800
O	0.70895900	1.71007000	-0.54547900
H	0.88968700	1.53984300	1.40901300
C	1.16084000	-1.18515100	0.01880600
N	2.00550200	-0.38459100	-0.56552700
H	1.49788500	0.67756900	-0.72216200
O	0.81716900	1.09648800	2.27239100
H	0.28669200	1.69001200	2.81255000
H	1.50798100	-2.03620700	0.61421800
C	3.43340100	-0.60875600	-0.48607700
H	3.65959600	-1.52306700	0.07501400
H	3.86221700	-0.70330100	-1.48897600
H	3.91849800	0.23511500	0.01519900

**S-TSIM2**

C	1.94172800	-1.61899300	-0.26749900
C	1.80281000	-0.74175400	0.97379000
C	0.60659900	0.14142100	0.62379400
C	0.49522900	-1.94338400	-0.61251500
H	2.40636800	-1.04646700	-1.08242300
H	2.54381600	-2.51673800	-0.10275100
H	2.69071300	-0.14917200	1.20699200
H	1.55499200	-1.35624600	1.84801500
H	0.02737000	0.45327000	1.50543900
H	0.13330300	-2.80226200	-0.02534400
H	0.34011600	-2.16424700	-1.67482700
N	-0.21913500	-0.72051700	-0.22233000
C	1.04208700	1.43417100	-0.06596000
O	1.98445500	2.08507400	0.31830500
O	0.31407300	1.83197800	-1.11362100
C	-1.58803700	-0.68382400	-0.16173800
N	-2.23084700	0.30478000	0.32190300
H	-0.41741300	1.20898200	-1.25965600

C	-3.67311300	0.22311600	0.32037100
H	-4.05294400	0.29851600	1.34633500
H	-4.09610500	1.06855900	-0.23543100
H	-4.06031300	-0.71093800	-0.12152700
H	-2.07206200	-1.57403400	-0.60076800

**S-TS6c-6d**

C	0.98722000	2.09034500	0.11872800
C	1.07651100	1.18241200	-1.10229200
C	0.60204000	-0.16560500	-0.55163700
C	-0.31871900	1.64065200	0.74803400
H	1.83012000	1.91023700	0.80051300
H	0.98163100	3.15502700	-0.13290300
H	2.07231900	1.11399600	-1.54974000
H	0.37369100	1.52205700	-1.87324000
H	0.08380400	-0.75302800	-1.31995100
H	-1.17430700	2.06875500	0.20443500
H	-0.41321600	1.89752500	1.80891900
N	-0.30093900	0.16472400	0.57873200
C	1.77778100	-1.00993000	-0.06328700
O	2.63618800	-1.42289800	-0.80848300
O	1.78495100	-1.24634900	1.24758900
C	-1.59519200	-0.43740200	0.50895900
N	-2.42134100	-0.13224200	-0.39530600
H	0.97823600	-0.78735600	1.58800100
C	-3.70603200	-0.79268900	-0.38952500
H	-3.81940600	-1.52938700	0.42168300
H	-4.49724300	-0.04027300	-0.30015100
H	-3.85503500	-1.29608400	-1.35096300
H	-1.81540100	-1.18155900	1.29267600

**S-TS6d-6b**

C	-1.64325100	-1.56972100	0.99399800
C	-2.17292200	-1.24610000	-0.40348700
C	-1.17283600	-0.20685800	-0.89328500
C	-0.11864600	-1.50452500	0.85935100
H	-1.98711100	-0.80686200	1.70351000
H	-1.97846400	-2.54155100	1.36694900
H	-3.19326400	-0.85562100	-0.40288100
H	-2.13585100	-2.13055700	-1.05188000
H	-1.13251300	-0.12086800	-1.98682600
H	0.34623700	-2.48955100	0.72092100
H	0.35123100	-1.02797400	1.72414800
N	0.08876900	-0.73087600	-0.37860400
C	-1.49184800	1.20051700	-0.32049600
O	-2.55219700	1.69477300	-0.69761300
O	-0.65756600	1.74014100	0.48975700
C	1.26642500	-0.38224500	-0.88247900
N	2.34868500	-0.32409800	-0.15448200
H	0.45420600	1.39188300	1.05375200
O	1.45053400	1.18192800	1.53723200
H	2.03483800	0.28592800	0.86021900
H	1.37396800	1.07796000	2.49086800

H	1.27290500	-0.09657200	-1.94322000
C	3.61991000	-0.02524900	-0.78654000
H	4.31853800	-0.85882800	-0.66024700
H	3.50360800	0.16645200	-1.86103500
H	4.06233800	0.86132900	-0.32006300

**S-TS6a-7**

N	-0.34828400	0.65231900	0.60723000
H	-0.04523700	-0.27115900	0.20882500
H	-0.61211200	0.54598300	1.58647300
C	-2.70549600	0.31465800	-0.05266300
C	-2.67867400	-1.00824800	-0.50891500
C	-3.87326400	0.81682600	0.52215900
C	-3.80752800	-1.81071700	-0.38569100
H	-1.76543200	-1.40481000	-0.95594700
C	-5.00559800	0.01315500	0.64067700
H	-3.89896900	1.84778500	0.87468700
C	-4.97333300	-1.30221800	0.18756500
H	-3.77925800	-2.83728800	-0.74303700
H	-5.91228700	0.41606300	1.08625400
H	-5.85544500	-1.93171300	0.27764500
C	-1.47895500	1.17744000	-0.17421800
H	-1.70096300	2.20194600	0.15187900
H	-1.14095400	1.21878600	-1.21790900
C	3.06983300	-1.41606300	1.74314600
C	3.84745400	-1.12941000	0.46179600
C	2.85263300	-0.31341700	-0.36371300
C	2.33360000	-0.10560500	2.00934300
H	2.34407400	-2.21909000	1.56385700
H	3.70462700	-1.71439100	2.58278700
H	4.16582500	-2.02764500	-0.07318300
H	4.73605800	-0.52290400	0.68210700
H	3.38060700	0.34520000	-1.06755200
H	2.90612100	0.56307100	2.67115300
H	1.35289300	-0.27605100	2.47654300
N	2.20797300	0.49443600	0.67915300
C	1.92274000	-1.23959400	-1.19914600
O	2.48961600	-1.81671000	-2.13996600
O	0.70391400	-1.32478100	-0.85985800
C	1.30307500	1.48456000	0.43892100
N	1.35523000	2.10856600	-0.77831100
H	1.51220300	1.52436200	-1.58978500
C	0.77544300	3.41495500	-1.01158800
H	0.65127100	3.92942000	-0.05341000
H	1.44766800	4.02058500	-1.62768100
H	-0.20245500	3.37491500	-1.50821500
H	1.16750900	2.18368900	1.27057000

**S-TS6a-8**

C	2.54672200	-2.11585900	-1.72029400
C	2.83778800	-2.07995200	-0.22069400
C	1.80634100	-1.09281000	0.27880700
C	2.21656100	-0.66239500	-2.07139600

H	3.37516200	-2.50292400	-2.32086300
H	1.67433500	-2.75540200	-1.91084300
H	3.84118500	-1.69049000	-0.00764900
H	2.74396400	-3.05627000	0.26368900
H	0.80927700	-1.57639300	0.23133300
H	1.39488500	-0.58147600	-2.80031800
H	3.08753400	-0.13852400	-2.48863600
N	1.85737400	-0.05741200	-0.77981800
C	1.92104100	-0.55464900	1.71935600
O	2.87134800	-0.93172600	2.41483500
O	0.97596600	0.23605400	2.04031300
C	1.50595500	1.25060500	-0.72259900
N	2.00461700	2.11330900	0.21285200
H	2.01320600	1.72826800	1.15877200
N	-0.37401100	1.17587900	-0.28724900
H	-0.20238900	0.81256500	0.67079700
H	-0.82097400	2.08871400	-0.21417600
C	-2.52629200	-0.04365600	-0.48869000
C	-2.60484100	-0.57486000	0.80318300
C	-3.70336100	0.20197100	-1.19485200
C	-3.84139800	-0.85303000	1.37478100
H	-1.69197400	-0.76389700	1.37080900
C	-4.94368700	-0.07944200	-0.62399900
H	-3.64936700	0.61489300	-2.20187800
C	-5.01437900	-0.60667500	0.66170000
H	-3.89016700	-1.26364800	2.38036800
H	-5.85439100	0.11803900	-1.18465700
H	-5.98080000	-0.82358400	1.11036000
C	-1.18293200	0.25877400	-1.09780400
H	-1.30328400	0.69099800	-2.09953600
H	-0.59797500	-0.66407100	-1.21520000
C	1.62167000	3.50860800	0.13359500
H	2.33862900	4.11301000	0.69418000
H	1.64500200	3.83838200	-0.91107400
H	0.61945700	3.70951900	0.54177200
H	1.41918600	1.70546400	-1.71549000

#### S-TS6a-11

C	-1.48784200	0.77635900	-1.14622900
N	-2.05347600	1.85054700	-0.47548100
N	0.41031700	0.96179700	-0.83659800
H	0.90187800	0.74511200	-1.70447200
H	0.56024500	1.95346700	-0.61772600
C	2.41768200	-0.08728000	0.13021200
C	2.91912800	-1.33507200	-0.24294500
C	3.30796200	0.97204800	0.33252400
C	4.28918100	-1.52521200	-0.41253400
H	2.22857500	-2.16613400	-0.38835800
C	4.67558400	0.78485700	0.16418200
H	2.91812400	1.94690500	0.62803000
C	5.16822200	-0.46523200	-0.21048900
H	4.66955600	-2.50303400	-0.69850100
H	5.36106700	1.61272100	0.32929900

H	6.23791400	-0.61212600	-0.33952100
C	0.93914000	0.13037200	0.26535200
H	0.66186900	0.61805800	1.20819800
H	0.40794100	-0.82938600	0.25818900
O	0.14990200	3.45441300	0.64194700
H	0.22241900	3.28720000	1.58872900
H	-0.73423200	3.12382200	0.39608600
N	-1.80535000	-0.48550400	-0.80076700
C	-1.64275000	-2.82048400	-0.70584800
C	-2.85780100	-2.37120600	0.10067300
C	-2.59688200	-0.89877100	0.38787400
C	-1.37158000	-1.62726200	-1.61083300
H	-0.79646200	-2.98365300	-0.02628500
H	-1.81096500	-3.74146100	-1.27184500
H	-2.97445700	-2.92969300	1.03224700
H	-3.77226000	-2.48068800	-0.49808800
H	-3.52895700	-0.31454000	0.40180300
H	-1.96204900	-1.67311800	-2.53969000
H	-0.31269100	-1.52836100	-1.89194700
C	-1.82027100	-0.59084800	1.70376600
O	-1.35192600	-1.54521200	2.34335000
O	-1.72054700	0.64575100	1.95491800
H	-2.26290000	1.58483200	0.50334900
C	-3.10527600	2.55205200	-1.20461200
H	-3.43261900	3.41246400	-0.61622100
H	-2.71660900	2.92670000	-2.15850400
H	-3.98057100	1.91737400	-1.40975600
H	-1.37168000	0.94012000	-2.22336700

S-TS11-12

C	-1.00027800	0.93598200	-0.97518100
N	-1.46391000	1.96930600	-0.10418700
N	0.54922500	0.82568200	-0.77163000
H	0.97000900	0.42719000	-1.61304000
H	0.86974800	1.86312900	-0.64372300
C	2.46409500	-0.25856300	0.29778200
C	2.88368800	-1.52762700	-0.10533700
C	3.41877400	0.73255100	0.54177200
C	4.23976100	-1.80408300	-0.26349700
H	2.14125000	-2.30622200	-0.28241300
C	4.77285800	0.45836200	0.38338800
H	3.09230300	1.72391200	0.85546400
C	5.18464000	-0.81073900	-0.02050600
H	4.55803700	-2.79721200	-0.57104200
H	5.50931600	1.23433500	0.57688900
H	6.24355600	-1.02612600	-0.14091200
C	1.00339900	0.05083600	0.42110000
H	0.78146600	0.66596500	1.30045600
H	0.39860700	-0.86118800	0.48567000
O	0.61036500	3.30880000	-0.22654400
H	1.00088200	3.71546500	0.55177700
H	-0.52319300	2.74596000	-0.01513100
N	-1.59157900	-0.32915600	-0.75004700

C	-2.11970400	-2.56802600	-1.05761400
C	-3.31445500	-1.88933500	-0.39421700
C	-2.75828000	-0.56241600	0.11598200
C	-1.40784300	-1.39885200	-1.71741800
H	-1.46803200	-3.01358700	-0.29316100
H	-2.40282600	-3.35208100	-1.76594700
H	-3.75135900	-2.47527600	0.41795500
H	-4.09335600	-1.69199600	-1.14166300
H	-3.50667400	0.23880600	0.00995700
H	-1.85638100	-1.14591100	-2.69699900
H	-0.33819400	-1.60178000	-1.88671100
C	-2.33626000	-0.58933800	1.59275600
O	-2.45607200	-1.57456500	2.29614500
O	-1.83428700	0.54583000	2.03605800
H	-1.73576700	1.23194400	1.24523600
H	-1.06121200	1.22713400	-2.04807400
C	-2.57020800	2.71565300	-0.69593000
H	-2.88184000	3.50098600	-0.00082700
H	-2.27377800	3.20002300	-1.64161000
H	-3.44987600	2.08875800	-0.90486500

#### S-TS6b-18

N	-0.42939600	0.40103000	-0.72762900
H	-1.02777000	0.62817800	-1.52161400
H	-0.01933300	-0.55593800	-0.82558100
C	-2.57205700	-0.06071000	0.40260100
C	-3.66563300	0.80577000	0.40142300
C	-2.78562500	-1.43161800	0.22768400
C	-4.95861000	0.31332600	0.23209000
H	-3.50366300	1.87513900	0.54052500
C	-4.07477900	-1.92413700	0.05846900
H	-1.93046000	-2.10760800	0.22213100
C	-5.16397500	-1.05235500	0.06044400
H	-5.80452500	0.99678600	0.23593400
H	-4.23180700	-2.99196300	-0.07363900
H	-6.17135100	-1.44037600	-0.07036200
C	-1.17224100	0.46782700	0.53646700
H	-0.60003800	-0.12303300	1.26430300
H	-1.19657800	1.50814100	0.89535800
C	3.31043900	-0.28799500	1.79752200
C	4.05179400	-0.52049300	0.48431800
C	2.92508100	-0.43571800	-0.54239500
C	2.34501900	0.84253500	1.45423000
H	2.74554500	-1.18971100	2.06758600
H	3.96436600	-0.03190700	2.63606600
H	4.56177000	-1.48435900	0.42720200
H	4.78483200	0.27991200	0.31415400
H	3.29491900	-0.12862200	-1.53084300
H	2.80757000	1.82810100	1.62740400
H	1.41324100	0.79108100	2.03504200
N	2.10210600	0.65019500	0.02286100
C	2.21921000	-1.81260900	-0.71893800
O	2.98016500	-2.72512700	-1.07802700

O	0.97600800	-1.87893200	-0.49853900
C	1.23868300	1.38412500	-0.69676200
N	0.91217900	2.64713600	-0.27060500
H	1.35625900	1.29544600	-1.77961800
H	0.88238700	2.78421900	0.73253500
C	-0.05712000	3.40557000	-1.03376700
H	-0.02744200	4.45222400	-0.72356900
H	0.20499200	3.36254100	-2.09615300
H	-1.08762900	3.03459900	-0.91704600

**S-TS7-19**

N	-0.43332500	0.46734000	0.24565000
H	0.58752500	-1.48554500	0.65642000
H	-0.57400600	0.09708900	1.18628900
C	-2.86786700	0.37734100	-0.01668400
C	-2.86721200	-0.95104400	-0.45312600
C	-4.05148900	0.91992300	0.48693700
C	-4.02838200	-1.71542600	-0.39020000
H	-1.94657400	-1.38485300	-0.83981200
C	-5.21597300	0.15841400	0.54531800
H	-4.05968900	1.95128900	0.83870900
C	-5.20731200	-1.16314600	0.10733800
H	-4.01178900	-2.74818600	-0.73080500
H	-6.12962000	0.59628100	0.94115800
H	-6.11359300	-1.76213100	0.15633900
C	-1.62896100	1.22768600	-0.10828100
H	-1.75693200	2.12526700	0.52655500
H	-1.51424400	1.59377300	-1.13857700
C	4.18931300	0.01297200	1.00060800
C	3.92266200	-0.30773200	-0.46458400
C	2.41832100	-0.56635900	-0.46571800
C	2.99869700	0.89135100	1.33250700
H	4.17298900	-0.90660700	1.60296800
H	5.14627500	0.51442700	1.17443300
H	4.48560700	-1.15904400	-0.85503700
H	4.13807600	0.57228000	-1.08414300
H	1.97536600	-0.28485800	-1.43217800
H	3.17569000	1.90812600	0.93680600
H	2.78675400	0.97221000	2.40575900
N	1.86701700	0.25911200	0.63022500
C	2.09826700	-2.05200300	-0.29892100
O	2.78130000	-2.93363300	-0.76885400
O	0.96967400	-2.33196400	0.35531100
C	0.82119700	1.21448400	0.26447200
N	1.07293400	1.91818000	-0.97137300
H	0.65137800	1.44651800	-1.76561900
C	0.80763300	3.34716300	-0.98658700
H	1.41753100	3.84157500	-0.22155200
H	1.10665000	3.75903400	-1.95517000
H	-0.24587700	3.62292300	-0.80856600
H	0.82093700	1.98104300	1.06438200

**S-TS19-20**



N	0.60163600	-0.36904800	-0.04964200
H	-1.10275300	1.58160800	0.65873700
H	0.64199200	0.17682200	0.80801600
C	3.05139900	-0.41568500	-0.00424000
C	3.21885200	0.75169200	-0.75551400
C	4.08496500	-0.83080700	0.83630600
C	4.39841300	1.48392700	-0.66929200
H	2.40876400	1.08523600	-1.40140600
C	5.26919900	-0.10102500	0.92133700
H	3.96035400	-1.73480900	1.43180500
C	5.42844300	1.05889200	0.16883700
H	4.51416300	2.39141600	-1.25752100
H	6.06502800	-0.43701600	1.58225400
H	6.34971900	1.63270300	0.23685200
C	1.78614500	-1.22135300	-0.11540000
H	1.77618800	-2.00547200	0.66659300
H	1.78107200	-1.75489100	-1.07818400
C	-3.69248500	-0.06952600	1.79140900
C	-4.07116500	0.03428500	0.31830900
C	-2.72761500	0.35513600	-0.34684400
C	-2.36543100	-0.80531700	1.72666600
H	-3.55667300	0.93218800	2.22299000
H	-4.43400600	-0.59685800	2.39915100
H	-4.83138300	0.78897200	0.09830700
H	-4.43998600	-0.93330800	-0.04692700
H	-2.65484200	-0.04124200	-1.36727600
H	-2.53492200	-1.89203700	1.62025000
H	-1.74035800	-0.65504100	2.61619500
N	-1.71207800	-0.25994600	0.52259100
C	-2.53665000	1.86500300	-0.46863000
O	-3.26968600	2.56423000	-1.13080200
O	-1.50918200	2.36258100	0.21994000
C	-0.65497700	-1.09692500	-0.06639100
N	-0.94611000	-1.50622800	-1.41258100
H	-0.12624900	-1.47155900	-2.00498000
C	-1.70325600	-2.73425800	-1.53499800
H	-2.70791100	-2.60054900	-1.11099100
H	-1.83026300	-2.98644400	-2.59125400
H	-1.23660000	-3.59339900	-1.02054700
H	-0.58955800	-1.99848100	0.59292400

#### S-TS20-21

N	0.72897700	0.05593200	-0.03694300
H	-2.19831000	1.03074200	1.46023000
H	0.84702300	-0.95046200	0.03903800
C	3.15587800	0.19609200	-0.27022900
C	3.46626900	0.46292300	1.06698200
C	4.10278100	-0.44755500	-1.06657100
C	4.69916900	0.09576400	1.59411000
H	2.72426600	0.95618400	1.69277800
C	5.34127300	-0.81515700	-0.54186900
H	3.86792800	-0.66347100	-2.10848800
C	5.64173000	-0.54438300	0.78944000

H	4.92807200	0.31026500	2.63562400
H	6.06946200	-1.31685400	-1.17502500
H	6.60609300	-0.83233000	1.20137200
C	1.82330000	0.60795100	-0.83087600
H	1.75853600	0.31433500	-1.89635300
H	1.74112000	1.70527300	-0.80816200
C	-2.71667600	-2.53823900	-0.04986400
C	-3.51951200	-1.53385900	-0.86286200
C	-2.96669100	-0.20051100	-0.36409000
C	-1.33329100	-1.91486300	-0.08379400
H	-3.08918100	-2.57946000	0.98319700
H	-2.73261800	-3.55323100	-0.45775400
H	-4.60253100	-1.59947200	-0.73259200
H	-3.29121800	-1.64969800	-1.93070800
H	-2.99344200	0.55756100	-1.16255200
H	-0.85525900	-2.12762000	-1.06163000
H	-0.67717700	-2.29053600	0.71060500
N	-1.57996200	-0.47215400	0.06978700
C	-3.81490600	0.38087500	0.77006600
O	-5.02132300	0.27976500	0.80441000
O	-3.14621900	1.04416100	1.70889300
C	-0.58356600	0.40070700	-0.54105700
N	-0.88208200	1.78201100	-0.21226600
H	-0.20377800	2.11154400	0.46861300
C	-1.04296200	2.71645400	-1.31467900
H	-1.93602300	2.46865000	-1.90041100
H	-1.19153600	3.72142700	-0.91018400
H	-0.18537900	2.74531700	-2.00836500
H	-0.63100800	0.29272400	-1.65794400

#### S-TS21-22

N	0.75434600	-0.06272000	-0.09432900
H	-1.90264700	1.57020300	0.93895500
H	0.89182400	-0.53552100	0.79317600
C	3.16186600	0.31529200	-0.22950100
C	4.07979900	0.92772100	0.62316700
C	3.53442300	-0.84965500	-0.90684800
C	5.35439800	0.39136500	0.79651800
H	3.79514000	1.83399000	1.15676800
C	4.80439800	-1.38832500	-0.73349200
H	2.81879900	-1.33207200	-1.57104000
C	5.71798500	-0.76787500	0.11865700
H	6.06048100	0.87811800	1.46486600
H	5.08534800	-2.29322400	-1.26713700
H	6.71088200	-1.19030600	0.25303900
C	1.79213300	0.90365400	-0.42307900
H	1.64269400	1.19563100	-1.47363200
H	1.70581900	1.82576200	0.17708200
C	-2.77548300	-2.29284700	1.00599300
C	-3.31497600	-2.06576400	-0.40715500
C	-2.84760400	-0.64502300	-0.72109300
C	-1.41424300	-1.59123800	1.00255300
H	-3.43796800	-1.82070700	1.73983100

H	-2.68757200	-3.35182700	1.26610500
H	-4.40173100	-2.15787100	-0.47891800
H	-2.85812700	-2.77301900	-1.11204000
H	-2.76174000	-0.46422500	-1.80107100
H	-0.59014100	-2.30032500	0.83204800
H	-1.22422000	-1.05560300	1.94604300
N	-1.50542200	-0.65980900	-0.12225000
C	-3.84191400	0.39245200	-0.12916100
O	-4.90223800	0.49824000	-0.76713000
O	-3.50337100	0.99022000	0.93298800
C	-0.54899000	0.23327000	-0.41920700
N	-0.98090600	1.85844100	0.53893900
H	-0.31590900	2.05309800	1.28466300
C	-1.16977500	3.00890900	-0.34239400
H	-1.96171500	2.77033100	-1.06080200
H	-1.47800000	3.90473600	0.20688200
H	-0.24965300	3.23063600	-0.89549100
H	-0.66492100	0.72151500	-1.39244400

#### S-TS8-23

C	-3.12275300	-0.59318900	2.24705400
C	-2.87613500	-1.63629300	1.15998500
C	-1.69210700	-1.09036500	0.35472300
C	-2.80578900	0.69175400	1.50537100
H	-4.14415000	-0.62383000	2.63944700
H	-2.42492700	-0.72002200	3.08503500
H	-3.74480800	-1.69777600	0.49378900
H	-2.68194700	-2.64180400	1.54577400
H	-0.75532700	-1.60088400	0.64407800
H	-2.59178100	1.54963900	2.15677300
H	-3.65826100	0.96128200	0.85409400
N	-1.60959500	0.31904400	0.76319700
C	-1.85482900	-1.34846400	-1.15627000
O	-2.89277000	-1.68925600	-1.67585800
O	-0.72295100	-1.27935400	-1.86571500
C	-0.92690700	1.28520800	-0.04709500
N	-1.56003000	1.55817000	-1.32878600
H	-0.87584500	1.76275000	-2.04987100
N	0.42285300	0.78097500	-0.31163500
H	-0.05863800	-0.75070300	-1.36010500
H	0.90034000	1.42397100	-0.94192800
C	2.63713900	0.21591300	0.53088000
C	2.88586800	-1.08353800	0.07814600
C	3.69733600	1.11965700	0.60423300
C	4.16811900	-1.46994100	-0.29498200
H	2.06380100	-1.79778100	0.02283300
C	4.98517400	0.73573900	0.23397400
H	3.51208300	2.13247000	0.96150700
C	5.22168600	-0.55926400	-0.21731800
H	4.34846400	-2.48395500	-0.64402700
H	5.80324000	1.44922300	0.30025800
H	6.22555200	-0.86162300	-0.50593200
C	1.24302200	0.63442100	0.89790200

H	1.26841800	1.57366100	1.47823700
H	0.76530700	-0.11697000	1.53835200
C	-2.59888200	2.57282900	-1.29807700
H	-2.85178600	2.86094300	-2.32199700
H	-3.51324300	2.17865700	-0.84152500
H	-2.30593400	3.48279400	-0.74271000
H	-0.89301300	2.21471400	0.56992300

**S-TS23-24**

C	-3.15876400	-0.56782600	2.01511800
C	-2.07302800	-1.58011300	1.66825200
C	-1.40436600	-0.99361400	0.42625500
C	-2.47366900	0.75016100	1.70421500
H	-4.02199200	-0.70123800	1.34894900
H	-3.50570200	-0.63865300	3.05051100
H	-2.45252800	-2.58873000	1.48636300
H	-1.33390700	-1.62697700	2.47951200
H	-0.31798200	-1.18170400	0.44414300
H	-1.81260100	1.06288900	2.53844100
H	-3.18465700	1.56646000	1.52007400
N	-1.71329300	0.43627500	0.50393700
C	-1.92263500	-1.58259500	-0.88349200
O	-2.82625500	-2.38278100	-0.96818400
O	-1.28116100	-1.15960700	-1.97880000
C	-0.95149300	1.45842700	-0.15501200
N	-1.55419000	1.86225600	-1.42358300
H	-1.08053000	2.69810000	-1.75953700
N	0.38363000	0.97858000	-0.47457400
H	-0.65104300	-0.44251100	-1.75251200
H	0.78837200	1.54110100	-1.22021600
C	2.62600400	0.36828600	0.33430000
C	2.73929300	-0.75634800	-0.48884400
C	3.78759200	0.93096600	0.86632100
C	3.98658500	-1.30782200	-0.76514700
H	1.84231900	-1.19808800	-0.92015000
C	5.03707000	0.37878000	0.59458100
H	3.71166900	1.81381000	1.50054700
C	5.13962800	-0.74372800	-0.22248500
H	4.05770900	-2.18269000	-1.40733700
H	5.93175800	0.83071500	1.01679100
H	6.11381700	-1.17571500	-0.43899500
C	1.28180200	0.95115700	0.67532200
H	1.41552300	1.95576600	1.11713100
H	0.80043400	0.34457700	1.46019800
C	-2.98575900	2.11150600	-1.36701200
H	-3.27835500	2.86609700	-0.61449300
H	-3.32541200	2.45562900	-2.34776600
H	-3.51233900	1.17826600	-1.13815200
H	-0.90782200	2.31881100	0.55766700

**S-TS24-25**

C	3.20995100	-1.48377300	-1.36297100
C	1.83341800	-2.13377700	-1.24800900

C	1.07541200	-1.16384500	-0.34515300
C	2.89066100	0.00272100	-1.48362200
H	3.78849600	-1.67150900	-0.45151100
H	3.79160800	-1.84652700	-2.21531100
H	1.85307400	-3.13831200	-0.81826400
H	1.35001800	-2.18786100	-2.23379300
H	-0.00783400	-1.25057400	-0.47413000
H	2.81426500	0.32182200	-2.53197600
H	3.62649400	0.64053000	-0.97974000
N	1.56856900	0.13977300	-0.84238500
C	1.38854600	-1.44188600	1.15680900
O	0.84666600	-2.47377200	1.58513600
O	2.15518200	-0.64315900	1.75745100
C	1.05808600	1.33167100	-0.58533000
N	1.79047700	2.02722800	1.24268700
H	1.12248200	2.58203500	1.77101600
N	-0.28985000	1.44540100	-0.28906700
H	1.87840200	1.08223900	1.65888000
H	-0.52899400	2.37581200	0.03330800
C	-2.53953900	0.44866100	-0.53166400
C	-2.47891100	-0.24465700	0.67966700
C	-3.78260000	0.66691900	-1.12776400
C	-3.64285000	-0.72084200	1.27520600
H	-1.51582000	-0.41080700	1.15972300
C	-4.94832400	0.19044400	-0.53306900
H	-3.83779600	1.21701500	-2.06719200
C	-4.87997200	-0.50634000	0.67049000
H	-3.58007100	-1.26536400	2.21418400
H	-5.91058300	0.36852900	-1.00780300
H	-5.78848600	-0.87873300	1.13796000
C	-1.28850700	0.91744600	-1.22681000
H	-1.54891000	1.67375600	-1.98366600
H	-0.82889700	0.08898400	-1.77923500
C	3.08814800	2.67950400	1.13193100
H	3.09146600	3.41070400	0.31156300
H	3.38333200	3.20003800	2.05048800
H	3.84952200	1.92174000	0.92122500
H	1.59795400	2.16163800	-1.05333000

#### S-TS12-26

C	-0.65520600	0.25894200	-0.67771100
N	-0.77626900	1.92971100	0.39906400
N	0.68810000	-0.05458000	-0.65163400
H	1.21937500	0.57292200	-1.24629800
C	2.90365200	-0.33496800	0.29233500
C	3.47419100	-1.27914800	-0.56652300
C	3.71584200	0.64838400	0.85732800
C	4.83434200	-1.23989900	-0.85255200
H	2.84123000	-2.04634100	-1.01090700
C	5.08028600	0.68749900	0.57524900
H	3.27846400	1.38635800	1.52970400
C	5.64024900	-0.25567400	-0.28089500
H	5.26862500	-1.97957900	-1.52083000

H	5.70417300	1.45631300	1.02443200
H	6.70409100	-0.22658700	-0.50329700
C	1.42857700	-0.37057700	0.57478900
H	1.18987400	0.34714500	1.37681400
H	1.13817400	-1.36513800	0.93127600
H	-0.74030100	1.74107600	1.39815800
N	-1.61408600	-0.54843100	-0.21115300
C	-2.85254500	-2.09954700	1.04299800
C	-3.50696800	-1.91161100	-0.32067400
C	-2.99881500	-0.54875600	-0.75916900
C	-1.44002800	-1.57471000	0.82296200
H	-3.37559500	-1.48343800	1.78455400
H	-2.85455100	-3.13524800	1.39540600
H	-4.59761000	-1.92327200	-0.27451400
H	-3.16439600	-2.68794300	-1.01903400
H	-2.92921300	-0.45898400	-1.85249100
H	-0.77478800	-2.36786100	0.44844700
H	-0.99862100	-1.15143600	1.73512200
C	-3.84575500	0.66253500	-0.26058800
O	-4.92931300	0.42124000	0.29244500
O	-3.33369300	1.79190600	-0.51481900
H	-1.76228000	2.12936900	0.14132100
H	-0.94755900	0.79632300	-1.58144800
C	0.15576400	2.97030700	-0.00542600
H	0.06939700	3.12491900	-1.08719400
H	-0.03816400	3.93091200	0.48601100
H	1.18799300	2.67176000	0.21708000

#### S-TS14-27

N	0.34656600	0.61194000	0.47874800
H	0.84503100	0.85175300	1.33159700
H	-0.40548000	-1.10238500	-0.64848700
C	2.56970700	0.11711000	-0.36358200
C	3.66167900	0.92126600	-0.03423900
C	2.72313600	-1.27230900	-0.35530000
C	4.89116400	0.35257100	0.29306400
H	3.54580400	2.00562100	-0.03938200
C	3.94984900	-1.84278200	-0.03223100
H	1.87419100	-1.91001000	-0.60116700
C	5.03665700	-1.03162500	0.29250100
H	5.73497800	0.99084700	0.54476100
H	4.05901800	-2.92471400	-0.03455700
H	5.99540600	-1.47991000	0.54254500
C	1.24221700	0.74849700	-0.67391500
H	0.78143100	0.26662100	-1.55136500
H	1.40949400	1.80069400	-0.96234200
C	-4.20671300	-0.08282600	-0.50505700
C	-3.78223000	-0.69818800	0.82004000
C	-2.26705700	-0.75121700	0.66162600
C	-3.17107200	1.01376500	-0.66825500
H	-4.12268600	-0.82551200	-1.31149300
H	-5.23011100	0.30445100	-0.50674200
H	-4.20557600	-1.68425900	1.02644800

H	-4.04315900	-0.02378500	1.64652600
H	-1.74862000	-0.67252800	1.63100900
H	-3.43420400	1.87568800	-0.03294600
H	-3.07348300	1.37991000	-1.69582300
N	-1.90886800	0.39627500	-0.20591400
C	-1.81082400	-2.08921400	0.07730800
O	-2.38384200	-3.13604300	0.27431900
O	-0.68880900	-2.03751300	-0.64226500
C	-0.94650100	1.30598800	0.40552100
N	-0.96385500	2.57166600	-0.27938400
H	-1.22920100	1.52298200	1.45912900
H	-0.71394100	2.46667100	-1.25926400
C	-0.18823600	3.60653700	0.37704800
H	-0.22766800	4.52386500	-0.21688200
H	-0.63217400	3.82563300	1.35613500
H	0.87460700	3.35221400	0.54453300

### S-TS27-28

N	-0.35157100	0.80057800	-0.82370400
H	-0.86107000	1.27640200	-1.56162100
H	2.89580100	0.59511000	1.10800900
C	-2.49917600	0.11007200	0.13087100
C	-3.65572200	0.65075100	0.69544100
C	-2.60726900	-1.04731700	-0.64605600
C	-4.89528600	0.04649000	0.49950700
H	-3.58372600	1.55685400	1.29643800
C	-3.84444900	-1.65204300	-0.84510400
H	-1.71240700	-1.46922500	-1.09999400
C	-4.99273300	-1.10776900	-0.27234800
H	-5.78630100	0.48218500	0.94591600
H	-3.91264300	-2.55335600	-1.45019400
H	-5.95951000	-1.58035300	-0.42962100
C	-1.16275400	0.75528600	0.38732700
H	-0.62450100	0.17673300	1.15547000
H	-1.33464000	1.75046200	0.83555300
C	3.49804400	-1.33134000	-1.38042000
C	2.37877500	-2.09480500	-0.68103000
C	1.64196300	-1.00085800	0.11352700
C	2.80509000	-0.03033000	-1.72965200
H	4.33305100	-1.14341700	-0.69140600
H	3.89257300	-1.85339600	-2.25725900
H	2.71589000	-2.91401200	-0.03888900
H	1.69171900	-2.51459000	-1.42641500
H	0.56200900	-1.19149100	0.08812200
H	2.14947900	-0.16987300	-2.61081200
H	3.49156300	0.79816700	-1.94244200
N	2.01071100	0.26306300	-0.53067100
C	2.06854500	-0.99660700	1.57919900
O	1.77097100	-1.87697000	2.35468900
O	2.80744500	0.05545800	1.93464900
C	1.00960400	1.32271100	-0.71597900
N	1.23544700	2.38013800	0.25347500
H	1.22669400	1.77477000	-1.69602600

H	1.02420200	2.07438500	1.20091900
C	0.54805300	3.61986900	-0.06363900
H	0.75113900	4.35995200	0.71543400
H	0.94204400	4.01733800	-1.00783300
H	-0.54690700	3.52834000	-0.17161300

**S-TS28-29**

N	-0.64523700	0.72513500	-0.84681700
H	-1.14450900	1.52429200	-1.23108500
H	3.39904200	0.21459600	-0.90506400
C	-2.68746200	0.09755600	0.32995500
C	-3.56699100	0.66786700	1.25001500
C	-3.20456500	-0.71022500	-0.68777700
C	-4.93851100	0.43428300	1.16279800
H	-3.17420600	1.30333300	2.04328800
C	-4.57230700	-0.94441300	-0.77820700
H	-2.51959300	-1.14688000	-1.41333800
C	-5.44430900	-0.37259800	0.14823900
H	-5.61180700	0.88752900	1.88676800
H	-4.96143200	-1.57629400	-1.57354600
H	-6.51398800	-0.55473400	0.07634500
C	-1.20361100	0.32735800	0.43665300
H	-0.71478400	-0.61245400	0.73698100
H	-1.01701000	1.04826400	1.25645200
C	1.97658700	-2.56169000	-0.71619500
C	1.92966400	-2.12932100	0.74757000
C	2.00798400	-0.59367000	0.67752400
C	1.14326200	-1.48395600	-1.38810800
H	3.00792800	-2.53898700	-1.09392400
H	1.58082400	-3.56885200	-0.87785500
H	2.72274400	-2.55300100	1.37132200
H	0.96918900	-2.42213600	1.19145300
H	1.41101700	-0.13290100	1.47495400
H	0.06524000	-1.68291300	-1.26357700
H	1.33497500	-1.37740600	-2.46408300
N	1.55199600	-0.26960200	-0.67911300
C	3.44006100	-0.11620000	0.90660800
O	3.96342400	-0.12342300	1.99824100
O	4.08699700	0.25206300	-0.19835600
C	0.79020900	0.94834100	-0.92702000
N	1.32846900	2.01542600	-0.09686500
H	0.97082200	1.22392000	-1.98100500
H	0.70782900	2.22087400	0.67926200
C	1.67479300	3.22850800	-0.81749000
H	2.02663600	3.98567500	-0.11121700
H	2.50124800	3.02150000	-1.50849300
H	0.84104300	3.65970700	-1.40053300

**S-TS29-30**

N	-0.31618300	1.06576400	-0.89008700
H	-0.71536500	1.55163700	-1.68501200
H	2.48805200	0.37269700	1.37619600
C	-2.51314300	0.48670800	0.04705700



C	-3.63562500	0.93919200	0.74563200
C	-2.65623900	-0.59934100	-0.82005800
C	-4.87003200	0.31528200	0.59538600
H	-3.53740500	1.79248500	1.41660900
C	-3.89156800	-1.22429300	-0.97416200
H	-1.79188700	-0.94922300	-1.38207700
C	-5.00184600	-0.77168400	-0.26645900
H	-5.73232100	0.68135000	1.14811700
H	-3.98580400	-2.06988000	-1.65197800
H	-5.96626100	-1.25905200	-0.38929200
C	-1.18159500	1.15573800	0.27815300
H	-0.67011100	0.67884000	1.12730500
H	-1.36542100	2.19393600	0.60692800
C	3.14815100	-1.70046200	-1.25111400
C	1.80377900	-2.22417000	-0.76222600
C	1.27543300	-1.05747500	0.07998500
C	2.80696100	-0.25827700	-1.57112000
H	3.89669100	-1.74859100	-0.44762500
H	3.54211800	-2.24455200	-2.11479900
H	1.85074200	-3.15590800	-0.19171900
H	1.13210700	-2.37857900	-1.61741800
H	0.18189300	-1.00895100	0.00838200
H	2.28356500	-0.20383400	-2.54437800
H	3.68077700	0.40492300	-1.62213000
N	1.91295300	0.14531800	-0.47503300
C	1.60382700	-1.24468500	1.55956300
O	1.22946700	-2.20617500	2.19320700
O	2.32810100	-0.26995300	2.10547100
C	1.09373700	1.33775300	-0.75505200
N	1.37027600	2.34031100	0.26488100
H	1.43204600	1.69377600	-1.74934400
H	0.68591500	3.08820300	0.18381100
C	2.70776800	2.90458300	0.16193900
H	2.82934400	3.70123100	0.90095000
H	3.46373200	2.13961500	0.37465700
H	2.93008700	3.31592100	-0.84009200

#### S-TS30-31

N	0.17163000	-1.72565000	-0.93774300
H	0.23909900	-2.57641300	-1.47766300
H	-1.96338900	-1.79775600	0.81409400
C	2.27453200	-0.80126300	0.04335100
C	3.23770700	-0.79608400	1.05666600
C	2.47621500	-0.00088300	-1.08046300
C	4.37902800	-0.00936500	0.94866300
H	3.08380800	-1.41287700	1.94218400
C	3.62076500	0.78804800	-1.19153000
H	1.72732200	0.00577000	-1.87040300
C	4.57562200	0.78636900	-0.17967800
H	5.11715700	-0.01537400	1.74738200
H	3.76327500	1.40839200	-2.07374200
H	5.46683400	1.40338400	-0.26530300
C	1.04307200	-1.65668400	0.22805300

H	0.45621100	-1.31046000	1.09341600
H	1.35531500	-2.68096900	0.47102800
C	-2.20188200	2.37540500	-0.87087900
C	-0.90768400	2.44224700	-0.06834100
C	-0.70184000	1.00452100	0.37930800
C	-2.02984600	1.09666400	-1.67170800
H	-3.05060100	2.28534400	-0.18072500
H	-2.37049500	3.24537800	-1.51249600
H	-0.96773400	3.11304300	0.79095500
H	-0.07274900	2.75222900	-0.71430900
H	0.36363000	0.79336200	0.53380500
H	-1.48827100	1.28653100	-2.61244500
H	-2.98026500	0.60870000	-1.92184100
N	-1.20314500	0.24494900	-0.79546700
C	-1.45524800	0.61618000	1.68926800
O	-2.01831000	1.51912500	2.32468500
O	-1.39047200	-0.61579900	1.98638000
C	-1.00412900	-1.04641200	-1.13650000
N	-2.30638200	-2.05600700	-0.13102800
H	-1.44330000	-1.28351500	-2.10825600
H	-2.20460100	-3.05532000	-0.29482600
C	-3.68548400	-1.60316700	-0.28530500
H	-4.37579400	-2.15177700	0.36459100
H	-3.73180400	-0.54553900	-0.00462100
H	-4.01307300	-1.71525100	-1.32511200

#### S-TS22-32

N	-0.68462400	-0.08051500	-0.05684100
H	-0.78870800	0.37920200	0.84199200
C	-3.10492900	-0.40367600	-0.21390000
C	-4.10863700	-1.08646400	0.47342100
C	-3.39117400	0.84964600	-0.76365600
C	-5.38070500	-0.53368400	0.60599900
H	-3.89203400	-2.06139100	0.90868200
C	-4.65859700	1.40603300	-0.62779100
H	-2.61083700	1.38798200	-1.29921600
C	-5.65748400	0.71473700	0.05641800
H	-6.15362500	-1.07694700	1.14439500
H	-4.86953400	2.38156900	-1.05983700
H	-6.64800100	1.15075700	0.16245100
C	-1.74639800	-1.02613100	-0.37992300
H	-1.58904700	-1.33953900	-1.42205000
H	-1.67096000	-1.93828300	0.23042100
C	2.98779800	1.85081000	1.18307300
C	3.45785000	1.80832500	-0.26940100
C	2.90698600	0.46513100	-0.74082300
C	1.57375900	1.27303100	1.12166100
H	3.63066300	1.20682900	1.79736400
H	3.00617400	2.85314600	1.61939000
H	4.54219100	1.86042300	-0.38281300
H	2.99773800	2.61856400	-0.84898300
H	2.78933100	0.42095500	-1.83218900
H	0.81420900	2.06466800	1.03987600

H	1.33719800	0.65227800	1.99955300
N	1.58593300	0.46735600	-0.10312000
C	3.85878100	-0.68486200	-0.33729200
O	5.03922200	-0.55516800	-0.63670600
O	3.37310900	-1.71124200	0.28132100
C	0.59239000	-0.37400800	-0.43786500
H	0.68045600	-0.82818400	-1.42579400
O	0.99281900	-2.00171300	0.35589600
H	2.22563100	-1.85529900	0.35596500
H	0.67094500	-1.99295400	1.26690300

**S-TS32-33**

N	0.66915800	-0.81858300	-0.46916800
H	1.02202700	-1.43187400	-1.19815100
C	2.92324500	-0.31570400	0.36804600
C	4.01725500	-0.93371200	0.97494600
C	3.15184300	0.73134700	-0.52952500
C	5.31621700	-0.51139600	0.70095300
H	3.84927000	-1.75770000	1.66764500
C	4.44853700	1.15261900	-0.80798300
H	2.30310100	1.20784400	-1.01763900
C	5.53501600	0.53355700	-0.19213600
H	6.15777300	-1.00580400	1.18069500
H	4.61260200	1.96591400	-1.51136300
H	6.54810600	0.86134800	-0.41285400
C	1.52530200	-0.75509900	0.70604300
H	1.07576600	-0.02987100	1.40459800
H	1.56300100	-1.71654500	1.25007500
C	-2.17798900	2.42584700	-0.26782200
C	-2.91377100	1.75882800	0.89054900
C	-2.70383100	0.25789500	0.65540500
C	-0.98602100	1.51072400	-0.47183800
H	-2.80197700	2.43105700	-1.17139500
H	-1.88508000	3.45785900	-0.05520100
H	-3.97786500	2.00053900	0.94166400
H	-2.45677200	2.04991300	1.84333300
H	-2.38015800	-0.23884100	1.58420700
H	-0.22709100	1.65228300	0.31233600
H	-0.49519200	1.59724000	-1.44424600
N	-1.58659800	0.16709700	-0.33372400
C	-3.97424300	-0.49431600	0.23818800
O	-5.06745600	-0.08203200	0.55353800
O	-3.83286200	-1.65344800	-0.38997900
C	-0.69650400	-1.10839700	-0.22899700
H	-0.86236800	-1.53854900	0.78262700
O	-1.31347700	-1.76919900	-1.25637000
H	-2.90115600	-1.87364100	-0.68177900
H	-1.80189600	-0.54649000	-1.32680700

**S-TS25-34**

C	3.40771700	-1.20001300	-0.43173100
C	2.18144600	-1.55605800	-1.26710500
C	1.09033300	-0.70225800	-0.62473400

C	3.24077600	0.29393800	-0.15700900
H	3.38993600	-1.76345100	0.50957500
H	4.35312200	-1.42440300	-0.93352400
H	1.92359500	-2.61690300	-1.24639900
H	2.31653300	-1.24408700	-2.31041300
H	0.23573500	-0.58327400	-1.29563300
H	3.85604700	0.91391000	-0.82200900
H	3.49205900	0.55203700	0.88218700
N	1.81347800	0.56646400	-0.42626000
C	0.55956800	-1.40316000	0.64633400
O	0.09127000	-2.52245700	0.49334000
O	0.66774500	-0.81335000	1.79629300
C	1.32633700	1.75364600	0.00058900
N	0.17749900	2.30292700	-0.48404000
H	0.84625100	0.30239500	1.82810100
H	-0.08407500	3.15721000	-0.01210800
C	-1.83537600	0.77681000	-0.66063300
C	-2.01704600	0.74807800	0.72026300
C	-2.61867600	-0.05352800	-1.46783100
C	-2.96631400	-0.10174400	1.28548500
H	-1.39159300	1.36472200	1.36363700
C	-3.57026500	-0.89590200	-0.90474300
H	-2.47304800	-0.04499300	-2.54887700
C	-3.74660300	-0.92180600	0.47808400
H	-3.08214400	-0.13088800	2.36621700
H	-4.16626300	-1.54339500	-1.54369500
H	-4.47845000	-1.59168500	0.92253400
C	-0.83699900	1.69850400	-1.32489000
H	-1.37516800	2.53655700	-1.78713700
H	-0.34129200	1.18862500	-2.16190600
H	2.11159600	2.48635400	0.18980400
O	0.97659100	1.57557100	1.82070600
H	1.75609900	1.81837800	2.33655900

#### S-TS34-35

C	-0.76641100	-2.11732800	1.54629400
C	-0.86140200	-2.09438800	0.02310100
C	-1.32665400	-0.67169100	-0.30357400
C	-0.27499100	-0.71680200	1.85680000
H	-1.75703000	-2.27592800	1.99329400
H	-0.09383200	-2.89213400	1.92592300
H	-1.54955900	-2.83551000	-0.39022800
H	0.12954400	-2.26336700	-0.41749100
H	-0.72975800	-0.22082300	-1.11373600
H	0.79582600	-0.61385700	1.62184000
H	-0.44512100	-0.38353800	2.88571500
N	-1.06070400	0.12369900	0.92747700
C	-2.77196800	-0.57984900	-0.79265900
O	-3.31735600	-1.51976400	-1.32626900
O	-3.38504400	0.59656100	-0.69610800
C	-0.66110900	1.63494200	0.73652600
N	-0.16988300	1.97244400	-0.54921700
H	-2.88175000	1.29274800	-0.19301400

H	-0.74947900	2.70141800	-0.95180900
C	2.07496200	0.97490000	-0.52645400
C	1.97671400	-0.03384500	-1.49015000
C	2.91425300	0.77775900	0.56988900
C	2.68647100	-1.22125900	-1.34928800
H	1.33387600	0.11935400	-2.35703000
C	3.63112700	-0.41007900	0.71444700
H	3.00203600	1.56084400	1.32302600
C	3.51278500	-1.41464000	-0.24126500
H	2.59929100	-1.99726700	-2.10669800
H	4.28041100	-0.54965800	1.57560300
H	4.06823800	-2.34291300	-0.13107000
C	1.26269000	2.23623500	-0.66245700
H	1.42950700	2.68276600	-1.65010600
H	1.60301100	2.97092400	0.08804900
H	0.09981100	1.81585100	1.52451300
O	-1.91182800	2.11428000	1.01027000
H	-1.98589200	0.84573900	1.33499900

#### S-TS26-36

C	0.59258200	-0.37453600	-0.43666100
N	-0.68456700	-0.08033700	-0.05605300
H	-0.78854100	0.38009900	0.84242800
C	-3.10488200	-0.40371100	-0.21321500
C	-4.10902000	-1.08613500	0.47384900
C	-3.39079200	0.84932000	-0.76380700
C	-5.38116900	-0.53330000	0.60536100
H	-3.89267500	-2.06082200	0.90977900
C	-4.65830400	1.40576900	-0.62899700
H	-2.61012100	1.38737500	-1.29915900
C	-5.65761100	0.71483700	0.05495600
H	-6.15441500	-1.07628100	1.14357500
H	-4.86897300	2.38108500	-1.06167500
H	-6.64818700	1.15092100	0.16017100
C	-1.74629000	-1.02634100	-0.37809300
H	-1.58869700	-1.34115500	-1.41976800
H	-1.67106000	-1.93772900	0.23342700
H	0.67263900	-1.98957900	1.26929700
N	1.58606400	0.46741700	-0.10265000
C	2.98835800	1.85071700	1.18314000
C	3.45809700	1.80823300	-0.26941900
C	2.90694000	0.46517900	-0.74077700
C	1.57408800	1.27356400	1.12182300
H	3.63106200	1.20631500	1.79717400
H	3.00726500	2.85295700	1.61965900
H	4.54242000	1.86015600	-0.38305100
H	2.99796600	2.61858800	-0.84882700
H	2.78882600	0.42119900	-1.83212300
H	0.81494000	2.06556000	1.03965000
H	1.33714100	0.65338300	2.00001100
C	3.85859400	-0.68525900	-0.33816100
O	5.03938500	-0.55485500	-0.63596200
O	3.37229900	-1.71315500	0.27732000

H	2.22446500	-1.85617600	0.35430400
H	0.68051500	-0.82858700	-1.42470200
O	0.99224300	-2.00035100	0.35748600

**S-TS36-37**

C	0.59376600	-0.74662400	-0.16024700
N	-0.71130800	-0.22513700	0.07122700
H	-0.91046600	-0.28068300	1.07107100
C	-3.11453300	-0.40333500	-0.35510500
C	-4.09958900	-1.20754400	0.21725800
C	-3.41492600	0.93199900	-0.64194000
C	-5.36557700	-0.69329800	0.49421400
H	-3.87205000	-2.24772000	0.44783700
C	-4.67550700	1.44911900	-0.36584200
H	-2.64592600	1.56492000	-1.08291000
C	-5.65589900	0.63594700	0.20357200
H	-6.12346700	-1.33357500	0.93964200
H	-4.89769600	2.48856900	-0.59718700
H	-6.64249400	1.03985500	0.41842500
C	-1.75188300	-0.95911600	-0.65876000
H	-1.53367500	-0.85265600	-1.73165200
H	-1.73285000	-2.03817500	-0.43054600
H	1.69259800	-0.72872800	1.08590100
N	1.68531100	0.23152400	0.31215500
C	2.71413900	2.28674200	0.76828000
C	3.36160900	1.75573400	-0.50560800
C	2.89698400	0.30087600	-0.57654100
C	1.35736000	1.61070000	0.74239300
H	3.28165500	1.96630000	1.65246000
H	2.63807500	3.37723100	0.79326700
H	4.45209400	1.81590900	-0.51022000
H	2.98426700	2.30607100	-1.37529100
H	2.59036400	0.03414300	-1.59851200
H	0.68688200	2.06192900	-0.00078100
H	0.83746300	1.58187200	1.70418300
C	3.98509900	-0.71815800	-0.20344700
O	5.15801500	-0.42620000	-0.26356500
O	3.59355800	-1.94716800	0.09597600
H	2.60125700	-2.05763400	0.20582100
H	0.70821800	-0.92304000	-1.24463500
O	1.00861000	-1.78632700	0.64510000

**S-TS31-38**

N	-0.04119100	2.11573500	-0.16547000
H	-0.04217600	3.12431000	-0.09887300
C	-2.02326200	0.66443100	0.31783900
C	-2.59393300	-0.31532700	1.13424200
C	-2.54844100	0.87615600	-0.95675500
C	-3.68022500	-1.06225300	0.68945600
H	-2.17066000	-0.50408100	2.12099300
C	-3.63559500	0.12775500	-1.40361900
H	-2.09256500	1.62332900	-1.60326300
C	-4.20665400	-0.84034300	-0.58167900

H	-4.10862600	-1.82663800	1.33328000
H	-4.03602800	0.30008600	-2.40028400
H	-5.05279600	-1.42644200	-0.93230000
C	-0.87915300	1.48634700	0.85714800
H	-0.26643800	0.88657000	1.54290300
H	-1.28383800	2.29650700	1.47674900
C	2.88478700	-1.42650000	-1.43345200
C	1.45159800	-1.89908200	-1.20665900
C	0.90048100	-0.83294400	-0.26270700
C	2.76099900	0.09546100	-1.49820100
H	3.51052200	-1.71909800	-0.58059800
H	3.34078600	-1.84244600	-2.33622900
H	1.37747300	-2.89725000	-0.76974600
H	0.88101600	-1.87984900	-2.14330200
H	-0.19516700	-0.80599900	-0.29907400
H	2.73582500	0.47020500	-2.53058400
H	3.58600900	0.59727800	-0.97272600
N	1.46989000	0.38525400	-0.84816000
C	1.31143700	-1.13555900	1.19318400
O	0.97035600	-2.21744100	1.65234800
O	1.98662400	-0.24868800	1.85923500
C	1.20337800	1.66789200	-0.51588300
H	1.73951200	2.38350900	-1.13923700
O	2.18864800	1.99470100	1.01069900
H	2.13895400	0.81217500	1.44920200
H	3.09977800	2.23613400	0.80275600

#### S-TS38-39

N	0.21668300	2.08482000	-0.59511800
H	0.29521000	2.74827500	-1.35188300
C	-1.97098800	0.99142300	-0.10076000
C	-2.46700900	0.24126100	0.96465800
C	-2.33319100	0.63203000	-1.40328000
C	-3.28875500	-0.86239800	0.73756200
H	-2.18869000	0.50816100	1.98340200
C	-3.15504600	-0.46543200	-1.63504300
H	-1.95034100	1.21087000	-2.24386000
C	-3.63011500	-1.22080700	-0.56250600
H	-3.64838000	-1.44945700	1.57913100
H	-3.42427600	-0.73586200	-2.65377200
H	-4.26269200	-2.08663400	-0.74275000
C	-1.04653900	2.16050400	0.14081600
H	-0.82779200	2.25257500	1.21183900
H	-1.54997800	3.09084900	-0.15403800
C	3.18473700	-1.35001400	-1.14551300
C	1.69969500	-1.69129300	-1.20659900
C	1.06073500	-0.71933800	-0.21246200
C	3.14903300	0.15900900	-1.00186300
H	3.64799200	-1.80132800	-0.25764600
H	3.74489600	-1.67907300	-2.02564300
H	1.46641000	-2.72661900	-0.94707400
H	1.31067500	-1.49468500	-2.21318100
H	0.13175000	-0.28966500	-0.62254100

H	2.89234300	0.63508600	-1.96247100
H	4.06984600	0.61278900	-0.62152100
N	2.04451400	0.38797900	-0.05051700
C	0.66863600	-1.36747000	1.11775000
O	0.47810500	-2.55806600	1.21720800
O	0.47996200	-0.55861200	2.15851500
C	1.44744200	1.85747000	0.05694100
H	2.22793000	2.47321900	-0.42803500
O	1.47452900	1.86799800	1.42328200
H	0.67651000	0.39687200	1.96992000
H	2.18763200	0.82478700	1.10932300

**T-IM1**

C	1.56455000	2.39672800	0.29847900
C	1.89556700	1.49777800	-0.89854800
C	0.97465500	0.27514300	-0.76476500
C	0.15535200	1.98093500	0.67006700
H	2.24269100	2.19577200	1.13730300
H	1.63366500	3.46323600	0.06780300
H	2.94108000	1.18012600	-0.91912300
H	1.69530300	2.01255900	-1.84376600
H	0.22418400	0.27837000	-1.56800300
H	-0.58415900	2.36987700	-0.04170200
H	-0.15498700	2.21945000	1.69273200
N	0.18466000	0.50614400	0.49696900
C	1.66808200	-1.09997700	-0.79757500
O	2.76176900	-1.18497600	-1.33888200
O	1.00556400	-2.08399800	-0.28961100
H	-0.06703400	-1.83404200	0.19189500
C	-1.27489300	-0.19379900	0.56001300
N	-1.99852600	0.19998400	-0.60707000
O	-1.06221500	-1.49431400	0.75153500
H	0.67140900	0.09696700	1.31507600
O	0.44358600	-0.84431600	2.98533600
H	1.10137100	-1.40801500	3.40457700
H	-0.14925400	-1.43497900	2.48092700
C	-2.28141100	-0.85822000	-1.56788400
H	-2.62497200	-0.39660100	-2.49998500
H	-1.38894300	-1.44914300	-1.78824000
H	-3.06038800	-1.54917800	-1.20774500
C	-3.17169900	1.02110700	-0.34926000
H	-2.93322800	1.83735100	0.34069100
H	-3.51536100	1.46972700	-1.28760300
H	-4.00642700	0.43738400	0.07733100
H	-1.69873100	0.31089800	1.44835400

**T-5a**

C	-2.36049700	-1.59681700	-0.01556000
C	-2.14447200	-0.67132700	-1.21297300
C	-0.93801300	0.16076900	-0.76864700
C	-0.94809000	-1.85956000	0.52425200
H	-2.96619500	-1.08639300	0.74467200
H	-2.88483900	-2.51991500	-0.27909900



H	-3.01332600	-0.05334900	-1.45339200
H	-1.86083700	-1.24267500	-2.10419800
H	-0.41481500	0.60048900	-1.62802500
H	-0.57171700	-2.86077600	0.26111300
H	-0.92980800	-1.78156800	1.62517100
N	-0.12383900	-0.84194100	-0.12193600
C	-1.41956700	1.32363100	0.11466300
O	-2.23171000	2.12489000	-0.29180000
O	-0.93449300	1.41571700	1.35454500
H	-0.19908800	0.78390700	1.52989900
C	1.23656800	-0.73248400	0.25752300
N	2.04779200	0.00872800	-0.66021100
O	1.36299500	-0.15250400	1.60209400
H	1.38792000	-0.85479200	2.26220500
H	1.63709900	-1.75637000	0.32088700
C	3.42444600	-0.46506800	-0.67338800
H	3.45787500	-1.53657900	-0.89589900
H	3.97413300	0.05802700	-1.46300400
H	3.94508500	-0.28070000	0.28450800
C	2.03234900	1.45903200	-0.49879100
H	1.01548700	1.85381100	-0.44461700
H	2.57033900	1.78544100	0.40618500
H	2.51433600	1.91005100	-1.37255800

#### T-5b

C	0.91419500	2.47353700	-0.31305400
C	2.05814700	1.48324500	-0.46548500
C	1.34675400	0.13199000	-0.49288700
C	0.01280500	1.73449000	0.66160900
H	1.23541700	3.45364200	0.05419900
H	0.39520600	2.62360300	-1.27125600
H	2.72294300	1.52304500	0.40591700
H	2.67349300	1.63481100	-1.35761700
H	1.12201700	-0.15264900	-1.53711800
H	-1.02503700	2.07608300	0.66910900
H	0.40807300	1.81775400	1.68462800
N	0.06922400	0.31519100	0.24480300
C	2.17919300	-0.99507900	0.11578400
O	3.21147200	-0.82573300	0.72091300
O	1.69519400	-2.22570700	-0.07922000
H	0.81875600	-2.16597800	-0.51705100
C	-1.07288600	-0.17306000	-0.50054800
O	-0.92542900	-1.59814200	-0.66642700
H	-1.14461500	-2.00477500	0.18588400
N	-2.30698000	0.20393400	0.10523800
H	-1.08546200	0.19564500	-1.54510100
C	-3.46201500	-0.04307800	-0.73933800
H	-4.33876600	0.44374900	-0.29834100
H	-3.29998800	0.38301400	-1.73513200
H	-3.68651200	-1.11829300	-0.85374900
C	-2.51523900	-0.27384600	1.46290300
H	-1.61797300	-0.11279700	2.06713400
H	-3.34316100	0.28329100	1.91471100

H -2.78571900 -1.34656900 1.50747700

**T-6a**

C -2.46674200 -1.21209400 -0.20917600  
C -2.52140700 0.22975800 -0.70012600  
C -1.06873400 0.69979800 -0.59847800  
C -1.19821900 -1.73052600 -0.85890900  
H -2.36641900 -1.24310300 0.88292200  
H -3.34443000 -1.80029200 -0.49213600  
H -3.17618800 0.87889400 -0.11311000  
H -2.85974800 0.26145300 -1.74452100  
H -0.85362000 1.45201700 -1.36187400  
H -1.37617300 -2.03252400 -1.89988500  
H -0.72399500 -2.55463800 -0.31591200  
N -0.30194500 -0.54860700 -0.84823900  
C -0.77362300 1.32631800 0.79888400  
O -1.23622700 2.47140200 0.92493500  
O -0.12582500 0.63733600 1.62839400  
H 0.40374400 -1.00360300 1.82245200  
C 0.98961700 -0.74244400 -0.70406400  
N 1.98734900 0.12564300 -0.69258500  
O 0.77296300 -1.91932200 1.80604500  
H 0.89108200 -2.17560900 2.72457400  
H 1.29200100 -1.78142700 -0.58240800  
C 3.27758100 -0.31641800 -0.17379500  
H 3.28047400 -1.40019800 -0.04473800  
H 4.07503900 -0.02170600 -0.86313900  
H 3.45370400 0.14658200 0.80467500  
C 1.86915500 1.56583700 -0.89427400  
H 1.12009600 1.78842300 -1.65350000  
H 1.61969000 2.07766000 0.04217700  
H 2.83385500 1.93212800 -1.25518900

**T-6b**

C 1.73212800 2.32636100 0.19546500  
C 2.47986500 1.00073000 0.16315200  
C 1.55395000 0.07262500 -0.61961300  
C 0.29550700 1.88847500 0.43015100  
H 2.08314300 3.00910700 0.97475700  
H 1.81342300 2.83977700 -0.77176900  
H 2.61065900 0.61158900 1.18252300  
H 3.46944000 1.05751700 -0.29513200  
H 1.76398300 0.13337900 -1.69733500  
H -0.45145700 2.61602000 0.09913300  
H 0.13239600 1.65656400 1.49211200  
N 0.20820800 0.65567300 -0.37160800  
C 1.69482400 -1.41230200 -0.18850700  
O 2.83290200 -1.86741500 -0.37696500  
O 0.67503500 -1.98167700 0.28248300  
H -0.63843100 -1.56412700 1.37708600  
C -0.84793800 0.00289000 -0.79776800  
O -1.42058100 -1.27279000 1.89924100  
H -1.43423000 -1.84328700 2.67253700

N	-2.13209000	0.21704200	-0.57107700
H	-0.63085300	-0.83423900	-1.45795800
C	-3.10852700	-0.65919500	-1.20880000
H	-3.92322700	-0.05742300	-1.62427900
H	-2.64256700	-1.22523600	-2.01719500
H	-3.51289200	-1.35562300	-0.46472900
C	-2.68860100	1.09944600	0.44865000
H	-1.96641800	1.27955400	1.24078300
H	-3.03297000	2.04164100	0.00725700
H	-3.53891100	0.58665600	0.90654400

**T-7**

N	0.38919400	0.47724200	-0.65855200
H	-0.03759800	-1.20169500	-0.90977200
H	0.97566700	0.84516000	-1.40437500
C	2.55115300	0.07768100	0.36611500
C	2.83772300	-1.28884300	0.31894700
C	3.57907300	0.99538700	0.14092600
C	4.13102000	-1.72867000	0.05546300
H	2.03934400	-2.01150200	0.48470800
C	4.87509300	0.55781900	-0.12447600
H	3.36008700	2.06320500	0.17951100
C	5.15216300	-0.80586800	-0.16621900
H	4.34314000	-2.79465300	0.02397500
H	5.66785700	1.28280500	-0.29378800
H	6.16325000	-1.15050200	-0.36982500
C	1.14796900	0.56029800	0.60094300
H	1.17528800	1.58557200	0.99564900
H	0.65560500	-0.06367200	1.36064200
C	-4.17454700	-0.61430700	-0.32823600
C	-3.42406300	-1.02566100	0.93463000
C	-1.96004200	-0.89664000	0.51571000
C	-3.34549300	0.55902000	-0.82153900
H	-4.15270600	-1.43324200	-1.06008000
H	-5.22005000	-0.34982200	-0.14394500
H	-3.65508200	-2.03435200	1.28413300
H	-3.63852700	-0.31842400	1.74688200
H	-1.32954500	-0.64257400	1.38548600
H	-3.63647100	1.49053500	-0.30358500
H	-3.44183100	0.74083900	-1.90178000
N	-1.97988300	0.16310200	-0.49472600
C	-1.41408700	-2.22884200	-0.03081700
O	-1.90348800	-3.30154200	0.25508100
O	-0.34249400	-2.15078300	-0.80928300
C	-0.94348100	1.12295800	-0.74337100
N	-1.12340900	2.36826200	-0.02095500
C	-0.30091500	3.46561000	-0.46378800
H	0.74371200	3.43048600	-0.09557400
H	-0.26638100	3.48712800	-1.56084400
H	-0.73483300	4.41463500	-0.12440900
C	-1.43973700	2.36523700	1.38797500
H	-2.11364100	1.53427400	1.61828500
H	-0.56350900	2.29171400	2.05724400

H	-1.96792200	3.29477100	1.64016900
H	-1.03027900	1.40660000	-1.80902000

**T-8**

N	-0.33784100	0.45065900	-0.58581800
H	-0.83445200	0.77987500	-1.41177000
H	-0.18009900	-1.31891400	-0.34946700
C	-2.57624400	0.10989100	0.32127200
C	-3.52897500	0.94370800	-0.27023200
C	-2.92137700	-1.21125300	0.61527400
C	-4.80318800	0.46910400	-0.56884700
H	-3.26677800	1.98041900	-0.48893500
C	-4.19619500	-1.68769100	0.32075300
H	-2.18316100	-1.86932000	1.07199000
C	-5.13856600	-0.85016800	-0.27180100
H	-5.53629100	1.13059900	-1.02469100
H	-4.45453100	-2.71720400	0.55755500
H	-6.13450900	-1.22376500	-0.49793700
C	-1.19881500	0.64323600	0.59717600
H	-0.73775200	0.11933000	1.44526300
H	-1.27730400	1.70485600	0.86868600
C	4.21287700	-0.50091700	0.20801400
C	3.60446800	-1.33027400	-0.91223100
C	2.10559300	-1.11110400	-0.73023700
C	3.31692200	0.71938500	0.19101300
H	4.12270500	-1.02882800	1.16646400
H	5.26658900	-0.25294500	0.04670900
H	3.86699300	-2.39055500	-0.87754700
H	3.91668600	-0.92614100	-1.88406000
H	1.59888900	-1.02488400	-1.70703600
H	3.57146600	1.36722600	-0.66943200
H	3.39052700	1.32931000	1.09658700
N	1.96186400	0.15837800	0.03453000
C	1.43247000	-2.25051300	0.03419200
O	2.03052900	-3.16240600	0.55978100
O	0.10400100	-2.17527500	0.07561200
C	1.00467700	1.08257200	-0.54759900
N	1.11109400	2.37447300	0.07526200
H	1.25191400	1.25118100	-1.62108200
C	0.45857700	3.45004200	-0.62980000
H	0.83677800	4.41117100	-0.26065900
H	0.68082400	3.39329600	-1.70259700
H	-0.64330700	3.45878800	-0.50856100
C	1.09707100	2.51793400	1.51997800
H	1.32578500	1.56272300	2.00029100
H	1.85604500	3.25110500	1.83053500
H	0.12514800	2.86585700	1.90716300

**T-9**

N	0.35661800	0.61915600	-0.70192000
H	-1.01649200	-1.43093900	-1.49227300
H	0.92120500	1.05417500	-1.42503200
C	2.50592500	0.16882100	0.30104900

C	2.74813200	-1.15869400	-0.06574700
C	3.57743800	1.05722600	0.38644400
C	4.04344500	-1.58940700	-0.32849400
H	1.90936400	-1.85010000	-0.14778000
C	4.87749800	0.62867600	0.12033200
H	3.39020100	2.09398900	0.66749000
C	5.11145500	-0.69602500	-0.23549500
H	4.22308000	-2.62565900	-0.60559100
H	5.70547600	1.33030700	0.19235600
H	6.12431500	-1.03494000	-0.44087100
C	1.10028100	0.63421400	0.55751700
H	1.12847500	1.62973300	1.03074000
H	0.61935100	-0.04295600	1.27824400
C	-4.07292900	-0.92221100	-0.40875900
C	-3.33353400	-1.23367600	0.88975400
C	-1.86873100	-0.88463800	0.56631600
C	-3.35747700	0.32834600	-0.88673600
H	-3.94336800	-1.73671700	-1.13449400
H	-5.14619100	-0.76951800	-0.26143100
H	-3.44122300	-2.26459000	1.23976100
H	-3.69249000	-0.57410600	1.69046000
H	-1.37507700	-0.47320900	1.45777900
H	-3.73100300	1.22427100	-0.36193200
H	-3.45888500	0.51175800	-1.96477600
N	-1.95824300	0.04938500	-0.55779900
C	-1.08746500	-2.14989200	0.21109300
O	-0.80615900	-2.98454100	1.04275300
O	-0.76438000	-2.28486500	-1.07148600
C	-1.01089000	1.12585200	-0.77352100
N	-1.33754900	2.34050200	-0.03599600
C	-0.53525700	3.47858000	-0.42126900
H	0.50278200	3.45403900	-0.03676100
H	-0.48209500	3.54310800	-1.51587800
H	-1.00287900	4.40046600	-0.05505400
C	-1.64661500	2.27938500	1.37594700
H	-2.41775100	1.52641400	1.57063400
H	-0.78603100	2.06967800	2.03601400
H	-2.06391000	3.24704000	1.68156100
H	-1.13598200	1.41037300	-1.83387500

#### T-10

N	0.51172100	0.49421600	-0.59140200
H	-3.37860500	0.24496400	-0.68623100
H	1.09140100	1.01106800	-1.24728200
C	2.62548700	-0.26924600	0.29446600
C	2.84302100	-1.46629200	-0.39430600
C	3.71995400	0.52777500	0.62878600
C	4.13171200	-1.86108300	-0.73511500
H	1.98696800	-2.08459900	-0.66426000
C	5.01428200	0.13544200	0.28905200
H	3.55439100	1.46411500	1.16218900
C	5.22134000	-1.05950700	-0.39298400
H	4.28967100	-2.79701600	-1.26620000

H	5.86008500	0.76417100	0.55781800
H	6.22974500	-1.36881900	-0.65787200
C	1.22806400	0.16623200	0.63531500
H	1.28269700	0.99092800	1.36711400
H	0.69788000	-0.65999000	1.13217600
C	-2.71043600	-0.72918800	2.17350300
C	-2.08101100	-1.87002900	1.37747200
C	-1.80467000	-1.22757500	0.00849000
C	-1.90269500	0.47584200	1.71554100
H	-3.76641500	-0.60315900	1.89748800
H	-2.66225600	-0.88203200	3.25567200
H	-2.70832500	-2.76270400	1.29556700
H	-1.13206200	-2.17322500	1.83790900
H	-0.88541300	-1.62084500	-0.44979200
H	-0.94792600	0.51863600	2.26824800
H	-2.42181600	1.42985100	1.86193700
N	-1.72656400	0.20757000	0.28446300
C	-2.94289200	-1.53308200	-0.96651100
O	-3.11165200	-2.62573600	-1.45669300
O	-3.75593300	-0.50342600	-1.20941700
C	-0.85774600	0.99262800	-0.57645300
N	-1.05930200	2.42473000	-0.34717000
C	-0.97601200	3.18663600	-1.58376600
H	0.03930700	3.18157300	-2.02884700
H	-1.68217000	2.79703800	-2.32427600
H	-1.24155000	4.23053900	-1.38394800
C	-0.20455800	3.03278100	0.65850000
H	-0.29708400	2.52518700	1.62290300
H	0.86447700	3.03948900	0.36768800
H	-0.51579000	4.07338400	0.80226300
H	-1.22056300	0.82112100	-1.60456400

#### T-11

N	0.79496200	0.28828800	-0.58074700
H	-2.72822200	1.33955600	0.09892600
H	1.29955100	1.11851400	-0.88127100
C	2.97642700	-0.42914500	0.16248000
C	3.46391800	-1.17416800	-0.91532000
C	3.86975200	0.33503000	0.91383300
C	4.81837700	-1.16014800	-1.22916600
H	2.76696200	-1.76489900	-1.50836900
C	5.22892200	0.35183700	0.60275400
H	3.49526400	0.92079500	1.75374000
C	5.70500200	-0.39613700	-0.46960600
H	5.18641300	-1.74826500	-2.06686000
H	5.91383000	0.95051400	1.19894200
H	6.76450000	-0.38661400	-0.71470300
C	1.50704800	-0.41771000	0.47766400
H	1.36930900	0.01990700	1.48298400
H	1.11701800	-1.44426400	0.51657200
C	-2.67453300	-1.83498300	1.58884600
C	-2.87921200	-2.30994100	0.14985700
C	-2.51633000	-1.06384900	-0.65222500

C	-1.55665100	-0.78009600	1.50480500
H	-3.59710700	-1.37362500	1.96344200
H	-2.42357100	-2.65214400	2.27148500
H	-3.89376800	-2.66057200	-0.05557000
H	-2.17270300	-3.10727200	-0.10626300
H	-2.25365800	-1.31178900	-1.69025400
H	-0.62928900	-1.11956600	1.98529100
H	-1.87638800	0.13891900	2.02095900
N	-1.35111500	-0.57582300	0.06475800
C	-3.73686900	-0.13015000	-0.73338400
O	-4.76437800	-0.50888400	-1.25388400
O	-3.64547100	1.09065000	-0.21093000
C	-0.62899000	0.53655600	-0.49250100
N	-1.01930000	1.84642100	0.12270900
C	-0.97270500	2.93304800	-0.85404100
H	0.05271900	3.14543500	-1.20680500
H	-1.59918100	2.69320700	-1.72005900
H	-1.36521700	3.84770000	-0.39709300
C	-0.26028500	2.23229300	1.30844500
H	-0.29385300	1.45628000	2.07679700
H	0.79908300	2.44419900	1.07593800
H	-0.70035000	3.14317000	1.72837500
H	-0.98759200	0.62986300	-1.52938600

#### T-12

N	0.39284900	-0.27214800	-0.49837400
H	-0.59223900	2.60356700	-0.22537800
H	0.83733700	0.64933200	-0.64238000
C	2.57830900	-1.03063500	0.21146700
C	3.20298600	-1.44398000	-0.96804000
C	3.34086700	-0.43166000	1.21372900
C	4.56967300	-1.25859700	-1.14333400
H	2.60868700	-1.91268000	-1.75201900
C	4.71127500	-0.24498300	1.04065200
H	2.85882300	-0.11122100	2.13701800
C	5.32591700	-0.65653900	-0.13792100
H	5.04788300	-1.58606800	-2.06329800
H	5.29676200	0.22284100	1.82833000
H	6.39494600	-0.51200600	-0.27378000
C	1.09528100	-1.20942300	0.37935100
H	0.81655900	-1.03752000	1.42874100
H	0.80247600	-2.23196500	0.11158100
C	-3.35587100	-2.16094300	0.90249900
C	-4.15176700	-1.59200600	-0.26692700
C	-3.26027400	-0.46186400	-0.75023400
C	-1.92063000	-2.15136300	0.39087900
H	-3.44567200	-1.49381400	1.76983900
H	-3.67336100	-3.16176500	1.20877900
H	-5.13367400	-1.20718200	0.01671200
H	-4.28211800	-2.35050600	-1.05083600
H	-3.40258000	-0.23858900	-1.81524500
H	-1.68357200	-3.06658800	-0.16815200
H	-1.18665000	-2.02662800	1.19000300

N	-1.89501600	-1.00061600	-0.53483600
C	-3.45541700	0.88632700	0.04125000
O	-4.64168800	1.22412800	0.18035500
O	-2.40373200	1.47598100	0.39778500
C	-0.89347500	-0.19747100	-0.80118800
N	0.43023800	2.59535500	-0.21432900
C	0.95701700	3.76881300	-0.89242200
H	2.05148500	3.70394400	-0.93836900
H	0.57944900	3.81446500	-1.91864100
H	0.69808000	4.71403100	-0.38418400
C	0.84587300	2.54223500	1.18063100
H	0.32591500	1.71954900	1.68618500
H	1.92940900	2.36685100	1.24088700
H	0.62142200	3.47074600	1.73294100
H	-1.14108900	0.66472300	-1.41344100

### T-13

N	-0.27559800	0.76510500	-0.71775700
H	-0.71377100	1.20215200	-1.52260800
H	1.24358400	-0.78088700	1.54301200
C	-2.48469600	0.30798500	0.19558800
C	-3.61233100	1.12669100	0.13885500
C	-2.63677000	-1.06726200	-0.00926900
C	-4.87370500	0.58755400	-0.11205100
H	-3.50159200	2.19916200	0.29885800
C	-3.89283300	-1.60886700	-0.25668200
H	-1.76341400	-1.71764600	0.03077900
C	-5.01564200	-0.78226400	-0.30930100
H	-5.74411700	1.23870500	-0.15062300
H	-3.99756600	-2.68115000	-0.40515200
H	-5.99775400	-1.20866500	-0.50062000
C	-1.12647100	0.89704900	0.46238500
H	-0.64986300	0.36022300	1.29383100
H	-1.24988600	1.94328400	0.79021700
C	3.96228600	-1.10419900	-0.05179900
C	3.02678900	-1.84179200	-1.00052100
C	1.64911700	-1.28851000	-0.61326400
C	3.35639400	0.28709800	-0.04126400
H	3.92694100	-1.54863400	0.95297000
H	5.00634400	-1.10384600	-0.37927700
H	3.06787900	-2.93293400	-0.93136100
H	3.25004300	-1.56298900	-2.03843600
H	0.97162800	-1.22965100	-1.47337100
H	3.63954600	0.83794300	-0.95600400
H	3.66190300	0.89784700	0.81474600
N	1.89801100	0.04591200	-0.02864900
C	0.96100200	-2.19949500	0.39733200
O	0.55325100	-3.30430800	0.11872800
O	0.85500400	-1.68646400	1.62472600
C	1.12817600	1.12906600	-0.64406600
N	1.50816600	2.38395500	-0.02282300
H	1.44182900	1.23054900	-1.70580800
C	1.01444500	3.54558600	-0.72553100



H	1.52928400	4.44126600	-0.35779500
H	1.22187400	3.45635400	-1.79905700
H	-0.07299100	3.71113800	-0.59888200
C	1.42560100	2.52707500	1.41851800
H	1.70118000	1.59238000	1.91574900
H	2.13537100	3.29984300	1.74308100
H	0.42529200	2.82264100	1.77914100

**T-14**

N	0.56824100	0.60992900	0.82539700
H	1.10671500	0.89115800	1.63868700
H	-3.43705900	0.40660400	0.03483300
C	2.67568700	0.15734900	-0.29998800
C	3.87243500	0.87265200	-0.30968100
C	2.72347500	-1.23745100	-0.21260200
C	5.09811700	0.21040600	-0.23695500
H	3.84455900	1.95980900	-0.37771300
C	3.94191600	-1.90204200	-0.14244500
H	1.79019500	-1.79955800	-0.19991000
C	5.13445000	-1.17752000	-0.15358700
H	6.02345000	0.78194000	-0.24516000
H	3.96531600	-2.98769500	-0.08180100
H	6.08859500	-1.69647500	-0.09826600
C	1.34999500	0.86510700	-0.38143100
H	0.79493800	0.49646200	-1.25534300
H	1.53071400	1.93860000	-0.56563300
C	-2.37108400	-2.19681400	1.54109400
C	-1.60416500	-2.35587200	0.23515800
C	-1.67891600	-0.94324600	-0.35703300
C	-1.86921500	-0.84815800	2.01895900
H	-3.45340200	-2.16672200	1.35344900
H	-2.17596600	-2.99675300	2.26138900
H	-2.00495600	-3.11163000	-0.44644100
H	-0.55596700	-2.60222900	0.44788500
H	-0.80479000	-0.73949000	-0.98674500
H	-0.86621100	-0.96479200	2.46535500
H	-2.52188400	-0.36308900	2.75503000
N	-1.78700600	-0.02663400	0.79306500
C	-2.91706000	-0.81428500	-1.24885100
O	-3.05063800	-1.44029400	-2.27671400
O	-3.83827900	0.02967700	-0.79161300
C	-0.82280600	1.07224100	0.94309900
N	-1.22731400	2.25754400	0.21426800
H	-0.93081100	1.36212200	1.99849600
C	-0.63923700	3.47713200	0.72556000
H	-1.18189600	4.33767200	0.31596400
H	-0.72947500	3.51402600	1.81783100
H	0.42865300	3.60497800	0.46528100
C	-1.32207100	2.26799800	-1.23424200
H	-1.69150000	1.31794600	-1.62490600
H	-2.04570200	3.03598800	-1.53630200
H	-0.36873500	2.49521600	-1.74080700

**T-15**

N	-0.44773900	0.31518700	-0.84894400
H	-1.07773900	0.79104400	-1.48671100
H	1.53272900	1.20078600	1.33368500
C	-2.56371600	-0.18852100	0.20919400
C	-2.94657800	-1.34156300	-0.48343100
C	-3.54916300	0.69300100	0.65283600
C	-4.28967100	-1.60806200	-0.72391200
H	-2.17699100	-2.03047000	-0.83090100
C	-4.89729000	0.42785200	0.41520100
H	-3.25882700	1.59023900	1.19946900
C	-5.26899500	-0.72199400	-0.27454500
H	-4.57601000	-2.51040600	-1.25941600
H	-5.65614000	1.12041600	0.77198000
H	-6.31991500	-0.93175800	-0.45976600
C	-1.10701900	0.09571300	0.44296100
H	-0.65350000	-0.76734400	0.94694400
H	-1.00882700	0.94569000	1.13792900
C	3.30534400	-1.89255400	-1.47214200
C	3.11740700	-1.95967800	0.05041600
C	1.86636700	-1.10986600	0.31471300
C	2.30787200	-0.82953000	-1.93541600
H	4.33239200	-1.61159200	-1.72637200
H	3.10468900	-2.85478600	-1.95423700
H	3.97234800	-1.51111800	0.57049200
H	2.99350400	-2.97259900	0.44146700
H	0.97441700	-1.75020000	0.15598800
H	1.40377000	-1.30338700	-2.36381400
H	2.71601600	-0.14391100	-2.68936600
N	1.96358500	-0.08460000	-0.72239800
C	1.83493900	-0.68730800	1.77839200
O	1.89534100	-1.54684300	2.63442200
O	1.75904500	0.59462900	2.10423300
C	0.88625700	0.86279100	-0.94402000
N	1.13088500	2.04924100	-0.08517000
H	0.98523100	1.19146500	-1.99830400
C	2.42354200	2.65904500	-0.41406300
H	2.59051200	3.52135300	0.23874400
H	3.22774700	1.93578900	-0.26668500
H	2.44472300	3.00382500	-1.46429300
C	0.08684600	3.05752600	-0.24330400
H	-0.89181000	2.68309300	0.06685900
H	0.32793700	3.92457900	0.37868100
H	0.01467900	3.39709700	-1.29331500

**T-16**

N	-0.37447500	-0.46780700	-1.71272600
H	-0.96989700	0.08709900	-2.31736900
H	0.86165500	1.66173000	0.50682200
C	-2.35461200	-0.87065500	-0.35875800
C	-3.58358400	-1.02601000	-1.00108000
C	-2.27340900	-0.10255200	0.80675200
C	-4.72768500	-0.41715600	-0.48898400

H	-3.64664600	-1.63602000	-1.90245800
C	-3.41737200	0.50284900	1.31655800
H	-1.30896200	0.01684900	1.30633500
C	-4.64334600	0.34964400	0.66995400
H	-5.68355200	-0.54651600	-0.99127700
H	-3.35174200	1.09520300	2.22627100
H	-5.53514600	0.82307400	1.07428400
C	-1.11218000	-1.48642300	-0.94142600
H	-1.36804200	-2.30836600	-1.62155900
H	-0.47570600	-1.89050000	-0.15278800
C	3.94396400	-0.24885000	0.15852400
C	3.44737000	-1.68461900	0.29995200
C	1.95008900	-1.56884400	0.00871800
C	3.19109600	0.24941600	-1.06302000
H	3.65842000	0.33786500	1.03958300
H	5.02753200	-0.17761000	0.02820600
H	3.62021000	-2.11781700	1.28919500
H	3.93063800	-2.33162600	-0.44448200
H	1.54653100	-2.49307200	-0.42040900
H	3.70867200	-0.02081000	-1.99339600
H	2.98480700	1.32564200	-1.06068000
N	1.90693200	-0.48866100	-0.99831300
C	1.16055300	-1.21616200	1.30636300
O	0.83616000	-2.21115400	1.97892800
O	0.94726900	0.00081300	1.52632800
C	0.87549400	-0.02797300	-1.65529300
N	0.83139300	2.49193500	-0.09492800
H	1.07128600	0.84588300	-2.27394300
C	1.72714600	3.49606600	0.45167200
H	1.38499900	3.90189100	1.42186000
H	2.72690700	3.07074800	0.60279900
H	1.82059500	4.33967100	-0.24599100
C	-0.53261600	2.98377600	-0.16123500
H	-1.20920200	2.19314200	-0.51045500
H	-0.91729900	3.33922500	0.81387900
H	-0.59587500	3.82373300	-0.86689700

#### T-17

N	0.63337900	-0.32663200	1.28226200
H	-2.23799400	-2.02972200	-0.24516900
H	1.09603800	-0.56695000	2.15265800
C	2.68063300	-0.38020800	-0.07680000
C	3.00783800	0.93947000	0.24535500
C	3.66604900	-1.19811100	-0.63432800
C	4.28904200	1.43017700	0.00731500
H	2.24738000	1.57796400	0.69161600
C	4.94675600	-0.70922900	-0.87708000
H	3.42438300	-2.23200600	-0.88053300
C	5.26293200	0.60895100	-0.55652400
H	4.52809800	2.46005000	0.26408000
H	5.70084100	-1.36190500	-1.31127800
H	6.26367500	0.99289600	-0.74031200
C	1.28978300	-0.92071300	0.12456000

H	1.32998900	-2.02101500	0.18110200
H	0.66761800	-0.68975700	-0.75217900
C	-2.22052600	2.30335800	-0.46587900
C	-3.37107500	1.63226100	0.27192800
C	-2.91475200	0.18042200	0.34367000
C	-1.01368700	1.63159200	0.16270900
H	-2.27368600	2.07082500	-1.53786600
H	-2.20087900	3.39142400	-0.35333500
H	-4.34045900	1.73168200	-0.22201400
H	-3.45200700	2.03871900	1.28887100
H	-3.26847200	-0.31459200	1.26315900
H	-0.78882800	2.08491700	1.14621500
H	-0.10510500	1.69794700	-0.44648300
N	-1.43682300	0.23152900	0.32240900
C	-3.43157300	-0.65543500	-0.83272200
O	-4.27464100	-0.26898500	-1.61032700
O	-2.90768900	-1.87617100	-0.94654800
C	-0.77558100	-0.48846000	1.37282100
H	-1.08425700	-0.13859800	2.38257200
H	-1.10964900	-2.33219400	2.04819400
O	-1.22611900	-1.84714200	1.22285700

**T-19**

N	-0.44378000	1.01358500	-0.71259400
H	-1.04675300	1.72837700	-1.10819200
H	1.77251400	0.81675000	1.55211300
C	-2.50335000	0.08089700	0.17228500
C	-2.76365200	-0.92069100	-0.76803700
C	-3.57624000	0.71549800	0.79716700
C	-4.07100000	-1.28333800	-1.07166900
H	-1.92812100	-1.41407700	-1.26354500
C	-4.88901800	0.35549600	0.49464000
H	-3.38111200	1.49690900	1.53082400
C	-5.13815400	-0.64456000	-0.43976300
H	-4.26009700	-2.06765900	-1.80113900
H	-5.71612300	0.85806200	0.99089700
H	-6.16105100	-0.92825300	-0.67645700
C	-1.08778900	0.47253900	0.49123300
H	-0.53476400	-0.41515300	0.82875800
H	-1.07610700	1.18880800	1.32665800
C	4.07192800	-0.34006100	-0.90902300
C	3.01807400	-1.43985400	-1.04299800
C	1.81673800	-0.82947600	-0.31607700
C	3.26989400	0.96625100	-0.97500700
H	4.57408900	-0.42443700	0.06376100
H	4.84684500	-0.39473800	-1.67894000
H	3.32476700	-2.39675200	-0.61284600
H	2.74565900	-1.59650300	-2.09295500
H	0.87408200	-1.29152900	-0.64095500
H	3.34708000	1.46209800	-1.95593900
H	3.62931000	1.68321600	-0.21670500
N	1.89162000	0.54772900	-0.74305700
C	1.94728600	-1.08550700	1.19461900

O	2.04479700	-2.21015000	1.63275600
O	1.97036000	-0.03100100	2.01237500
C	0.88337500	1.53307700	-0.59803000
H	1.03020500	2.28081700	-1.39296200
O	1.02650100	2.24250500	0.67892100
H	1.62289000	2.99240600	0.56872700

**T-TS3-IM1**

C	1.54165800	2.39480800	0.46855400
C	1.85592900	1.59693400	-0.80218300
C	0.96425600	0.34633200	-0.72907200
C	0.14721700	1.92537300	0.83352500
H	2.24101400	2.13823800	1.27421400
H	1.59185800	3.47703700	0.32017500
H	2.90726500	1.30853100	-0.87832900
H	1.61158200	2.17605900	-1.69863600
H	0.20055200	0.38115000	-1.52087800
H	-0.60923000	2.35616400	0.16421200
H	-0.15018500	2.08626800	1.87468200
N	0.19264800	0.47130700	0.55058200
C	1.69656200	-0.99625800	-0.86985700
O	2.79828700	-1.02705900	-1.38948200
O	1.05406600	-2.05361300	-0.46387200
H	0.06033700	-1.87064100	-0.01839200
C	-1.30417600	-0.28176000	0.55699800
N	-2.01997100	0.21765000	-0.56733300
O	-1.05428300	-1.57029900	0.61746400
H	0.68052600	-0.00222900	1.33074100
O	0.45581800	-1.15135300	2.88223300
H	1.09273700	-1.78354300	3.22905300
H	-0.14763600	-1.65352000	2.29673200
C	-2.31223700	-0.73732000	-1.62623500
H	-2.59895800	-0.18343700	-2.52731400
H	-1.43996700	-1.35136400	-1.86194000
H	-3.13572300	-1.41700500	-1.35367700
C	-3.16196000	1.06452000	-0.26518900
H	-2.92253200	1.77006400	0.53688900
H	-3.43357600	1.64811900	-1.15220900
H	-4.04566900	0.47817000	0.04213200
H	-1.70572900	0.16205800	1.48980600

**T-TS3-5b-H<sub>2</sub>O**

C	0.96230900	2.65930600	0.02350900
C	2.10936200	1.67064000	-0.09535900
C	1.39662200	0.40154900	-0.52226000
C	-0.11027300	1.83447600	0.71263600
H	1.21792300	3.55956200	0.58954000
H	0.62186300	2.97474400	-0.97250900
H	2.59976200	1.51038000	0.87348200
H	2.88365000	1.95571400	-0.81260600
H	1.15361100	0.46375000	-1.59667100
H	-1.13630900	2.13478900	0.48901800
H	0.02748500	1.82857200	1.80114900

N	0.08946100	0.42550200	0.23026600
C	2.23874500	-0.86780500	-0.35270000
O	3.40355700	-0.80268800	-0.03006000
O	1.66763700	-2.02102600	-0.66505300
H	0.67479600	-1.93997300	-0.77613000
C	-1.05075900	-0.22390500	-0.60318000
O	-0.91287300	-1.57585900	-0.43509200
H	0.13027800	-0.34404700	1.15020200
O	-0.19423900	-1.43238800	1.82541100
H	0.54265400	-2.00105400	2.07520900
H	-0.65355300	-1.72604200	0.72805200
N	-2.32063800	0.34442400	-0.25416700
C	-2.84972700	-0.07965300	1.03608200
H	-3.75423500	0.50005200	1.24824000
H	-3.10759600	-1.15132500	1.05280300
H	-2.12867700	0.10192800	1.83932000
C	-3.29939300	0.12326300	-1.31006200
H	-4.21200000	0.68049600	-1.07274800
H	-2.91550500	0.49252000	-2.26738800
H	-3.56277200	-0.94287600	-1.42330900
H	-0.85710800	0.06179200	-1.65200400

#### T-TSIM1-5a

C	0.44655400	2.69012400	0.07843200
C	1.52189600	1.85571200	-0.60033000
C	0.91504200	0.46277800	-0.57798900
C	0.02555800	1.78762600	1.22578700
H	0.80555300	3.66260700	0.42776700
H	-0.39434400	2.86458500	-0.60654600
H	2.45417200	1.86439400	-0.02082000
H	1.76370600	2.17464900	-1.61788900
H	0.16132700	0.38462100	-1.38108100
H	-0.99113100	1.95836300	1.59355900
H	0.70624600	1.89348500	2.08004100
N	0.15293700	0.38907900	0.70942600
C	1.92071900	-0.66205500	-0.79452900
O	3.06186600	-0.43934500	-1.13122500
O	1.46637200	-1.90535800	-0.67568300
H	0.53323300	-1.93763700	-0.32645900
C	-1.20410700	-0.41035800	0.58591100
N	-1.93642900	-0.02330400	-0.58054500
O	-0.86038400	-1.72157100	0.62657300
H	0.64781400	-0.31850300	1.56623600
O	0.65386700	-1.31487600	2.40158400
H	1.47050300	-1.82343200	2.44364900
H	-0.15265000	-1.76172800	1.59008200
H	-1.73877500	-0.08225600	1.49880100
C	-2.20916900	-1.06972700	-1.55581800
H	-1.29781700	-1.60289600	-1.83708300
H	-2.93609700	-1.81185300	-1.18777600
H	-2.61489100	-0.59845700	-2.45761400
C	-3.11722300	0.78076100	-0.31013300
H	-2.88010600	1.61632900	0.35583500

H	-3.48961100	1.20616300	-1.24818000
H	-3.93207500	0.19116800	0.14732900

#### T-TS5a-6a

C	-2.41748600	-1.48384300	0.11605300
C	-2.34832200	-0.49758300	-1.04385500
C	-1.02586600	0.22497200	-0.78366500
C	-0.97625400	-1.95965500	0.26150600
H	-2.73754700	-0.96280600	1.02757100
H	-3.11225500	-2.31047400	-0.05642400
H	-3.18477600	0.20366300	-1.08526600
H	-2.28683100	-1.02923200	-2.00166200
H	-0.64400400	0.66119100	-1.71352900
H	-0.78840200	-2.89395100	-0.28630500
H	-0.70025600	-2.11946100	1.31267500
N	-0.17130800	-0.87616400	-0.33558100
C	-1.23650100	1.36993100	0.23012900
O	-1.99519800	2.26981600	-0.10596500
O	-0.63164400	1.31996800	1.37593200
H	0.22012800	0.57734200	1.56152100
C	1.14877200	-0.84468300	-0.03050900
N	2.08069400	-0.08739900	-0.69067600
O	1.23140600	-0.17390900	1.68419800
H	1.07972100	-0.86141300	2.34348500
H	1.52908600	-1.83657100	0.21798300
C	3.45732600	-0.44503800	-0.36397100
H	3.57318000	-1.53230700	-0.34443000
H	4.12086300	-0.04630800	-1.13706700
H	3.75598400	-0.03393700	0.61190600
C	1.93607900	1.36387500	-0.78961800
H	0.96086700	1.66051100	-1.17139500
H	2.09738400	1.84130900	0.18762300
H	2.68816100	1.73252600	-1.49262000

#### T-TS5b-6b

C	-1.20736200	2.51856900	0.06948100
C	-2.22392800	1.38875100	0.06299100
C	-1.41347900	0.17131600	0.50625100
C	0.04141000	1.85629700	-0.49456200
H	-1.51793600	3.38776700	-0.51782200
H	-1.01550800	2.85319900	1.09770100
H	-2.60732000	1.21972700	-0.95243100
H	-3.08480800	1.55254300	0.71384200
H	-1.38322300	0.12360300	1.60943000
H	0.96810400	2.32335300	-0.14384300
H	0.03341000	1.87276300	-1.59524300
N	-0.05230100	0.48201500	0.01597800
C	-2.08316100	-1.13722800	0.05414500
O	-3.27805400	-1.23261500	0.31368300
O	-1.38731600	-2.05279100	-0.52870200
H	-0.22112000	-1.93732200	-0.63596600
C	0.99645400	-0.27132000	0.41118200
O	0.98589500	-1.79682100	-0.67301900

H	1.20831800	-1.52978800	-1.57442700
N	2.28288700	0.19205000	0.35559200
H	0.79345400	-0.90585700	1.27774600
C	3.23867900	-0.57022500	1.15038800
H	4.16854900	0.00159500	1.22403000
H	2.85263700	-0.72637900	2.16092500
H	3.45331300	-1.54571200	0.68820800
C	2.84533000	0.57966200	-0.93289700
H	2.07836600	0.94744300	-1.61644800
H	3.58950000	1.36984700	-0.78951000
H	3.34230700	-0.28234300	-1.40475500

**T-TS6a-7**

N	-0.34716300	0.41252300	0.42996200
H	-0.01118500	-0.43576700	-0.22388500
H	-0.55604900	-0.01609600	1.33443100
C	-2.76779600	0.29284400	0.02640600
C	-2.83719500	-0.87060700	-0.74725400
C	-3.84372400	0.63576100	0.84512800
C	-3.96954900	-1.67583000	-0.69754000
H	-1.99723800	-1.15048600	-1.38381200
C	-4.98145300	-0.16747000	0.88912800
H	-3.79391000	1.54179500	1.44822500
C	-5.04449400	-1.32432100	0.11823800
H	-4.01349900	-2.57963700	-1.30006200
H	-5.81708300	0.11111800	1.52661600
H	-5.93053000	-1.95369600	0.15127500
C	-1.54171300	1.15789200	-0.02590300
H	-1.66436300	2.04924800	0.60394000
H	-1.34227800	1.49699500	-1.04862800
C	3.10982500	-1.53049500	1.81744100
C	3.85656900	-1.08129200	0.56307900
C	2.75104900	-0.41846900	-0.25477300
C	2.07696600	-0.42349800	2.05840800
H	2.59708600	-2.47994400	1.61627400
H	3.76377100	-1.68643000	2.68071000
H	4.32629700	-1.90316900	0.01768700
H	4.62191600	-0.33570700	0.81245200
H	3.16982400	0.29296300	-0.98041500
H	2.36158600	0.25570700	2.87762500
H	1.10333300	-0.86869800	2.33020300
N	2.04092400	0.31404200	0.79595000
C	1.94114700	-1.46651800	-1.06644000
O	2.59578500	-2.22700100	-1.78454800
O	0.66153200	-1.45057100	-0.96675700
C	0.99390200	1.23695300	0.58512200
N	1.16067400	2.15574900	-0.47245000
C	0.91261200	3.55940800	-0.23152300
H	-0.11854500	3.86455100	-0.48929100
H	1.10086600	3.81200900	0.81653600
H	1.59511300	4.16461500	-0.84225300
C	1.09495700	1.77697500	-1.87170600
H	2.00955600	2.07135000	-2.40530900



H	0.95830500	0.69955900	-1.99515000
H	0.24822400	2.27740700	-2.37114400
H	0.84261400	1.80868800	1.51331400

**T-TS6b-8**

N	0.21830700	1.01146600	0.62601600
H	0.60903000	1.88859000	0.97166600
H	0.38007600	0.25943900	1.32333100
C	2.32303700	0.29243500	-0.45535900
C	3.27522500	1.29830300	-0.63799100
C	2.73497200	-0.98444900	-0.06232100
C	4.62679500	1.04026100	-0.42682500
H	2.95337200	2.29103400	-0.95605400
C	4.08727900	-1.23975500	0.14936200
H	1.98926200	-1.76880200	0.08456000
C	5.03312500	-0.23198500	-0.03076800
H	5.36184500	1.82801500	-0.57582500
H	4.40333100	-2.23413000	0.45568200
H	6.08808700	-0.43937900	0.13406300
C	0.86376800	0.59904000	-0.63908100
H	0.32319000	-0.28881900	-0.99041700
H	0.72694300	1.39721600	-1.37891800
C	-2.66239000	-1.75491700	-1.64586300
C	-2.96670500	-2.30161200	-0.25613400
C	-2.09792900	-1.46601600	0.66870900
C	-2.51227800	-0.25453000	-1.42344000
H	-1.71314400	-2.17400600	-1.99990900
H	-3.43710300	-1.98180200	-2.38471500
H	-2.73477900	-3.36578700	-0.16327600
H	-4.02601900	-2.14721700	-0.00918500
H	-2.57067800	-1.29839100	1.64672100
H	-3.46997500	0.28124400	-1.52079900
H	-1.80314800	0.18019700	-2.13934300
N	-2.02797000	-0.15881000	-0.04359700
C	-0.65958000	-1.99162100	0.92187300
O	-0.20400300	-2.86259600	0.15863200
O	-0.06311400	-1.40550700	1.87274300
C	-1.68027900	0.96077100	0.63030900
N	-2.12310900	2.22680300	0.27057300
H	-1.72534500	0.80758800	1.71094600
C	-2.04858600	3.21326600	1.33822300
H	-2.70197700	4.05580100	1.09064600
H	-2.39154500	2.78421100	2.28317800
H	-1.02758800	3.61212800	1.47488200
C	-1.74946600	2.81223000	-1.00613800
H	-1.83796800	2.10058700	-1.82621500
H	-2.41635500	3.65401300	-1.21677500
H	-0.71511600	3.19835500	-0.98353200

**T-TS7-9**

N	0.39057700	0.55757600	-0.70468700
H	-0.64173200	-1.34327800	-1.31722700
H	0.98763300	1.03217700	-1.37623500

C	2.52344300	0.05604400	0.31792900
C	2.81498200	-1.25642300	-0.06484200
C	3.56109000	0.98403100	0.40928900
C	4.12398600	-1.63317600	-0.34430400
H	2.00405300	-1.97981500	-0.14604000
C	4.87428200	0.60957400	0.12808400
H	3.33668700	2.00872800	0.70747100
C	5.15659500	-0.70028800	-0.24855200
H	4.34136400	-2.65820200	-0.63565700
H	5.67534300	1.34106700	0.20654500
H	6.18024900	-0.99616100	-0.46630000
C	1.10253200	0.47054600	0.57444100
H	1.09631700	1.42238300	1.12972100
H	0.61261800	-0.27453800	1.21803400
C	-4.11023000	-0.76952700	-0.53844600
C	-3.47291600	-1.05922900	0.81693800
C	-1.97676000	-0.82567500	0.55479900
C	-3.30946600	0.43001700	-1.01027700
H	-3.95955100	-1.61757200	-1.22092700
H	-5.18386300	-0.56962900	-0.47532000
H	-3.66653200	-2.06121700	1.20884900
H	-3.83051700	-0.33357800	1.55906200
H	-1.48820100	-0.44675600	1.46554300
H	-3.68639400	1.36182700	-0.55263200
H	-3.32520900	0.56855500	-2.09996800
N	-1.95217100	0.11593400	-0.56459500
C	-1.27909400	-2.15588500	0.24670900
O	-1.30460800	-3.08149100	1.02821100
O	-0.64546000	-2.24158800	-0.91865800
C	-0.95451700	1.13933800	-0.76083400
N	-1.20706500	2.36045100	-0.00677600
C	-0.32573100	3.45045800	-0.35306200
H	0.69881200	3.35521200	0.05697800
H	-0.24070200	3.52903000	-1.44499000
H	-0.74303700	4.39471600	0.01715000
C	-1.56989200	2.30229200	1.39176100
H	-2.39023500	1.59401900	1.54637600
H	-0.74743100	2.03364600	2.07948600
H	-1.93987200	3.28940500	1.69626400
H	-1.05846900	1.44431100	-1.81799900

#### T-TS9-10

N	0.41416600	0.34800400	-0.00899600
H	-2.69228500	-0.74771700	-1.52046300
H	0.43270400	-0.66898800	-0.04265400
C	2.83075500	0.17529300	-0.25979700
C	3.31145400	0.46027400	1.02206900
C	3.52034300	-0.74183200	-1.05198100
C	4.46265200	-0.15625400	1.49865300
H	2.76732600	1.17182400	1.64342900
C	4.67523800	-1.36252900	-0.57779200
H	3.14957400	-0.97040700	-2.05079400
C	5.14831800	-1.07003800	0.69764500

H	4.82948200	0.07581400	2.49601000
H	5.20391300	-2.07547500	-1.20621200
H	6.04975000	-1.55161700	1.06941300
C	1.57597600	0.83509600	-0.75328300
H	1.46703200	0.67017700	-1.84321000
H	1.64916600	1.92102900	-0.60540000
C	-4.00286100	-0.20325900	1.16449700
C	-3.06762200	-1.34918600	1.53439800
C	-1.89909300	-1.20470700	0.53642000
C	-3.02785900	0.89969300	0.79422700
H	-4.62302800	-0.46907900	0.29713500
H	-4.67203700	0.08025000	1.98266000
H	-3.52597000	-2.34237000	1.49271400
H	-2.68225200	-1.20503700	2.55070800
H	-0.95756600	-1.43367600	1.05347800
H	-2.63053900	1.37187500	1.70925800
H	-3.46682400	1.68888100	0.17714100
N	-2.00202000	0.16630000	0.04337700
C	-2.03869900	-2.21397700	-0.60099500
O	-1.73563400	-3.37990500	-0.49689800
O	-2.56122900	-1.70470500	-1.72030700
C	-0.83923800	0.86314400	-0.54939000
N	-0.96368000	2.28370600	-0.38461900
C	-0.78539500	3.13534600	-1.53756200
H	0.27259400	3.38862800	-1.74156800
H	-1.20246700	2.66139400	-2.43203500
H	-1.32282600	4.08035600	-1.38227400
C	-0.49949200	2.87354200	0.85270900
H	-0.55380300	2.14875500	1.66881300
H	0.54773900	3.22474800	0.79279300
H	-1.12593300	3.73909000	1.10986200
H	-0.86496500	0.68871300	-1.64840200

#### T-TS10-11

N	0.69837400	0.39156200	-0.59011400
H	-3.08690600	0.97893100	-0.19295000
H	1.23699000	1.13466400	-1.02948300
C	2.85301900	-0.38944200	0.18897300
C	3.23118100	-1.33533900	-0.76853900
C	3.83897800	0.39382000	0.78974100
C	4.56900100	-1.50136700	-1.10891500
H	2.46141300	-1.94021500	-1.24617800
C	5.18185200	0.23124800	0.45103100
H	3.54953200	1.13561800	1.53456700
C	5.54868100	-0.71778200	-0.49817300
H	4.85157000	-2.24516200	-1.85051200
H	5.94033400	0.84616800	0.93015700
H	6.59533800	-0.84938400	-0.76258600
C	1.40489200	-0.19773700	0.54039000
H	1.34590800	0.39907700	1.46822200
H	0.93410700	-1.16869800	0.75627500
C	-2.68823100	-1.32167100	1.96419600
C	-2.49679300	-2.23942800	0.75892900

C	-2.21454100	-1.23905300	-0.36196000
C	-1.65567700	-0.21079300	1.75021500
H	-3.70301400	-0.90154700	1.95384800
H	-2.55616100	-1.83318200	2.92200800
H	-3.35681100	-2.87998800	0.54377400
H	-1.61140100	-2.87407500	0.89154800
H	-1.65994700	-1.70311500	-1.19106000
H	-0.72398700	-0.42015600	2.30230500
H	-2.03649000	0.76070200	2.10073800
N	-1.44321500	-0.21937400	0.30467500
C	-3.53050300	-0.71380000	-0.95265100
O	-4.28136300	-1.41268600	-1.59268500
O	-3.81912100	0.57072100	-0.70278000
C	-0.70924900	0.74612700	-0.46380300
N	-1.01363000	2.12414500	-0.02906900
C	-0.99495200	3.06382400	-1.14246200
H	0.01304100	3.20092100	-1.58082100
H	-1.67582300	2.73240400	-1.93417800
H	-1.33800400	4.04382100	-0.79330600
C	-0.18069100	2.63198900	1.05184400
H	-0.20657200	1.97346800	1.92484800
H	0.87686600	2.76078000	0.74992200
H	-0.56062800	3.61161300	1.36180900
H	-1.11799400	0.69517800	-1.48656400

#### T-TS11-12

N	0.77388000	0.04793300	-0.58750800
H	-1.93268600	1.63401200	0.61150500
H	1.29967900	0.77150100	-1.06076000
C	3.00729600	-0.55052600	0.10646800
C	3.60856000	-0.99029900	-1.07657400
C	3.77847100	0.12923100	1.04949900
C	4.95789800	-0.75073700	-1.31343400
H	3.00913200	-1.52690900	-1.81155600
C	5.13170100	0.36671100	0.81649500
H	3.31659600	0.47016500	1.97585600
C	5.72195100	-0.07087000	-0.36562800
H	5.41652600	-1.09998500	-2.23539400
H	5.72418500	0.89431600	1.55996700
H	6.77765000	0.11438600	-0.54842100
C	1.54097700	-0.78539400	0.33458500
H	1.29332200	-0.57406100	1.38554400
H	1.29368000	-1.83863800	0.14041900
C	-2.75861200	-1.96938700	1.38517700
C	-3.26678700	-2.17134900	-0.03956000
C	-2.77402300	-0.91257900	-0.74731400
C	-1.37259200	-1.35096000	1.19541100
H	-3.41007200	-1.26379100	1.91186500
H	-2.71478700	-2.89643900	1.96492100
H	-4.35377100	-2.27172900	-0.10554000
H	-2.80823200	-3.06067300	-0.49283500
H	-2.67146700	-1.06291500	-1.82907900
H	-0.58515800	-2.11268900	1.25254200

H	-1.16532900	-0.58392800	1.95390900
N	-1.42879600	-0.75664000	-0.15205200
C	-3.77080600	0.25318000	-0.50611000
O	-4.74186200	0.25987100	-1.28152100
O	-3.53522800	1.03578700	0.45933600
C	-0.58630400	0.17652400	-0.64769100
N	-0.97516500	1.87113500	0.27596200
C	-1.06454600	2.92782900	-0.72393200
H	-0.11475000	3.01128600	-1.27153300
H	-1.86893200	2.69793800	-1.42988800
H	-1.28119400	3.90033300	-0.26313400
C	-0.03803400	2.18373400	1.34131100
H	-0.11740600	1.44550700	2.14442400
H	0.99056500	2.17056400	0.95426900
H	-0.22988300	3.17978100	1.76288000
H	-0.93127600	0.58905200	-1.59950600

#### T-TS8-13

N	-0.37493800	0.45043300	-0.53490600
H	-0.82534900	0.54193400	-1.44095400
H	0.31686000	-1.09208900	0.85176600
C	-2.65819200	0.14243800	0.23792800
C	-3.76146200	0.91552000	-0.12509700
C	-2.79920800	-1.24742600	0.30955200
C	-4.98831500	0.31712000	-0.40807600
H	-3.65836700	1.99912800	-0.18245100
C	-4.02162800	-1.84704400	0.02779100
H	-1.94339100	-1.86236300	0.58709900
C	-5.11976800	-1.06599600	-0.33174900
H	-5.84062300	0.93267900	-0.68652100
H	-4.11960800	-2.92825300	0.09152400
H	-6.07585900	-1.53672700	-0.54876700
C	-1.33386000	0.79788800	0.51838700
H	-0.94660500	0.46003500	1.49334800
H	-1.48724600	1.88437900	0.61128400
C	4.20811200	-0.42790000	0.02817400
C	3.51339400	-1.21216800	-1.07369500
C	2.05128200	-1.10307500	-0.66050100
C	3.27737400	0.76038800	0.18038900
H	4.23965400	-1.01994700	0.95390900
H	5.23203900	-0.12963800	-0.21721800
H	3.83370800	-2.25270000	-1.16806100
H	3.66097900	-0.71180600	-2.04036500
H	1.37663100	-1.12968800	-1.53044000
H	3.45953500	1.48810400	-0.63013200
H	3.39739500	1.29197000	1.13068300
N	1.91889600	0.19000100	0.05529700
C	1.61513000	-2.27687300	0.21606700
O	2.12986200	-3.37082100	0.19209100
O	0.56467900	-2.02473400	1.00199100
C	0.94521800	1.09911400	-0.54623300
N	1.06511000	2.40483600	0.04537700
H	1.18859800	1.24075000	-1.62339300

C	0.46190300	3.48049700	-0.70246500
H	0.85209500	4.43927200	-0.33893900
H	0.71992100	3.39558900	-1.76516600
H	-0.64219600	3.51953500	-0.62312100
C	1.01225000	2.57523900	1.48472000
H	1.26315500	1.63637800	1.98686000
H	1.74314000	3.33540000	1.79692000
H	0.02235400	2.89928500	1.84795100

**T-TS13-14**

N	0.52974900	0.57607000	0.67630600
H	1.11671900	0.91490600	1.43234500
H	-3.21522500	0.36847500	-0.75880000
C	2.63331600	-0.03647900	-0.33779900
C	3.75410000	0.75761200	-0.09237700
C	2.76657600	-1.42686100	-0.30080500
C	4.99055300	0.17666900	0.18363300
H	3.65366500	1.84326200	-0.12225500
C	3.99925900	-2.01110500	-0.03019200
H	1.89336700	-2.05156000	-0.48775000
C	5.11420500	-1.20945300	0.21408000
H	5.85702600	0.80657700	0.37123000
H	4.09301900	-3.09441900	-0.01088600
H	6.07834000	-1.66695600	0.42355900
C	1.29424600	0.60208900	-0.57215400
H	0.74347000	0.05627100	-1.35282600
H	1.44571700	1.62345400	-0.95720200
C	-3.12752700	-1.43969000	1.76757000
C	-1.99617000	-2.12719400	1.01307100
C	-1.62873400	-1.07151800	-0.03372200
C	-2.59511900	-0.02264000	1.88139700
H	-4.05766800	-1.46932900	1.18340600
H	-3.33402300	-1.88311800	2.74630100
H	-2.26089600	-3.08848400	0.56318700
H	-1.13416500	-2.27661300	1.67716100
H	-0.58351600	-1.17662300	-0.33758900
H	-1.87987700	0.02704900	2.72160000
H	-3.36870600	0.73590900	2.05255600
N	-1.88978600	0.22852900	0.60255400
C	-2.49863900	-1.25580300	-1.27586000
O	-2.40601800	-2.21731500	-2.00488600
O	-3.39491700	-0.28814500	-1.47706900
C	-0.79095300	1.20364500	0.75018600
N	-1.03823100	2.39528700	-0.04047900
H	-0.85464000	1.56016900	1.78967100
C	-0.26358400	3.54075500	0.38125600
H	-0.67458700	4.44674900	-0.08036300
H	-0.32802100	3.66056500	1.47004600
H	0.80888300	3.48778300	0.10828100
C	-1.17265300	2.30935800	-1.48239200
H	-1.63530200	1.36566200	-1.78130400
H	-1.82617100	3.11831100	-1.83510300
H	-0.21531500	2.40012000	-2.02363400

**T-TS14-15**

N	-0.62219800	0.92805300	-0.69628400
H	-1.08084400	1.70679900	-1.15673000
H	3.33576900	-0.22744600	-0.86274700
C	-2.70943900	0.18182200	0.33248000
C	-3.71750300	0.79464900	1.07665000
C	-3.06290300	-0.79672300	-0.60144900
C	-5.05332000	0.43721900	0.89851700
H	-3.45360200	1.56178900	1.80410200
C	-4.39316000	-1.15798500	-0.78159900
H	-2.28034000	-1.27056600	-1.19252000
C	-5.39388900	-0.54051400	-0.03067200
H	-5.82763900	0.92730200	1.48429900
H	-4.65246400	-1.92405300	-1.50895500
H	-6.43478200	-0.82174400	-0.17243800
C	-1.26455700	0.55423000	0.55150500
H	-0.73182900	-0.31390900	0.95989400
H	-1.22547900	1.33382000	1.33177000
C	1.38649000	-2.70341300	-0.68748600
C	1.27575100	-2.22441400	0.75727100
C	1.78672400	-0.78139700	0.66849800
C	0.92542600	-1.48302300	-1.47093200
H	2.43062000	-2.94518700	-0.93037300
H	0.78181200	-3.59072100	-0.89713600
H	1.84208500	-2.81984300	1.47934300
H	0.22257400	-2.22787000	1.07053600
H	1.35793500	-0.13058500	1.44010000
H	-0.17396100	-1.44078300	-1.52743700
H	1.31135200	-1.45506700	-2.49861500
N	1.45095700	-0.34790700	-0.69747800
C	3.29859600	-0.74355100	0.90087600
O	3.80162300	-1.01723100	1.96732900
O	4.01612900	-0.41822100	-0.17174200
C	0.80737500	0.94336500	-0.91000800
N	1.61205400	1.95959800	-0.20609500
H	0.89766800	1.14147100	-1.99539700
C	2.48462400	2.66748000	-1.12664500
H	3.19295500	3.28739500	-0.56712900
H	3.06964000	1.96201100	-1.72741500
H	1.92293200	3.32271500	-1.82229100
C	0.90662700	2.88464600	0.65744600
H	0.12929300	3.47845800	0.13859000
H	0.44191400	2.36996600	1.50324600
H	1.63563400	3.58711400	1.07489500

**T-TS15-16**

N	-0.48183900	0.25799200	-1.09088100
H	-1.14712600	0.95354000	-1.40786200
H	0.94910700	1.27028500	1.19825000
C	-2.56596100	-0.52094000	-0.09844100
C	-3.28520400	-0.79488600	-1.26661200
C	-3.26067800	-0.13953200	1.05041900

C	-4.67115200	-0.67935600	-1.28659000
H	-2.75106500	-1.11023600	-2.16270400
C	-4.64959100	-0.03023200	1.03434100
H	-2.70828800	0.06185100	1.96773400
C	-5.35674000	-0.29640900	-0.13458300
H	-5.21980200	-0.89914700	-2.19952000
H	-5.17888700	0.26150600	1.93831600
H	-6.44066100	-0.21213000	-0.14792100
C	-1.06908300	-0.64717900	-0.08413000
H	-0.78756000	-1.68143900	-0.31691500
H	-0.67801400	-0.42499700	0.91819700
C	4.17354200	-0.48147900	-0.71423700
C	3.39397800	-1.78128100	-0.55268300
C	1.98084600	-1.31094800	-0.18951500
C	3.18264600	0.38821400	-1.46424900
H	4.39159500	-0.04243300	0.26931500
H	5.11807600	-0.60168100	-1.25319100
H	3.78667600	-2.45320700	0.21390600
H	3.37858400	-2.32427800	-1.50745400
H	1.24153800	-2.01165100	-0.59730100
H	3.19856600	0.16192400	-2.54314500
H	3.35883600	1.46209500	-1.34392300
N	1.88846500	-0.01541300	-0.89254400
C	1.77534200	-1.27602800	1.35310700
O	1.82087300	-2.39852300	1.88245500
O	1.57778700	-0.16086400	1.91391600
C	0.79910400	0.76207500	-1.04840700
N	0.79164100	1.99595800	0.46841700
H	0.94086700	1.56478400	-1.77894000
C	1.94872800	2.88122800	0.44030200
H	1.91558600	3.60340700	1.26687400
H	2.86003400	2.28632200	0.54741300
H	1.97815600	3.44232800	-0.50462600
C	-0.46250200	2.71936900	0.59547400
H	-1.29674000	2.02399300	0.72982200
H	-0.44667800	3.40352300	1.45424900
H	-0.63960300	3.31528700	-0.31165800

#### T-TS12-17

N	-0.72662400	-0.12822100	-0.74273400
H	2.09535200	-1.94424600	0.12121600
H	-1.23808800	-0.74085600	-1.36977500
C	-2.92289700	0.04743400	0.27741200
C	-3.48522900	1.07850700	-0.48112700
C	-3.75217100	-0.95175800	0.78586900
C	-4.85405300	1.10881600	-0.72345200
H	-2.84010600	1.85945400	-0.88181800
C	-5.12532400	-0.92080300	0.54843400
H	-3.31996800	-1.76062000	1.37360200
C	-5.67759200	0.10849500	-0.20724500
H	-5.28187700	1.91636000	-1.31277800
H	-5.76181700	-1.70441300	0.95210700
H	-6.74816100	0.13355600	-0.39530100



C	-1.44172100	0.02005100	0.53078600
H	-1.20384700	-0.80155600	1.22614000
H	-1.13385500	0.95262900	1.01400500
C	2.79270600	1.82495600	1.14859200
C	3.45502500	1.74303800	-0.22361500
C	2.95695600	0.39345900	-0.72654500
C	1.39193600	1.26137200	0.90984600
H	3.33978600	1.19225000	1.85976000
H	2.76176700	2.83730300	1.56102400
H	4.54492300	1.78367500	-0.18786300
H	3.08671600	2.54058400	-0.88121900
H	2.98982200	0.31301900	-1.82213000
H	0.67151700	2.06331400	0.69737200
H	1.02715100	0.67667700	1.76535800
N	1.55488400	0.42032800	-0.28340800
C	3.82181000	-0.75837600	-0.15971000
O	5.03749500	-0.61891400	-0.20155700
O	3.22603000	-1.80389300	0.31448800
C	0.62282500	-0.36797000	-0.84689500
H	0.90539500	-0.72678100	-1.83597600
H	0.39391100	-2.19907400	0.66128300
O	0.88896500	-2.07211300	-0.15744500

#### T-TS17-18

N	0.70013200	-0.52485400	0.80400500
H	-2.74496200	-2.05691800	-0.03433100
H	1.14084500	-0.73440100	1.69266400
C	2.92491000	-0.36348600	-0.18929600
C	3.13721400	0.99324700	0.07627100
C	4.03168900	-1.19870200	-0.34494500
C	4.42786000	1.50142200	0.17884700
H	2.27722800	1.64868600	0.20762000
C	5.32653600	-0.69284700	-0.24487900
H	3.87567100	-2.25798000	-0.54584200
C	5.52756200	0.65875500	0.01780600
H	4.57875900	2.55904100	0.38405700
H	6.17804100	-1.35816000	-0.36752900
H	6.53632900	1.05673800	0.09955300
C	1.53352100	-0.91636500	-0.32896900
H	1.57261600	-2.00786700	-0.45776900
H	1.07059900	-0.52146800	-1.24644300
C	-2.26031700	2.27304100	-0.64205200
C	-3.17741000	1.82307300	0.48887000
C	-2.91488800	0.32321700	0.58280200
C	-1.01206500	1.45068100	-0.38390200
H	-2.69641700	2.00947100	-1.61534600
H	-2.06278700	3.34870100	-0.64040100
H	-4.23588400	2.02571200	0.31073900
H	-2.88195100	2.30789800	1.42715000
H	-2.90327500	-0.01960100	1.62813300
H	-0.42647600	1.84517800	0.45862900
H	-0.34537400	1.34840900	-1.24597000
N	-1.54336500	0.12510600	0.00067300

C	-3.97256600	-0.53557300	-0.12439600
O	-5.03863300	-0.08247000	-0.47208300
O	-3.68770400	-1.82410900	-0.26965300
C	-0.66345500	-0.90987900	0.78386800
H	-1.03035900	-0.94691300	1.82345200
H	-1.45897100	-0.90644500	-0.67610300
O	-1.02273100	-1.96608900	-0.01515900

**T-TS16-19**

N	0.49552300	-1.13607400	0.15811800
H	1.13925800	-1.66521100	0.73713800
H	-1.44824700	0.52985500	1.70984000
C	2.53129700	0.14416400	-0.15746500
C	3.14981100	-0.51996600	-1.22095300
C	3.32194300	0.71843700	0.83768500
C	4.53603000	-0.60555700	-1.28817500
H	2.53393000	-0.96951700	-1.99933400
C	4.71165600	0.63762300	0.77034800
H	2.84320900	1.23520300	1.66822400
C	5.32002300	-0.02516900	-0.29139500
H	5.00809100	-1.12039100	-2.12176200
H	5.31809400	1.09358800	1.54925000
H	6.40420000	-0.08809200	-0.34591700
C	1.03279200	0.21645300	-0.08070800
H	0.63853900	0.60644800	-1.02549800
H	0.73292600	0.90223700	0.72331600
C	-4.20359900	-0.61484300	-0.41990500
C	-3.40970000	0.04374600	-1.54331100
C	-2.04253800	0.26175400	-0.89546900
C	-3.18878200	-1.54814100	0.23533900
H	-4.53586000	0.14723100	0.29660100
H	-5.09053600	-1.14940900	-0.77126700
H	-3.83770600	0.98247500	-1.90207500
H	-3.30049500	-0.64129400	-2.39327900
H	-1.26433800	0.35503300	-1.66077400
H	-3.26006000	-2.57585200	-0.14737600
H	-3.30396600	-1.58242000	1.32742000
N	-1.87937400	-0.98184000	-0.13851600
C	-2.04577500	1.56107000	-0.06164500
O	-2.25901400	2.60266300	-0.66820300
O	-1.84843600	1.49226200	1.21785300
C	-0.79203400	-1.38440500	0.55516000
H	-0.90912200	-2.38270100	0.97735200
O	-0.89578800	-0.49627600	2.17669200
H	-1.48180100	-0.95197600	2.79314500

**T-TS19-20**

N	0.43609100	-1.03786400	-0.35151000
H	1.00142400	-1.49551600	-1.05702100
H	-1.42616200	-0.50253900	1.96345000
C	2.57350200	-0.09780300	0.29536700
C	2.68789000	1.16368600	-0.29478600
C	3.70754600	-0.90554700	0.38870400

C	3.91292200	1.61068000	-0.77831600
H	1.80610300	1.80046700	-0.36564500
C	4.93700600	-0.46210800	-0.09512400
H	3.62478800	-1.88813800	0.85255700
C	5.04113000	0.79664300	-0.67988900
H	3.99153500	2.59802000	-1.22763800
H	5.81418300	-1.09945500	-0.01150800
H	6.00002700	1.14770300	-1.05390800
C	1.24459300	-0.59244200	0.78984800
H	0.72292300	0.22047500	1.31353600
H	1.38643900	-1.40110200	1.52116700
C	-3.77243100	0.14631400	-1.67183600
C	-2.81883900	1.27093400	-1.27939100
C	-1.92716100	0.64119300	-0.20403100
C	-2.86854200	-1.06774000	-1.59433600
H	-4.58633800	0.05453900	-0.94040300
H	-4.21854900	0.28098500	-2.66146400
H	-3.31588900	2.16746400	-0.90173900
H	-2.20646700	1.55924700	-2.14207800
H	-0.86424900	0.87353100	-0.39038500
H	-2.17721600	-1.09566700	-2.45204400
H	-3.38326800	-2.03141000	-1.52591600
N	-2.08774200	-0.82965900	-0.36440000
C	-2.23014900	1.12925800	1.21553800
O	-2.76249100	2.19718000	1.41564300
O	-1.82133900	0.37197300	2.23002400
C	-0.78872400	-1.70583000	-0.12367000
H	-0.89832300	-2.52622800	-0.85707200
O	-1.12620000	-2.02686400	1.16199000
H	-2.22161500	-1.49146800	0.67776000