

Electronic Supplementary Information for
New Insights into the Degradation Mechanism of Ibuprofen in
UV/H₂O₂ Process: Role of Natural Dissolved Matter in
Hydrogen Transfer Reactions

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Table S1. Energy barriers (ΔG^* , in kcal mol⁻¹) of R1-R5 calculated by M06-2X, CBS-QB3, MPWB1K and WB97XD methods with the same basis set mentioned in the main text. ‘SD’ refers to the standard deviation of each method with respect to CBS-QB3.

	$\Delta G^*_{\text{M06-2X}}$	$\Delta G^*_{\text{CBS-QB3}}$	$\Delta G^*_{\text{MPWB1K}}$	$\Delta G^*_{\text{WB97XD}}$
R1	8.02	8.66	9.27	6.74
R2	7.31	8.03	9.02	5.00
R3	9.47	9.91	11.54	7.03
R4	10.65	11.74	10.23	9.11
R5	9.68	10.30	9.94	8.23
SD	0.33	0	0.51	1.14

Table S2. Gibbs free energies of all species, calculated at the CBS-QB3//M06-2X-D3/6-311+g(d,p) level, involved in this work. The unit is Hartree.

Species	Gibbs free energies
IBU	-656.413830
IM1	-655.776276
IM2	-655.766375
IM3	-655.757868
IM4	-655.757161
IM5	-655.756776
IM6	-806.138560
IM7	-806.130100
IM8	-806.121445
IM9	-498.625887
IM10	-806.125156
IM11	-688.314564
IM12	-498.605691
IM13	-806.126072
IM14	-806.139939
IM15	-806.137947
P1	-806.784109
P2	-730.461379
P3	-612.626087
P4	-615.926389
P5	-731.641281
P6	-574.522844
P7	-806.780807
P8	-691.185421
P9	-731.617306
P10	-655.214036
P11	-655.219827
IMs1	-655.742047
IMs2	-655.741191
IMs3	-655.743040
IMs4	-655.741678
IMs5	-655.735514
IMs6a	-732.170967
IMs6s	-732.175795
IMs7a	-732.171276
IMs7s	-732.170292
IMs8a	-732.171323

IMs8s	-732.172237
IMs9a	-732.168237
IMs9s	-732.172518
IMs10a	-732.170652
IMs10s	-732.170321
IMs11a	-732.169999
IMs11s	-732.175506
IMs12	-732.152323
IBU ⁺	-656.168671
TS1 (IBU→IM1)	-732.146542
TS2 (IBU→IM2)	-732.147550
TS3 (IBU→IM3)	-732.144561
TS4 (IBU→IM4)	-732.141633
TS5 (IBU→IM5)	-732.143932
TS6 (P1→P2)	-806.717519
TS6-H ₂ O (P1→P2)	-883.172662
TS6-NH ₃ (P1→P2)	-863.291346
TS6-CH ₃ OH (P1→P2)	-922.432498
TS6-C ₂ H ₅ OH (P1→P2)	-961.717875
TS6-HCOOH (P1→P2)	-996.501869
TS6-CH ₃ COOH (P1→P2)	-1035.795477
TS7 (P1→P3)	-806.693484
TS8 (IM1→P4)	-655.719630
TS9 (IM1→IM6)	-806.097642
TS10 (IM6→IM7)	-806.082509
TS10-H ₂ O (IM6→IM7)	-882.527737
TS10-NH ₃ (IM6→IM7)	-862.638896
TS10-CH ₃ OH (IM6→IM7)	-921.789819
TS10-C ₂ H ₅ OH (IM6→IM7)	-961.075025
TS10-HCOOH (IM6→IM7)	-995.858325
TS10-CH ₃ COOH (IM6→IM7)	-1035.150404
TS11 (IM7→P2)	-806.109562
TS12 (IM6→IM8)	-806.093044
TS12-H ₂ O (IM6→IM8)	-882.530837
TS12-NH ₃ (IM6→IM8)	-862.644836
TS12-CH ₃ OH (IM6→IM8)	-921.793819
TS12-C ₂ H ₅ OH (IM6→IM8)	-961.077885
TS12-HCOOH (IM6→IM8)	-995.860325
TS12-CH ₃ COOH (IM6→IM8)	-1035.153403
TS13 (IM8→IM9)	-806.079934
TS14 (IM6→IM10)	-806.098329
TS14-H ₂ O (IM6→IM10)	-882.535237

TS14-NH ₃ (IM6→IM10)	-862.657638
TS14-CH ₃ OH (IM6→IM10)	-921.798519
TS14-C ₂ H ₅ OH (IM6→IM10)	-961.083025
TS14-HCOOH (IM6→IM10)	-995.865325
TS14-CH ₃ COOH (IM6→IM10)	-1035.162402
TS15 (IM10→IM11)	-806.089904
TS16 (IM11→P3)	-688.312293
TS17 (P7→P8)	-806.643168
TS18 (IM2→IM12)	-655.706172
TS19 (IM2→IM13)	-806.095632
TS20 (IM13→IM14)	-806.073697
TS20-H ₂ O (IM13→IM14)	-882.508640
TS20-NH ₃ (IM13→IM14)	-862.634639
TS20-CH ₃ OH (IM13→IM14)	-921.780952
TS20-C ₂ H ₅ OH (IM13→IM14)	-961.064598
TS20-HCOOH (IM13→IM14)	-995.849912
TS20-CH ₃ COOH (IM13→IM14)	-1035.141901
TS21 (IM14→P10)	-806.098646
TS22 (IM13→IM15)	-806.094807
TS22-H ₂ O (IM13→IM15)	-882.529890
TS22-NH ₃ (IM13→IM15)	-862.651939
TS22-CH ₃ OH (IM13→IM15)	-921.801002
TS22-C ₂ H ₅ OH (IM13→IM15)	-961.085028
TS22-HCOOH (IM13→IM15)	-995.866128
TS22-CH ₃ COOH (IM13→IM15)	-1035.159203
TS23 (IM15→P11)	-806.104630
TS24 (IBU→IMs1)	-732.138015
TS25 (IBU→IMs2)	-732.139312
TS26 (IBU→IMs3)	-732.140048
TS27 (IBU→IMs4)	-732.139730
TS28 (IBU→IMs5)	-732.133981
TS29 (IBU→IMs6a)	-732.141475
TS30 (IBU→IMs6s)	-732.142105
TS31 (IBU→IMs7a)	-732.143671
TS32 (IBU→IMs7s)	-732.142340
TS33 (IBU→IMs8a)	-732.144479
TS34 (IBU→IMs8s)	-732.144223
TS35 (IBU→IMs9a)	-732.136411
TS36 (IBU→IMs9s)	-732.144362
TS37 (IBU→IMs10a)	-732.144057
TS38 (IBU→IMs10s)	-732.143442
TS39 (IBU→IMs11a)	-732.142711

TS40 (IBU→IMs11s)	-732.142810
TS41 (IBU→IMs12)	-732.122162
·OH	-75.746516
OH ⁻	-75.949068
H ₂ O	-76.433568
HO ₂	-150.920137
(CH ₃) ₂ C=CH ₂	-157.108341
O ₂	-150.335287
CH ₃	-39.809189
CH ₃ CHOHCH ₃	-194.260230
CH ₃ CH=CH ₂	-117.823333
(CH ₃) ₂ C=CHOOH	-307.467840
NH ₃	-56.538567
CH ₃ OH	-115.690550
C ₂ H ₅ OH	-154.974756
HCOOH	-189.761056
CH ₃ COOH	-229.055131

Table S3. The ΔG^* (in kcal/mol) of H transfer reactions in the subsequent reactions of IM2 catalyzed by NDM.

Reactions	NDM	ΔG^*
IM13 \rightarrow IM14	H ₂ O	32.00
IM13 \rightarrow IM14	NH ₃	18.83
IM13 \rightarrow IM14	CH ₃ OH	22.38
IM13 \rightarrow IM14	C ₂ H ₅ OH	22.73
IM13 \rightarrow IM14	HCOOH	23.35
IM13 \rightarrow IM14	CH ₃ COOH	24.66
IM13 \rightarrow IM15	H ₂ O	31.22
IM13 \rightarrow IM15	NH ₃	20.52
IM13 \rightarrow IM15	CH ₃ OH	22.35
IM13 \rightarrow IM15	C ₂ H ₅ OH	22.46
IM13 \rightarrow IM15	HCOOH	25.73
IM13 \rightarrow IM15	CH ₃ COOH	26.36

Table S4. Estimated values for acute and chronic toxicity of IBU and its degradation products.

Compounds	Fish		Daphnid		Green Algae	
	LC ₅₀	ChV	LC ₅₀	ChV	EC ₅₀	ChV
IBU	41.6	4.94	27.8	4.31	41.1	15.6
P1	11.1	9.45	30.8	16.4	5.05	2.03
P2	736	75.4	435	47.4	382	110
P3	175	30.9	167	1.72	93.4	34.4
P4	142	15.7	89.6	11.8	104	34.6
P5	402	37.6	328	57.8	157	84.8
P6	618	57.4	201	19.7	763	97
P7	10.8	8.91	29.7	15.5	4.91	1.98
P8	6830	620	3640	299	2100	478
P9	1000	101	584	61.4	486	135
P10	49.1	5.78	32.6	4.94	46.7	17.4
P11	41.7	4.95	27.9	4.31	41.2	15.6

Note: the acute (LC₅₀/EC₅₀) and chronic (ChV) toxicity classification (mg L⁻¹) are defined as follows:

Classification	Acute toxicity ¹	Chronic toxicity ²
Not harmful	LC ₅₀ >100 or EC ₅₀ >100	ChV>10
Harmful	10< LC ₅₀ <100 or 10< EC ₅₀ <100	1< ChV <10
Toxic	1< LC ₅₀ <10 or 1< EC ₅₀ <10	0.1< ChV <1

¹ Criteria set by the European Union (described in Annex VI of Directive 67/548/EEC); ²Criteria set by the Chinese hazard evaluation guidelines for new chemical substances (HJ/T 154–2004).

Table S5. Estimated values for developmental toxicity, mutagenicity and bioconcentration factors of IBU and its degradation products.

Compounds	Developmental toxicity	Mutagenicity	Bioconcentration factors
IBU	0.90	-0.05	19.80
P1	0.82	0.53	N/A
P2	0.96	0.38	2.74
P3	0.84	0.53	N/A
P4	0.86	0.16	7.84
P5	0.88	0.02	4.10
P6	0.52	0.37	1.18
P7	0.77	0.58	N/A
P8	0.87	-0.04	2.88
P9	0.69	0.01	6.03
P10	0.89	-0.01	10.13
P11	0.91	0.13	6.91

Note: Developmental toxicity < 0.50: developmental non-toxicant, and developmental toxicity > 0.50: developmental toxicant. Ames mutagenicity \leq 0.50: Ames mutagenicity negative, and Ames mutagenicity > 0.50: mutagenicity positive.

Table S6. Estimated health effects of IBU and its degradation products.

Compounds	Genotoxic carcinogenicity	Skin irritation and corrosion
IBU	Negative	Irritating to skin
P1	Negative	Irritating to skin
P2	Negative	Irritating to skin
P3	Structural Alert	Irritating or Corrosive to skin
P4	Negative	Irritating to skin
P5	Negative	Irritating to skin
P6	Negative	Irritating or Corrosive to skin
P7	Negative	Irritating to skin
P8	Negative	Irritating to skin
P9	Negative	Irritating to skin
P10	Negative	Irritating to skin
P11	Structural Alert	Irritating to skin

Figure S1

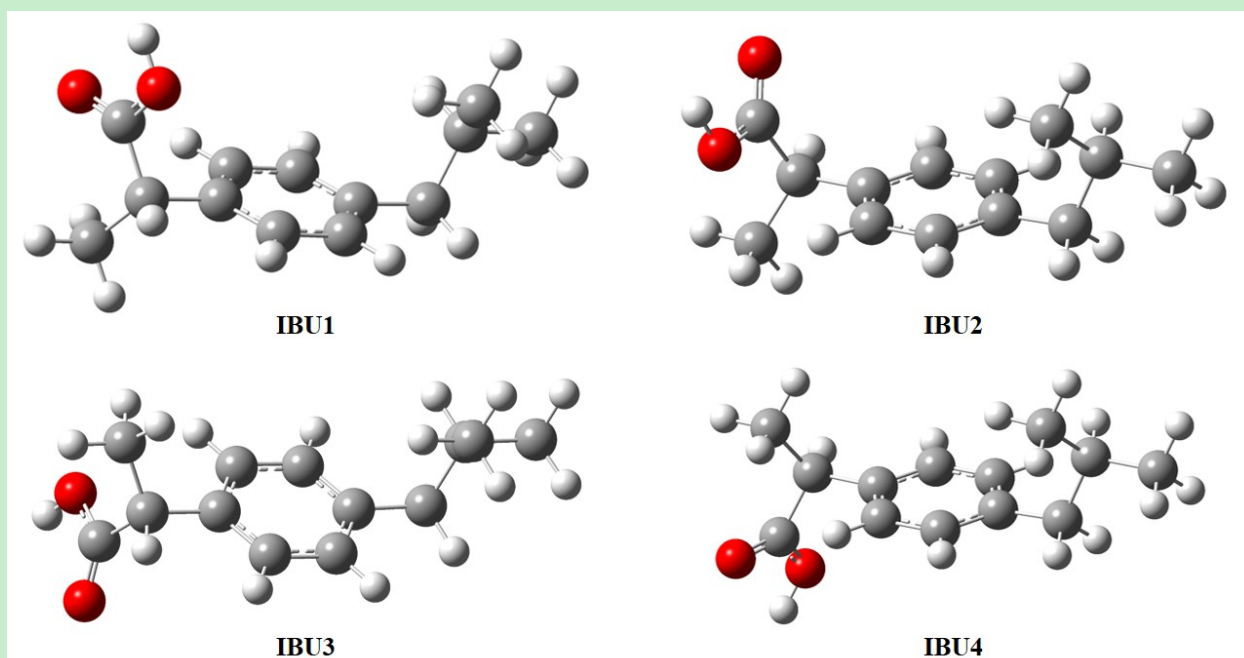


Figure S1. Four stable isomers of IBU. White ball, grey ball and red ball denote H atom, C atom and O atom, respectively.

Figure S2

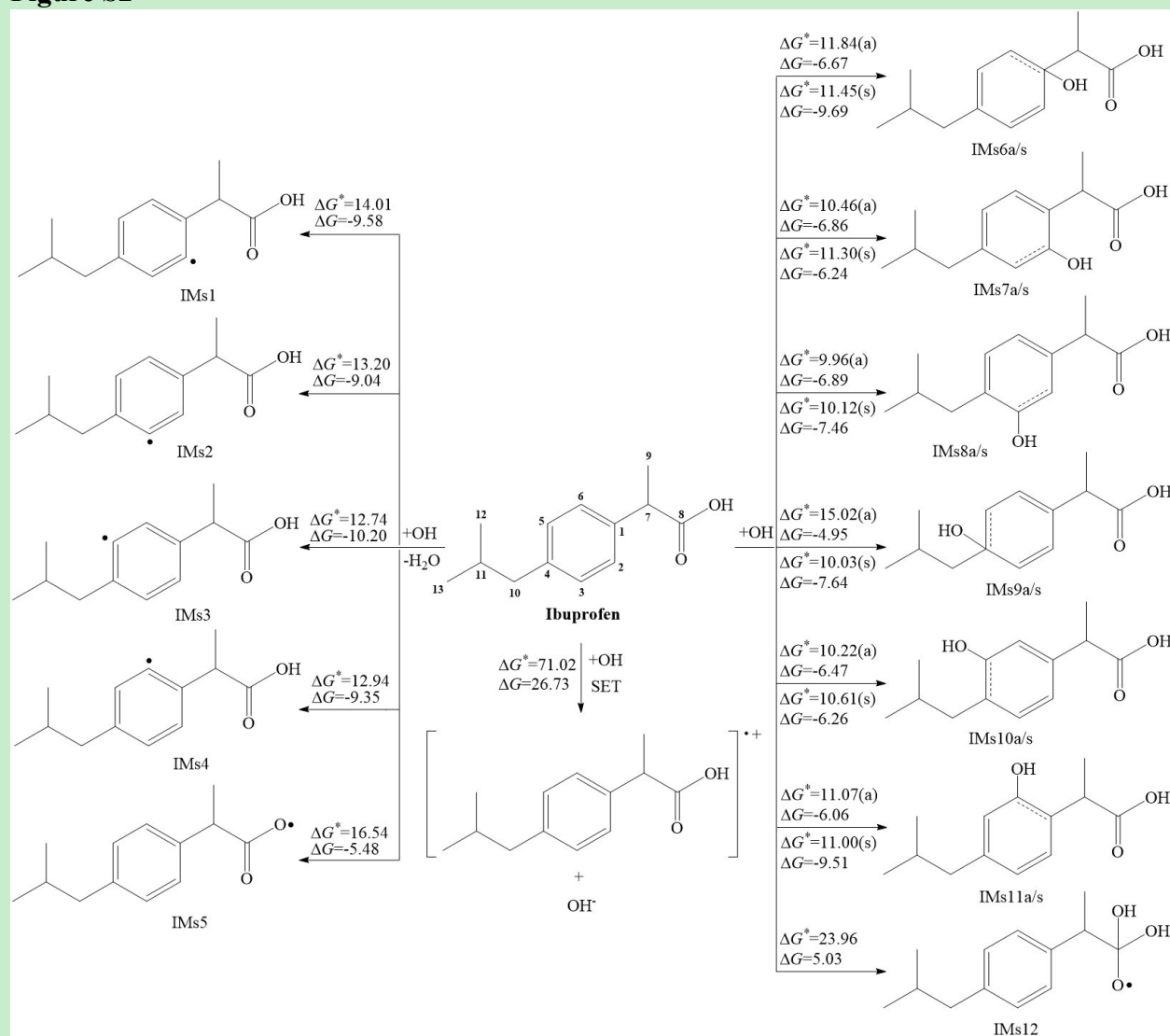


Figure S2. The H-abstraction and OH-addition at benzene ring and carboxyl group and SET of initial reaction of IBU and $\cdot\text{OH}$ embedded with ΔG^* (in kcal/mol) and ΔG (in kcal/mol). The ‘a’ and ‘s’ denote *anti*- and *syn*-position with respect to the carboxyl group, respectively.

Figure S3

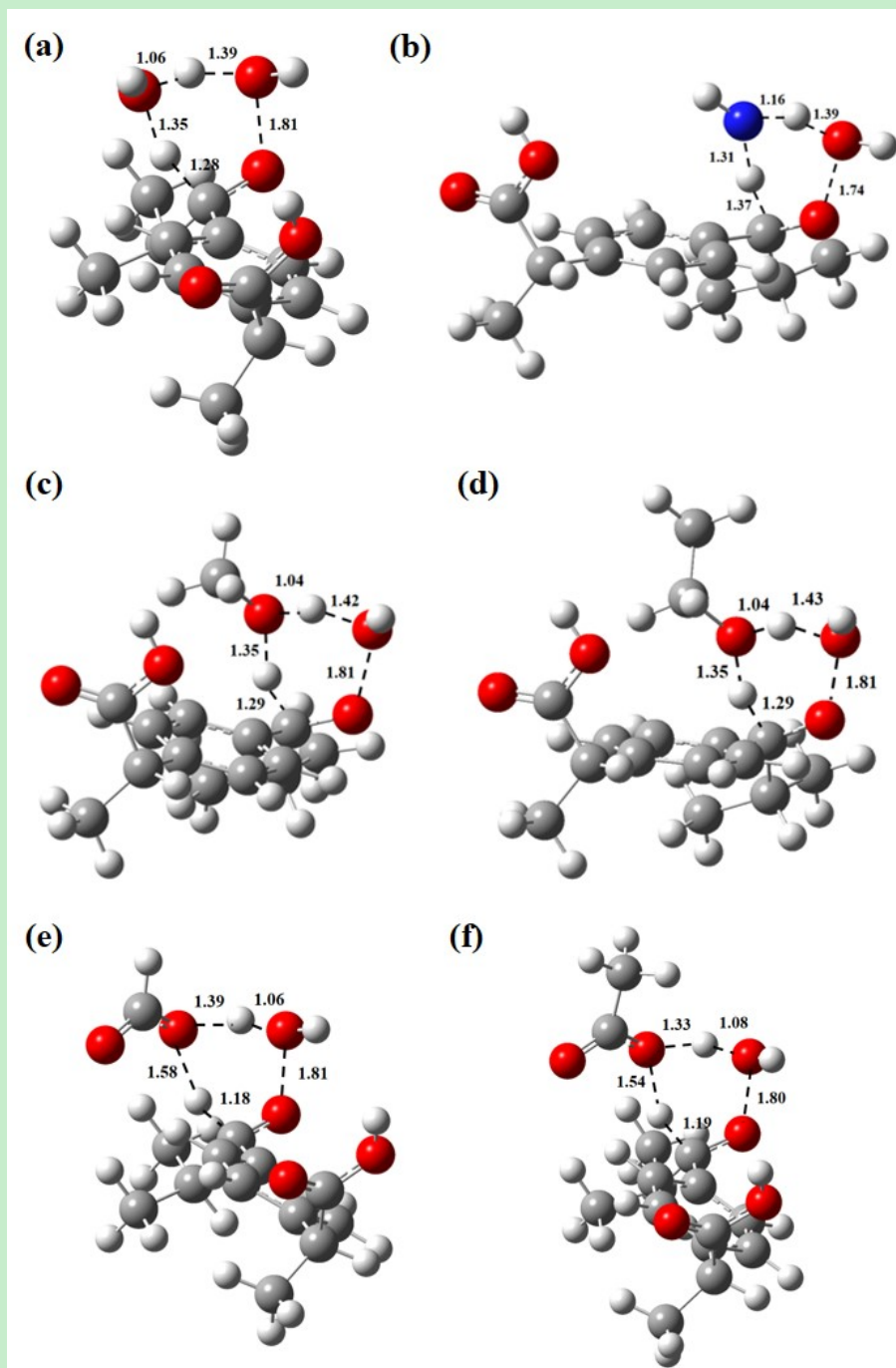


Figure S3. Structures of the transition states of the reaction $P1 \rightarrow P2 + H_2O$ catalyzed by NDM.

The NDM in (a), (b), (c), (d), (e) and (f) are H_2O , NH_3 , CH_3OH , C_2H_5OH , $HCOOH$ and CH_3COOH , respectively. The unit of distance is angstrom (\AA).

Text S1.

The Cartesian coordinates of optimized structures involved in this work.

IBU

C	-0.87683900	-0.94775400	0.98266200
C	0.44931300	-0.66587100	1.29525900
C	1.25848700	0.02561700	0.39488300
C	0.71455500	0.41853600	-0.82840100
C	-0.61110000	0.13182700	-1.13813900
C	-1.42923700	-0.55207900	-0.23707200
H	-1.49180100	-1.48719200	1.69672000
H	0.85885600	-0.98693200	2.24748600
H	1.33032300	0.95083500	-1.54722300
H	-1.01802900	0.44747200	-2.09365900
C	-2.88116600	-0.82281500	-0.54003000
H	-3.06748200	-0.67647500	-1.60974300
H	-3.11172700	-1.86881900	-0.31220800
C	-3.84368300	0.07830500	0.25538600
H	-3.64622500	-0.08399500	1.32204600
C	-5.29007900	-0.31756700	-0.03597000
H	-5.46960100	-1.36946400	0.20003300
H	-5.98662700	0.28785700	0.54899500
H	-5.51906500	-0.16426900	-1.09560000
C	-3.61284600	1.55558300	-0.06011200
H	-2.59701600	1.86845300	0.19216400
H	-3.76850500	1.74378300	-1.12795300
H	-4.31061500	2.18450600	0.49808600
C	2.70121500	0.36186200	0.74133500
H	2.93355300	-0.10377300	1.70205500
C	2.94435000	1.86826400	0.81203200
H	2.29103800	2.30796800	1.56666400
H	3.98151100	2.08248200	1.07542600
H	2.73190000	2.33831400	-0.14923800

C	3.60115800	-0.28601600	-0.29076800
O	4.14106500	0.28510800	-1.20419300
O	3.71551700	-1.60771200	-0.09756400
H	4.26209000	-1.97727200	-0.80638000

IM1

C	-1.00191100	0.52752600	0.80672900
C	0.33957400	0.82162200	0.98982700
C	1.30447000	0.40279300	0.07057600
C	0.88739700	-0.33224700	-1.04963100
C	-0.44531900	-0.63506500	-1.24157700
C	-1.44029800	-0.21546000	-0.31879300
H	-1.72187500	0.87570300	1.53786500
H	0.64630600	1.39114100	1.86123700
H	1.62236700	-0.67302100	-1.77294600
H	-0.74840300	-1.20798900	-2.11175100
C	-2.80041200	-0.54311900	-0.54104000
H	-3.04115200	-1.09058100	-1.44869200
C	-3.93847300	-0.13717400	0.34298100
H	-3.61456200	-0.19301300	1.38888300
C	-5.13035200	-1.07855500	0.15954200
H	-4.85814800	-2.11115000	0.38911400
H	-5.95692800	-0.78721300	0.81118300
H	-5.48559300	-1.04171500	-0.87472200
C	-4.35453600	1.31775300	0.05697400
H	-3.51833200	2.00602300	0.19744000
H	-4.70420900	1.41224400	-0.97495200
H	-5.16740800	1.61917700	0.72277000
C	2.77036000	0.75140000	0.25987200
H	2.88237500	1.22501300	1.23810700
C	3.29129100	1.67820400	-0.83807500
H	2.71489400	2.60412000	-0.83643700

H	4.34374900	1.91748800	-0.67688500
H	3.19230500	1.20778100	-1.81747600
C	3.56474200	-0.53880900	0.30114700
O	4.22379200	-0.98174300	-0.60491100
O	3.42878000	-1.17519600	1.47326600
H	3.91484600	-2.01170600	1.42922700

IM2

C	-0.99658800	-0.60587000	0.98937700
C	0.31967100	-0.30032600	1.31634700
C	1.21127000	0.13539500	0.33531000
C	0.75772300	0.25000800	-0.97814200
C	-0.55995500	-0.06233200	-1.30254200
C	-1.45536400	-0.49349400	-0.32460600
H	-1.68263400	-0.93545700	1.76394400
H	0.65885500	-0.39886100	2.34231500
H	1.43658200	0.58430400	-1.75698400
H	-0.89649300	0.03286500	-2.32983900
C	-2.89683800	-0.81936100	-0.65042900
H	-3.04013800	-0.73646800	-1.73979400
H	-3.09652400	-1.86572200	-0.39517400
C	-3.88392300	0.05998900	0.06573500
C	-5.24661600	-0.48960400	0.33450700
H	-5.20224700	-1.52464000	0.68311700
H	-5.77711100	0.10756800	1.08078200
H	-5.86562800	-0.48372600	-0.57710500
C	-3.73712300	1.54112100	-0.06945000
H	-2.69051700	1.85263900	-0.02338400
H	-4.13544200	1.88813300	-1.03659700
H	-4.29168300	2.06904500	0.71066500
C	2.64549300	0.49863700	0.68972700
H	2.80578200	0.25362300	1.74233200

C	2.94846900	1.97521200	0.44144400
H	2.27886000	2.59116800	1.04305200
H	3.97950400	2.21066000	0.71069200
H	2.80368200	2.22771300	-0.60994700
C	3.57336000	-0.38862900	-0.11483600
O	4.18852200	-0.05030200	-1.09413700
O	3.61768700	-1.63797100	0.36928800
H	4.18801100	-2.17113700	-0.20393600

IM3

C	-0.90014100	-1.05829200	0.94866800
C	0.43154200	-0.80327700	1.26402100
C	1.22609000	-0.03507300	0.41482500
C	0.66194000	0.46536200	-0.76012700
C	-0.66763900	0.20578700	-1.07280600
C	-1.47052000	-0.55819600	-0.22270800
H	-1.50469900	-1.65875600	1.62183900
H	0.85585300	-1.20571600	2.17802500
H	1.26634600	1.06064200	-1.43823700
H	-1.09130700	0.60331800	-1.98985800
C	-2.92661100	-0.79371700	-0.52759100
H	-3.10931400	-0.66670700	-1.59935400
H	-3.19868900	-1.82110900	-0.26509700
C	-3.86559100	0.16998000	0.24846100
H	-3.66910000	0.01037300	1.31568900
C	-5.32431700	-0.18442600	-0.04836400
H	-5.53181200	-1.22875900	0.19661500
H	-6.00411300	0.44675200	0.52772200
H	-5.54037500	-0.03447300	-1.11057700
C	-3.57806800	1.59645000	-0.08451800
H	-2.77827400	2.13661800	0.40512400
H	-4.06136600	2.05986300	-0.93751100

C	2.67286500	0.27588500	0.76695900
H	2.93392100	-0.29769800	1.65951200
C	2.89825100	1.76652200	1.01339200
H	2.26409400	2.09940500	1.83604900
H	3.94032000	1.96546100	1.26905500
H	2.64709700	2.34607000	0.12387200
C	3.55736200	-0.23011400	-0.35404000
O	4.07625200	0.45500200	-1.19838400
O	3.68297400	-1.56462700	-0.32919700
H	4.21663600	-1.83963300	-1.08925100

IM4

C	0.72007700	-1.15413800	0.12319500
C	-0.63478200	-0.99325600	-0.10703800
C	-1.27612300	0.24025300	0.15708900
C	-0.46799800	1.28796700	0.65367400
C	0.88377600	1.10692200	0.89567000
C	1.50761400	-0.11581900	0.63434800
H	1.18345500	-2.11090400	-0.09741500
H	-1.20073500	-1.81885000	-0.51168600
H	-0.91182600	2.25103400	0.87270900
H	1.46909400	1.93028000	1.29212500
C	2.98416400	-0.31203100	0.84557500
H	3.37367400	0.48165200	1.49223800
H	3.15159400	-1.26370000	1.36067800
C	3.78827800	-0.31730800	-0.46930300
H	3.38223900	-1.11312800	-1.10539400
C	5.25510000	-0.62973200	-0.17791900
H	5.36300500	-1.59182200	0.32909800
H	5.83867600	-0.66215800	-1.10098300
H	5.68702700	0.14293700	0.46627200
C	3.65363700	1.01190400	-1.21037900

H	2.61456200	1.22573800	-1.47147600
H	4.02048000	1.83305800	-0.58506500
H	4.24050900	1.00215600	-2.13200900
C	-2.67497100	0.49834400	-0.09744400
C	-3.16948000	1.90701300	-0.20789300
H	-2.47657800	2.52410800	-0.78213600
H	-4.14757000	1.92800100	-0.68276100
H	-3.27285200	2.36410300	0.78374000
C	-3.70568100	-0.53448900	-0.20331600
O	-4.85332100	-0.31336700	-0.54612200
O	-3.32232900	-1.77907400	0.14756000
H	-4.09122500	-2.35675900	0.04300400

IM5

C	0.80174600	-1.07433400	-0.78989700
C	-0.51674600	-0.80897500	-1.14618200
C	-1.28293800	0.08273400	-0.39835500
C	-0.70903300	0.69980100	0.71325200
C	0.60793400	0.42729300	1.06752500
C	1.38522400	-0.46126400	0.32117000
H	1.38646300	-1.77080900	-1.38307900
H	-0.95311700	-1.29932500	-2.01006200
H	-1.29570700	1.39786600	1.30241200
H	1.04200900	0.91521400	1.93436000
C	2.82860800	-0.72531600	0.66682700
H	3.02594400	-0.40205200	1.69482300
H	3.02068100	-1.80223500	0.62404500
C	3.81833900	-0.01071200	-0.27234600
H	3.60719300	-0.34502200	-1.29536500
C	5.25075200	-0.40787900	0.08166400
H	5.38906200	-1.49030900	0.02255500
H	5.96664600	0.06551300	-0.59445500

H	5.49141200	-0.09108300	1.10160200
C	3.64758100	1.50658200	-0.21354100
H	2.64280300	1.81200100	-0.51405500
H	3.81943000	1.86759700	0.80626600
H	4.36503000	2.00243700	-0.87173500
C	-2.73815300	0.37915500	-0.77511300
H	-2.93205200	-0.12720300	-1.72692400
C	-3.01181700	1.83940000	-0.88835900
H	-3.63508400	2.34420700	-0.16518100
H	-2.51064000	2.40563700	-1.66018300
C	-3.62303500	-0.27844600	0.26827800
O	-4.17754400	0.29046200	1.17277300
O	-3.69216500	-1.60378400	0.09199500
H	-4.22316700	-1.98408500	0.80729200

IM6

C	0.59156400	-0.15695600	-1.20503900
C	-0.76437600	0.04713000	-1.43083600
C	-1.63292100	0.28814800	-0.36619600
C	-1.12161800	0.30873400	0.93136700
C	0.23284100	0.09005800	1.15967700
C	1.09966900	-0.13723200	0.09385800
H	1.25483000	-0.34073400	-2.04379600
H	-1.15119700	0.02290000	-2.44368900
H	-1.78542000	0.48894800	1.77133600
H	0.61789700	0.10118700	2.17369900
C	2.57448100	-0.31680600	0.33992500
H	2.77217800	-0.44365000	1.40849800
C	3.45748400	0.78645700	-0.24108100
H	3.31412300	0.78144600	-1.32801900
C	4.93013000	0.52354000	0.07559500
H	5.26581100	-0.43852500	-0.31383100

H	5.55308400	1.30518100	-0.36339400
H	5.09076500	0.53231600	1.15804800
C	3.01920000	2.14531200	0.30745500
H	1.99806100	2.39388100	0.01336200
H	3.07264700	2.15323900	1.40079400
H	3.68416000	2.92557800	-0.06693300
C	-3.10978500	0.55099300	-0.61426800
H	-3.31554500	0.35563000	-1.66940900
C	-3.50199000	1.98353900	-0.25628100
H	-2.91368800	2.68167600	-0.85308400
H	-4.56094500	2.15644400	-0.45389100
H	-3.31231000	2.18197100	0.79962300
C	-3.91840600	-0.45272900	0.18337900
O	-4.51717300	-0.21535000	1.20106700
O	-3.87228400	-1.67619700	-0.36121800
H	-4.36740800	-2.28651800	0.20480400
O	2.57543000	-2.61518600	0.30284100
O	3.01969200	-1.55978000	-0.30012100

IM7

C	0.61349200	1.68147000	0.37832900
C	-0.76025200	1.60152600	0.55923400
C	-1.42581900	0.38804500	0.38607700
C	-0.68910400	-0.74329700	0.03157600
C	0.68788500	-0.66873400	-0.13404500
C	1.35517800	0.54763600	0.03595900
H	1.12869200	2.62566300	0.50615500
H	-1.32138000	2.48719300	0.83602200
H	-1.19343300	-1.69266800	-0.11817600
H	1.22547700	-1.56290100	-0.41687200
C	2.83480000	0.71763500	-0.15836000
C	3.80764000	-0.44225200	0.01543500

H	4.76856000	0.05926400	0.15690000
C	3.91623000	-1.26606700	-1.27765500
H	4.14610000	-0.62459600	-2.13054000
H	4.72376100	-1.99329400	-1.17096500
H	3.00095900	-1.81631500	-1.50038800
C	3.54142900	-1.31233600	1.24771200
H	3.37774000	-0.70088100	2.13794300
H	2.67839000	-1.96645300	1.12208500
H	4.41285400	-1.94473700	1.42958700
C	-2.92539900	0.28646900	0.60932900
H	-3.31795600	1.29801500	0.73628000
C	-3.26124800	-0.56773400	1.83105100
H	-2.79978500	-0.13292600	2.71835300
H	-4.34043900	-0.61588500	1.98278800
H	-2.88587300	-1.58418700	1.70483900
C	-3.56358300	-0.27816400	-0.64509900
O	-3.98155700	-1.40043800	-0.77035300
O	-3.58835700	0.62061900	-1.63818000
H	-3.96858600	0.20333900	-2.42529300
O	3.28957385	1.87400592	-0.46223444
O	3.44708434	2.20159926	-1.69496236
H	2.87649407	2.00382586	-2.48700303

IM8

C	-0.58493200	-0.49289300	1.02644400
C	0.75977000	-0.31005400	1.33123700
C	1.65148100	0.15774700	0.36669400
C	1.17493500	0.42741900	-0.91698800
C	-0.16561800	0.23241400	-1.22873400
C	-1.05803700	-0.22553900	-0.25921100
H	-1.26769400	-0.85350500	1.78699300
H	1.11883100	-0.53040300	2.33091800

H	1.85670800	0.78207700	-1.68375500
H	-0.52094700	0.43524100	-2.23379500
C	-2.53280500	-0.34853000	-0.58727500
H	-2.65480900	-0.42151400	-1.67515400
C	-3.29820600	0.83269100	-0.06929200
H	-4.32894000	-2.38021000	-0.99007800
C	-3.26040300	2.07763800	-0.88997500
H	-3.28102200	1.85902800	-1.96094500
H	-4.10470000	2.72930800	-0.65025600
H	-2.34444300	2.65662600	-0.69348900
C	-3.56505000	0.93811000	1.39509400
H	-3.73693700	-0.04157400	1.84514300
H	-2.71748000	1.40322800	1.92196300
H	-4.43830700	1.56884300	1.58184400
C	3.11691700	0.38660700	0.70436300
H	3.28645500	0.03888000	1.72599600
C	3.51764200	1.85456300	0.57142100
H	2.90645000	2.46192900	1.24009900
H	4.56835800	1.99450000	0.82996000
H	3.36742100	2.20410000	-0.45084800
C	3.95476900	-0.49088500	-0.20404700
O	4.56141400	-0.11320400	-1.17379300
O	3.92429000	-1.77631200	0.17462800
H	4.43594500	-2.29826200	-0.46078800
O	-4.33613300	-1.75940200	-0.24825300
O	-2.95053100	-1.58158600	0.00964400

IM9

C	2.70487700	0.71838400	0.62664800
C	1.37316300	0.66406800	1.05288700
C	0.42548700	-0.06544200	0.33505500
C	0.80843500	-0.74542100	-0.82490500

C	2.13057100	-0.70217500	-1.27288600
C	3.01762600	0.03036800	-0.51969600
H	3.44316800	1.28193000	1.18522800
H	1.07677600	1.19505100	1.95160900
H	0.07207000	-1.31002900	-1.38935600
H	2.42852500	-1.22674800	-2.17318200
C	-1.01574700	-0.14137100	0.81818400
H	-1.12046600	0.53198600	1.67206800
C	-1.41922800	-1.56021100	1.21417500
H	-0.76366700	-1.91704700	2.00943300
H	-2.45026300	-1.58423500	1.57028900
H	-1.33536400	-2.23787400	0.36343200
C	-1.91637000	0.39658000	-0.27616600
O	-2.59718100	-0.27249800	-1.01108900
O	-1.85193700	1.73206500	-0.36493500
H	-2.41071500	2.02175200	-1.10110200

IM10

C	-0.51937200	-0.16269700	1.21339500
C	0.84350900	0.00200200	1.43588500
C	1.71396100	0.23098300	0.37116800
C	1.19670700	0.28001600	-0.92387500
C	-0.16342900	0.09939200	-1.14844100
C	-1.03482000	-0.11729400	-0.08233600
H	-1.18327300	-0.33521500	2.05353500
H	1.23341300	-0.04328700	2.44699900
H	1.86093400	0.45470900	-1.76487100
H	-0.55122100	0.13452300	-2.16092200
C	-2.51608400	-0.27618700	-0.32155000
H	-2.71125300	-0.36164900	-1.39591600
C	-3.33662600	0.89904400	0.26519700
H	-3.09948800	0.93185000	1.33513400

C	-4.80505000	0.69868100	0.09970600
H	-3.71359000	-2.71704600	-0.87882800
H	-5.37842800	0.14247100	0.82809800
H	-5.27096600	0.92839100	-0.85189300
C	-2.89211100	2.21184700	-0.39159900
H	-1.83710100	2.41937300	-0.20383900
H	-3.04551600	2.16543800	-1.47442600
H	-3.48244800	3.04346000	-0.00353600
C	3.19797200	0.45512700	0.61492100
H	3.40461200	0.23817600	1.66577400
C	3.62201000	1.88340500	0.27726700
H	3.05170600	2.58565400	0.88657600
H	4.68536400	2.02952600	0.47300100
H	3.43287100	2.10191800	-0.77481100
C	3.97901500	-0.55411300	-0.20256500
O	4.58158200	-0.31408000	-1.21752300
O	3.90344700	-1.78595200	0.31989900
H	4.38214000	-2.39763100	-0.25856800
O	-4.05682800	-2.02685600	-0.29390600
O	-2.86468200	-1.52584900	0.29596200

IM11

C	1.35335500	0.78375300	0.68856700
C	0.00489500	0.89111000	0.98330900
C	-0.92994700	0.00590500	0.43925100
C	-0.47689900	-1.00137700	-0.42663800
C	0.86212500	-1.12284000	-0.73685100
C	1.81649000	-0.23393200	-0.18019000
H	2.06205400	1.47525200	1.12683300
H	-0.33261100	1.67560300	1.65242800
H	-1.18874000	-1.69423000	-0.86464300
H	1.19510100	-1.90415400	-1.41103500

C	3.17757600	-0.38306700	-0.51269600
H	3.57457200	-1.16378200	-1.14801300
H	5.89228300	0.49987500	-0.44992500
C	-2.40454900	0.11629600	0.78614100
H	-2.53981400	1.00500300	1.40676000
C	-2.92496000	-1.12080800	1.51718300
H	-2.36118300	-1.26232200	2.43996400
H	-3.98195200	-1.00889900	1.76419900
H	-2.81064400	-2.01191400	0.89854800
C	-3.17608100	0.35364800	-0.49709900
O	-3.80593800	-0.47994800	-1.09723700
O	-3.05378000	1.61672100	-0.92905700
H	-3.52615200	1.70289700	-1.77018100
O	5.33203500	-0.06667300	0.10001400
O	4.05331700	0.54921900	-0.07506900

IM12

C	2.71244000	-0.50083300	-0.79989300
C	1.38098300	-0.33607700	-1.19651800
C	0.42641500	0.14914000	-0.30260300
C	0.80334700	0.47122900	1.00477200
C	2.12549200	0.31093000	1.42548800
C	3.01875500	-0.16833200	0.49652600
H	3.45525000	-0.87664300	-1.49397400
H	1.08978800	-0.58861800	-2.21089200
H	0.06291200	0.84741800	1.70500000
H	2.41880900	0.55708400	2.43940400
C	-1.01319300	0.35282000	-0.75098700
H	-1.11707300	-0.06942300	-1.75339000
C	-1.41128200	1.82735700	-0.75826700
H	-0.75280800	2.37945400	-1.42999700
H	-2.44129400	1.94878200	-1.09694600

H	-1.32606900	2.25521900	0.24176800
C	-1.92101500	-0.45332000	0.15658300
O	-2.61749300	-0.00024100	1.02852100
O	-1.84606300	-1.76634300	-0.10084000
H	-2.41271200	-2.23809400	0.52697500

IM13

C	0.47406100	1.24626200	-0.22380700
C	-0.83686900	1.37093300	0.22700300
C	-1.69470100	0.27329700	0.22670200
C	-1.21722500	-0.95163400	-0.24416200
C	0.09053500	-1.07241400	-0.69793900
C	0.95805900	0.02245400	-0.68782000
H	1.12760100	2.11265500	-0.21880300
H	-1.19549600	2.33210600	0.58000600
H	-1.87309700	-1.81676800	-0.26328300
H	0.44353900	-2.03059900	-1.06612400
C	2.38726000	-0.11631500	-1.14800400
H	2.46786300	-0.91951700	-1.88519800
H	2.71839000	0.80572500	-1.63146100
C	3.38909900	-0.44510200	-0.03063400
C	4.80567800	-0.52261500	-0.57474100
H	5.06277200	0.39058000	-1.11243100
H	5.51787500	-0.67427800	0.23845200
H	4.87814000	-1.36708200	-1.26225900
C	3.01587800	-1.66810300	0.78563900
H	2.04164500	-1.54070000	1.25956900
H	2.97354700	-2.54107000	0.13146600
H	3.76648600	-1.84827900	1.55716900
C	-3.11979900	0.39592800	0.74300400
H	-3.31501600	1.45089200	0.95010400
C	-3.35002500	-0.43915700	2.00104800

H	-2.66624100	-0.11201400	2.78524800
H	-4.37476200	-0.32785800	2.35878900
H	-3.16958300	-1.49608100	1.79965900
C	-4.06796000	-0.01536400	-0.36525800
O	-4.66514800	-1.06000100	-0.42220000
O	-4.15394300	0.91953800	-1.32193900
H	-4.73562600	0.59212200	-2.02360400
O	3.64152100	1.80856400	0.48881500
O	3.34357200	0.64704100	0.97238700

IM14

C	-0.58050900	-0.13018500	-0.88275800
C	0.75902500	-0.10443400	-1.23910300
C	1.76476000	-0.34845000	-0.30273800
C	1.39377000	-0.62026700	1.02248000
C	0.06555100	-0.64430400	1.39363400
C	-0.97250700	-0.40188500	0.45398100
H	-1.33192700	0.05598500	-1.63904900
H	1.02944100	0.10809100	-2.26821700
H	2.16044200	-0.80879100	1.76818000
H	-0.20134600	-0.85289400	2.42413000
C	-2.31887500	-0.43453700	0.90228200
H	-2.48475900	-0.67243900	1.94759900
H	-2.02221700	2.02093900	-0.22895900
C	-3.55233100	-0.20723500	0.07291600
C	-4.74590800	0.11835200	0.96395200
H	-4.54937600	1.01845300	1.54775600
H	-5.63338100	0.27648900	0.34858300
H	-4.93614100	-0.70890100	1.65055800
C	-3.85087400	-1.40582400	-0.83081400
H	-2.99253100	-1.64613300	-1.45952600
H	-4.08430600	-2.27286100	-0.21109400

H	-4.71291800	-1.18544700	-1.46451100
C	3.22757200	-0.34750100	-0.70790200
H	3.29217700	0.00622000	-1.73980100
C	3.85923300	-1.73369100	-0.58578500
H	3.32003200	-2.43665800	-1.22186400
H	4.90587400	-1.71061300	-0.89358800
H	3.81253400	-2.08917000	0.44466000
C	3.96396400	0.66375400	0.14866600
O	4.70091600	0.39879600	1.06379800
O	3.67736700	1.92351700	-0.20807500
H	4.14033600	2.52796000	0.39041800
O	-2.99109800	2.05623500	-0.20591200
O	-3.36083100	0.86482700	-0.88082800

IM15

C	-0.44928500	-1.26733900	-0.52649600
C	0.86160800	-1.44026200	-0.08966500
C	1.67654800	-0.33798400	0.15229600
C	1.15954700	0.94007800	-0.07172600
C	-0.14759800	1.10781900	-0.51087800
C	-0.98006600	0.00634700	-0.73072500
H	-1.05535900	-2.14226500	-0.74243700
H	1.25314600	-2.44113500	0.05798500
H	1.78638000	1.81159400	0.09200700
H	-0.52576000	2.10876500	-0.69113800
C	-2.40978300	0.17989800	-1.17402800
H	-2.48775600	1.00209100	-1.89139500
H	-2.74771800	-0.72575200	-1.68318500
C	-3.40397000	0.48388600	-0.03507300
C	-4.80148200	0.48573200	-0.55873500
H	-2.77244900	-2.24747900	0.65153800
H	-5.61688900	0.70843800	0.11799600

H	-5.02059300	0.21625500	-1.58314200
C	-3.09755000	1.78940200	0.69729500
H	-2.12126100	1.74101500	1.18238800
H	-3.10191300	2.61790300	-0.01303200
H	-3.86051700	1.97379200	1.45531400
C	3.09763100	-0.51454600	0.66419000
H	3.32520500	-1.58316300	0.66655600
C	3.27894800	0.06669200	2.06526000
H	2.59249000	-0.42522700	2.75552200
H	4.30039700	-0.08249400	2.41871600
H	3.06783500	1.13704800	2.06875100
C	4.04712900	0.13468000	-0.32242100
O	4.59590200	1.19612500	-0.16883900
O	4.19420400	-0.60135500	-1.43290000
H	4.77423200	-0.12568500	-2.04543100
O	-3.61094800	-1.77878100	0.54449700
O	-3.27660000	-0.48475400	1.03564400

P1

C	0.56973200	0.25831800	1.19819700
C	-0.78691200	0.06059000	1.43041400
C	-1.64531500	-0.27439300	0.38312200
C	-1.12177700	-0.39475200	-0.90461400
C	0.23367900	-0.18579500	-1.13728500
C	1.09200600	0.13444100	-0.08838600
H	1.22710700	0.51961400	2.02060000
H	-1.18307400	0.16491700	2.43482400
H	-1.77663600	-0.64418800	-1.73387400
H	0.62740600	-0.27534900	-2.14460800
C	2.57453600	0.30075900	-0.32738500
H	2.76803700	0.38650200	-1.40497400
C	3.41321500	-0.85177600	0.24373500

H	3.26637500	-0.84805800	1.33041000
C	4.89750800	-0.64856800	-0.06424800
H	5.27267300	0.28729500	0.35002400
H	5.48419400	-1.47001100	0.35238300
H	5.05926300	-0.63526900	-1.14678700
C	2.92704100	-2.19044200	-0.31378800
H	1.89726500	-2.40469000	-0.02343700
H	2.98121700	-2.19325800	-1.40726100
H	3.56217800	-2.99783200	0.05571700
C	-3.12365900	-0.52493300	0.63874700
H	-3.33388600	-0.27251200	1.68073900
C	-3.51848200	-1.97368700	0.35738200
H	-2.93606200	-2.64009500	0.99471300
H	-4.57916600	-2.13268400	0.55773600
H	-3.32394900	-2.23040800	-0.68489400
C	-3.92691700	0.43489900	-0.21574200
O	-4.51547300	0.14573400	-1.22634700
O	-3.88931100	1.68504500	0.26625700
H	-4.38065500	2.26359600	-0.33536000
O	3.06678300	1.47630000	0.31763900
O	2.43167000	2.60772700	-0.26122700
H	3.11043300	2.93601300	-0.86742000

P2

C	-0.79368700	0.82474700	0.72407100
C	0.55856900	1.14968400	0.75895600
C	1.48033700	0.43070300	0.00221200
C	1.02878900	-0.63140500	-0.78721100
C	-0.31607000	-0.96310900	-0.81468700
C	-1.24494100	-0.23666300	-0.06246200
H	-1.48290400	1.40778900	1.32235700
H	0.89644400	1.97273700	1.37870000

H	1.73591000	-1.20244700	-1.38084700
H	-0.66557100	-1.78840500	-1.42288300
C	-2.68959700	-0.64492000	-0.13237000
C	-3.74750900	0.27841400	0.44803400
H	-3.40909700	0.60707200	1.43493000
C	-5.08636600	-0.43504600	0.59335900
H	-5.00065200	-1.31826800	1.22862200
H	-5.81798900	0.24261500	1.03745400
H	-5.45875200	-0.75414100	-0.38191000
C	-3.87678200	1.51270400	-0.46234300
H	-2.93597700	2.05601900	-0.56132700
H	-4.20333100	1.20795300	-1.46013500
H	-4.62523500	2.19335000	-0.05266200
C	2.95097900	0.81194800	0.00214400
H	3.10572400	1.56528500	0.77814100
C	3.39599700	1.35287500	-1.35579800
H	2.80264200	2.23146200	-1.61189400
H	4.44980600	1.63423900	-1.33168500
H	3.25907400	0.60036100	-2.13374400
C	3.76692900	-0.40291500	0.39999400
O	4.43221600	-1.07178300	-0.34823200
O	3.64427500	-0.67835800	1.70521100
H	4.14704600	-1.48254400	1.90186600
O	-2.99611800	-1.68175700	-0.68552600

P3

C	-1.85922400	0.95705600	0.49323800
C	-0.50845900	1.26942500	0.48651200
C	0.41330600	0.41371200	-0.12357400
C	-0.03483700	-0.76476400	-0.72392900
C	-1.38643700	-1.08243900	-0.71543700
C	-2.30216900	-0.22229200	-0.10879600

H	-2.58048700	1.61715500	0.96101600
H	-0.16050100	2.18385200	0.95395700
H	0.67578000	-1.43610400	-1.19510800
H	-1.73438700	-2.00006900	-1.17883300
C	-3.73713000	-0.57859300	-0.11153800
H	-3.98290300	-1.53057200	-0.61588000
C	1.88906600	0.77397300	-0.16276100
H	2.03869600	1.66014500	0.45834900
C	2.37081400	1.04041500	-1.58824000
H	1.79422900	1.85805300	-2.02236800
H	3.42703300	1.31354800	-1.59202100
H	2.24281200	0.15362000	-2.21052300
C	2.67767800	-0.35092800	0.47989400
O	3.33689800	-1.16594300	-0.11189900
O	2.53598000	-0.35853600	1.81170900
H	3.02332500	-1.11411100	2.17197700
O	-4.60778400	0.09461500	0.38984200

P4

C	-1.31990600	-1.07548700	-0.18178400
C	0.03644400	-1.35586800	-0.07943200
C	0.95142700	-0.35800000	0.25781500
C	0.47607600	0.93442900	0.48040600
C	-0.88046000	1.21566500	0.37485300
C	-1.80661600	0.21640900	0.05226700
H	-1.99992800	-1.87253400	-0.45870500
H	0.39080200	-2.36360200	-0.26935600
H	1.16967900	1.73072500	0.73267000
H	-1.23254600	2.22726100	0.54834700
C	-3.23661800	0.56669900	-0.03164100
H	-3.45239000	1.63363700	-0.01114800
C	-4.25985100	-0.28738000	-0.10747700

H	-4.06968200	-1.35832000	-0.10568100
C	-5.69686900	0.12510300	-0.18959900
H	-6.26923500	-0.29674200	0.64129600
H	-5.80028000	1.21101700	-0.16812800
H	-6.15406700	-0.24973300	-1.10983300
C	2.43325900	-0.67032500	0.39270200
H	2.58917700	-1.70635200	0.08270500
C	2.93939800	-0.46430400	1.81929700
H	2.38303400	-1.11013900	2.49972400
H	4.00109500	-0.70531800	1.89318100
H	2.80049300	0.57180700	2.13093500
C	3.19464600	0.20066200	-0.58612200
O	3.82363200	1.18764900	-0.29994400
O	3.06698500	-0.23456000	-1.84740700
H	3.53332600	0.37798200	-2.43491600

P5

C	0.74053100	-0.88910200	1.02660700
C	-0.63530400	-0.88687500	1.22955400
C	-1.50513200	-0.53801800	0.19645100
C	-0.97074500	-0.19273400	-1.04551100
C	0.40566900	-0.19506400	-1.24674900
C	1.27563800	-0.53884900	-0.21322800
H	1.40673000	-1.16790300	1.83596300
H	-1.03802000	-1.15898000	2.19942400
H	-1.63207900	0.07964500	-1.86238500
H	0.80807600	0.07696700	-2.21733400
C	2.77608200	-0.49893100	-0.41278100
H	2.98367900	-0.41008500	-1.48859200
C	3.42838000	0.69345600	0.29794100
H	3.23932000	0.56401200	1.37089200
C	2.80569100	2.01224600	-0.16031700

H	1.74559300	2.07399700	0.09251700
H	3.31818200	2.85363200	0.31057200
H	2.90325200	2.12557400	-1.24524600
C	4.93783700	0.69952800	0.05613400
H	5.40097900	-0.22571400	0.39865300
H	5.14830000	0.81486800	-1.01227400
H	5.40356200	1.53625200	0.58171100
C	-3.01138300	-0.55883300	0.40721200
H	-3.20137700	-0.74972900	1.46605500
C	-3.69947400	-1.61907400	-0.45088900
H	-3.29845800	-2.60306600	-0.20505900
H	-4.77596900	-1.62329400	-0.27312200
H	-3.52773900	-1.42789900	-1.51108700
C	-3.55510300	0.82350500	0.10664300
O	-4.15270000	1.13780600	-0.89105300
O	-3.26744800	1.69693800	1.08201400
H	-3.59830200	2.56964000	0.82317500
O	3.39249300	-1.67905800	0.09781000
H	2.97938200	-2.44093100	-0.32044400

P6

C	-2.17741700	-0.80869600	0.80181500
C	-0.82003000	-0.81281600	1.11100100
C	0.07374100	0.01399400	0.43632100
C	-0.42128600	0.84992200	-0.56860300
C	-1.77051400	0.86177300	-0.89072900
H	-2.86229200	-1.45593300	1.33938200
H	-0.45810300	-1.47179100	1.89289900
H	0.25688600	1.49937500	-1.11355700
H	-2.15412400	1.50801100	-1.67103500
C	1.55190000	0.02683500	0.79437700
H	1.72579700	-0.75994000	1.53205400

C	2.00467500	1.37696900	1.34711400
H	1.42895900	1.61587200	2.24219600
H	3.06480000	1.35583000	1.60568000
H	1.84786600	2.16700700	0.61123600
C	2.34295700	-0.34622700	-0.44291600
O	2.92326700	0.42895500	-1.16006100
O	2.30178200	-1.66362300	-0.68726600
H	2.77819800	-1.84035800	-1.51168600
C	-2.65259100	0.03016500	-0.20201900
O	-3.96740300	0.08090300	-0.55532800
H	-4.47777400	-0.53946300	-0.02409500

P7

C	0.38258600	0.18002200	-1.29719400
C	-0.91102000	0.68728300	-1.22039800
C	-1.76634300	0.30052100	-0.19014400
C	-1.30339800	-0.61347700	0.75771000
C	-0.01280600	-1.12327500	0.67447500
C	0.85234000	-0.72980600	-0.34895600
H	1.03777000	0.49522400	-2.10170400
H	-1.25922300	1.39043900	-1.96987000
H	-1.95648400	-0.93550300	1.56330200
H	0.32946700	-1.83805700	1.41619000
C	2.26081700	-1.26537100	-0.41174100
H	2.31636100	-2.21566500	0.12558700
H	2.54289200	-1.46126000	-1.45042100
C	3.33545400	-0.34349000	0.19429100
C	4.68661700	-1.04724300	0.18457900
H	4.91873800	-1.41066100	-0.81901800
H	5.47187100	-0.36101400	0.50380000
H	4.67045800	-1.89711100	0.87004800
C	2.96621500	0.14313900	1.58996500

H	2.06937400	0.76559500	1.55950200
H	2.76686700	-0.71367100	2.23797400
H	3.78521300	0.71578400	2.02773100
C	-3.16946100	0.87736300	-0.08407400
H	-3.36412600	1.46195300	-0.98658200
C	-3.33775100	1.75236900	1.15668300
H	-2.62746500	2.57919100	1.11745500
H	-4.34874400	2.15910700	1.21244900
H	-3.14918000	1.17518800	2.06314400
C	-4.16142200	-0.26762400	-0.08311100
O	-4.75077800	-0.68139300	0.88263600
O	-4.29893900	-0.81125000	-1.30090900
H	-4.90998000	-1.55990000	-1.23778800
O	4.31681800	1.72430700	-0.31675400
H	3.76507100	2.39997300	0.10004900
O	3.35916800	0.76182900	-0.73551700

P8

C	-0.93803400	-0.79915200	1.17495500
C	0.39508200	-0.47726500	1.41538300
C	1.18374300	0.07307000	0.40786300
C	0.61418800	0.28907200	-0.84924200
C	-0.71488700	-0.03743300	-1.08788400
C	-1.50879000	-0.58381800	-0.07789800
H	-1.53853300	-1.22604700	1.97161600
H	0.82403500	-0.65695500	2.39538100
H	1.21474600	0.71000700	-1.64990500
H	-1.14177500	0.13257900	-2.07091000
C	-2.95618800	-0.89891300	-0.32688500
H	-3.11289300	-1.24349900	-1.35516000
H	-3.30510900	-1.71022900	0.31917100
C	-3.89112400	0.28783200	-0.12509900

C	-5.36287000	-0.03122700	-0.17522300
H	-5.63283100	-0.56987700	0.73762300
H	-5.94645600	0.88485600	-0.24033400
H	-5.58653300	-0.68830000	-1.01759000
C	2.63273900	0.45268600	0.67141500
H	2.89592900	0.10437600	1.67301000
C	2.86278700	1.95886700	0.56059100
H	2.22717600	2.47797000	1.27890800
H	3.90455600	2.20866800	0.76749800
H	2.61757100	2.31377900	-0.44138600
C	3.51316700	-0.30674700	-0.30077600
O	4.05026200	0.16307100	-1.27143600
O	3.61280400	-1.60367900	0.02340900
H	4.15000500	-2.04994200	-0.64762000
O	-3.48166200	1.40945500	0.06759100

P9

C	0.63029400	-1.07772000	-0.83627500
C	-0.69069600	-0.82203200	-1.19219600
C	-1.50676300	-0.03751100	-0.37897800
C	-0.97575300	0.47857400	0.80432000
C	0.34276800	0.21650100	1.15924300
C	1.16871300	-0.56006100	0.34259700
H	1.25506600	-1.68491700	-1.48144800
H	-1.09117800	-1.23732500	-2.11111300
H	-1.59693000	1.08416000	1.45750700
H	0.73820600	0.62164400	2.08538600
C	2.60600200	-0.81585000	0.71722400
H	2.72666700	-0.71316700	1.79893500
H	2.88144800	-1.84050800	0.45060600
C	3.62156900	0.12061700	0.03930600
C	5.02452700	-0.20663100	0.54685600

H	5.25367000	-1.26013900	0.37227300
H	5.76665000	0.40224900	0.02330700
H	5.10862300	-0.00049000	1.61625800
C	3.29300600	1.59168200	0.27993600
H	2.31818200	1.84297300	-0.14147800
H	3.27957700	1.81492200	1.34976100
H	4.05017200	2.22603100	-0.18976100
C	-2.94239300	0.26844100	-0.77791900
H	-3.17625900	-0.31740400	-1.67004800
C	-3.15999600	1.75542500	-1.05229400
H	-2.49699400	2.07797700	-1.85599500
H	-4.19220400	1.94946800	-1.34807700
H	-2.94122600	2.34707000	-0.16226000
C	-3.86194200	-0.22318400	0.32141400
O	-4.42178400	0.47382400	1.12919700
O	-3.96967900	-1.55965200	0.32339200
H	-4.53159400	-1.82333900	1.06681400
O	3.54253000	-0.16950700	-1.36200500
H	4.14356800	0.42397200	-1.82473700

P10

C	-1.03391300	0.62770900	0.80644500
C	0.30377400	1.01140500	0.81451600
C	1.23541400	0.36651500	0.00466800
C	0.80307200	-0.68901700	-0.80211700
C	-0.52944600	-1.07678100	-0.80380400
C	-1.47973000	-0.41222400	-0.01630600
H	-1.73331700	1.12710600	1.46643100
H	0.62578600	1.81813700	1.46458400
H	1.51523100	-1.21641400	-1.42978800
H	-0.84593400	-1.90450500	-1.42998600
C	-2.88586900	-0.86157400	-0.04811500

H	-3.01952100	-1.93784500	-0.13927500
C	-3.98893400	-0.10077500	-0.01165200
C	-5.35378900	-0.73391500	-0.02504800
H	-5.29718900	-1.82282500	-0.01819900
H	-5.93029000	-0.40917200	0.84727200
H	-5.91482200	-0.41570500	-0.90925100
C	-3.99795000	1.40437600	0.01675100
H	-3.05352800	1.83626800	-0.31298900
H	-4.79699800	1.77689200	-0.62971200
H	-4.20986800	1.77302400	1.02603100
C	2.68956700	0.80937400	-0.01852600
H	2.83094700	1.54683800	0.77525000
C	3.08445500	1.40528500	-1.36879100
H	2.45074800	2.26568100	-1.58750200
H	4.12676300	1.72854100	-1.36130700
H	2.95890800	0.66922700	-2.16433300
C	3.56202900	-0.38043900	0.32587500
O	4.21185000	-1.02074600	-0.46095100
O	3.51216500	-0.67759400	1.63215500
H	4.04888800	-1.46817000	1.78976100

P11

C	-1.06355800	-0.98218700	0.78901900
C	0.24547400	-0.73840400	1.19017900
C	1.11413600	-0.01358100	0.37461900
C	0.64701400	0.45328800	-0.85442400
C	-0.66087500	0.20092200	-1.25619900
C	-1.53430400	-0.51766200	-0.43992300
H	-1.73058700	-1.54168000	1.43798900
H	0.59567400	-1.11325400	2.14628900
H	1.30856800	1.01630600	-1.50620400
H	-1.00830300	0.56945800	-2.21606200

C	-2.97282400	-0.76162600	-0.84444800
H	-3.08649800	-0.53071000	-1.90878300
H	-3.22241700	-1.81614900	-0.70414600
C	-3.93408600	0.09385400	-0.04703600
C	-4.85717200	-0.45027400	0.74525800
H	-5.54348400	0.16635200	1.31613600
H	-4.95311100	-1.52662000	0.84330800
C	-3.77222400	1.58063800	-0.20302900
H	-2.78456700	1.89882500	0.14413500
H	-3.84294200	1.86395600	-1.25807100
H	-4.53163000	2.12549800	0.35828700
C	2.53575500	0.28628700	0.82361200
H	2.72427300	-0.27193100	1.74404700
C	2.76280800	1.77855200	1.05755300
H	2.07020100	2.13738900	1.81993700
H	3.78398700	1.96839300	1.39201400
H	2.59171200	2.34207600	0.13922300
C	3.49381600	-0.25379500	-0.21870800
O	4.09715800	0.40860800	-1.02394200
O	3.58223100	-1.59070400	-0.17170400
H	4.17025100	-1.88721200	-0.88174900

IMs1

C	0.87713500	-0.92409600	-1.05032000
C	-0.43665100	-0.59853000	-1.27595000
C	-1.27723700	0.04816100	-0.39966700
C	-0.71323500	0.38406700	0.83762600
C	0.61447600	0.07541200	1.12096200
C	1.43090100	-0.57458000	0.19128500
H	1.47750300	-1.43654400	-1.79600300
H	-1.32044700	0.88865700	1.58403400
H	1.02870500	0.34851000	2.08578100

C	2.88338400	-0.85924900	0.47707800
H	3.06915200	-0.76800600	1.55281800
H	3.11389200	-1.89163400	0.19498500
C	3.84253900	0.08448800	-0.27196600
H	3.64993600	-0.02849100	-1.34582500
C	5.28974000	-0.31789000	0.00621200
H	5.47429700	-1.35787600	-0.27436800
H	5.98481600	0.31496100	-0.55062900
H	5.51546000	-0.20917000	1.07196600
C	3.60243800	1.54380700	0.11244200
H	2.58828800	1.86568800	-0.13508500
H	3.74636500	1.68049000	1.18973000
H	4.30386200	2.20089500	-0.40726700
C	-2.71676800	0.39406000	-0.74825200
H	-2.92729400	-0.02008800	-1.73667700
C	-2.96518800	1.90075800	-0.73638700
H	-2.30691300	2.38442700	-1.45892900
H	-4.00073600	2.12373700	-0.99837400
H	-2.76496700	2.31699200	0.25187500
C	-3.62241500	-0.31772900	0.23696400
O	-4.16403100	0.19763200	1.18138100
O	-3.73599500	-1.62349600	-0.04000300
H	-4.28641500	-2.03770700	0.64077400

IMs2

C	-0.89245900	-0.58954100	1.07657400
C	0.40124800	-0.27746200	1.40860300
C	1.25102600	0.12835200	0.37019200
C	0.74241600	0.18707900	-0.92849700
C	-0.58207400	-0.14775700	-1.20065300
C	-1.45459100	-0.55406600	-0.18200900
H	0.76532000	-0.33781900	2.42913900

H	1.38919400	0.49723200	-1.74327000
H	-0.95215600	-0.09199900	-2.21991500
C	-2.90259200	-0.89240000	-0.43036700
H	-3.10114600	-0.86281700	-1.50707100
H	-3.09564400	-1.91601500	-0.09347700
C	-3.87309000	0.05907200	0.28908500
H	-3.64028400	0.01845500	1.36068700
C	-5.31238200	-0.41021500	0.08572900
H	-5.45388200	-1.42876400	0.45566100
H	-6.01430700	0.24356700	0.60884300
H	-5.57022300	-0.39756000	-0.97828700
C	-3.69621100	1.49800000	-0.19268600
H	-2.67868400	1.85749400	-0.02168600
H	-3.90289900	1.56534100	-1.26627100
H	-4.38555400	2.16879100	0.32562300
C	2.69325600	0.51706400	0.65767600
H	2.89935800	0.29824700	1.70811800
C	2.96341500	1.99171400	0.36436700
H	2.30828600	2.61169900	0.97762900
H	4.00045500	2.24657800	0.58908100
H	2.77463100	2.21711800	-0.68619400
C	3.60008400	-0.37713000	-0.16410300
O	4.17418800	-0.05129000	-1.17160900
O	3.67574200	-1.61504300	0.34371900
H	4.22981300	-2.15514300	-0.23894700

IMs3

C	-0.87550300	-0.97989500	0.98118400
C	0.45443900	-0.69116100	1.27947200
C	1.25611900	0.02160200	0.38788400
C	0.70255200	0.44210500	-0.83104400
C	-0.61118600	0.12476300	-1.06650400

C	-1.45501700	-0.56882200	-0.22650500
H	-1.47745100	-1.53751400	1.69320900
H	0.87544300	-1.02758300	2.22078200
H	1.29878200	0.99244800	-1.55306900
C	-2.90576700	-0.83198000	-0.54226100
H	-3.07228800	-0.70944900	-1.61759600
H	-3.14556900	-1.86978300	-0.29015900
C	-3.86489000	0.10200600	0.21767700
H	-3.68456200	-0.03726000	1.29057700
C	-5.31175000	-0.28276900	-0.08648300
H	-5.50732700	-1.32762100	0.16728600
H	-6.00836300	0.34215300	0.47730400
H	-5.52423600	-0.14710500	-1.15185500
C	-3.60932100	1.56742000	-0.13166000
H	-2.59732700	1.87735000	0.13857300
H	-3.73510200	1.72728700	-1.20807200
H	-4.31466700	2.21816900	0.39076500
C	2.70077400	0.35622800	0.72696600
H	2.94173500	-0.12576500	1.67727600
C	2.93919700	1.86197400	0.82101600
H	2.29052000	2.28706200	1.58778200
H	3.97776300	2.07369700	1.08034400
H	2.71903600	2.34775900	-0.13059300
C	3.59183900	-0.27190000	-0.32575800
O	4.11558300	0.31647900	-1.23722000
O	3.71459700	-1.59506400	-0.15307100
H	4.25325300	-1.95259800	-0.87412700

IMs4

C	0.80743300	-1.07037400	-0.78524300
C	-0.51261500	-0.80097600	-1.13475100
C	-1.28566600	0.08997500	-0.38015300

C	-0.64938400	0.64801400	0.70661200
C	0.64553300	0.41815200	1.09667000
C	1.40929000	-0.47207700	0.32582500
H	1.38587700	-1.76199100	-1.38944500
H	-0.95379900	-1.28214400	-2.00224100
H	1.07927700	0.90291900	1.96565100
C	2.85652000	-0.74122500	0.65031800
H	3.06334900	-0.44966700	1.68578800
H	3.04950000	-1.81590200	0.57114600
C	3.83241800	0.00647200	-0.27768200
H	3.60626500	-0.29265000	-1.30847600
C	5.26906300	-0.40274800	0.04285500
H	5.40661900	-1.48218200	-0.05876700
H	5.97584400	0.09583800	-0.62473500
H	5.52348200	-0.12434800	1.07073300
C	3.66282800	1.52065000	-0.16375400
H	2.65435500	1.83709600	-0.43954200
H	3.85000300	1.84632800	0.86539500
H	4.37118700	2.03849900	-0.81479800
C	-2.73131000	0.40892400	-0.72147400
H	-2.94808100	-0.01681700	-1.70365800
C	-3.01102900	1.90856600	-0.70737000
H	-2.37515600	2.40679800	-1.44000300
H	-4.05517600	2.11087500	-0.95043800
H	-2.79878800	2.32440900	0.27907900
C	-3.60555000	-0.31637600	0.28408600
O	-4.12390600	0.18723100	1.24719800
O	-3.71591100	-1.62141300	0.00075300
H	-4.24141100	-2.04547800	0.69507000

IMs5

C	0.64121800	0.50952200	1.13390300
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C	-0.73642700	0.38840000	1.01155000
C	-1.35724500	0.54484400	-0.23365900
C	-0.56346700	0.82674000	-1.34470000
C	0.81620500	0.95060500	-1.21624100
C	1.44053100	0.79233300	0.02225600
H	1.10544200	0.38624400	2.10725000
H	-1.33376000	0.17294100	1.89212900
H	-1.02784400	0.95223100	-2.31710900
H	1.41847800	1.17020500	-2.09171100
C	2.93810400	0.87661000	0.16491900
H	3.36571900	1.36288800	-0.71856000
H	3.18523400	1.50026800	1.03001600
C	3.60650700	-0.50000200	0.34244700
H	3.16977800	-0.97051800	1.23163700
C	5.10627000	-0.32282000	0.57457400
H	5.30179700	0.30798200	1.44525000
H	5.59373300	-1.28735300	0.73488000
H	5.57209500	0.14863200	-0.29674500
C	3.34782600	-1.40495800	-0.86127100
H	2.28084500	-1.58793700	-1.00751800
H	3.73942600	-0.94249800	-1.77374200
H	3.84374800	-2.37002500	-0.73312700
C	-2.86294400	0.42295900	-0.36436700
H	-3.13095700	0.52991100	-1.42152600
C	-3.64824600	1.45478700	0.45034400
H	-3.38410300	2.45648600	0.10974500
H	-4.72051300	1.30796800	0.31906000
H	-3.41181500	1.37600900	1.51279400
C	-3.30519700	-0.97791200	-0.01049000
O	-4.43326400	-1.36981400	0.17869800
O	-2.32999900	-1.86519500	0.06651300

IMs6a

C	0.60074800	-0.22979500	-1.21570800
C	-0.60687500	0.37929700	-1.34695700
C	-1.36435600	0.95500900	-0.18407800
C	-0.59586100	0.83124000	1.10008700
C	0.61659600	0.22736200	1.17763600
C	1.25281400	-0.34849400	0.04101400
H	1.09639000	-0.62829000	-2.09592700
H	-1.08458600	0.47045900	-2.31731100
H	-1.04816900	1.27589900	1.97939300
H	1.12687800	0.17922000	2.13539800
C	2.60678500	-0.97648500	0.16957300
H	2.61426000	-1.65394800	1.03094500
H	2.82310300	-1.57781600	-0.72016800
C	3.74178700	0.05419400	0.35304500
H	3.51993600	0.63797300	1.25432500
C	3.82008600	1.00973200	-0.83676700
H	2.89477300	1.57768700	-0.95999100
H	4.64033200	1.72011800	-0.70905800
H	3.99861900	0.45011300	-1.76127800
C	5.07131700	-0.66964000	0.55835400
H	5.02864700	-1.34298500	1.41796000
H	5.32012600	-1.26465100	-0.32618400
H	5.88270100	0.04332200	0.72270300
C	-2.78279200	0.30487900	-0.10024600
H	-3.27479200	0.55956500	-1.04164100
C	-3.60766600	0.81028700	1.08241400
H	-3.60562100	1.89976200	1.09667700
H	-4.63941000	0.46574300	0.99472500
H	-3.20508700	0.43829300	2.02486600
C	-2.64354200	-1.20110000	-0.03871900
O	-2.35607700	-1.82689900	0.95020100
O	-2.87519500	-1.79050600	-1.22029200

H	-2.74791600	-2.74558900	-1.11663200
O	-1.66497400	2.34296100	-0.43885700
H	-0.82446100	2.81176300	-0.49511200

IMs6s

C	-1.00232600	-1.37180700	0.83196200
C	0.33801300	-1.37689000	1.03873600
C	1.31932400	-0.79785600	0.05985400
C	0.64711100	-0.33873700	-1.20157000
C	-0.70258400	-0.35498800	-1.36232000
C	-1.58052900	-0.83448800	-0.35414900
H	-1.66181100	-1.79851700	1.58247500
H	0.76469900	-1.80265000	1.94173600
H	1.29814500	0.02701500	-1.98728900
H	-1.13177000	0.00490300	-2.29283500
C	-3.06846900	-0.75177700	-0.49923700
H	-3.33176900	-0.58612400	-1.54970300
H	-3.52164300	-1.70145600	-0.19243800
C	-3.69176900	0.37932600	0.34768500
H	-3.43467300	0.18852600	1.39674700
C	-5.21261200	0.35480200	0.20789400
H	-5.62351100	-0.61222200	0.50846900
H	-5.67396600	1.12888400	0.82580900
H	-5.50153600	0.53764100	-0.83216400
C	-3.12956900	1.74361100	-0.04869000
H	-2.04928400	1.79633200	0.10774500
H	-3.32729500	1.94270600	-1.10759000
H	-3.59724000	2.53916500	0.53646900
C	2.11025800	0.35164300	0.75949800
H	2.47696100	-0.05671400	1.70390400
C	1.24349000	1.58398000	1.00848600
H	0.34464800	1.30143200	1.55997000

H	1.78899700	2.32547200	1.59418400
H	0.94414100	2.03785700	0.06250600
C	3.31488800	0.71600300	-0.08146100
O	3.27196600	1.32855700	-1.11999300
O	4.46831000	0.30035500	0.45736300
H	5.19173100	0.56551400	-0.13001900
O	2.33797300	-1.77082900	-0.24867600
H	1.90782000	-2.51935600	-0.67765800

IMs7a

C	0.88692800	0.72268200	-1.13942600
C	-0.53274900	1.11216400	-0.86861200
C	-1.24463800	0.17374300	0.06332400
C	-0.60932400	-0.91023000	0.59767900
C	0.73840300	-1.19857200	0.29942400
C	1.48932700	-0.35698300	-0.57559300
H	1.44323400	1.37738200	-1.80372500
H	-1.09332400	1.16474900	-1.81270300
H	-1.14969600	-1.57199300	1.26856300
H	1.21129700	-2.06848400	0.73995300
C	2.94491800	-0.67051400	-0.81383600
H	3.04212900	-1.71601100	-1.12631100
H	3.32260300	-0.05038100	-1.63376400
C	3.82656600	-0.44138100	0.42715800
H	3.44694300	-1.07758800	1.23571100
C	3.76783600	1.01359000	0.89035900
H	2.75275300	1.30824100	1.16657300
H	4.41605700	1.17074800	1.75579000
H	4.10554500	1.67991400	0.08917000
C	5.26583500	-0.85623400	0.12424300
H	5.31998900	-1.90153100	-0.19000100
H	5.67717300	-0.23908200	-0.68101900

H	5.90299900	-0.73023100	1.00276100
C	-2.69524600	0.49204700	0.37582400
H	-2.96274600	1.39869800	-0.17202800
C	-2.95543800	0.69120200	1.86769900
H	-2.34557100	1.51765900	2.23480000
H	-4.00670300	0.92097000	2.04889500
H	-2.69956300	-0.20759500	2.42985200
C	-3.53912600	-0.63374300	-0.18574400
O	-4.06678000	-1.50398100	0.45861400
O	-3.60858000	-0.58106700	-1.52479000
H	-4.11225900	-1.34625400	-1.83930800
O	-0.60587500	2.46521800	-0.37413800
H	-0.08074000	2.50280800	0.43430300

IMs7s

C	0.86761200	-1.10531900	-0.30378600
C	-0.54317500	-0.86489200	-0.73685500
C	-1.12948600	0.41951400	-0.21198400
C	-0.37302500	1.28234000	0.52054100
C	0.97509600	0.99826000	0.84751600
C	1.58766300	-0.21722100	0.43695900
H	1.31168400	-2.04450500	-0.62272400
H	-0.58487600	-0.83819100	-1.83688800
H	-0.80226900	2.21109800	0.87947100
H	1.54195900	1.70677500	1.43993900
C	3.02901900	-0.49402000	0.79167500
H	3.30525600	0.08241000	1.68195300
H	3.14240500	-1.55247800	1.04464800
C	4.01269300	-0.15053100	-0.34146600
H	3.73382000	-0.75497700	-1.21321300
C	5.43424200	-0.52418200	0.07611000
H	5.50532500	-1.58243300	0.33999900

H	6.14495200	-0.32413000	-0.72931100
H	5.73975100	0.06304800	0.94824300
C	3.93589100	1.32487200	-0.73174700
H	2.94140000	1.59810000	-1.09200200
H	4.16889500	1.95859900	0.13100100
H	4.65675600	1.55228700	-1.52094200
C	-2.57508700	0.64929400	-0.56692500
H	-2.72177100	0.36804600	-1.61506300
C	-3.06941100	2.08939200	-0.36837700
H	-2.44941400	2.77800000	-0.94350000
H	-4.10089900	2.18221400	-0.71085200
H	-3.03027800	2.37673600	0.68385200
C	-3.47991500	-0.25207500	0.25632300
O	-3.33379600	-0.50546100	1.42564800
O	-4.53121600	-0.68702500	-0.45031700
H	-5.10550400	-1.20013300	0.13730800
O	-1.38997400	-1.98595600	-0.41918100
H	-1.39000800	-2.08551800	0.54098300

IMs8a

C	0.79793800	1.38397900	-0.28098400
C	-0.65625600	1.41614200	0.07602100
C	-1.41788300	0.29823500	0.18370500
C	-0.84796900	-0.97850500	-0.09584800
C	0.50269800	-1.08471600	-0.48139100
C	1.32366100	0.00524600	-0.58587800
H	0.97445500	2.02466600	-1.15628000
H	-1.07888500	2.39538300	0.27967600
H	-1.45927700	-1.87075800	-0.01963900
H	0.90641900	-2.06771500	-0.70541300
C	2.75802700	-0.11940200	-1.01188000
H	2.87158000	-1.03530200	-1.60384200

H	3.01077900	0.72386600	-1.66563000
C	3.79846600	-0.16898000	0.13045000
H	3.74056800	0.77369400	0.68134900
C	5.19744400	-0.29759700	-0.47163300
H	5.41078400	0.52363800	-1.16068600
H	5.96047200	-0.29303200	0.31058400
H	5.28926700	-1.23741200	-1.02599900
C	3.52153700	-1.32069400	1.09507400
H	2.55458100	-1.21178200	1.59158700
H	3.51719700	-2.27589000	0.55811800
H	4.29512700	-1.37213000	1.86535400
C	-2.87132800	0.37681100	0.62279100
H	-3.15312000	1.43189600	0.66540500
C	-3.09529800	-0.28510200	1.98098600
H	-2.47939400	0.21061000	2.73238600
H	-4.14208500	-0.21184400	2.27969200
H	-2.82312800	-1.34130100	1.94961100
C	-3.73613500	-0.26395300	-0.44485000
O	-4.29405700	-1.32727000	-0.34781100
O	-3.79966100	0.48622400	-1.55385900
H	-4.33463100	0.01960900	-2.21245100
O	1.57381600	2.03088900	0.74862700
H	1.44909800	1.52627100	1.56115500

IMs8s

C	0.92846800	0.79879600	0.77530700
C	-0.52527500	0.65726800	1.10633200
C	-1.38243900	-0.09945900	0.37466400
C	-0.91275900	-0.79087300	-0.77916700
C	0.43359600	-0.66564900	-1.18310200
C	1.33808500	0.08809200	-0.48982400
H	1.52009200	0.39645200	1.61115200

H	-0.87089800	1.19526500	1.98365200
H	-1.59735700	-1.39396700	-1.36454500
H	0.75724200	-1.17681300	-2.08444700
C	2.76379600	0.24399400	-0.93094500
H	2.92727200	-0.35678600	-1.83219800
H	2.94302500	1.29106000	-1.20196100
C	3.80131800	-0.15884100	0.13362400
H	3.67394100	0.50126700	0.99939800
C	5.21167300	0.04773600	-0.41597800
H	5.36679600	1.08295200	-0.72986700
H	5.96449100	-0.19710200	0.33702200
H	5.38045100	-0.59815900	-1.28353700
C	3.59974500	-1.60559800	0.58221900
H	2.61247900	-1.76096900	1.02532800
H	3.69017000	-2.28185500	-0.27451500
H	4.35214200	-1.89287400	1.32050300
C	-2.84255600	-0.23960900	0.77543300
H	-3.03428600	0.45555900	1.59639200
C	-3.18384600	-1.66629400	1.20089000
H	-2.55927900	-1.95163200	2.04823700
H	-4.23185600	-1.74286300	1.49407700
H	-3.00580700	-2.36830900	0.38495500
C	-3.70945100	0.20501400	-0.38619200
O	-4.36180600	-0.52251800	-1.09092900
O	-3.65658800	1.53176000	-0.57058700
H	-4.20049200	1.75869900	-1.33911000
O	1.31578700	2.18342200	0.74704200
H	0.81059100	2.61129200	0.04569000

IMs9a

C	0.53288000	1.36719000	-1.21861100
C	-0.81631800	1.21001700	-1.25913700

C	-1.51879300	0.57383800	-0.20461800
C	-0.78218300	0.14149900	0.93328900
C	0.56681300	0.27499900	1.00927300
C	1.40338700	0.84795300	-0.10509000
H	1.05538800	1.87273200	-2.02457400
H	-1.37711400	1.59121500	-2.10668800
H	-1.31834400	-0.29845600	1.76933100
H	1.08758300	-0.04468100	1.90238900
C	2.38047500	-0.19871700	-0.70356400
H	1.83441000	-1.14404200	-0.80150800
H	2.62202200	0.12921500	-1.72054200
C	3.70868200	-0.43915300	0.02820300
H	4.26599600	0.50197000	0.01788400
C	4.50888800	-1.48107000	-0.75845700
H	4.64055300	-1.18040700	-1.80089700
H	5.49833400	-1.62437600	-0.31778300
H	3.99291300	-2.44663100	-0.74804600
C	3.55660500	-0.88400000	1.48266400
H	3.17189000	-0.07944700	2.11057100
H	2.88135300	-1.74270700	1.56075500
H	4.52703200	-1.18402900	1.88656100
C	-3.02127200	0.41336900	-0.25047700
H	-3.36636300	0.71609500	-1.24200600
C	-3.72750300	1.23862500	0.82720900
H	-3.49256200	2.29457100	0.68919800
H	-4.80898300	1.10716400	0.76615100
H	-3.40102300	0.93511200	1.82264200
C	-3.34600000	-1.06210700	-0.10399900
O	-3.77343900	-1.58795600	0.89170300
O	-3.06622300	-1.74729500	-1.22168400
H	-3.25108000	-2.68503100	-1.06473400
O	2.22985400	1.91744600	0.39522900
H	1.64248900	2.60951800	0.71919800

IMs9s

C	-0.90279600	-0.97044400	1.23286600
C	0.30753200	-0.38866000	1.44510600
C	1.11856100	0.05442300	0.36779000
C	0.65574700	-0.13968300	-0.96290400
C	-0.55655300	-0.69504900	-1.21581200
C	-1.47511800	-1.19453600	-0.13662100
H	-1.50661000	-1.31364200	2.06744700
H	0.67349600	-0.26112400	2.45904700
H	1.28347300	0.17704600	-1.79114200
H	-0.90331500	-0.83334300	-2.23519100
C	-2.90024200	-0.61749900	-0.25157900
H	-3.19963700	-0.67458600	-1.30569300
H	-3.54842400	-1.30431300	0.30361300
C	-3.13240700	0.80287200	0.27560000
H	-2.92183300	0.80284500	1.35156300
C	-4.60632100	1.16559100	0.08269600
H	-5.26348600	0.42747700	0.54939500
H	-4.82612400	2.14315600	0.51816100
H	-4.85091300	1.20919400	-0.98358300
C	-2.23882800	1.85671100	-0.38049300
H	-1.18801700	1.72431400	-0.11676400
H	-2.32311500	1.80889300	-1.47160600
H	-2.54282900	2.85735300	-0.06220800
C	2.43786900	0.74691400	0.62205500
H	2.66329700	0.67231500	1.68876200
C	2.40168300	2.21543600	0.19342600
H	1.62014500	2.73657600	0.74808000
H	3.35896000	2.70055200	0.39116100
H	2.18703500	2.30057900	-0.87298700
C	3.53208400	-0.00730000	-0.11057900

O	4.07962200	0.35886600	-1.11871300
O	3.81360600	-1.17626900	0.48224600
H	4.48881400	-1.63341000	-0.04028000
O	-1.67374000	-2.61744300	-0.34225200
H	-0.80409700	-3.03376200	-0.33732000

IMs10a

C	-0.79931700	-1.30326600	-0.71160200
C	0.55773100	-1.53597700	-0.40036000
C	1.39353800	-0.46489200	0.01111500
C	0.88621100	0.79518600	0.09286000
C	-0.54418400	1.12380000	-0.20398600
C	-1.36853700	-0.06346300	-0.63108600
H	-1.41209000	-2.14227500	-1.02809100
H	0.96505900	-2.53721000	-0.47246300
H	1.50940700	1.62790200	0.40842900
H	-0.58863000	1.88019200	-1.00087800
C	-2.81093400	0.17262000	-0.97577300
H	-2.90271200	1.13807000	-1.48721500
H	-3.13649100	-0.60143100	-1.68075500
C	-3.79749800	0.16429300	0.21443700
H	-3.52137700	0.98016200	0.88768600
C	-3.74005500	-1.15255700	0.98647000
H	-2.75399600	-1.32486600	1.42382200
H	-4.47563600	-1.15600700	1.79469300
H	-3.96542200	-1.99455800	0.32245500
C	-5.21184100	0.41989500	-0.30549400
H	-5.27000900	1.36463400	-0.85206300
H	-5.52011400	-0.38298000	-0.98324800
H	-5.92893800	0.45828200	0.51807600
C	2.83853800	-0.75256800	0.39959800
H	3.08884300	-1.75632800	0.04729300

C	3.04746800	-0.65836000	1.90983000
H	2.38146700	-1.35997600	2.41424700
H	4.07803400	-0.89766000	2.17736900
H	2.82262800	0.34954100	2.26191700
C	3.74577100	0.20695600	-0.34049400
O	4.29506000	1.16400200	0.14296300
O	3.86038700	-0.11227200	-1.63769500
H	4.41565600	0.55224200	-2.07107900
O	-1.13762800	1.80901800	0.91687500
H	-1.10957400	1.20628500	1.66956800

IMs10s

C	0.85105100	-0.33444800	1.48142700
C	-0.50276600	-0.73295400	1.44652500
C	-1.30821700	-0.44148000	0.31341700
C	-0.78290600	0.25331400	-0.73296300
C	0.61344400	0.79193700	-0.73116700
C	1.43102600	0.35688100	0.45589400
H	1.45084000	-0.59440100	2.34904000
H	-0.93013000	-1.27226400	2.28312600
H	-1.38930700	0.48979400	-1.60309500
H	1.13021000	0.49679600	-1.65322900
C	2.89289800	0.70295200	0.45549500
H	3.08219300	1.49349000	-0.27869300
H	3.17962900	1.09657500	1.43603800
C	3.79822000	-0.50474300	0.13245200
H	3.62853400	-1.25888500	0.90994700
C	5.26484500	-0.07986900	0.17612300
H	5.52419000	0.35292700	1.14547000
H	5.92373900	-0.93250500	-0.00477700
H	5.46608500	0.67081500	-0.59474400
C	3.45280400	-1.12387700	-1.22139400

H	2.42726800	-1.50230200	-1.24280800
H	3.56078300	-0.38204400	-2.02001700
H	4.12169800	-1.95811700	-1.44582500
C	-2.74902400	-0.93728500	0.27086000
H	-3.00204100	-1.32396800	1.26102800
C	-2.95076600	-2.02315600	-0.78374800
H	-2.28311300	-2.86061700	-0.57683300
H	-3.98023400	-2.38470200	-0.77853300
H	-2.72547500	-1.63589500	-1.77835100
C	-3.65821700	0.24721500	0.02044700
O	-4.21286500	0.49663300	-1.01955800
O	-3.76578300	1.03205100	1.10248900
H	-4.32213300	1.79249600	0.87868700
O	0.59172800	2.23422200	-0.82484400
H	0.11826600	2.56264100	-0.05133200

IMs11a

C	-0.84652500	-1.09747300	0.91888600
C	0.50042800	-0.81609000	1.23918200
C	1.25876100	0.03112600	0.48374100
C	0.63787800	0.79111200	-0.65979500
C	-0.71663900	0.27805700	-1.04236100
C	-1.44249700	-0.56690700	-0.25899300
H	-1.42379400	-1.75725900	1.55606900
H	0.95027300	-1.31324700	2.09311500
H	1.31226500	0.77787200	-1.52361300
H	-1.14939300	0.69475700	-1.94772300
C	-2.87262500	-0.90995600	-0.60148000
H	-2.95346700	-1.09744500	-1.67651500
H	-3.16133200	-1.83502500	-0.08951100
C	-3.86888400	0.19870200	-0.21749300
H	-3.58300000	1.10202400	-0.77010100

C	-3.81961200	0.51106300	1.27753100
H	-2.83217200	0.86266400	1.58660900
H	-4.54900000	1.28332000	1.53408600
H	-4.05773900	-0.38479400	1.86137100
C	-5.28148600	-0.20348400	-0.63865700
H	-5.33040200	-0.41845500	-1.70911300
H	-5.59667400	-1.10190600	-0.09814200
H	-5.99795500	0.59094100	-0.41636600
C	2.74407900	0.18354200	0.74310700
H	2.96440200	-0.29882100	1.69771600
C	3.26296500	1.62177800	0.74624600
H	2.73392700	2.20447400	1.50033100
H	4.33017400	1.62933100	0.97645800
H	3.11086600	2.09580600	-0.22251700
C	3.44428500	-0.62756900	-0.33559300
O	3.81215100	-0.19511900	-1.39887300
O	3.57507000	-1.91709000	0.00385600
H	3.97181200	-2.39280600	-0.74097000
O	0.53207800	2.20139700	-0.34516400
H	-0.09394600	2.28166900	0.38433500

IMs11s

C	1.03101700	-0.67616000	-1.17720400
C	-0.31187400	-0.35452400	-1.47049500
C	-1.14340600	0.18838800	-0.53575700
C	-0.64677800	0.50357100	0.84954300
C	0.76801900	0.07897200	1.08952000
C	1.56104200	-0.46844700	0.13100400
H	1.65572200	-1.12110200	-1.94284900
H	-0.69706800	-0.56571800	-2.46333500
H	-0.72291900	1.58796900	1.01639300
H	1.15215600	0.24799800	2.09125000

C	2.99685100	-0.84117600	0.40339000
H	3.19120400	-0.78232100	1.47967100
H	3.16178800	-1.88086100	0.10005200
C	4.00967700	0.05440900	-0.33220200
H	3.80944600	-0.01910900	-1.40788200
C	5.42980700	-0.44656700	-0.07224000
H	5.54755100	-1.48678500	-0.38595700
H	6.16331300	0.15782100	-0.61108700
H	5.66394300	-0.38663400	0.99553600
C	3.86550700	1.51661300	0.08671600
H	2.87057800	1.90499000	-0.14221800
H	4.02706100	1.61883100	1.16529100
H	4.60181400	2.14068800	-0.42538800
C	-2.58850900	0.50382200	-0.83189600
H	-2.75688100	0.29849300	-1.89569600
C	-2.96111900	1.95804900	-0.53435500
H	-2.27146400	2.62923300	-1.04799600
H	-3.97509000	2.16776100	-0.87361000
H	-2.91561600	2.15774300	0.53773000
C	-3.54332900	-0.43683800	-0.11097800
O	-4.59218200	-0.11407100	0.38394100
O	-3.12362800	-1.71236200	-0.13402400
H	-3.79898000	-2.26061400	0.29176100
O	-1.53770200	-0.03506400	1.84464000
H	-1.47988400	-0.99707300	1.79160700

IMs12

C	-1.14691200	-0.97550000	0.91002800
C	0.17209200	-0.67192500	1.22937200
C	0.94660300	0.13115200	0.39095900
C	0.36223100	0.62007400	-0.77944600
C	-0.95648600	0.30836700	-1.10019900

C	-1.73391700	-0.49038800	-0.26107300
H	-1.73047200	-1.60186800	1.57831000
H	0.60871200	-1.06656800	2.14123600
H	0.93653000	1.25027700	-1.44935400
H	-1.39074200	0.69980400	-2.01494800
C	-3.17912500	-0.78759400	-0.57081400
H	-3.38158200	-0.57132100	-1.62575600
H	-3.37235700	-1.85445200	-0.41714100
C	-4.16417300	0.01977400	0.29491300
H	-3.94813600	-0.20922600	1.34577700
C	-5.59837100	-0.40909800	-0.01019600
H	-5.73832100	-1.47918300	0.16234900
H	-6.31118300	0.13393400	0.61502300
H	-5.84220100	-0.20022900	-1.05704700
C	-3.99202300	1.52299400	0.08244400
H	-2.98533500	1.85521200	0.34588900
H	-4.16830900	1.78000200	-0.96787200
H	-4.70557000	2.08430700	0.69054100
C	2.38458500	0.45404500	0.74786600
H	2.57790900	0.08361400	1.75875400
C	2.68133800	1.95324300	0.69113600
H	1.95850900	2.49192600	1.30547300
H	3.68342400	2.16549000	1.06286200
H	2.60731000	2.32737600	-0.33187500
C	3.33544100	-0.33370700	-0.15831000
O	3.19445600	-0.02835800	-1.50964600
O	3.12899100	-1.68912900	0.04972300
H	3.48278100	-2.17974000	-0.70293700
O	4.65087100	0.06257800	0.10209000
H	5.25678700	-0.51870500	-0.37668800

IBU⁺

C	-0.90838300	-0.59152800	1.32116400
C	0.39407200	-0.24987400	1.52803400
C	1.23513300	0.05529100	0.42180600
C	0.70519100	0.00608200	-0.90590500
C	-0.59459400	-0.33979200	-1.11411700
C	-1.44341500	-0.65154000	-0.00737100
H	-1.55793900	-0.83170500	2.15469400
H	0.80611000	-0.20939500	2.52870900
H	1.35174700	0.24373300	-1.74356600
H	-1.00450200	-0.38620400	-2.11563000
C	-2.86881800	-0.97303600	-0.20468700
H	-3.06547800	-1.24764900	-1.24314400
H	-3.14771100	-1.80482100	0.45003200
C	-3.76951100	0.25077900	0.17301400
H	-3.57944100	0.49025900	1.22410100
C	-5.23128700	-0.15741700	0.01459600
H	-5.47625100	-1.02185400	0.63470100
H	-5.88141200	0.67060100	0.30554400
H	-5.44691200	-0.40762600	-1.02801800
C	-3.43789300	1.46871600	-0.68635800
H	-2.41777700	1.82544100	-0.52242900
H	-3.55178100	1.23190200	-1.74871600
H	-4.11933700	2.28828500	-0.44997700
C	2.65120600	0.48049700	0.64104500
H	2.92904400	0.25792100	1.67591500
C	2.80400700	1.98920000	0.38583300
H	2.15093000	2.55055700	1.05316900
H	3.83883700	2.27205400	0.57623900
H	2.55832200	2.23781300	-0.64746700
C	3.61564000	-0.32226300	-0.22826200
O	4.56918300	0.13454200	-0.79178800
O	3.27858400	-1.61501500	-0.25230200
H	3.92333400	-2.10621600	-0.78419200

TS1

C	0.69783900	0.36307000	1.06584400
C	-0.65115500	0.19666200	1.35643500
C	-1.54584100	-0.20854300	0.36583200
C	-1.06375400	-0.43017300	-0.92469100
C	0.28455800	-0.25491800	-1.21581400
C	1.18716000	0.13428900	-0.22319700
H	1.37843500	0.68317900	1.84850700
H	-1.01381700	0.38362000	2.36168300
H	-1.74569100	-0.73865100	-1.71127600
H	0.64426400	-0.42932000	-2.22453800
C	2.64756200	0.28783700	-0.51914000
H	2.83973700	0.20421400	-1.59367100
H	2.93293300	1.35694000	-0.22975400
C	3.57697300	-0.64751000	0.26045000
H	3.39370400	-0.49643000	1.33037100
C	5.03754100	-0.31538100	-0.03680500
H	5.26577100	0.72284900	0.21592000
H	5.70634400	-0.96239800	0.53529300
H	5.25225400	-0.46376800	-1.09990200
C	3.26849600	-2.10738200	-0.08280500
H	2.23594400	-2.36694200	0.16195200
H	3.41990200	-2.28490100	-1.15251900
H	3.93114700	-2.77798700	0.46939200
C	-3.01724100	-0.42471800	0.68436200
H	-3.19155300	-0.09956700	1.71272600
C	-3.43425700	-1.88432800	0.51326800
H	-2.83657500	-2.51391400	1.17362100
H	-4.48913300	-2.01811700	0.75784300
H	-3.27687900	-2.21128800	-0.51545400
C	-3.83672000	0.48421100	-0.20941100

O	-4.44727700	0.13599400	-1.18782300
O	-3.78570000	1.76154500	0.19379400
H	-4.28692300	2.30362200	-0.43298800
O	3.36058000	2.80397100	0.10316800
H	3.91234900	2.93808600	-0.68628700

TS2

C	0.68076800	0.90714500	-0.68966900
C	-0.61561600	1.25929400	-0.32829200
C	-1.51603700	0.29190000	0.11652800
C	-1.09276800	-1.03569800	0.18699400
C	0.20337100	-1.38538800	-0.17802200
C	1.10916700	-0.41999400	-0.62009400
H	1.37284700	1.67295300	-1.02601700
H	-0.93125300	2.29544600	-0.39294300
H	-1.78050500	-1.80469600	0.52589700
H	0.51646000	-2.42284700	-0.11736100
C	2.52910300	-0.77737400	-0.98037100
H	2.61979500	-1.86372400	-1.09957200
H	2.78991600	-0.32468600	-1.94214900
C	3.55577100	-0.32722300	0.06744200
H	3.42585100	0.80574800	0.14694300
C	4.97901100	-0.59076800	-0.40229500
H	5.17161600	-0.11663200	-1.36758400
H	5.70852300	-0.21782300	0.32066300
H	5.14093200	-1.66805300	-0.51534000
C	3.28715200	-0.90039500	1.45091800
H	2.29165700	-0.63389200	1.81142500
H	3.35373300	-1.99396700	1.41690100
H	4.02472500	-0.53885400	2.17077200
C	-2.92810400	0.67367400	0.53401000
H	-3.06839600	1.73557100	0.31861600

C	-3.19084900	0.39782100	2.01332700
H	-2.48356300	0.96350800	2.62107900
H	-4.20503800	0.69203600	2.28855000
H	-3.07069600	-0.66346900	2.23533600
C	-3.90448600	-0.08522500	-0.34124800
O	-4.53393200	-1.05661500	-0.00632600
O	-3.97592000	0.43074200	-1.57645000
H	-4.57907700	-0.11298100	-2.10421500
O	3.58532500	2.35440100	0.23645700
H	4.51979900	2.32153300	0.50418800

TS3

C	-0.34933500	-1.05917200	1.15068100
C	0.92347400	-0.56067800	1.41006000
C	1.66611500	0.04785800	0.39956400
C	1.11136900	0.13783800	-0.87807300
C	-0.15887700	-0.36620700	-1.13464200
C	-0.91096100	-0.96887000	-0.12421600
H	-0.91305700	-1.53010000	1.95041800
H	1.34332900	-0.64689400	2.40683500
H	1.67606400	0.60328600	-1.68061800
H	-0.57515300	-0.28740400	-2.13403400
C	-2.31045400	-1.46656100	-0.38020800
H	-2.46561100	-1.60328400	-1.45568800
H	-2.44587500	-2.44376200	0.09411900
C	-3.40211200	-0.51621400	0.15910800
H	-3.23181000	-0.39011300	1.23464000
C	-4.78421800	-1.12961200	-0.05671700
H	-4.86368200	-2.10295800	0.43268200
H	-5.56485300	-0.47906400	0.34344600
H	-4.97420800	-1.27026100	-1.12551500
C	-3.30193900	0.84414000	-0.50901400

H	-2.36174100	1.36532200	-0.31931300
H	-3.49562400	0.79538700	-1.58423100
H	-4.11525100	1.53927300	-0.06102600
C	3.04451000	0.62468900	0.68293300
H	3.32536600	0.34481200	1.70128600
C	3.07569100	2.14374100	0.52546800
H	2.35821000	2.59531900	1.21181100
H	4.06949700	2.53734200	0.74497000
H	2.81109000	2.42957000	-0.49367500
C	4.04150600	-0.03927200	-0.24459200
O	4.52910400	0.46581800	-1.22362200
O	4.31141100	-1.29822000	0.12896100
H	4.91555000	-1.69020900	-0.51868100
O	-5.28437500	2.32753300	0.31103400
H	-5.80996400	2.12261600	-0.48052000

TS4

C	0.92343300	-1.02458400	0.49219600
C	-0.41616300	-0.93966500	0.14258300
C	-1.01558300	0.30310900	-0.09439000
C	-0.23440000	1.45276400	0.02432000
C	1.10869700	1.35973000	0.38032900
C	1.70962600	0.12519500	0.62075100
H	1.36952400	-1.99830200	0.67025900
H	-1.00673700	-1.84443500	0.04739800
H	-0.66573400	2.43030200	-0.15388100
H	1.69890900	2.26621200	0.46925800
C	3.17173200	0.01406300	0.96628200
H	3.54036700	0.98180600	1.32383800
H	3.29574100	-0.70236500	1.78477600
C	4.04556500	-0.43812600	-0.21901700
H	3.66189400	-1.40506900	-0.56692700

C	5.48903700	-0.62631600	0.24505200
H	5.55373100	-1.35334700	1.05846100
H	6.12195400	-0.97332300	-0.57516200
H	5.89742800	0.32305500	0.60666000
C	3.97596200	0.55639200	-1.37666000
H	2.95879600	0.66070000	-1.76082200
H	4.31623200	1.54426900	-1.04768500
H	4.61839000	0.23603200	-2.20043100
C	-2.48388400	0.37467700	-0.45643300
H	-2.64884300	-0.42348900	-1.27620900
C	-2.97954300	1.70158800	-1.00309500
H	-2.37092200	2.01046700	-1.85348400
H	-4.01652700	1.61022500	-1.32848700
H	-2.93457100	2.47608700	-0.23468700
C	-3.31429900	-0.07331600	0.73117000
O	-3.78218600	0.66689500	1.55444500
O	-3.45495300	-1.40708300	0.78467000
H	-3.94563400	-1.64376900	1.58639900
O	-3.00992800	-1.60723100	-2.08112200
H	-3.34853500	-2.12877100	-1.33174200

TS5

C	-0.94963800	-0.56864000	1.29267600
C	0.38864800	-0.20680100	1.40903900
C	1.18973100	-0.08722400	0.27342900
C	0.63022600	-0.35461200	-0.97648900
C	-0.70746000	-0.71888400	-1.08629200
C	-1.52017400	-0.82536200	0.04414900
H	-1.56019200	-0.65062300	2.18660500
H	0.81256300	-0.00841500	2.38807700
H	1.24081000	-0.27716200	-1.87097700
H	-1.12981700	-0.91608200	-2.06631000

C	-2.98594700	-1.15626600	-0.06947300
H	-3.19334700	-1.57004700	-1.06249400
H	-3.24260900	-1.92820700	0.66331700
C	-3.89793600	0.06368400	0.15803100
H	-3.68909400	0.45340200	1.16192800
C	-5.36329100	-0.36495800	0.10093900
H	-5.57612300	-1.14755700	0.83351500
H	-6.02626500	0.48006300	0.30144500
H	-5.60672400	-0.75552100	-0.89242800
C	-3.61621900	1.16953200	-0.85818400
H	-2.58945100	1.53588000	-0.78404600
H	-3.76888200	0.79626400	-1.87668100
H	-4.29054200	2.01541300	-0.70456000
C	2.63367700	0.37829800	0.38963100
H	2.87371200	0.49008500	1.44910400
C	2.86642500	1.68947800	-0.34199400
H	2.08584000	2.47189100	0.07165500
H	3.84447300	2.12939800	-0.14575800
H	2.67212600	1.62229900	-1.41180200
C	3.53630300	-0.71030700	-0.16371400
O	4.03351800	-0.70877400	-1.26005100
O	3.69167600	-1.71362000	0.70739100
H	4.23287400	-2.40309200	0.29469100
O	0.94161500	3.10741600	0.54233700
H	0.35010100	2.33421800	0.51682400

TS6

C	-0.38492300	-0.30048700	1.46478100
C	0.99165800	-0.13930900	1.58218600
C	1.76059000	0.20942700	0.47362500
C	1.12767200	0.38842300	-0.75879100
C	-0.24565700	0.22187500	-0.87826600

C	-1.01717500	-0.12044600	0.23405700
H	-0.97506300	-0.56712100	2.33501700
H	1.47029300	-0.28233700	2.54508800
H	1.71305800	0.65237200	-1.63439200
H	-0.71995700	0.35361300	-1.84514500
C	-2.51466600	-0.29460500	0.14294600
H	-2.74603200	-0.79000200	-0.98416400
C	-3.41266900	0.97096600	0.19587500
H	-3.29951300	1.36416500	1.21381700
C	-4.87486300	0.60512900	-0.03923100
H	-5.21488200	-0.16075600	0.65761400
H	-5.50146700	1.49080100	0.08405800
H	-5.01353300	0.22762000	-1.05651200
C	-2.94841400	2.03970200	-0.79079900
H	-1.92731700	2.36833300	-0.59232800
H	-2.99727700	1.66430100	-1.81791000
H	-3.60296300	2.91094000	-0.72062800
C	3.25958000	0.42455900	0.60361200
H	3.56309600	0.09661800	1.60078900
C	3.64690100	1.88660100	0.38883200
H	3.13658200	2.51036500	1.12369200
H	4.72396800	2.02206300	0.49878400
H	3.35912100	2.21820000	-0.60993600
C	3.96623000	-0.47856500	-0.38752100
O	4.48362600	-0.11872600	-1.41376500
O	3.93064400	-1.76284600	-0.00612000
H	4.35944400	-2.30073500	-0.68790600
O	-2.98575200	-1.34442700	0.76500900
O	-3.27936900	-2.17839100	-0.88071200
H	-3.64635300	-3.02295400	-1.21306400

TS6-H₂O

C	-0.11541800	0.09497800	-1.56842400
C	1.27109500	0.00913300	-1.63752100
C	2.02105000	-0.28499900	-0.50010900
C	1.35615100	-0.48332400	0.71154000
C	-0.02811700	-0.38932400	0.78179700
C	-0.78425800	-0.10553600	-0.35923700
H	-0.68797900	0.32164200	-2.46088300
H	1.77364700	0.16701200	-2.58599000
H	1.92338600	-0.70279500	1.61100000
H	-0.52156700	-0.53617400	1.73710000
C	-2.29227400	-0.00240500	-0.31029000
H	-2.53017100	0.45999200	0.86076000
C	-3.14431600	-1.30778800	-0.24772600
H	-3.02224200	-1.79512300	-1.22304800
C	-4.61842600	-0.96489600	-0.04589400
H	-4.97689300	-0.27485700	-0.80977900
H	-5.22068100	-1.87487200	-0.08924900
H	-4.77187300	-0.50399800	0.93473800
C	-2.65719600	-2.26634900	0.83609000
H	-1.62365800	-2.57730800	0.67773200
H	-2.73282400	-1.80437600	1.82599800
H	-3.28183600	-3.16250200	0.83750000
C	3.53412500	-0.41152500	-0.57448000
H	3.84921900	-0.11002500	-1.57631700
C	4.00841400	-1.83285000	-0.27826900
H	3.56260200	-2.52336500	-0.99524000
H	5.09487000	-1.90188100	-0.35237800
H	3.71376500	-2.13633300	0.72734000
C	4.14677400	0.58040200	0.39427500
O	4.64137300	0.30412700	1.45716100
O	4.05265500	1.83991500	-0.05409500
H	4.42182300	2.43481700	0.61512000
O	-2.79211200	0.89203500	-1.12771000

O	-3.36022700	2.39857200	-0.29084000
H	-2.67205300	2.97156900	-0.65069400
O	-2.93855600	1.32729400	1.81225600
H	-3.13784700	2.00035600	1.02420700
H	-2.17036800	1.63957900	2.30738300

TS6-NH₃

C	-0.11049200	-0.29765800	1.55896200
C	1.27739200	-0.23132100	1.63009400
C	2.02522300	0.21113500	0.54061300
C	1.35209600	0.56671600	-0.62965500
C	-0.03342300	0.48924200	-0.70262800
C	-0.79547800	0.06887800	0.39534900
H	-0.67812400	-0.63779200	2.41752500
H	1.78414200	-0.51637000	2.54654800
H	1.91571600	0.89489300	-1.49809200
H	-0.52568100	0.75434400	-1.63209700
C	-2.29966000	-0.02413300	0.33451700
H	-2.50298600	-0.53670800	-0.93051000
C	-3.14456200	1.27472100	0.28630700
H	-3.08101200	1.73573400	1.28213000
C	-4.61112100	0.93695100	0.01355100
H	-4.98200900	0.18728600	0.71299300
H	-5.22888300	1.83390900	0.10230000
H	-4.73730400	0.54680700	-1.00168400
C	-2.64101000	2.30007000	-0.72887800
H	-1.62456900	2.63087000	-0.51081500
H	-2.65804900	1.89235200	-1.74527000
H	-3.29045100	3.17897200	-0.71502800
C	3.53905800	0.32919300	0.62476500
H	3.85960400	-0.09739200	1.57826500
C	4.00840300	1.77871400	0.51028600

H	3.56673600	2.36806100	1.31491000
H	5.09545600	1.84378300	0.58159900
H	3.69990600	2.20735400	-0.44437200
C	4.14636600	-0.52670400	-0.46761000
O	4.59995200	-0.11601100	-1.50584300
O	4.09756200	-1.83260500	-0.16832500
H	4.45649800	-2.33352100	-0.91539400
O	-2.80175800	-0.91769000	1.15984900
O	-3.37350300	-2.33223400	0.32160700
H	-3.78202500	-2.72311600	1.10178300
H	-3.32426400	-1.98283200	-1.63683900
N	-2.75260300	-1.22629900	-2.01559300
H	-3.25224900	-0.71900100	-2.74146500
H	-1.89701700	-1.61005500	-2.40967900

TS6-CH₃OH

C	-0.02880100	-0.63387500	1.58245600
C	-1.41887100	-0.68449400	1.59232800
C	-2.14371000	-0.53039100	0.41231600
C	-1.44875200	-0.31455000	-0.77938900
C	-0.06097600	-0.25545000	-0.78708400
C	0.67083100	-0.42112400	0.39265700
H	0.52217100	-0.75978400	2.50742700
H	-1.94407200	-0.85266700	2.52663000
H	-1.99436600	-0.17932300	-1.70819800
H	0.45546700	-0.07514200	-1.72368300
C	2.18288700	-0.36342700	0.40732500
H	2.46088100	0.53998000	-0.46420200
C	3.00266400	-1.55555300	-0.17569100
H	2.86196000	-2.39043200	0.52203000
C	4.48631800	-1.19543300	-0.22149900
H	4.84391700	-0.85533100	0.75043500

H	5.07229300	-2.06683600	-0.52153600
H	4.66310400	-0.40014000	-0.95218000
C	2.51213400	-1.99153600	-1.55395300
H	1.47463500	-2.32758000	-1.53602200
H	2.60002400	-1.17307600	-2.27641200
H	3.12750200	-2.81990600	-1.91251100
C	-3.66153900	-0.61843400	0.41255900
H	-3.99531800	-0.68623900	1.45060900
C	-4.16860100	-1.81860400	-0.38502400
H	-3.76106500	-2.73717000	0.03889300
H	-5.25810800	-1.87079800	-0.35598000
H	-3.85649200	-1.74750500	-1.42792500
C	-4.21451200	0.67807600	-0.14437400
O	-4.65905000	0.82757300	-1.25398400
O	-4.12639900	1.68040700	0.74083300
H	-4.45177000	2.49167900	0.32372500
O	2.68492700	0.08752900	1.53254700
O	3.35033400	1.76252300	1.40207200
H	2.68265600	2.17989500	1.96041500
O	2.90787700	1.70478800	-0.96763600
H	3.16618700	1.96148300	0.00823600
C	1.84562600	2.54028900	-1.44128100
H	1.47954600	2.12853700	-2.38017600
H	1.03003000	2.57967700	-0.71400300
H	2.23111600	3.54515700	-1.61431000

TS6-C₂H₅OH

C	-0.23909100	-1.16320100	1.44809800
C	-1.62899500	-1.10889400	1.43694000
C	-2.31392400	-0.67594400	0.30327100
C	-1.57858900	-0.29135700	-0.81998000
C	-0.19070400	-0.33731100	-0.80514600

C	0.50077200	-0.77957100	0.32727300
H	0.28153700	-1.50311900	2.33598500
H	-2.18653900	-1.40952500	2.31784800
H	-2.09312800	0.06042100	-1.70897000
H	0.35905400	-0.01738300	-1.68383400
C	2.01316600	-0.82588800	0.36814300
H	2.35147500	0.22678300	-0.28849200
C	2.77756100	-1.91439500	-0.44396600
H	2.57740100	-2.86850100	0.05937700
C	4.27927800	-1.63856600	-0.39701500
H	4.63582200	-1.54558200	0.62888400
H	4.82281400	-2.45267600	-0.88136100
H	4.51436800	-0.71133600	-0.92891700
C	2.29598800	-2.02313100	-1.88862000
H	1.24176800	-2.29571300	-1.95295800
H	2.44368200	-1.07727900	-2.42056200
H	2.87360400	-2.79143900	-2.40766300
C	-3.83364000	-0.63635300	0.27722200
H	-4.19543600	-0.88522800	1.27762600
C	-4.41946300	-1.60250100	-0.75106800
H	-4.10109400	-2.61943600	-0.51861300
H	-5.50984300	-1.56407200	-0.74063100
H	-4.07742100	-1.35071600	-1.75584700
C	-4.26754200	0.78815900	-0.00533700
O	-4.67302200	1.19767500	-1.06327900
O	-4.11960000	1.57870200	1.06697700
H	-4.37245700	2.48103900	0.82231900
O	2.51463100	-0.65216700	1.56864200
O	3.29829100	0.95899900	1.79474700
H	2.65561700	1.29334900	2.43297800
O	2.85605500	1.45107600	-0.53150100
H	3.14059000	1.46500900	0.46850900
C	1.81809400	2.42498900	-0.74467900

H	1.40259300	2.23141300	-1.73399000
H	1.02792600	2.27283800	-0.00148100
C	2.38923300	3.82611900	-0.65584700
H	1.60145000	4.55955000	-0.83830600
H	2.80674700	4.00831200	0.33661800
H	3.17577500	3.96609400	-1.39892800

TS6-HCOOH

C	-0.24531100	-1.55208600	1.01720700
C	-1.63177600	-1.55281600	0.91537700
C	-2.27816400	-0.66884100	0.05245700
C	-1.51381200	0.22286400	-0.70373700
C	-0.12825100	0.22855600	-0.60165100
C	0.51591900	-0.66292400	0.25830100
H	0.25017400	-2.24617700	1.68785000
H	-2.21640600	-2.24856400	1.50740900
H	-2.00468000	0.92371300	-1.37190000
H	0.45873900	0.93032300	-1.18750500
C	2.01452500	-0.67198500	0.37080800
H	2.44863100	0.33924800	-0.04134500
C	2.83671500	-1.62896700	-0.60941400
H	2.57040800	-2.64641200	-0.30740600
C	4.33099400	-1.40180900	-0.43924900
H	4.65456300	-1.58125300	0.58552300
H	4.87590100	-2.08252000	-1.09657800
H	4.59533400	-0.37695400	-0.71485400
C	2.38357200	-1.38322700	-2.04376500
H	1.32542000	-1.60531400	-2.18457500
H	2.56473700	-0.34314700	-2.33246000
H	2.95886900	-2.02949500	-2.71056000
C	-3.79207600	-0.68631800	-0.08566600
H	-4.19126100	-1.37930600	0.65880000

C	-4.23614800	-1.10489200	-1.48623800
H	-3.85111600	-2.10103100	-1.70750500
H	-5.32467400	-1.12422300	-1.55697000
H	-3.85590600	-0.40943100	-2.23582800
C	-4.32193600	0.68971500	0.26697900
O	-4.72552500	1.50534100	-0.52197300
O	-4.26657800	0.92274900	1.58541100
H	-4.57903100	1.82371800	1.75470800
O	2.47755800	-0.81874400	1.59912000
O	2.83618000	0.77517300	2.37079100
H	1.98142900	0.94913100	2.79206900
O	3.05206000	1.77454500	0.19825500
H	2.94022600	1.40742300	1.53195000
C	2.62340300	2.76107700	-0.52572200
O	2.16912800	2.65623100	-1.64967200
H	2.71013100	3.74783200	-0.04041200

TS6-CH₃COOH

C	-0.49853800	-1.65942300	1.11012800
C	-1.88185700	-1.55253700	1.02134900
C	-2.46711900	-0.68418100	0.10063700
C	-1.64325900	0.08337400	-0.72613100
C	-0.26051300	-0.01724200	-0.63581000
C	0.32276500	-0.89395900	0.28162800
H	-0.05184400	-2.34230100	1.82501200
H	-2.51223900	-2.15360300	1.66791800
H	-2.08439300	0.77197700	-1.44017600
H	0.37193800	0.59150300	-1.27561400
C	1.81907000	-1.02033200	0.38297800
H	2.31735700	-0.04648600	-0.07735400
C	2.55097600	-2.06906400	-0.55760700
H	2.20383800	-3.05223500	-0.22391400

C	4.06067400	-1.96477800	-0.39155100
H	4.36729000	-2.13436400	0.64027300
H	4.54653800	-2.71154200	-1.02290400
H	4.41075500	-0.97603300	-0.70129500
C	2.12661200	-1.84217400	-2.00439200
H	1.05313100	-1.97549600	-2.14306600
H	2.39737100	-0.83299800	-2.33085300
H	2.64366500	-2.55990700	-2.64503000
C	-3.97947700	-0.58883700	-0.02212600
H	-4.42184300	-1.18778400	0.77731100
C	-4.47802300	-1.07391400	-1.38235000
H	-4.17628500	-2.11110400	-1.53292100
H	-5.56584700	-1.01178600	-1.43961500
H	-4.05750500	-0.46781900	-2.18595300
C	-4.39024100	0.84884800	0.22733200
O	-4.71879400	1.63739900	-0.62145000
O	-4.31948000	1.17049600	1.52640300
H	-4.55360700	2.10478000	1.62800300
O	2.27675800	-1.13051900	1.61832200
O	2.83088500	0.45273200	2.27353300
H	2.01871900	0.72523300	2.72503300
O	3.03808400	1.30367200	0.06582700
H	2.95304300	1.03368000	1.36985500
C	2.60859100	2.32491800	-0.63849100
O	2.14862100	2.19815200	-1.75954900
C	2.73865200	3.66463600	0.04716100
H	2.15212300	3.65321000	0.96842300
H	3.78086900	3.83499700	0.32111800
H	2.38845900	4.46061500	-0.60546300

TS7

C	0.35046500	1.15867200	0.11750400
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C	-1.02682700	1.01572600	0.18790100
C	-1.69310000	0.11152300	-0.64624300
C	-0.95455100	-0.64008800	-1.55716100
C	0.42797000	-0.49854800	-1.63148500
C	1.08686900	0.39676400	-0.79200800
H	0.86900200	1.85830800	0.76351900
H	-1.59327400	1.60865500	0.89945900
H	-1.46086000	-1.33847300	-2.21435300
H	0.99228100	-1.07983700	-2.35429000
C	2.56628700	0.54124100	-0.87610800
H	3.06789200	0.03723600	-1.71558700
C	3.25224600	-1.00287600	0.26461700
H	4.20857100	-0.48764000	0.28994700
C	3.13979900	-2.24591500	-0.53737600
H	3.68462900	-2.20178100	-1.47885700
H	3.59864900	-3.03269200	0.07916400
H	2.10098400	-2.53734500	-0.70040300
C	2.46228300	-0.88280000	1.50386300
H	2.38025600	0.15801600	1.81699600
H	1.49954400	-1.39047300	1.44516600
H	3.08376200	-1.36873900	2.27505500
C	-3.20582400	-0.02142000	-0.57843600
H	-3.50082500	-0.85375400	-1.22154300
C	-3.91392200	1.26008600	-1.01490500
H	-3.63401800	1.50011400	-2.04142800
H	-4.99715000	1.13933400	-0.96456200
H	-3.63122900	2.09522700	-0.37249200
C	-3.59107800	-0.40275900	0.83721700
O	-4.06172400	0.34357300	1.65701700
O	-3.31742900	-1.68802300	1.09941200
H	-3.54559100	-1.87172500	2.02264800
O	3.14632000	1.54523000	-0.38754200
O	4.10538000	1.40144800	1.46699500

H	4.49329600	2.21012100	1.12021300
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TS8

C	-1.00219600	-0.10365000	1.01293100
C	0.35190500	-0.21885100	1.29865200
C	1.31664900	0.27690500	0.42106600
C	0.89043100	0.88684000	-0.76134100
C	-0.46121300	0.99958000	-1.05128200
C	-1.44158600	0.51472800	-0.16904800
H	-1.72127900	-0.50774200	1.71628200
H	0.66492600	-0.70530300	2.21672000
H	1.62241700	1.27089800	-1.46542600
H	-0.77312000	1.47186400	-1.97711100
C	-2.85095300	0.64756900	-0.52154300
H	-3.05440800	1.02827100	-1.52038900
C	-3.90518800	0.25628800	0.24536300
H	-3.73849200	0.02118500	1.29260200
C	-3.93873100	-2.03459700	-0.07658400
H	-2.88764600	-2.26703500	0.03461200
H	-4.60098600	-2.30888300	0.73497500
H	-4.34871100	-2.04013700	-1.07789300
C	-5.32834400	0.55368300	-0.14308900
H	-5.65036400	1.49991700	0.30268500
H	-5.42700500	0.63870500	-1.22719300
H	-6.01110700	-0.22154600	0.20748500
C	2.79870000	0.16333200	0.74103000
H	2.90084900	-0.40104800	1.67080900
C	3.47255000	1.52801400	0.87551800
H	2.99135200	2.09432300	1.67387100
H	4.53185900	1.41547800	1.11210100
H	3.38771000	2.09312700	-0.05359500
C	3.45282200	-0.66025900	-0.34994600

O	4.10780000	-0.21907300	-1.25979800
O	3.19168100	-1.96833700	-0.21621300
H	3.58908700	-2.44029800	-0.96279500

TS9

C	0.69888100	0.82390500	-0.87612400
C	-0.65922900	0.98236100	-1.09712500
C	-1.59297000	0.63166800	-0.11762500
C	-1.13424900	0.10794000	1.09452600
C	0.22188400	-0.05766900	1.32183600
C	1.17503600	0.30938400	0.34892900
H	1.39722500	1.10524800	-1.65566800
H	-1.00560100	1.38203500	-2.04429700
H	-1.84579300	-0.18093500	1.86200400
H	0.56555400	-0.47058200	2.26452800
C	2.55487100	0.04415400	0.59040900
H	2.82539100	-0.25763200	1.59895400
C	3.67575700	0.44542900	-0.31519100
H	3.39472200	0.21894800	-1.34990300
C	4.95363600	-0.32417700	0.02462800
H	4.80902100	-1.40152200	-0.06922900
H	5.76556400	-0.02655500	-0.64190400
H	5.26185500	-0.10664500	1.05161600
C	3.91980200	1.96178500	-0.20113000
H	3.02780000	2.53420200	-0.46243600
H	4.20383200	2.22072100	0.82267700
H	4.73286000	2.26090100	-0.86690900
C	-3.08071100	0.82397200	-0.35641900
H	-3.21901700	1.14275200	-1.39225200
C	-3.69112000	1.84989800	0.59744100
H	-3.19231400	2.81103700	0.46751400
H	-4.75649400	1.97665300	0.39871200

H	-3.57120800	1.53192600	1.63397800
C	-3.76293900	-0.52293100	-0.21601900
O	-4.41776500	-0.87779900	0.73063500
O	-3.52912800	-1.31381300	-1.27230800
H	-3.94988000	-2.17203300	-1.11580100
O	1.26955000	-2.54557000	-0.07364200
O	2.41291700	-2.14067300	-0.04598400

TS10

C	-0.41830900	-0.82987500	1.21691700
C	0.95498800	-0.70670500	1.39553100
C	1.72340800	0.03785400	0.50344500
C	1.09296700	0.65532500	-0.58075400
C	-0.27710500	0.54078700	-0.76044800
C	-1.04960200	-0.19468100	0.14497500
H	-1.00525200	-1.41871500	1.91119000
H	1.43273900	-1.19763700	2.23629100
H	1.67938600	1.22303100	-1.29621700
H	-0.74757600	1.01062400	-1.61616800
C	-2.52481500	-0.31379300	-0.01318000
H	-2.77289900	-0.81559300	-1.19472400
C	-3.45740200	0.86418100	0.24021300
H	-3.45614100	0.97116000	1.33528700
C	-4.88378200	0.55157400	-0.21327800
H	-5.23502500	-0.39696000	0.19283300
H	-5.55597800	1.34411500	0.11995400
H	-4.93179300	0.50137400	-1.30483000
C	-2.96598700	2.17205300	-0.37534000
H	-1.98903300	2.46991200	0.00660800
H	-2.90652800	2.09020400	-1.46464400
H	-3.67755900	2.96556400	-0.14011900
C	3.22062500	0.19561300	0.70961900

H	3.51901900	-0.45539200	1.53472400
C	3.60626300	1.64250900	1.01368300
H	3.08569000	1.97742600	1.91161800
H	4.68153900	1.72898200	1.17667500
H	3.33114400	2.29718400	0.18554300
C	3.93266200	-0.31021800	-0.52979200
O	4.44325900	0.38262900	-1.37199100
O	3.90734500	-1.64738300	-0.60862400
H	4.33761300	-1.91771500	-1.43314100
O	-3.25427200	-1.99497800	-0.85410700
O	-3.03543500	-1.51593200	0.50091800

TS10-H₂O

C	-0.41652127	-0.84141483	1.20893274
C	0.95679006	-0.71860774	1.38768640
C	1.72345479	0.03714759	0.50354054
C	1.09123638	0.66630208	-0.57287865
C	-0.27886159	0.55214288	-0.75261562
C	-1.04960200	-0.19468100	0.14497500
H	-1.00208668	-1.43895406	1.89690777
H	1.43593430	-1.21861292	2.22228405
H	1.67628393	1.24295255	-1.28228562
H	-0.75071391	1.03123610	-1.60242240
C	-2.52481500	-0.31379300	-0.01318000
H	-2.40850335	-0.56935967	-1.30910950
C	-3.45740200	0.86418100	0.24021300
H	-3.45614100	0.97116000	1.33528700
C	-4.88378200	0.55157400	-0.21327800
H	-5.23502500	-0.39696000	0.19283300
H	-5.55597800	1.34411500	0.11995400
H	-4.93179300	0.50137400	-1.30483000
C	-2.96598700	2.17205300	-0.37534000

H	-1.98903300	2.46991200	0.00660800
H	-2.90652800	2.09020400	-1.46464400
H	-3.67755900	2.96556400	-0.14011900
C	3.22066925	0.19437733	0.71013689
H	3.51101237	-0.42221418	1.56404586
C	3.61414454	1.65063842	0.95336615
H	3.09152507	2.02725483	1.83341267
H	4.68917679	1.73740146	1.11780547
H	3.34711344	2.27062098	0.09638209
C	3.93525202	-0.36892913	-0.50273515
O	4.45422275	0.28370885	-1.37151503
O	3.90173382	-1.70806859	-0.52389462
H	4.33412094	-2.01642989	-1.33382852
O	-3.40715554	-2.53885316	-0.73084445
O	-3.03543500	-1.51593200	0.50091800
O	-2.64780507	-1.02465399	-2.53280576
H	-3.52890250	-0.67734460	-2.68978826
H	-3.12496288	-1.96195049	-1.76294617

TS10-NH₃

C	-0.38310344	-1.03309351	1.04158309
C	0.99056674	-0.91710607	1.22212563
C	1.72446557	0.02423032	0.50384077
C	1.05895149	0.84806521	-0.40862886
C	-0.31170312	0.74081591	-0.58837783
C	-1.04960200	-0.19468100	0.14497500
H	-0.94298273	-1.77456320	1.59836625
H	1.49578153	-1.56805179	1.92722513
H	1.61833178	1.57355343	-0.99071578
H	-0.80949053	1.37465149	-1.31281322
C	-2.52481500	-0.31379300	-0.01318000
H	-2.40850335	-0.56935967	-1.30910950

C	-3.45740200	0.86418100	0.24021300
H	-3.51145541	0.92691806	1.33738001
C	-4.86159216	0.58734057	-0.29788225
H	-5.24273244	-0.37248130	0.05066991
H	-5.54210587	1.37386277	0.03271748
H	-4.85383877	0.58175449	-1.39160047
C	-2.92191110	2.18977173	-0.29549408
H	-1.96299225	2.46018423	0.14767079
H	-2.80726740	2.15117711	-1.38277744
H	-3.63669075	2.98168817	-0.06466565
C	3.22181606	0.17107165	0.71699219
H	3.54106952	-0.60243997	1.41941780
C	3.58987455	1.55395988	1.25255986
H	3.07658031	1.72663380	2.19922012
H	4.66584973	1.63049504	1.41590683
H	3.29379533	2.33198834	0.54749640
C	3.92445844	-0.11031942	-0.59682440
O	4.41317400	0.72102370	-1.31798399
O	3.91806228	-1.41619283	-0.89602233
H	4.34110038	-1.53887750	-1.75859144
O	-3.40715554	-2.53885316	-0.73084445
O	-3.03543500	-1.51593200	0.50091800
H	-3.52890250	-0.67734460	-2.68978826
H	-3.12496288	-1.96195049	-1.76294617
N	-2.61109268	-1.03912521	-2.52626482
H	-1.89166371	-1.09582760	-3.38760592

TS10-CH₃OH

C	-0.46291529	-0.49070282	1.37754618
C	0.91021816	-0.35855383	1.55092329
C	1.72253049	0.05609302	0.49789361
C	1.13628745	0.33148174	-0.74093402

C	-0.23328782	0.20712778	-0.91786858
C	-1.04960200	-0.19468100	0.14497500
H	-1.08436955	-0.82265467	2.20025646
H	1.35326311	-0.58331011	2.51494269
H	1.75686024	0.63686936	-1.57741024
H	-0.66953694	0.40703165	-1.88950207
C	-2.52481500	-0.31379300	-0.01318000
H	-2.40850335	-0.56935967	-1.30910950
C	-3.45740200	0.86418100	0.24021300
H	-3.57149787	0.88001249	1.33445459
C	-4.83248799	0.62929601	-0.38580991
H	-5.24256543	-0.33966581	-0.10126815
H	-5.52185384	1.40957902	-0.05878482
H	-4.76420034	0.67101259	-1.47663868
C	-2.87895057	2.20463017	-0.20645615
H	-1.94323454	2.44302736	0.30014594
H	-2.70465130	2.21169614	-1.28645045
H	-3.59694164	2.99507350	0.01940111
C	3.22020250	0.22600211	0.69067287
H	3.46981029	-0.09761000	1.70389343
C	3.66370790	1.67216923	0.47484133
H	3.13826404	2.32284363	1.17483025
H	4.73775530	1.77447193	0.63676350
H	3.43758083	1.99733355	-0.54164299
C	3.93700380	-0.71255296	-0.26028011
O	4.49763022	-0.38348641	-1.27391646
O	3.85312827	-1.98818885	0.14044878
H	4.28961082	-2.54930751	-0.51732555
O	-3.40715554	-2.53885316	-0.73084445
O	-3.03543500	-1.51593200	0.50091800
O	-2.64780507	-1.02465399	-2.53280576
H	-3.12496288	-1.96195049	-1.76294617
C	-3.70224398	-0.97039870	-3.49723043

H	-4.44555374	-0.27184829	-3.17409279
H	-3.30646357	-0.65888335	-4.44127283
H	-4.14370007	-1.93986789	-3.59795781

TS10-C₂H₅OH

C	-0.45581474	-0.55224943	1.35766764
C	0.91731614	-0.42151850	1.53213676
C	1.72262740	0.05309927	0.49924441
C	1.12937105	0.39039838	-0.72079246
C	-0.24026096	0.26766069	-0.89841508
C	-1.04960200	-0.19468100	0.14497500
H	-1.07175496	-0.93096742	2.16416621
H	1.36587726	-0.69451304	2.48103323
H	1.74451685	0.74331496	-1.54244335
H	-0.68192166	0.51628146	-1.85626163
C	-2.52481500	-0.31379300	-0.01318000
H	-2.40850335	-0.56935967	-1.30910950
C	-3.39153143	0.90952580	0.25856071
H	-3.48883597	0.92604108	1.35441299
C	-4.78581790	0.74888568	-0.34814938
H	-5.24126051	-0.19895903	-0.06148415
H	-5.42914858	1.56214722	-0.00793833
H	-4.73123276	0.79218900	-1.43968782
C	-2.75110474	2.22043736	-0.19120357
H	-1.79709925	2.40782515	0.30256026
H	-2.59229456	2.22361437	-1.27360234
H	-3.42395604	3.04580202	0.04831184
C	3.22016925	0.22122993	0.69457714
H	3.47606726	-0.15421123	1.68815899
C	3.65464600	1.67935706	0.55395406
H	3.12869280	2.28893148	1.28964773
H	4.72881397	1.77915675	0.71663672

H	3.42220499	2.05665754	-0.44290159
C	3.93796672	-0.66139475	-0.30779093
O	4.49225012	-0.27578471	-1.30484672
O	3.86298013	-1.95695369	0.02502992
H	4.29966232	-2.47985490	-0.66338944
O	-3.40715554	-2.53885316	-0.73084445
O	-3.03543500	-1.51593200	0.50091800
O	-2.64780507	-1.02465399	-2.53280576
H	-3.12496288	-1.96195049	-1.76294617
C	-3.66740576	-0.99292545	-3.53495731
H	-4.42913263	-0.29886985	-3.24693128
H	-4.09476876	-1.96823724	-3.63997059
C	-3.05403645	-0.55395771	-4.87759852
H	-2.29231043	-1.24801435	-5.16562431
H	-3.81695474	-0.53021529	-5.62745982
H	-2.62667215	0.42135349	-4.77258510

TS10-HCOOH

C	-0.47430464	-0.38424995	1.40360858
C	0.89886222	-0.24983788	1.57496971
C	1.72241882	0.06098754	0.49524896
C	1.14740243	0.22944164	-0.76776059
C	-0.22210469	0.10244017	-0.94333692
C	-1.04960200	-0.19468100	0.14497500
H	-1.10462435	-0.63517824	2.24799101
H	1.33306782	-0.39121575	2.55864415
H	1.77667023	0.45268606	-1.62347585
H	-0.64971037	0.21832013	-1.93231200
C	-2.52481500	-0.31379300	-0.01318000
H	-2.40850335	-0.56935967	-1.30910950
C	-3.46940867	0.81084850	0.39237342
H	-3.57187730	0.68989049	1.48118125

C	-4.84809719	0.63600697	-0.24526717
H	-5.24281475	-0.36626000	-0.07891360
H	-5.54368811	1.36031923	0.18197664
H	-4.79212009	0.81301103	-1.32315724
C	-2.91277993	2.20407377	0.10951099
H	-1.97473413	2.39105308	0.63310645
H	-2.75025146	2.34682747	-0.96288060
H	-3.63821240	2.95056018	0.43788441
C	3.22035868	0.23358996	0.68350139
H	3.45982215	-0.00002240	1.72356257
C	3.67969349	1.65034180	0.34217252
H	3.15599160	2.36611152	0.97688739
H	4.75357712	1.75678183	0.50250624
H	3.46374672	1.88498857	-0.70109808
C	3.93424996	-0.79320340	-0.17385264
O	4.50501887	-0.56173038	-1.20859343
O	3.83495557	-2.02685875	0.33908087
H	4.27030604	-2.64881994	-0.26231125
O	-3.40715554	-2.53885316	-0.73084445
O	-3.01463983	-1.57716347	0.35306363
O	-2.76031418	-0.93852230	-2.79628769
H	-3.12496288	-1.96195049	-1.76294617
C	-2.96627680	-0.57887991	-4.07258403
H	-2.25616347	-1.07378659	-4.70163605
O	-3.81093042	0.19001731	-4.54092960

TS10-CH₃COOH

C	-0.54419326	-0.27876880	1.44441841
C	0.81643531	-0.11686925	1.67999619
C	1.69696188	0.11686722	0.62610101
C	1.19220748	0.17956588	-0.67601482
C	-0.16457778	0.02476118	-0.91617196

C	-1.04960200	-0.19468100	0.14497500
H	-1.21903894	-0.46924138	2.26998073
H	1.19600260	-0.17599276	2.69418093
H	1.86680487	0.34154067	-1.51072864
H	-0.53710321	0.05812019	-1.93325528
C	-2.52481500	-0.31379300	-0.01318000
H	-2.40850335	-0.56935967	-1.30910950
C	-3.46940867	0.81084850	0.39237342
H	-3.52623738	0.72580219	1.48789648
C	-4.86975257	0.59517824	-0.18248345
H	-5.24214665	-0.40619157	0.03337688
H	-5.55859828	1.32396101	0.24807376
H	-4.85978890	0.73596074	-1.26709946
C	-2.94589034	2.20117085	0.04044207
H	-1.99054528	2.41895389	0.51890812
H	-2.82873062	2.30939310	-1.04186075
H	-3.66885652	2.94831589	0.37273338
C	3.18099073	0.31947682	0.88234723
H	3.36354707	0.17078634	1.94921605
C	3.64990983	1.70980916	0.45600172
H	3.08725216	2.46765506	1.00238883
H	4.71251277	1.83980834	0.66632918
H	3.49100570	1.85952633	-0.61284808
C	3.94786099	-0.76389504	0.14939653
O	4.57397887	-0.60839061	-0.86738278
O	3.82772491	-1.95444186	0.75191731
H	4.29973575	-2.61708755	0.22642260
O	-3.40715554	-2.53885316	-0.73084445
O	-3.01463983	-1.57716347	0.35306363
O	-2.72215157	-0.83545043	-2.65979535
H	-3.12496288	-1.96195049	-1.76294617
C	-2.92655858	-0.47393188	-3.93581169
O	-3.76991485	0.29653003	-4.40392375

C	-1.88747032	-1.19811449	-4.85628529
H	-0.89659399	-0.92193395	-4.56168659
H	-2.00524415	-2.25746710	-4.76246964
H	-2.05045982	-0.90984887	-5.87375143

TS11

C	0.62993948	1.65604624	0.48132481
C	-0.74289492	1.57577164	0.66886663
C	-1.42410161	0.38874179	0.39976349
C	-0.70391765	-0.71609683	-0.05742505
C	0.67224132	-0.64252261	-0.23023126
C	1.35517800	0.54763600	0.03595900
H	1.15724445	2.58027602	0.68385810
H	-1.29109021	2.44058475	1.02588550
H	-1.22061734	-1.64373145	-0.28235644
H	1.19674817	-1.51503508	-0.59374942
C	2.83480000	0.71763500	-0.15836000
C	3.81410900	-0.42531358	0.07951106
H	4.77088010	0.08925037	0.20079957
C	3.93580316	-1.31281797	-1.16951704
H	4.16659942	-0.71382678	-2.05251236
H	4.74739601	-2.02819606	-1.02153256
H	3.02548331	-1.87985652	-1.36923913
C	3.54618791	-1.23364706	1.35278885
H	3.37319252	-0.57900784	2.20993681
H	2.68819219	-1.89914434	1.25560744
H	4.42060470	-1.85007973	1.57141435
C	-2.92261471	0.28465821	0.62894552
H	-3.30219160	1.28585339	0.84567684
C	-3.25696487	-0.66701991	1.77680469
H	-2.78223109	-0.31452175	2.69314733
H	-4.33518139	-0.71630599	1.93496872

H	-2.89461820	-1.67298171	1.56056800
C	-3.57898004	-0.16394766	-0.66241662
O	-4.01111498	-1.26686617	-0.87856456
O	-3.60256391	0.81652111	-1.57497308
H	-3.99493526	0.47205994	-2.39083753
O	3.28385121	1.86019471	-0.51789157
O	3.49902448	2.30970382	-2.09733466
H	2.73629191	1.94525739	-2.62405452

TS12

C	0.51987000	-0.83698900	-0.94234600
C	-0.82471100	-0.66265800	-1.25430600
C	-1.67076100	0.03763800	-0.39656000
C	-1.15095700	0.55020900	0.79389100
C	0.18661300	0.36272600	1.11705800
C	1.03453000	-0.32637800	0.24883500
H	1.16597700	-1.37989400	-1.62181200
H	-1.21802000	-1.07243300	-2.17840800
H	-1.79739300	1.08889400	1.47970700
H	0.57463300	0.75131600	2.05331900
C	2.48935700	-0.44664400	0.59816800
H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500
H	4.37382100	-0.16925400	0.08371000
C	3.61075100	1.85062900	0.96139200
H	3.88723900	1.53064300	1.96782600
H	4.38111900	2.51798900	0.57095300
H	2.68265300	2.43343400	1.03648300
C	3.19860800	1.01716000	-1.41234400
H	3.12932900	0.11632200	-2.02522300
H	2.27117500	1.58851800	-1.54122500
H	4.02430900	1.63216700	-1.77432200

C	-3.13223500	0.25836200	-0.75325700
H	-3.34680400	-0.30524400	-1.66425800
C	-3.45697400	1.73688600	-0.95860800
H	-2.83858000	2.13737300	-1.76280700
H	-4.50725900	1.86935500	-1.22265600
H	-3.25760600	2.30579200	-0.04942500
C	-3.98619800	-0.34136100	0.34607600
O	-4.55310100	0.28109900	1.20747900
O	-4.02022100	-1.67918200	0.27781500
H	-4.53878100	-2.01489600	1.02381900
O	4.41881700	-1.46144500	0.20327800
O	3.04511200	-1.61980000	0.00989700

TS12-H₂O

C	0.52956256	-0.78855335	-0.96603640
C	-0.81574104	-0.61477800	-1.27517836
C	-1.67229724	0.03730073	-0.39027831
C	-1.16220485	0.50152162	0.82397188
C	0.17619197	0.31403112	1.14369294
C	1.03453000	-0.32637800	0.24883500
H	1.18386533	-1.29353265	-1.66657757
H	-1.20138310	-0.98689920	-2.21824678
H	-1.81681284	1.00199729	1.53066638
H	0.55673292	0.66438841	2.09793856
C	2.48935700	-0.44664400	0.59816800
H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500
H	4.47148164	-0.00724197	0.10021004
C	3.75735548	1.76251395	1.02092139
H	4.11180860	1.35093036	1.96786805
H	4.52032331	2.42453018	0.60752879
H	2.87198604	2.37766379	1.23158191

C	3.07795610	1.14119520	-1.35637425
H	2.90407377	0.29637725	-2.02568501
H	2.17317849	1.76128849	-1.34902368
H	3.89594639	1.74636021	-1.75097662
C	-3.13483428	0.25817714	-0.74249571
H	-3.34012575	-0.26629100	-1.67865968
C	-3.47486851	1.74086838	-0.88271376
H	-2.85807148	2.18357385	-1.66572736
H	-4.52560727	1.87382017	-1.14470585
H	-3.28482822	2.27055012	0.05181142
C	-3.98604717	-0.39929470	0.32550285
O	-4.56264337	0.17784640	1.21167189
O	-4.00532962	-1.73299890	0.19727085
H	-4.52279977	-2.10732631	0.92544251
O	3.48860444	-2.65957417	-0.06967464
O	2.45919146	-1.86206007	0.43412902
O	5.34888910	-0.92129671	0.44387257
H	6.04613076	-1.09219091	-0.19350428
H	4.38483947	-1.74169006	0.25288801

TS12-NH₃

C	0.52419296	-0.81579694	-0.95305347
C	-0.82070580	-0.64169419	-1.26376873
C	-1.67143529	0.03752617	-0.39379037
C	-1.15596247	0.52894341	0.80741555
C	0.18197016	0.34143698	1.12906429
C	1.03453000	-0.32637800	0.24883500
H	1.17395084	-1.34212306	-1.64201620
H	-1.21059626	-1.03499772	-2.19643683
H	-1.80603934	1.05092347	1.50264322
H	0.56665317	0.71329484	2.07346202
C	2.48935700	-0.44664400	0.59816800

H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500
H	4.47148164	-0.00724197	0.10021004
C	3.70827982	1.79320295	1.00342374
H	4.03786250	1.41206963	1.97185478
H	4.47399368	2.45676261	0.59765323
H	2.80701391	2.39897047	1.16904891
C	3.11692970	1.09966749	-1.37743087
H	2.97825129	0.23511641	-2.02954209
H	2.20285633	1.70481031	-1.41569692
H	3.93789860	1.70779057	-1.76114981
C	-3.13337531	0.25834345	-0.74851448
H	-3.34381717	-0.28817372	-1.67082007
C	-3.46481654	1.73908310	-0.92519066
H	-2.84706034	2.15828632	-1.72029000
H	-4.51529985	1.87177672	-1.18833550
H	-3.26959781	2.29086327	-0.00462363
C	-3.98621778	-0.36699443	0.33733348
O	-4.55743940	0.23565238	1.20990055
O	-4.01376954	-1.70335274	0.24262598
H	-4.53190881	-2.05617575	0.98098765
O	3.48860444	-2.65957417	-0.06967464
O	2.45919146	-1.86206007	0.43412902
H	6.11100828	-1.07665387	-0.19362661
H	4.38483947	-1.74169006	0.25288801
N	5.37716144	-0.89678773	0.47721252
H	5.43896062	-0.96436970	1.53887014

TS12-CH₃OH

C	0.51441614	-0.86284316	-0.92853384
C	-0.82977371	-0.68826628	-1.24203815
C	-1.66993369	0.03769623	-0.39998534

C	-1.14466603	0.57607272	0.77659591
C	0.19245966	0.38866243	1.10163830
C	1.03453000	-0.32637800	0.24883500
H	1.15592683	-1.42594201	-1.59581030
H	-1.22739344	-1.11812932	-2.15510351
H	-1.78651706	1.13510965	1.45032405
H	0.58469235	0.79767467	2.02738604
C	2.48935700	-0.44664400	0.59816800
H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500
H	4.47148164	-0.00724197	0.10021004
C	3.81618614	1.72415630	1.03870167
H	4.19883793	1.27634841	1.95782719
H	4.57550854	2.38464504	0.61625291
H	2.95196819	2.34865294	1.30289388
C	3.03309577	1.19098687	-1.32807988
H	2.81676451	0.37111401	-2.01578520
H	2.14171309	1.82720908	-1.26602782
H	3.84699267	1.79304841	-1.73567967
C	-3.13083717	0.25824818	-0.75911756
H	-3.35058998	-0.32612909	-1.65568117
C	-3.44737735	1.73321019	-0.99983955
H	-2.82833860	2.11032858	-1.81476884
H	-4.49742094	1.86537584	-1.26499737
H	-3.24279815	2.32293085	-0.10519310
C	-3.98598610	-0.30946300	0.35617516
O	-4.54745067	0.33713572	1.20323964
O	-4.02795172	-1.64832735	0.32063267
H	-4.54690217	-1.96269895	1.07561033
O	3.48860444	-2.65957417	-0.06967464
O	2.45919146	-1.86206007	0.43412902
O	5.35495114	-0.99369277	0.52470145
H	4.38483947	-1.74169006	0.25288801

C	6.39355069	-1.24825392	-0.42472448
H	7.29569538	-0.77130247	-0.10292909
H	6.55567450	-2.30309176	-0.50175042
H	6.10641578	-0.86084325	-1.37990326

TS12-C₂H₅OH

C	0.55027626	-0.67226302	-1.01226474
C	-0.79671263	-0.50028463	-1.31500678
C	-1.67591913	0.03537896	-0.37585624
C	-1.18658951	0.38348751	0.88488789
C	0.15376537	0.19660612	1.19666411
C	1.03453000	-0.32637800	0.24883500
H	1.22223388	-1.08572647	-1.75482456
H	-1.16593945	-0.78190200	-2.29527983
H	-1.85878295	0.79182734	1.63309857
H	0.51836269	0.45529963	2.18575098
C	2.48935700	-0.44664400	0.59816800
H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500
H	4.47148164	-0.00724197	0.10021004
C	3.88521034	1.67696585	1.05510788
H	4.29869475	1.18704563	1.93871121
H	4.63976279	2.33611235	0.62214675
H	3.04872976	2.30977931	1.38147211
C	2.98305590	1.24941889	-1.29062783
H	2.71657576	0.46061106	-1.99681467
H	2.11052778	1.90206456	-1.16437185
H	3.79142142	1.84845623	-1.71340827
C	-3.14098025	0.25579339	-0.71772097
H	-3.32611146	-0.17361326	-1.70511692
C	-3.51742244	1.73627832	-0.70707455
H	-2.90635569	2.27274169	-1.43394556

H	-4.56925787	1.86997256	-0.96424383
H	-3.34765722	2.17066621	0.27908077
C	-3.98301552	-0.52949760	0.26805192
O	-4.58047081	-0.06163645	1.20346825
O	-3.96758578	-1.84278118	0.00228833
H	-4.48069282	-2.30314115	0.68267072
O	3.48860444	-2.65957417	-0.06967464
O	2.45919146	-1.86206007	0.43412902
O	5.35495114	-0.99369277	0.52470145
H	4.38483947	-1.74169006	0.25288801
C	6.31045650	-1.34609489	-0.47915225
H	6.43487579	-2.40870660	-0.49577117
H	5.96326245	-1.01265537	-1.43475382
C	7.66009093	-0.67614187	-0.16095441
H	8.00728457	-1.00958127	0.79464736
H	8.37504953	-0.93982747	-0.91208963
H	7.53567130	0.38646980	-0.14433555

TS12-HCOOH

C	0.53012922	-0.78561589	-0.96738500
C	-0.81521779	-0.61187807	-1.27635909
C	-1.67238985	0.03727107	-0.38990281
C	-1.16286531	0.49855946	0.82570262
C	0.17558143	0.31107369	1.14521741
C	1.03453000	-0.32637800	0.24883500
H	1.18491230	-1.28829132	-1.66913330
H	-1.20041137	-0.98171487	-2.22050881
H	-1.81795206	0.99671457	1.53359207
H	0.55568546	0.65911338	2.10048474
C	2.48935700	-0.44664400	0.59816800
H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500

H	4.47148164	-0.00724197	0.10021004
C	3.92351891	1.64974592	1.06211665
H	4.35305553	1.13663614	1.92464935
H	4.67519203	2.30835923	0.62337428
H	3.10380740	2.28592821	1.42268756
C	2.95650427	1.28185489	-1.26783914
H	2.66202911	0.51113431	-1.98282410
H	2.09591775	1.94243889	-1.10593841
H	3.76145689	1.87950419	-1.69901248
C	-3.13499113	0.25814988	-0.74185186
H	-3.33973745	-0.26393563	-1.67946589
C	-3.47595036	1.74099279	-0.87816546
H	-2.85926587	2.18619573	-1.65985055
H	-4.52671670	1.87397041	-1.14003380
H	-3.28645823	2.26828644	0.05782039
C	-3.98601593	-0.40273461	0.32418848
O	-4.56318002	0.17165414	1.21177498
O	-4.00441003	-1.73610193	0.19237285
H	-4.52179963	-2.11271588	0.91942187
O	3.48860444	-2.65957417	-0.06967464
O	2.45919146	-1.86206007	0.43412902
O	5.55164216	-0.94673956	0.09802677
H	4.38483947	-1.74169006	0.25288801
C	6.87232736	-1.22015384	-0.37729968
H	7.57543186	-1.06552694	0.41430287
O	7.25779206	-1.57945625	-1.48870363

TS12-CH₃COOH

C	0.53728935	-0.74740250	-0.98404812
C	-0.80861831	-0.57419118	-1.29086858
C	-1.67358921	0.03679329	-0.38507246
C	-1.17124046	0.45993057	0.84728276

C	0.16785345	0.27255826	1.16414142
C	1.03453000	-0.32637800	0.24883500
H	1.19815347	-1.22006898	-1.70079016
H	-1.18814235	-0.91430193	-2.24839572
H	-1.83238715	0.92786457	1.57000502
H	0.54244007	0.59045895	2.13201041
C	2.48935700	-0.44664400	0.59816800
H	2.62331900	-0.48827700	1.68506100
C	3.39310800	0.68255700	0.04391500
H	4.47148164	-0.00724197	0.10021004
C	3.84548828	1.70441254	1.04625629
H	4.24152731	1.23867569	1.95068334
H	4.60285100	2.36427190	0.61932986
H	2.99265863	2.33279065	1.33692584
C	3.01150947	1.21579070	-1.31274416
H	2.77393468	0.40886753	-2.00870575
H	2.12771534	1.85931602	-1.22343949
H	3.82315468	1.81648671	-1.72679755
C	-3.13702381	0.25763475	-0.73356395
H	-3.33485310	-0.23336454	-1.68928235
C	-3.48999032	1.74144078	-0.81954061
H	-2.87492671	2.21850426	-1.58350669
H	-4.54111603	1.87471998	-1.07980850
H	-3.30745373	2.23757529	0.13468489
C	-3.98538876	-0.44674888	0.30642362
O	-4.56974086	0.09179546	1.21160495
O	-3.99228248	-1.77486249	0.12852242
H	-4.50847978	-2.18066982	0.84055550
O	3.48860444	-2.65957417	-0.06967464
O	2.45919146	-1.86206007	0.43412902
O	5.53516049	-0.96840707	0.12073622
H	4.38483947	-1.74169006	0.25288801
C	6.86407885	-1.07226668	-0.39703708

O	7.25543048	-1.33540768	-1.53303915
C	7.87694674	-0.79194924	0.72862751
H	7.71975780	0.19441897	1.11238445
H	7.74351561	-1.50583896	1.51441222
H	8.87131242	-0.86966181	0.34120312

TS13

C	-0.24936800	-1.52168800	-0.49074000
C	1.13445500	-1.61708300	-0.31600600
C	1.86596600	-0.53247800	0.16945900
C	1.20681800	0.66099100	0.47687400
C	-0.17344200	0.77479800	0.30014300
C	-0.85356100	-0.32435000	-0.17704300
H	-0.82066800	-2.36782600	-0.85849800
H	1.64572600	-2.54425800	-0.55528100
H	1.77223800	1.50953400	0.85186900
H	-0.68529300	1.70215100	0.53619900
C	-3.14503700	-0.13654500	-0.54088400
H	-2.96362000	-0.32039800	-1.59653200
C	-3.45029200	1.08900100	-0.05859100
H	-4.32233600	-2.64622200	-0.63970100
C	-3.27013200	2.29436100	-0.92930600
H	-2.91791900	2.02781000	-1.92668600
H	-4.21793600	2.83372800	-1.02479400
H	-2.55453400	2.99266400	-0.48267300
C	-3.86718800	1.31715500	1.36040100
H	-4.05717400	0.38138600	1.88323300
H	-3.08835100	1.86895600	1.89903900
H	-4.76940700	1.93506800	1.39022100
C	3.36762500	-0.64987400	0.38813900
H	3.69309800	-1.61382200	-0.00983800
C	3.74636700	-0.53490900	1.86356100

H	3.24918500	-1.32439700	2.42865900
H	4.82508100	-0.63229500	1.99676200
H	3.43646900	0.43019000	2.26678400
C	4.05379300	0.42025300	-0.43637600
O	4.50291300	1.45228300	-0.00626000
O	4.08155200	0.10767900	-1.73956600
H	4.48740400	0.84115500	-2.22478000
O	-4.60449100	-1.84515700	-0.17639000
O	-3.34347200	-1.27870600	0.22324500

TS14

C	-0.49425400	-0.30612900	1.16059100
C	0.86389100	-0.14036000	1.40816600
C	1.73725600	0.20145200	0.37633600
C	1.22941200	0.35999100	-0.91363300
C	-0.12582800	0.17912200	-1.16552500
C	-0.99929300	-0.14884100	-0.13017600
H	-1.16154300	-0.56442700	1.97552900
H	1.24818800	-0.27151100	2.41387400
H	1.89586900	0.61941300	-1.73028200
H	-0.50779700	0.29749200	-2.17388500
C	-2.47114400	-0.30176900	-0.39602500
H	-2.67223200	-0.30844200	-1.47327200
C	-3.33243000	0.79438800	0.28584300
H	-3.07399300	0.77728800	1.34874600
C	-4.79340300	0.47016100	0.12271800
H	-4.73821800	-0.85946900	-0.02200600
H	-5.43607800	0.63553400	0.98406300
H	-5.23683900	0.76805000	-0.82767700
C	-2.98806400	2.16999500	-0.30162500
H	-1.94069100	2.41843400	-0.11827800
H	-3.16492300	2.17902100	-1.38062800

H	-3.61177900	2.94126500	0.15210900
C	3.21613100	0.42483300	0.65148900
H	3.41270300	0.14503300	1.68919200
C	3.63111500	1.87458200	0.40758900
H	3.04753100	2.53360700	1.05162600
H	4.69074800	2.01641100	0.62517000
H	3.45367400	2.15636500	-0.63128400
C	4.01395100	-0.52563200	-0.21886500
O	4.61448300	-0.22026400	-1.21730600
O	3.95538200	-1.78548500	0.23387700
H	4.44281600	-2.35726300	-0.37725000
O	-4.14703300	-1.85799000	-0.31328200
O	-2.86926700	-1.56595600	0.14333100

TS14-H₂O

C	-0.47710073	-0.42439473	1.13365498
C	0.88063899	-0.25897752	1.38367615
C	1.73624117	0.19989659	0.38284925
C	1.21123163	0.47656360	-0.88003653
C	-0.14338846	0.29660716	-1.13588557
C	-0.99929300	-0.14884100	-0.13017600
H	-1.13056932	-0.77479190	1.92505691
H	1.27845327	-0.48240211	2.36762665
H	1.86382952	0.82823384	-1.67302098
H	-0.53868178	0.50762328	-2.12377072
C	-2.47114400	-0.30176900	-0.39602500
H	-2.67223200	-0.30844200	-1.47327200
C	-3.33243000	0.79438800	0.28584300
H	-3.12503715	0.73132708	1.35815658
C	-4.79262889	0.52005206	0.04349196
H	-5.23006193	-0.69908714	-0.14331189
H	-5.47033041	0.67345079	0.87984360

H	-5.18214061	0.86507436	-0.91456035
C	-2.92209799	2.17934046	-0.23332511
H	-1.87796351	2.38960506	0.00729961
H	-3.04750371	2.23247752	-1.31824811
H	-3.54455721	2.95207668	0.21963803
C	3.21398844	0.42212024	0.66491163
H	3.42707497	0.04415300	1.66765338
C	3.60081258	1.89637118	0.56282177
H	3.01308318	2.47713968	1.27482598
H	4.66018570	2.03543188	0.78343403
H	3.40680511	2.27678162	-0.44106720
C	4.01845427	-0.42211184	-0.30334633
O	4.60229449	-0.00786486	-1.27200662
O	3.98699903	-1.72162434	0.02209651
H	4.47744500	-2.22064704	-0.64755809
O	-3.22048131	-2.77293451	-0.25739695
O	-2.37520784	-1.68966321	-0.06117950
O	-5.57256146	-1.88991012	-0.31972771
H	-6.06808941	-2.03526685	0.48954570
H	-4.51802394	-2.58083192	-0.15450438

TS14-NH₃

C	-0.48586169	-0.36596179	1.14854610
C	0.87207560	-0.20033823	1.39735478
C	1.73673385	0.20075353	0.37962862
C	1.22049087	0.41905795	-0.89821977
C	-0.13443029	0.23859699	-1.15211175
C	-0.99929300	-0.14884100	-0.13017600
H	-1.14637943	-0.67088740	1.95281787
H	1.26298875	-0.37818167	2.39329250
H	1.88015733	0.72518420	-1.70413985
H	-0.52291594	0.40383029	-2.15135073

C	-2.47114400	-0.30176900	-0.39602500
H	-2.66932330	-0.33643326	-1.47327398
C	-3.32891338	0.81646063	0.25367639
H	-3.12475705	0.78125398	1.32788567
C	-4.78977053	0.54274561	0.01461256
H	-5.23006193	-0.69908714	-0.14331189
H	-5.46899207	0.72183770	0.84459973
H	-5.17497504	0.86375776	-0.95347457
C	-2.91039595	2.18496148	-0.30134592
H	-1.86590545	2.39658699	-0.06347516
H	-3.03258061	2.20951400	-1.38765902
H	-3.53030029	2.97258623	0.12890777
C	3.21503032	0.42364139	0.65826830
H	3.41972918	0.09401448	1.67964022
C	3.61572836	1.88754082	0.48532141
H	3.02979589	2.50807930	1.16449961
H	4.67522054	2.02801645	0.70446056
H	3.43013539	2.21938249	-0.53721486
C	4.01655769	-0.47465092	-0.26262331
O	4.60890457	-0.11413489	-1.24747158
O	3.97169579	-1.75609149	0.12664867
H	4.46088379	-2.29202842	-0.51480662
O	-3.23293774	-2.76467559	-0.19318386
O	-2.38291285	-1.68060503	-0.02373200
H	-6.15098644	-2.03165247	0.48305824
H	-4.51802394	-2.58083192	-0.15450438
N	-5.63481149	-1.88023920	-0.35993490
H	-6.12943333	-2.17944524	-1.29379135

TS14-CH₃OH

C	-0.50016673	-0.26132664	1.16755406
C	0.85813729	-0.09549100	1.41421034

C	1.73765832	0.20186010	0.37387381
C	1.23573266	0.31564420	-0.92311653
C	-0.11975288	0.13453935	-1.17351350
C	-0.99929300	-0.14884100	-0.13017600
H	-1.17223919	-0.48466738	1.98886637
H	1.23776922	-0.19166664	2.42562677
H	1.90698718	0.54004998	-1.74618379
H	-0.49713378	0.21782892	-2.18709536
C	-2.47114400	-0.30176900	-0.39602500
H	-2.66697156	-0.36009557	-1.47268260
C	-3.32578839	0.83442337	0.22604217
H	-3.12426542	0.82280421	1.30126233
C	-4.78720654	0.56130440	-0.01025858
H	-5.23006193	-0.69908714	-0.14331189
H	-5.46760129	0.76197847	0.81380906
H	-5.16884072	0.86180250	-0.98631198
C	-2.90033888	2.18824090	-0.35891253
H	-1.85553640	2.40095724	-0.12339650
H	-3.01990708	2.18859954	-1.44579403
H	-3.51797863	2.98796004	0.05184626
C	3.21697691	0.42549034	0.64642760
H	3.40775998	0.18321124	1.69459685
C	3.64270930	1.86236414	0.35042640
H	3.06121022	2.54877208	0.96716854
H	4.70245988	2.00514527	0.56680872
H	3.47107449	2.10645406	-0.69890942
C	4.01157244	-0.56199818	-0.18477689
O	4.61789620	-0.29800800	-1.19148113
O	3.94275301	-1.80370766	0.31427887
H	4.42857453	-2.40106662	-0.27320552
O	-3.24357139	-2.75630410	-0.13912716
O	-2.38947047	-1.67213720	0.00770266
O	-5.55075318	-1.83900069	-0.32308669

H	-4.51802394	-2.58083192	-0.15450438
C	-6.49350473	-2.18654653	0.69442566
H	-5.97085296	-2.53015452	1.56256659
H	-7.07852541	-1.32704306	0.94721924
H	-7.13655106	-2.96249372	0.33484620

TS14-C₂H₅OH

C	-0.50761234	-0.20121562	1.17419756
C	0.85090960	-0.03534606	1.41962783
C	1.73821300	0.20225681	0.37057465
C	1.24374125	0.25598965	-0.93313951
C	-0.11208262	0.07465983	-1.18153393
C	-0.99929300	-0.14884100	-0.13017600
H	-1.18572629	-0.37759824	2.00194573
H	1.22466185	-0.08457921	2.43659327
H	1.92105563	0.43335612	-1.76269762
H	-0.48369033	0.11089599	-2.20001139
C	-2.47114400	-0.30176900	-0.39602500
H	-2.66697156	-0.36009557	-1.47268260
C	-3.32578839	0.83442337	0.22604217
H	-3.09114594	0.85144575	1.29445130
C	-4.78883637	0.53163671	0.04168963
H	-5.23006193	-0.69908714	-0.14331189
H	-5.44695294	0.74033872	0.88170191
H	-5.20542620	0.80272157	-0.92866592
C	-2.94199305	2.18096928	-0.40285881
H	-1.89428114	2.41645493	-0.20493324
H	-3.09489534	2.15377500	-1.48521247
H	-3.56045529	2.97978442	0.00842112
C	3.21814036	0.42606392	0.63965629
H	3.40154554	0.23440315	1.69955478
C	3.65836095	1.84267117	0.27510062

H	3.08008763	2.56393440	0.85393327
H	4.71828521	1.98664934	0.48983274
H	3.49412521	2.03591356	-0.78594984
C	4.00782109	-0.60841715	-0.13730562
O	4.62147299	-0.40005273	-1.15258310
O	3.92526621	-1.82318614	0.42229797
H	4.40853172	-2.45321753	-0.13224066
O	-3.24357139	-2.75630410	-0.13912716
O	-2.38947047	-1.67213720	0.00770266
O	-5.71526705	-2.01648847	-0.35133783
H	-4.51802394	-2.58083192	-0.15450438
C	-6.65801860	-2.36403431	0.66617452
H	-6.13536683	-2.70764230	1.53431545
H	-7.24303928	-1.50453084	0.91896810
C	-7.58352453	-3.48081811	0.14864894
H	-8.28748072	-3.74245295	0.91081224
H	-8.10787330	-3.13642267	-0.71815562
H	-6.99826559	-4.33952561	-0.10628911

TS14-HCOOH

C	-0.49216154	-0.32143607	1.15781157
C	0.86592981	-0.15569806	1.40570144
C	1.73712075	0.20129019	0.37717787
C	1.22718251	0.37511946	-0.90999209
C	-0.12797494	0.19434461	-1.16239538
C	-0.99929300	-0.14884100	-0.13017600
H	-1.15776037	-0.59166913	1.97025768
H	1.25187697	-0.29879625	2.40914604
H	1.89194446	0.64649636	-1.72413362
H	-0.51156827	0.32470214	-2.16865814
C	-2.47114400	-0.30176900	-0.39602500
H	-2.66331934	-0.39899022	-1.47052892

C	-3.32034841	0.86256218	0.17973750
H	-3.12294958	0.88979636	1.25544049
C	-4.78269777	0.59056471	-0.05205284
H	-5.23006193	-0.69908714	-0.14331189
H	-5.46479834	0.82643938	0.76121004
H	-5.15860421	0.85691040	-1.04017141
C	-2.88347934	2.19069801	-0.45366744
H	-1.83814212	2.40508862	-0.22207507
H	-2.99895889	2.15122838	-1.54027440
H	-3.49718787	3.00931779	-0.07554598
C	3.21584623	0.42456266	0.65322117
H	3.41445378	0.13198443	1.68700506
C	3.62716793	1.87826661	0.42732214
H	3.04293517	2.52765645	1.08049350
H	4.68676312	2.01975838	0.64530646
H	3.44768516	2.17288693	-0.60763142
C	4.01468055	-0.51285507	-0.23025394
O	4.61316808	-0.19336627	-1.22549879
O	3.95961629	-1.77852152	0.20642853
H	4.44754295	-2.34131486	-0.41259442
O	-3.26125687	-2.73977440	-0.05072157
O	-2.40033759	-1.65660342	0.05893184
O	-5.69265900	-1.95391287	0.07293994
H	-4.51802394	-2.58083192	-0.15450438
C	-6.71958381	-2.36363840	0.97983045
H	-6.40141069	-2.18108922	1.98498797
O	-7.85004533	-2.86625468	0.78505010

TS14-CH₃COOH

C	-0.48669428	-0.36020481	1.14984402
C	0.87126275	-0.19456439	1.39853365
C	1.73678332	0.20082851	0.37931160

C	1.22137355	0.41338262	-0.89984189
C	-0.13357785	0.23287769	-1.15354127
C	-0.99929300	-0.14884100	-0.13017600
H	-1.14788293	-0.66064690	1.95525107
H	1.26151978	-0.36791603	2.39552013
H	1.88171279	0.71501808	-1.70690350
H	-0.52141676	0.39360119	-2.15376655
C	-2.47114400	-0.30176900	-0.39602500
H	-2.66331934	-0.39899022	-1.47052892
C	-3.32034841	0.86256218	0.17973750
H	-3.08081953	0.92551891	1.24533934
C	-4.78490858	0.55567466	0.01524252
H	-5.23006193	-0.69908714	-0.14331189
H	-5.43872462	0.80240208	0.84827597
H	-5.20527682	0.78527430	-0.96414430
C	-2.93632609	2.17947947	-0.50892563
H	-1.88718931	2.42075465	-0.32609632
H	-3.09420249	2.10554979	-1.58837804
H	-3.55108182	2.99698615	-0.13009776
C	3.21513476	0.42377192	0.65761501
H	3.41903163	0.09892500	1.68067740
C	3.61720391	1.88646391	0.47777166
H	3.03147534	2.51080253	1.15363499
H	4.67670882	2.02707390	0.69676306
H	3.43241544	2.21350321	-0.54645614
C	4.01633573	-0.47967843	-0.25850235
O	4.60949295	-0.12446300	-1.24478793
O	3.97015405	-1.75917566	0.13695851
H	4.45919351	-2.29864609	-0.50164171
O	-3.26125687	-2.73977440	-0.05072157
O	-2.40033759	-1.65660342	0.05893184
O	-5.70077434	-1.93455133	0.11406705
H	-4.51802394	-2.58083192	-0.15450438

C	-6.72665060	-2.34666944	1.02106018
O	-7.70533873	-3.11479126	0.87730982
C	-6.50286946	-1.67502770	2.38869294
H	-5.65603742	-1.02346438	2.33176539
H	-7.37115848	-1.10902226	2.65442217
H	-6.32592825	-2.42593651	3.13012922

TS15

C	-0.43485500	-0.74480100	1.00430100
C	0.90362700	-0.51458700	1.30111600
C	1.75017200	0.09242400	0.37506400
C	1.22987300	0.46206400	-0.87061500
C	-0.09940700	0.22826300	-1.18052600
C	-0.95443000	-0.38181400	-0.24688100
H	-1.08168800	-1.20666600	1.74013600
H	1.29329200	-0.80670600	2.27060600
H	1.87612100	0.92978000	-1.60714000
H	-0.48645800	0.51493300	-2.15284900
C	-2.35955500	-0.54083100	-0.56390900
H	-2.67806300	-0.50158800	-1.60353100
C	-3.23859500	1.32669700	0.03507400
H	-2.31869500	1.84241900	-0.23273800
C	-3.48437800	1.13605800	1.37102900
H	-4.46972300	-2.38094200	-0.52950900
H	-2.69559400	1.23028000	2.10846800
H	-4.44988000	0.77688200	1.71104600
C	-4.37084900	1.47694300	-0.95449000
H	-4.07907300	1.17761200	-1.96319900
H	-5.23194600	0.88021700	-0.65200900
H	-4.67634500	2.52619600	-1.00333900
C	3.20562600	0.37236000	0.71305900
H	3.41890600	-0.07894000	1.68488400

C	3.51253300	1.86870200	0.74605300
H	2.88291300	2.35352200	1.49304400
H	4.55924200	2.04482400	0.99936700
H	3.31444200	2.32371800	-0.22550900
C	4.07612300	-0.33783800	-0.30389000
O	4.62869100	0.18737600	-1.23695100
O	4.14467700	-1.65623200	-0.07230200
H	4.67513800	-2.06552500	-0.77162400
O	-4.35127400	-1.52569200	-0.09219600
O	-2.95558400	-1.53318400	0.17414700

TS16

C	-1.39312000	-0.50726100	-0.86206100
C	-0.05744500	-0.84573100	-0.99741200
C	0.89418600	-0.40342200	-0.07381400
C	0.47682800	0.39347100	0.99997400
C	-0.85328200	0.74048000	1.14707300
C	-1.81631100	0.29407000	0.21758600
H	-2.12322800	-0.85821700	-1.58103600
H	0.25611900	-1.46489700	-1.83099800
H	1.20448500	0.74582500	1.72452100
H	-1.16476800	1.36002900	1.98101700
C	-3.17994600	0.67897700	0.38195800
H	-3.52294900	1.20958000	1.26621300
H	-5.92628300	-0.01423000	-0.09307500
C	2.35328000	-0.80107800	-0.21140800
H	2.47681600	-1.30759300	-1.17150000
C	2.81028300	-1.71068000	0.92838600
H	2.20167500	-2.61567300	0.93892600
H	3.85710800	-1.99113300	0.80246400
H	2.70309200	-1.20692000	1.89008800
C	3.19173400	0.46110300	-0.26983300

O	3.86272900	0.89474600	0.63122800
O	3.08119300	1.07931800	-1.45357900
H	3.59729200	1.89850700	-1.42566700
O	-5.13486100	-0.53790700	0.09969600
O	-4.07363700	0.36948600	-0.53530100

TS17

C	-0.41770500	-0.91790700	1.18969500
C	0.87346300	-0.44951400	1.40959000
C	1.64749600	0.02369300	0.35140400
C	1.10821100	0.00278000	-0.93559300
C	-0.18176200	-0.46765300	-1.15292000
C	-0.96743800	-0.92348100	-0.09231700
H	-1.01021400	-1.27553700	2.02445000
H	1.28291000	-0.45130900	2.41430200
H	1.70106500	0.34881200	-1.77691000
H	-0.58013400	-0.48293600	-2.16249800
C	-2.38301000	-1.37903000	-0.31706100
H	-2.53256700	-1.67710700	-1.35794800
H	-2.59567400	-2.26119400	0.29705100
C	-3.44567200	-0.33307400	0.07072800
C	-4.86673000	-0.63316200	-0.38880500
H	-5.21383900	-1.53327000	0.12594200
H	-5.52682600	0.19455200	-0.12881100
H	-4.91551000	-0.81526900	-1.46397000
C	-3.08955200	1.14143200	-1.39583200
H	-2.19930300	1.74301000	-1.50058600
H	-3.07131500	0.24937600	-2.01205100
H	-4.02305700	1.68578400	-1.38475400
C	3.04881300	0.56509500	0.58988600
H	3.29534500	0.40966300	1.64297100
C	3.16481500	2.04600200	0.23455300

H	2.46281800	2.62204400	0.83872000
H	4.17499400	2.41262500	0.42368000
H	2.93312500	2.20946900	-0.81877500
C	4.02612400	-0.26632800	-0.21577500
O	4.55849500	0.07802100	-1.24014400
O	4.22186000	-1.47573900	0.32868600
H	4.82086600	-1.97833800	-0.24265000
O	-2.66023900	1.88522300	0.66898400
H	-2.42326100	2.68634500	1.17769000
O	-3.33033200	0.19501400	1.21982800

TS18

C	0.81004000	-1.56454200	-0.30159100
C	-0.49302000	-1.35071900	-0.76200500
C	-1.22999000	-0.25122400	-0.32240400
C	-0.65648400	0.63909000	0.59083400
C	0.64161900	0.43648600	1.06216700
C	1.33226600	-0.66924300	0.60753100
H	1.38234500	-2.41691600	-0.65404700
H	-0.93395500	-2.04337300	-1.47240900
H	-1.22584500	1.49786000	0.93651600
H	1.08455800	1.13323000	1.76696700
C	3.65254700	-0.74241100	0.99086000
H	3.51105900	-0.47653600	2.03298200
H	3.64950900	-1.79966300	0.74698400
C	4.05977100	0.17580800	0.08932100
C	4.30884000	-0.18516400	-1.34490100
H	4.26693100	-1.26336100	-1.50444600
H	3.55568900	0.28884500	-1.98581900
H	5.28349700	0.18339600	-1.67902000
C	4.12837300	1.63573900	0.42577000
H	3.98753800	1.81305100	1.49269800

H	5.08820900	2.06282600	0.11953000
H	3.35007900	2.18198900	-0.12092000
C	-2.63407500	0.00096400	-0.85244000
H	-2.92647200	-0.86263800	-1.45468600
C	-2.71548900	1.27680300	-1.68866500
H	-2.02710200	1.20362400	-2.53152200
H	-3.72606500	1.42774300	-2.07163400
H	-2.44161900	2.14758000	-1.09109900
C	-3.58910700	0.05773100	0.32244300
O	-4.08007400	1.05986800	0.77671000
O	-3.81656100	-1.15671800	0.84286600
H	-4.39702400	-1.05875900	1.61180700

TS19

C	0.47574228	0.28290877	-1.24713020
C	-0.81797324	0.78985236	-1.17008370
C	-1.68000723	0.38683536	-0.15172213
C	-1.22364267	-0.54302454	0.78381493
C	0.06709758	-1.05239628	0.70026973
C	0.93891615	-0.64279338	-0.31109782
H	1.13617606	0.61081227	-2.04221588
H	-1.16098677	1.50553905	-1.91002711
H	-1.88198994	-0.87777059	1.57988308
H	0.40422195	-1.77957487	1.43222854
C	2.34739315	-1.17835838	-0.37388282
H	2.40293715	-2.12865238	0.16344518
H	2.62946815	-1.37424738	-1.41256282
C	3.42203015	-0.25647738	0.23214918
C	4.77319315	-0.96023038	0.22243718
H	5.00531415	-1.32364838	-0.78115982
H	5.55844715	-0.27400138	0.54165818
H	4.75703415	-1.81009838	0.90790618

C	3.05279115	0.23015162	1.62782318
H	2.15595015	0.85260762	1.59736018
H	2.85344315	-0.62665838	2.27583218
H	3.87178915	0.80279662	2.06558918
C	-3.08336871	0.96295412	-0.04494480
H	-3.27196815	1.56249249	-0.93889369
C	-3.25884212	1.81752357	1.20899104
H	-2.54775932	2.64432093	1.18784811
H	-4.26988701	2.22408218	1.26512325
H	-3.07635631	1.22533283	2.10697630
C	-4.07609818	-0.18111273	-0.06907009
O	-4.67178420	-0.61027904	0.88601472
O	-4.20634335	-0.70448520	-1.29650220
H	-4.81827963	-1.45359305	-1.24955976
O	4.32086632	1.91300062	-0.47548540
O	3.44979246	1.03753524	-0.85639022

TS20

C	-0.54169900	-0.20857000	0.87477900
C	0.78952200	-0.07342100	1.23807600
C	1.76182900	0.24224000	0.28666200
C	1.37462800	0.40731000	-1.04544000
C	0.04592800	0.26414700	-1.41465100
C	-0.94116300	-0.03265200	-0.46120900
H	-1.28125600	-0.46508300	1.62445100
H	1.08038300	-0.21561200	2.27313800
H	2.11830600	0.64360200	-1.80018300
H	-0.24002600	0.38848100	-2.45336400
C	-2.33472600	-0.20361500	-0.88965500
H	-2.47365000	-0.05585800	-1.95977100
H	-2.69602000	-1.40534000	-0.59898200
C	-3.52261200	0.31800700	-0.03327900

C	-4.78090300	0.36718400	-0.89080900
H	-4.95509600	-0.59376500	-1.37651900
H	-5.64158700	0.61426400	-0.26663000
H	-4.67611500	1.13425600	-1.66057700
C	-3.28231900	1.63125100	0.68734800
H	-2.42449900	1.57404900	1.35632600
H	-3.09858500	2.41672800	-0.04859000
H	-4.16824400	1.90277100	1.26522800
C	3.21467300	0.42414400	0.69104200
H	3.31443200	0.12971400	1.73840800
C	3.68372600	1.86584600	0.50052600
H	3.06656100	2.53225200	1.10432700
H	4.72510200	1.97646600	0.80628700
H	3.59885600	2.16334100	-0.54553300
C	4.06135400	-0.53830300	-0.11903200
O	4.75735300	-0.23746800	-1.05460100
O	3.92622500	-1.80072900	0.30851300
H	4.44981800	-2.38057500	-0.26415400
O	-3.52399200	-1.90359200	0.29599900
O	-3.64306000	-0.70084800	0.98258700

TS20-H₂O

C	-0.49259195	-0.43937729	0.80715259
C	0.83887962	-0.29470944	1.16583629
C	1.76261464	0.25957527	0.27718932
C	1.32702102	0.65568954	-0.98970457
C	-0.00164987	0.50448118	-1.35579994
C	-0.94116300	-0.03265200	-0.46120900
H	-1.19348413	-0.88209673	1.50536547
H	1.16816513	-0.61675514	2.14768625
H	2.03303824	1.07985384	-1.69691896
H	-0.32511972	0.81005934	-2.34481085

C	-2.33472600	-0.20361500	-0.88965500
H	-2.47365000	-0.05585800	-1.95977100
H	-2.48632856	-1.49886622	-0.84832536
C	-3.52261200	0.31800700	-0.03327900
C	-4.77492042	0.39218744	-0.89774022
H	-4.95581182	-0.55996876	-1.39809735
H	-5.63695749	0.63923524	-0.27541845
H	-4.65750366	1.16894187	-1.65588836
C	-3.27352258	1.61840867	0.70737190
H	-2.42055231	1.54297280	1.38072912
H	-3.07719117	2.41227821	-0.01620406
H	-4.16025930	1.89080547	1.28359189
C	3.21398692	0.44961295	0.68311067
H	3.36170151	-0.03576188	1.65068914
C	3.59339426	1.92722543	0.76984665
H	2.95716794	2.42397981	1.50334265
H	4.63532719	2.04100231	1.07253650
H	3.46039990	2.41627421	-0.19611889
C	4.09013758	-0.28262600	-0.31467636
O	4.73947128	0.23686325	-1.18571155
O	4.04069848	-1.60995410	-0.13994833
H	4.57949542	-2.03383758	-0.82430142
O	-4.02512120	-1.92261831	1.12225595
O	-3.88583433	-0.54060704	1.06917664
O	-2.81227449	-2.73852081	-0.82849543
H	-3.48920045	-2.96297656	-1.47113908
H	-3.44774840	-2.61593361	0.26562282

TS20-NH₃

C	-0.47795547	-0.49611089	0.78218443
C	0.85346892	-0.34884428	1.13998459
C	1.76260924	0.26434549	0.27530341

C	1.31255112	0.71733866	-0.96723968
C	-0.01602099	0.56396123	-1.33279080
C	-0.94116300	-0.03265200	-0.46120900
H	-1.16727248	-0.98470925	1.46105501
H	1.19419848	-0.71508117	2.10224528
H	2.00721970	1.18794595	-1.65607363
H	-0.35072854	0.91420916	-2.30307456
C	-2.33472600	-0.20361500	-0.88965500
H	-2.47365000	-0.05585800	-1.95977100
H	-2.48632856	-1.49886622	-0.84832536
C	-3.52261200	0.31800700	-0.03327900
C	-4.76255711	0.44044821	-0.90998681
H	-4.95583981	-0.49399581	-1.43832056
H	-5.62716855	0.68754705	-0.29126705
H	-4.62074259	1.23502368	-1.64514748
C	-3.25730129	1.59262218	0.74557924
H	-2.41427296	1.48203290	1.42655799
H	-3.03668262	2.40179973	0.04636815
H	-4.14554705	1.86679730	1.31862283
C	3.21352901	0.45641193	0.68188706
H	3.37514441	-0.07506399	1.62264752
C	3.57060828	1.93351928	0.84144887
H	2.93165410	2.38229565	1.60296220
H	4.61264142	2.04821195	1.14344736
H	3.42366491	2.46881437	-0.09759982
C	4.09426255	-0.21031328	-0.35694822
O	4.72969525	0.36290591	-1.20420891
O	4.06651461	-1.54541465	-0.24967104
H	4.60725220	-1.92545538	-0.95783090
O	-4.08282635	-1.94276835	1.05448614
O	-3.91597897	-0.56285850	1.04091622
H	-3.46290316	-3.03255949	-1.49457854
H	-3.44774840	-2.61593361	0.26562282

N	-2.75777195	-2.79875142	-0.82515807
H	-1.97242012	-3.52291569	-0.61940331

TS20-CH₃OH

C	-0.41276267	-0.70570091	0.65377119
C	0.91801595	-0.54771110	1.00939290
C	1.76172882	0.28417495	0.27025451
C	1.24709753	0.94767217	-0.84625547
C	-0.08071254	0.78545156	-1.21075653
C	-0.94116300	-0.03265200	-0.46120900
H	-1.05033997	-1.36425905	1.23217238
H	1.30968852	-1.07712472	1.87106891
H	1.89077530	1.59099318	-1.43815483
H	-0.46567454	1.30123829	-2.08363776
C	-2.33472600	-0.20361500	-0.88965500
H	-2.47365000	-0.05585800	-1.95977100
H	-2.48632856	-1.49886622	-0.84832536
C	-3.52261200	0.31800700	-0.03327900
C	-4.78618079	0.34404598	-0.88403642
H	-4.95400482	-0.62480524	-1.35609870
H	-5.64560087	0.59119164	-0.25814421
H	-4.69307234	1.10188312	-1.66438022
C	-3.29069900	1.64281889	0.66867799
H	-2.42857516	1.60250337	1.33334026
H	-3.11863136	2.42024729	-0.07854008
H	-4.17585455	1.91355473	1.24810293
C	3.21058351	0.48386384	0.68051346
H	3.43271189	-0.21430696	1.49096576
C	3.48390772	1.91865366	1.12938286
H	2.84336116	2.16297801	1.97765813
H	4.52615202	2.03733556	1.42910270
H	3.27624417	2.62116078	0.32110987

C	4.09671338	0.09786229	-0.48789121
O	4.67025675	0.86950412	-1.21302742
O	4.15182148	-1.23049826	-0.65280130
H	4.69194101	-1.42470325	-1.43310496
O	-3.96703453	-1.89949698	1.18874514
O	-3.85580649	-0.51700511	1.09645246
O	-2.78628220	-2.74341468	-0.89869312
H	-3.44774840	-2.61593361	0.26562282
C	-3.77597099	-3.11826762	-1.86041105
H	-4.56820633	-2.39907235	-1.85579318
H	-3.33228991	-3.15391965	-2.83343522
H	-4.16795278	-4.08229516	-1.61161156

TS20-C₂H₅OH

C	-0.37877646	-0.79337832	0.57821364
C	0.95144738	-0.63022496	0.93357941
C	1.76084103	0.29380251	0.26930045
C	1.21247324	1.04558727	-0.77270766
C	-0.11477828	0.87916623	-1.13734933
C	-0.94116300	-0.03265200	-0.46120900
H	-0.98928957	-1.52331918	1.09706974
H	1.36966231	-1.22785287	1.73614335
H	1.82934703	1.76184762	-1.30652944
H	-0.52603911	1.46451401	-1.95244800
C	-2.33472600	-0.20361500	-0.88965500
H	-2.47365000	-0.05585800	-1.95977100
H	-2.48632856	-1.49886622	-0.84832536
C	-3.52261200	0.31800700	-0.03327900
C	-4.77492042	0.39218744	-0.89774022
H	-4.95581182	-0.55996876	-1.39809736
H	-5.63695749	0.63923524	-0.27541846
H	-4.65750365	1.16894188	-1.65588836

C	-3.27352258	1.61840867	0.70737191
H	-2.42055231	1.54297279	1.38072913
H	-3.07719116	2.41227821	-0.01620405
H	-4.16025930	1.89080547	1.28359189
C	3.20859435	0.49675716	0.68183859
H	3.46156673	-0.26896399	1.41892237
C	3.44611544	1.88942318	1.26396983
H	2.81002535	2.03179379	2.13843264
H	4.48835207	2.01013976	1.56290273
H	3.20750364	2.65968532	0.52932279
C	4.09001831	0.25155243	-0.52744188
O	4.63131143	1.10615717	-1.18078569
O	4.18143121	-1.05258201	-0.82010387
H	4.71659080	-1.15463706	-1.62104548
O	-4.02512121	-1.92261831	1.12225594
O	-3.88583433	-0.54060704	1.06917663
O	-2.84099974	-2.77746333	-0.90419909
H	-3.44774840	-2.61593361	0.26562282
C	-3.85338909	-3.16091429	-1.88797600
H	-4.64562443	-2.44171902	-1.88335813
H	-3.40970801	-3.19656632	-2.86100017
C	-4.41754979	-4.54839317	-1.52989076
H	-4.86123189	-4.51274056	-0.55686708
H	-5.15808479	-4.82887786	-2.24949916
H	-3.62531427	-5.26758826	-1.53450666

TS20-HCOOH

C	-0.38901953	-0.76827517	0.60151331
C	0.94138487	-0.60665192	0.95690234
C	1.76113486	0.29094434	0.26948524
C	1.22293937	1.01743389	-0.79551571
C	-0.10449037	0.85225372	-1.16007287

C	-0.94116300	-0.03265200	-0.46120900
H	-1.00769508	-1.47775661	1.13875462
H	1.35160116	-1.18475282	1.77769079
H	1.84790515	1.71275825	-1.34730339
H	-0.50781889	1.41766152	-1.99301552
C	-2.33472600	-0.20361500	-0.88965500
H	-2.47365000	-0.05585800	-1.95977100
H	-2.48632856	-1.49886622	-0.84832536
C	-3.52261200	0.31800700	-0.03327900
C	-4.80215620	0.26587110	-0.85857942
H	-4.94723846	-0.72799388	-1.28386042
H	-5.65722112	0.51349612	-0.22693811
H	-4.74845824	0.99053305	-1.67338268
C	-3.32073475	1.67963053	0.60459304
H	-2.44539199	1.69646144	1.25278327
H	-3.18814680	2.42783862	-0.17958941
H	-4.20315931	1.94791252	1.18930081
C	3.20922164	0.49295808	0.68131421
H	3.45294100	-0.25358913	1.44084337
C	3.45705207	1.89954835	1.22435711
H	2.81929511	2.07236310	2.09209344
H	4.49929822	2.01965445	1.52350263
H	3.22772448	2.65057884	0.46718627
C	4.09252436	0.20565859	-0.51728002
O	4.64353650	1.03651328	-1.19275891
O	4.17341729	-1.10704568	-0.77230516
H	4.71035576	-1.23658407	-1.56806604
O	-3.87158096	-1.85544389	1.29431664
O	-3.80713660	-0.47565156	1.13877424
O	-2.85039453	-2.81054160	-0.88405941
H	-3.44774840	-2.61593361	0.26562282
C	-3.65765568	-3.45188711	-1.87497080
H	-4.54824860	-2.88051327	-2.03395562

O -3.47279548 -4.50606705 -2.52538384

TS20-CH₃COOH

C -0.35962170 -0.83747196 0.53350559
C 0.97023568 -0.67151359 0.88894400
C 1.76023495 0.29905362 0.26917644
C 1.19283507 1.09530886 -0.72867297
C -0.13406190 0.92662142 -1.09356352
C -0.94116300 -0.03265200 -0.46120900
H -0.95485881 -1.60339893 1.01703453
H 1.40340626 -1.30343252 1.65654640
H 1.79454741 1.84846242 -1.22790217
H -0.56016958 1.54704770 -1.87436876
C -2.33472600 -0.20361500 -0.88965500
H -2.47365000 -0.05585800 -1.95977100
H -2.48632856 -1.49886622 -0.84832536
C -3.52261200 0.31800700 -0.03327900
C -4.81416115 0.19470459 -0.83188378
H -4.93686767 -0.81962773 -1.21366047
H -5.66514538 0.44311814 -0.19506240
H -4.79627157 0.88646640 -1.67631752
C -3.35043349 1.71003532 0.54487800
H -2.46486478 1.77901693 1.17548754
H -3.25387244 2.42887102 -0.27138680
H -4.23019235 1.97635082 1.13448119
C 3.20736142 0.50367433 0.68308867
H 3.47754439 -0.29534779 1.37748137
C 3.42664150 1.86765296 1.33599773
H 2.79436644 1.95370371 2.22052513
H 4.46884477 1.98950520 1.63458595
H 3.17076127 2.67131540 0.64419023
C 4.08427937 0.33645505 -0.54265414

O	4.60739952	1.23276931	-1.15353194
O	4.19445525	-0.94891918	-0.90383050
H	4.72567604	-1.00020419	-1.71221952
O	-3.78344406	-1.80818925	1.38778906
O	-3.76293001	-0.43467858	1.17513675
O	-2.84871239	-2.71527155	-0.88240145
H	-3.44774840	-2.61593361	0.26562282
C	-3.65718358	-3.35798206	-1.87144014
O	-3.83836570	-3.09055556	-3.08146570
C	-4.37948048	-4.56278170	-1.24029435
H	-3.65584854	-5.25618518	-0.86552987
H	-5.00002828	-4.22556890	-0.43648594
H	-4.98442008	-5.04369173	-1.98034409

TS21

C	-0.53209200	-0.18332900	-0.86433800
C	0.80928600	-0.20671300	-1.22444200
C	1.80749000	-0.35132200	-0.26149700
C	1.43603900	-0.44679100	1.08307200
C	0.10049500	-0.40828400	1.44874100
C	-0.91498100	-0.30335000	0.48135000
H	-1.28856700	-0.02783200	-1.62304800
H	1.08462600	-0.10116400	-2.26832300
H	2.19899700	-0.54299800	1.84961800
H	-0.17247300	-0.47173700	2.49679400
C	-2.30134300	-0.26886900	0.92031500
H	-2.45957300	0.10933800	1.92788200
H	-2.87913500	2.61418700	0.06024000
C	-3.43073300	-0.59171800	0.18845200
C	-4.76576300	-0.51370900	0.87778300
H	-4.79167700	0.30227600	1.60060700
H	-5.55823900	-0.36284200	0.14283400

H	-4.96596600	-1.45394900	1.40093300
C	-3.39711700	-1.46888300	-1.03754700
H	-2.42273000	-1.92808600	-1.19728500
H	-4.13960900	-2.26230400	-0.92383900
H	-3.66643900	-0.89574100	-1.92975500
C	3.27211000	-0.41211900	-0.66018000
H	3.34124800	-0.19079800	-1.72808600
C	3.89196200	-1.77679700	-0.36404500
H	3.34806000	-2.55055400	-0.90715600
H	4.93879100	-1.80075700	-0.67104500
H	3.84207500	-1.99919000	0.70284100
C	4.01597400	0.69230800	0.06481000
O	4.75627600	0.53693500	1.00190600
O	3.73468700	1.90033400	-0.44280500
H	4.20233100	2.57094300	0.07635300
O	-3.75912900	2.22930100	-0.06256600
O	-3.55179400	1.13701300	-0.86208500

TS22

C	0.48197100	0.86011100	-0.88310000
C	-0.80796700	1.25142000	-0.53554200
C	-1.69659100	0.34142000	0.03313700
C	-1.27327900	-0.97319700	0.23616600
C	0.01237500	-1.36320700	-0.11967500
C	0.91091300	-0.44976800	-0.67563200
H	1.16400400	1.58172100	-1.31866000
H	-1.12536800	2.27435800	-0.70862000
H	-1.95483700	-1.70068100	0.66682700
H	0.32152700	-2.39224100	0.03460300
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500

C	3.34610100	-0.78097900	0.05459700
C	4.69500300	-0.74034000	-0.29659800
H	4.80442300	0.56994100	-0.17408500
H	5.41765700	-1.10003900	0.43091200
H	4.95198900	-0.89864800	-1.34102500
C	2.93045700	-1.09748300	1.45515000
H	2.04133200	-0.53702600	1.74589600
H	2.68272300	-2.16425400	1.51085500
H	3.73910100	-0.89545200	2.15753900
C	-3.09573500	0.77050600	0.44631400
H	-3.25677700	1.78902100	0.08503600
C	-3.29006200	0.70991200	1.96046400
H	-2.56695100	1.36596700	2.44667000
H	-4.29641900	1.02856400	2.23667600
H	-3.13946500	-0.30656200	2.32701100
C	-4.09975800	-0.11180600	-0.26745000
O	-4.72261200	-1.01095700	0.23745100
O	-4.20532200	0.20012100	-1.56674300
H	-4.82514300	-0.41624400	-1.98383700
O	4.34116900	1.75600800	0.09281000
O	3.15268400	1.40311100	0.35576000

TS22-H₂O

C	0.35384341	0.71430646	-1.20234001
C	-0.93550220	1.10801466	-0.85529378
C	-1.69494004	0.34806013	0.03176412
C	-1.14338135	-0.82217774	0.55612850
C	0.14096771	-1.21731308	0.20123078
C	0.91091300	-0.44976800	-0.67563200
H	0.93475299	1.31997670	-1.88886032
H	-1.35391945	2.01498413	-1.27889137
H	-1.72367294	-1.43484764	1.23959060

H	0.55030495	-2.13606743	0.60942327
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500
C	3.34610100	-0.78097900	0.05459700
C	4.69589936	-0.76665973	-0.29521066
H	5.44345816	0.24044900	-0.09164299
H	5.41194176	-1.12684683	0.43856828
H	4.95163828	-0.94438114	-1.33681696
C	3.25992182	-1.86121076	1.08423573
H	2.37598444	-1.74670141	1.71251184
H	3.17770168	-2.82576030	0.56910508
H	4.15438070	-1.87941818	1.70687828
C	-3.09111018	0.79002577	0.44140944
H	-3.36808694	1.64802969	-0.17579576
C	-3.16413928	1.15866932	1.92223810
H	-2.46686378	1.97135097	2.12972151
H	-4.17082785	1.48005873	2.19403499
H	-2.89731758	0.30348766	2.54491463
C	-4.06470820	-0.32224979	0.10832434
O	-4.56595823	-1.07369127	0.90546219
O	-4.29539984	-0.40737037	-1.20930245
H	-4.88834532	-1.15565983	-1.37218226
O	3.90027608	1.27921819	1.36454414
O	3.22561460	0.52143777	0.60508623
O	6.21170988	1.16608470	0.38578917
H	6.80299197	0.89714854	1.09265467
H	5.01440485	1.32490547	0.91763873

TS22-NH₃

C	0.33834793	0.69139230	-1.23486327
C	-0.95094550	1.08536394	-0.88792216

C	-1.69479410	0.34879009	0.03147800
C	-1.12770792	-0.79865483	0.58862706
C	0.15652440	-1.19435590	0.23393725
C	0.91091300	-0.44976800	-0.67563200
H	0.90703762	1.27889880	-1.94692413
H	-1.38156798	1.97417508	-1.33701077
H	-1.69574779	-1.39325305	1.29785681
H	0.57801989	-2.09553358	0.66811232
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500
C	3.34610100	-0.78097900	0.05459700
C	4.69633246	-0.83192567	-0.29008473
H	5.44345816	0.24044900	-0.09164299
H	5.39590378	-1.19247591	0.45923929
H	4.94764657	-1.05754328	-1.32346215
C	3.21525263	-1.81854095	1.12269219
H	2.33482508	-1.64682005	1.74281139
H	3.09685854	-2.79742260	0.64284939
H	4.10671138	-1.84860538	1.74916594
C	-3.09071172	0.79215449	0.44047185
H	-3.38138690	1.62681537	-0.20192855
C	-3.15235697	1.20907717	1.90896093
H	-2.46030489	2.03412226	2.08233474
H	-4.15912078	1.53069165	2.18021235
H	-2.87180688	0.37733161	2.55683941
C	-4.05764490	-0.33883605	0.15429648
O	-4.54429366	-1.06767837	0.98092003
O	-4.30059593	-0.46958390	-1.15737585
H	-4.88845757	-1.22790360	-1.28936532
O	3.97671017	1.30282527	1.29054839
O	3.27501115	0.54445549	0.55660740
H	6.82729786	0.88986636	1.09302397

H	5.07538686	1.32620305	0.89572402
N	6.21137902	1.17000819	0.35670575
H	6.48503154	1.90425348	-0.29597350

TS22-CH₃OH

C	0.44326554	0.82511230	-0.98996189
C	-0.84646016	1.21719183	-0.64248442
C	-1.69600024	0.34355108	0.03292800
C	-1.23397697	-0.93658548	0.34343815
C	0.05121246	-1.32823648	-0.01227866
C	0.91091300	-0.44976800	-0.67563200
H	1.09473393	1.51879470	-1.50957345
H	-1.19439632	2.21217832	-0.89947439
H	-1.88495206	-1.63655745	0.85869910
H	0.39055690	-2.33121967	0.22679812
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500
C	3.34610100	-0.78097900	0.05459700
C	4.69419112	-0.72309385	-0.29729558
H	5.44345816	0.24044900	-0.09164299
H	5.42116788	-1.08236673	0.42610664
H	4.95182712	-0.86865050	-1.34341600
C	3.29052572	-1.88788328	1.05767113
H	2.40550185	-1.81172203	1.69022214
H	3.23202515	-2.84138684	0.51926216
H	4.18671961	-1.89805043	1.67799772
C	-3.09406234	0.77680001	0.44542247
H	-3.29067897	1.75356151	-0.00302818
C	-3.24611834	0.85209427	1.96374213
H	-2.52721617	1.56673383	2.36643794
H	-4.25251530	1.17175476	2.23864012

H	-3.05985040	-0.12238778	2.41755326
C	-4.09400857	-0.19056360	-0.15483656
O	-4.67994749	-1.05320614	0.44837822
O	-4.24229403	-0.00267454	-1.47366696
H	-4.85713744	-0.66904118	-1.81421708
O	3.85001226	1.26033664	1.41348915
O	3.19329986	0.50405243	0.63699794
O	6.24130432	1.21642027	0.39236904
H	5.01440485	1.32490547	0.91763873
C	7.15173233	0.85225117	1.43323488
H	7.36677541	-0.19395372	1.36911148
H	8.05845396	1.41001909	1.32529585
H	6.71119667	1.06819809	2.38412670

TS22-C₂H₅OH

C	0.47126675	0.85133051	-0.91368882
C	-0.81860922	1.24285715	-0.56614573
C	-1.69641848	0.34202180	0.03309964
C	-1.26240362	-0.96396674	0.26688735
C	0.02311491	-1.35443979	-0.08893527
C	0.91091300	-0.44976800	-0.67563200
H	1.14484525	1.56592181	-1.37331234
H	-1.14445688	2.25876833	-0.76324801
H	-1.93550453	-1.68455449	0.72176277
H	0.34060967	-2.37699072	0.08959848
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500
C	3.34610100	-0.78097900	0.05459700
C	4.69632775	-0.78843218	-0.29376808
H	5.44345816	0.24044900	-0.09164299
H	5.40688753	-1.14887482	0.44519666

H	4.95080194	-0.98217026	-1.33282507
C	3.24486300	-1.84733841	1.09724357
H	2.36184513	-1.71371180	1.72303264
H	3.15066080	-2.81696500	0.59382943
H	4.13837458	-1.86952640	1.72111590
C	-3.09524504	0.77228613	0.44612605
H	-3.26618031	1.77992288	0.05976039
C	-3.27732260	0.74989095	1.96284325
H	-2.55501842	1.42326737	2.42602228
H	-4.28368468	1.06883989	2.23869381
H	-3.11680483	-0.25563861	2.35450623
C	-4.09864859	-0.13509536	-0.23639566
O	-4.71127557	-1.02495553	0.29669130
O	-4.21651642	0.14212130	-1.54248241
H	-4.83527285	-0.48908013	-1.93843257
O	3.92562274	1.28771829	1.33994912
O	3.24196142	0.52952065	0.58900363
O	6.22913759	1.13801621	0.32093066
H	5.05940655	1.32644250	0.90018373
C	7.31030640	1.03073790	1.25069697
H	7.67230747	0.02389911	1.26213710
H	6.96761389	1.29767741	2.22855439
C	8.44685163	1.98010925	0.82813456
H	9.25583769	1.89983875	1.52383435
H	8.78954442	1.71316908	-0.14972258
H	8.08484995	2.98694781	0.81669350

TS22-HCOOH

C	0.41426199	0.79342340	-1.06374299
C	-0.87532476	1.18605268	-0.71637059
C	-1.69561313	0.34507238	0.03264716
C	-1.20456374	-0.90371069	0.41741072

C	0.08032006	-1.29653537	0.06188405
C	0.91091300	-0.44976800	-0.67563200
H	1.04283719	1.46189345	-1.64136181
H	-1.24613028	2.15581810	-1.03126712
H	-1.83261690	-1.57873611	0.99109451
H	0.44233240	-2.27561175	0.35961570
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500
C	3.34610100	-0.78097900	0.05459700
C	4.69518711	-0.74487868	-0.29638659
H	5.44345816	0.24044900	-0.09164299
H	5.41670224	-1.10467584	0.43220446
H	4.95198006	-0.90653844	-1.34034755
C	3.27514384	-1.87472673	1.07104395
H	2.39053773	-1.77937391	1.70157423
H	3.20482512	-2.83390155	0.54424749
H	4.17049689	-1.88892691	1.69250450
C	-3.09297535	0.78127640	0.44439809
H	-3.31591588	1.72268359	-0.06341992
C	-3.21675497	0.95463998	1.95724591
H	-2.50317796	1.70637377	2.29694886
H	-4.22321823	1.27494653	2.23114735
H	-3.00409624	0.01568944	2.47047462
C	-4.08677844	-0.24040976	-0.06990584
O	-4.64516429	-1.07079626	0.60092061
O	-4.26410443	-0.14299404	-1.39492289
H	-4.87332113	-0.84070017	-1.67796436
O	3.87507072	1.27009033	1.38905930
O	3.20939288	0.51294776	0.62108552
O	6.17144993	1.23778159	0.33641669
H	5.01440485	1.32490547	0.91763873
C	7.30827177	1.90049798	-0.22335387

H	8.20335785	1.47806733	0.18318427
O	7.13258609	2.81396912	-1.04842875

TS22-CH₃COOH

C	0.38440390	0.75642527	-1.13465615
C	-0.90505594	1.14959837	-0.78742774
C	-1.69525913	0.34657795	0.03225854
C	-1.17431382	-0.86550989	0.48842814
C	0.11028938	-1.25949799	0.13317496
C	0.91091300	-0.44976800	-0.67563200
H	0.98941947	1.39550802	-1.76800588
H	-1.29939513	2.08997486	-1.15795464
H	-1.77876572	-1.51138510	1.11827437
H	0.49567235	-2.21045032	0.48737443
C	2.31140500	-0.87412100	-1.04391000
H	2.29794900	-1.93001800	-1.34454800
H	2.66791000	-0.30948400	-1.90898500
C	3.34610100	-0.78097900	0.05459700
C	4.68835351	-0.64568267	-0.29836073
H	5.46489502	0.26560561	-0.08577443
H	5.43464021	-1.00200451	0.40660303
H	4.94727411	-0.73370461	-1.35056948
C	3.34645833	-1.93170269	1.00870301
H	2.46198480	-1.92399446	1.64653976
H	3.32926131	-2.86265818	0.42947791
H	4.24520669	-1.92733534	1.62539115
C	-3.09198962	0.78569249	0.44305814
H	-3.34176244	1.68744646	-0.12110710
C	-3.18938212	1.05700554	1.94338769
H	-2.48302627	1.84147564	2.21790913
H	-4.19594275	1.37788938	2.21625367
H	-2.94982645	0.15788946	2.51300064

C	-4.07699503	-0.28437985	0.01796372
O	-4.60710322	-1.07763626	0.75354118
O	-4.28183649	-0.27812218	-1.30665145
H	-4.88374146	-1.00318238	-1.53036871
O	3.76219439	1.22061869	1.49957346
O	3.13718012	0.46917067	0.69281537
O	6.10336623	1.29739111	0.33798236
H	4.92618497	1.31755833	0.95863680
C	7.24012696	1.96185143	-0.21984156
O	7.07076017	2.99820811	-0.88566679
C	8.54961425	1.22888158	0.12598826
H	8.66750769	1.19159856	1.18881991
H	8.51475014	0.23315099	-0.26414643
H	9.37642312	1.75262419	-0.30642446

TS23

C	0.45631800	0.90026900	-1.20981500
C	-0.85269200	1.23376600	-0.86490100
C	-1.61523000	0.37491000	-0.08084500
C	-1.04975100	-0.83585000	0.32829300
C	0.25257800	-1.16730900	-0.02030500
C	1.03996500	-0.28987500	-0.77309700
H	1.01913900	1.56767900	-1.85720700
H	-1.28048100	2.16563300	-1.21917500
H	-1.63831400	-1.53323200	0.91707100
H	0.65421100	-2.12658500	0.28542400
C	2.46259600	-0.62352100	-1.16150800
H	2.47509200	-1.61118900	-1.63872000
H	2.80419600	0.09025600	-1.91454100
C	3.49453700	-0.67921500	-0.04424500
C	4.78416200	-0.29624300	-0.34665800
H	2.06918000	2.04257000	-0.03860600

H	5.59515100	-0.49510100	0.34312800
H	5.00229100	0.28748900	-1.23299300
C	3.26281800	-1.64088800	1.08994900
H	2.37131400	-1.36906300	1.65695600
H	3.12219100	-2.65202100	0.69714200
H	4.11741100	-1.64656600	1.76687900
C	-3.03124700	0.74242000	0.33251200
H	-3.31024400	1.65674400	-0.19663300
C	-3.15242900	0.94728000	1.84136800
H	-2.47899500	1.74540400	2.15606200
H	-4.17306800	1.21904000	2.11535800
H	-2.88493200	0.03499800	2.37657300
C	-3.97153900	-0.34515200	-0.14747200
O	-4.47981400	-1.18626700	0.54897100
O	-4.16195900	-0.29143700	-1.47298800
H	-4.73424800	-1.02779600	-1.73437700
O	2.95802800	2.05944100	0.34975600
O	3.03244500	0.88428800	1.05651100

TS24

C	0.87201100	1.08285800	-0.05532600
C	-0.43357600	0.90335600	0.35750400
C	-1.11307600	-0.30443300	0.26696100
C	-0.40471000	-1.38186400	-0.26973900
C	0.91579000	-1.22982600	-0.68442700
C	1.57699700	-0.00566200	-0.58389100
H	1.35018900	2.05351700	0.03054300
H	-1.01264000	1.85585800	0.81755700
H	-0.88305300	-2.34985700	-0.36799200
H	1.44379300	-2.08392800	-1.09562400
C	3.02035000	0.15079300	-0.98743000
H	3.31425700	-0.68972400	-1.62551700

H	3.13371500	1.06426000	-1.57991100
C	3.98147900	0.21777400	0.21419500
H	3.67776700	1.06796300	0.83718900
C	5.40764100	0.46133100	-0.27676500
H	5.47405400	1.38030600	-0.86445600
H	6.10170400	0.54186400	0.56316300
H	5.73854300	-0.36962200	-0.90808200
C	3.90951400	-1.05342700	1.05901800
H	2.91009500	-1.21048300	1.47128700
H	4.16582500	-1.92765500	0.45071700
H	4.61565400	-1.00343400	1.89122600
C	-2.56767300	-0.42450000	0.70355500
H	-2.75774000	0.37305600	1.42635300
C	-2.92638600	-1.77456500	1.31412700
H	-2.25654000	-1.99286800	2.14646300
H	-3.95200600	-1.75758700	1.68492700
H	-2.85055200	-2.57691100	0.58048000
C	-3.43575600	-0.13129000	-0.50684000
O	-4.02853700	-0.94602000	-1.16055100
O	-3.45249600	1.18290300	-0.80368500
H	-3.97451000	1.32151600	-1.60811800
O	-1.83824900	2.84378500	1.02541000
H	-2.49993200	2.59511800	0.35473600

TS25

C	0.77818500	0.98598500	0.20879700
C	-0.53069600	1.08211600	0.64542200
C	-1.42823600	0.06643500	0.30876200
C	-0.97255500	-0.99944800	-0.46868300
C	0.34728400	-1.05740300	-0.90386200
C	1.26274600	-0.05210900	-0.57540800
H	1.54570700	1.84099700	0.53366000

H	-0.85483000	1.92720700	1.24314800
H	-1.65899300	-1.79420600	-0.74460700
H	0.67842100	-1.89469800	-1.50993800
C	2.70703100	-0.10515800	-0.99968300
H	2.83122200	-0.86903000	-1.77446200
H	2.98878300	0.85643000	-1.44015700
C	3.66394500	-0.41473900	0.16600800
H	3.50950200	0.35329400	0.93311100
C	5.11081000	-0.33302600	-0.31711600
H	5.33418600	0.65264300	-0.73336100
H	5.80801000	-0.52409700	0.50210500
H	5.29437500	-1.07980700	-1.09641700
C	3.37081400	-1.78366200	0.77762900
H	2.35352500	-1.84084700	1.17206700
H	3.48561400	-2.56853700	0.02219100
H	4.06393400	-1.99831400	1.59447300
C	-2.86792500	0.10950400	0.79638500
H	-3.03121200	1.07418000	1.28275900
C	-3.18073200	-1.02890500	1.76554100
H	-2.51368400	-0.96877500	2.62633800
H	-4.21259900	-0.96756300	2.11486900
H	-3.03935300	-1.99676800	1.28229400
C	-3.78376100	0.06721700	-0.41088100
O	-4.42215600	-0.88934200	-0.76905400
O	-3.78672200	1.23031500	-1.07629500
H	-4.35122500	1.13823100	-1.85784800
O	2.31888400	2.91833800	0.60747000
H	2.02711100	3.36433300	-0.20465700

TS26

C	-0.69003100	-1.53472900	-0.60724400
C	0.64793200	-1.67580100	-0.25329800

C	1.40161600	-0.57752800	0.15932900
C	0.78789400	0.67783000	0.20441500
C	-0.54491300	0.78177000	-0.14838100
C	-1.32406400	-0.28833500	-0.56747100
H	-1.25640000	-2.40416000	-0.92747000
H	1.11419100	-2.65396000	-0.30311300
H	1.34723600	1.55636700	0.51123000
H	-1.06090900	1.85610300	-0.06426200
C	-2.78323000	-0.14322400	-0.91197400
H	-3.00542200	0.90782900	-1.12320000
H	-2.99588700	-0.71308400	-1.82174500
C	-3.71862300	-0.63053700	0.21029700
H	-3.48518900	-1.68412200	0.40653300
C	-5.17143700	-0.53165600	-0.25226900
H	-5.33771900	-1.10596200	-1.16709700
H	-5.85284700	-0.90623900	0.51516800
H	-5.43357900	0.51176400	-0.45535200
C	-3.50630900	0.16265300	1.49882100
H	-2.48886200	0.05160200	1.88073200
H	-3.68666600	1.22834200	1.32169900
H	-4.19777500	-0.17257500	2.27558300
C	2.85813500	-0.73287100	0.56853900
H	3.15042600	-1.76895300	0.38303400
C	3.08746400	-0.37304900	2.03528800
H	2.47358300	-1.01482600	2.66843700
H	4.13539200	-0.50858800	2.30744500
H	2.81595200	0.66635700	2.22483200
C	3.70012600	0.13574200	-0.34474900
O	4.15708800	1.21191000	-0.05542800
O	3.85840200	-0.41660700	-1.55527800
H	4.36005600	0.19687400	-2.11213100
O	-1.50155400	3.09308000	-0.25310900
H	-1.17442400	3.22856000	-1.15762400

TS27

C	-1.07051700	-1.53995000	0.08823600
C	0.24940900	-1.58709900	0.52274900
C	1.09001500	-0.47731500	0.39507200
C	0.53874700	0.65695400	-0.18737500
C	-0.76666400	0.72307400	-0.63857700
C	-1.60264100	-0.38967500	-0.49735600
H	-1.69938800	-2.41765600	0.20004400
H	0.63999800	-2.49661800	0.96753100
H	1.18158000	1.67134800	-0.32528300
H	-1.14384800	1.63340400	-1.09340600
C	-3.04679200	-0.34343500	-0.92446400
H	-3.19359200	0.47166400	-1.64141300
H	-3.29877700	-1.27623900	-1.43875300
C	-4.02041500	-0.14749400	0.25288100
H	-3.85260900	-0.96572700	0.96384500
C	-5.46104200	-0.22799100	-0.24959900
H	-5.65574400	-1.18268000	-0.74453600
H	-6.16988800	-0.11919900	0.57457400
H	-5.65679900	0.57302200	-0.96980000
C	-3.77030500	1.17782100	0.97051400
H	-2.76097800	1.23074100	1.38489800
H	-3.89431000	2.01438700	0.27438200
H	-4.48103600	1.31293800	1.78922900
C	2.52921800	-0.53426400	0.88426800
H	2.68908100	-1.52055600	1.32250300
C	2.84839300	0.55234100	1.91195500
H	2.18407900	0.44150200	2.76965300
H	3.88051700	0.46461400	2.25509900
H	2.70671300	1.54716600	1.48948200
C	3.43701400	-0.43419400	-0.32501800

O	3.85268400	0.59924500	-0.79744700
O	3.71277800	-1.62394500	-0.85664500
H	4.24957300	-1.49415700	-1.65336300
O	1.91059400	2.69310800	-0.66542800
H	2.74045800	2.19215100	-0.78823700

TS28

C	-1.28374900	-0.12992200	1.37697600
C	-0.00418200	0.39950700	1.50931500
C	0.82956400	0.52252500	0.39867500
C	0.36112800	0.09311300	-0.84377800
C	-0.91770500	-0.43890100	-0.96993200
C	-1.76163500	-0.55657000	0.13600900
H	-1.91975700	-0.21607100	2.25274400
H	0.34873300	0.72146700	2.48335700
H	0.99902900	0.16789900	-1.71918100
H	-1.26736400	-0.76758000	-1.94332800
C	-3.16584800	-1.08863600	0.00093600
H	-3.27578100	-1.59609500	-0.96388000
H	-3.34781000	-1.83495500	0.78122700
C	-4.24147000	0.00857000	0.10536900
H	-4.12143300	0.50059000	1.07827300
C	-5.63305600	-0.61942500	0.04729100
H	-5.76693700	-1.36421700	0.83580900
H	-6.41025500	0.14043900	0.15898700
H	-5.78454700	-1.11620700	-0.91657900
C	-4.07524300	1.05830300	-0.99224200
H	-3.10215500	1.55136000	-0.93414400
H	-4.15961700	0.59090600	-1.97934700
H	-4.85040000	1.82454000	-0.91451900
C	2.22097100	1.11954800	0.53901600
H	2.39636200	1.33606600	1.59509100

C	2.41021000	2.38347100	-0.29878100
H	1.69480300	3.13884200	0.02858600
H	3.41892100	2.78212200	-0.18027200
H	2.24067000	2.18041000	-1.35674400
C	3.21519500	0.02866900	0.18056500
O	3.70060000	-0.00467400	-0.97759100
O	3.50361700	-0.85356700	1.04471500
H	4.22272200	-1.51571800	0.37093400
O	4.87441300	-1.76223700	-0.63421400
H	4.33069800	-2.24149300	-1.27681200

TS29

C	0.74011100	-0.74328400	-1.06980800
C	-0.55787900	-0.28739700	-1.19491600
C	-1.21363800	0.36014700	-0.11424100
C	-0.52625700	0.41802400	1.12613200
C	0.76952500	-0.04198200	1.23749400
C	1.43037900	-0.62620700	0.14427200
H	1.23345400	-1.20340800	-1.91907500
H	-1.08772900	-0.39199100	-2.13530000
H	-1.01630400	0.85808400	1.98585300
H	1.28630000	0.03625400	2.18857400
C	2.85533300	-1.08293600	0.28115200
H	2.95730900	-1.66962600	1.20005000
H	3.11758900	-1.73562800	-0.55799700
C	3.86000000	0.08644100	0.33077800
H	3.58504100	0.72589700	1.17801000
C	3.80708400	0.92141800	-0.94759200
H	2.82066800	1.36491700	-1.10281200
H	4.53903600	1.73148500	-0.90891700
H	4.03788700	0.29800800	-1.81805500
C	5.26921800	-0.45430000	0.56624000

H	5.32167100	-1.03924600	1.48772200
H	5.57120700	-1.10059400	-0.26406200
H	5.99236200	0.36153900	0.63727600
C	-2.72339100	0.56400000	-0.18212100
H	-2.95487000	0.87887500	-1.20122400
C	-3.27193600	1.57021800	0.82298400
H	-2.71957900	2.50498600	0.74018800
H	-4.32697500	1.76045000	0.62011400
H	-3.19428900	1.19119400	1.84226300
C	-3.36273800	-0.79936900	0.02987200
O	-3.74636400	-1.22850100	1.08765400
O	-3.43164400	-1.50728300	-1.10551500
H	-3.79680300	-2.38158900	-0.90316800
O	-0.81712800	2.27537500	-0.77649500
H	0.14023800	2.18502500	-0.89607400

TS30

C	-1.06453900	-0.84500700	1.09434700
C	0.26908400	-0.59045900	1.34252900
C	1.12198300	-0.09486200	0.32359500
C	0.53369700	0.22010000	-0.92703700
C	-0.80148600	-0.04683600	-1.16428600
C	-1.62495300	-0.58485600	-0.16509300
H	-1.68999100	-1.25392200	1.88108300
H	0.69177300	-0.79543000	2.32036100
H	1.15423200	0.64741100	-1.70489300
H	-1.22726000	0.17337000	-2.13756800
C	-3.08790300	-0.83194300	-0.40653800
H	-3.28989800	-0.83664600	-1.48276000
H	-3.35582800	-1.81980800	-0.01810500
C	-3.99328300	0.22263800	0.26165100
H	-3.78388900	0.20875100	1.33795800

C	-5.45994500	-0.14690200	0.04749900
H	-5.68146300	-1.13967000	0.44681400
H	-6.11877000	0.57390700	0.53739000
H	-5.69914100	-0.14958800	-1.02074000
C	-3.70240700	1.62454200	-0.27171100
H	-2.67354000	1.93070500	-0.06812000
H	-3.85675100	1.65746000	-1.35558800
H	-4.37117400	2.35742400	0.18588600
C	2.47823200	0.45136700	0.72949300
H	2.78684800	-0.06444800	1.63935200
C	2.39118800	1.96279700	0.99388600
H	1.64256500	2.15826300	1.76323300
H	3.35169000	2.35319900	1.33574100
H	2.10206500	2.48861100	0.08204300
C	3.53879200	0.19655500	-0.32046300
O	3.51070300	0.61617700	-1.45076500
O	4.57612700	-0.49856100	0.16085600
H	5.23048600	-0.59626000	-0.54688400
O	1.92301200	-1.96370400	-0.19141700
H	1.11855700	-2.34743200	-0.57183100

TS31

C	-0.84657900	0.21281200	1.29232000
C	0.48590100	0.65822000	1.12411800
C	1.26295800	0.15566600	0.05175200
C	0.66259700	-0.69317100	-0.86970400
C	-0.66850600	-1.07295500	-0.71720700
C	-1.44292500	-0.62593400	0.36836300
H	-1.41267700	0.56741500	2.14714500
H	0.98536800	1.15299600	1.94740600
H	1.23337200	-1.07328500	-1.71032400
H	-1.11724700	-1.74040400	-1.44641300

C	-2.88810800	-1.03453600	0.48310100
H	-2.98033700	-2.10263400	0.26183900
H	-3.23290900	-0.88455600	1.51186200
C	-3.81181800	-0.24972200	-0.46724100
H	-3.43661100	-0.38991700	-1.48852900
C	-3.80310000	1.24428600	-0.14707200
H	-2.80435400	1.67675600	-0.24277000
H	-4.47225300	1.78700800	-0.81901300
H	-4.14612800	1.41300800	0.87948600
C	-5.23134400	-0.80965700	-0.39076600
H	-5.25344100	-1.87236500	-0.64476300
H	-5.63101600	-0.69501900	0.62199500
H	-5.89760100	-0.28031600	-1.07607600
C	2.70655700	0.59252600	-0.10319800
H	2.92670100	1.29976100	0.69979300
C	2.98356900	1.23712600	-1.45958700
H	2.32179300	2.09379500	-1.58968600
H	4.01916100	1.57554800	-1.51748300
H	2.81168500	0.52974200	-2.27142100
C	3.58847000	-0.62197200	0.12029800
O	4.16617400	-1.23302000	-0.74121100
O	3.63230000	-0.97187600	1.41320300
H	4.16865800	-1.77371700	1.50042600
O	0.22022900	2.51970300	0.32983100
H	-0.21782500	2.24158900	-0.48912800

TS32

C	-0.91735200	-0.99818700	0.70985200
C	0.43127800	-0.71094900	1.01961600
C	1.10835600	0.32900000	0.33022700
C	0.45301000	0.97372200	-0.70839100
C	-0.86053400	0.63649700	-1.03454700

C	-1.56664100	-0.35090200	-0.32810100
H	-1.43610500	-1.75905200	1.28408600
H	0.84870100	-1.08711900	1.94518400
H	0.96017100	1.74141500	-1.27978500
H	-1.35401700	1.15356000	-1.85137600
C	-3.00898300	-0.65539700	-0.64244300
H	-3.24420900	-0.31877100	-1.65804400
H	-3.16371900	-1.73837800	-0.61597400
C	-3.99307600	0.00985800	0.33803900
H	-3.73643200	-0.33271300	1.34797800
C	-5.42041800	-0.43374500	0.02230500
H	-5.51715200	-1.52145900	0.06624300
H	-6.13062200	0.00083100	0.72985400
H	-5.70618000	-0.10879300	-0.98334600
C	-3.87898700	1.53304200	0.29914300
H	-2.87927300	1.87242600	0.57991300
H	-4.09150600	1.90338800	-0.70966200
H	-4.59664800	1.99067500	0.98427200
C	2.54904500	0.60604600	0.68106800
H	2.75392800	0.18928000	1.66839100
C	2.91259300	2.09985900	0.68028900
H	2.26279200	2.63742700	1.37151800
H	3.94781000	2.23681200	0.99705200
H	2.79891400	2.53161200	-0.31493800
C	3.46582600	-0.09825400	-0.30557200
O	3.34309500	-0.07420500	-1.50322400
O	4.49239100	-0.70110900	0.30672700
H	5.06739300	-1.08965000	-0.36927900
O	1.46450700	-2.21440600	0.10180900
H	1.17150100	-2.02727300	-0.80349200

TS33

C	0.79360900	0.17671400	-1.27252200
C	-0.57908200	0.52174100	-1.29222100
C	-1.39649500	0.23170200	-0.21452300
C	-0.85239400	-0.47067300	0.87074000
C	0.47474500	-0.89829900	0.85928200
C	1.31059500	-0.61689300	-0.21415100
H	1.37082300	0.26677300	-2.18485500
H	-0.97172500	1.06057100	-2.14738400
H	-1.48009000	-0.70894400	1.72433000
H	0.85564700	-1.47754000	1.69364800
C	2.72726100	-1.11700900	-0.26599500
H	2.84970500	-1.92707900	0.46133000
H	2.91459500	-1.54094900	-1.25860500
C	3.79272000	-0.04008400	0.01763800
H	3.65445900	0.76643100	-0.70798600
C	5.18566300	-0.64232200	-0.16030200
H	5.31799900	-1.04939100	-1.16599400
H	5.95967200	0.11072200	0.00696000
H	5.34583500	-1.45398900	0.55692200
C	3.62778900	0.54138300	1.41966400
H	2.64762400	1.00610900	1.54456500
H	3.73339900	-0.24563400	2.17462100
H	4.39045300	1.29965800	1.61493700
C	-2.84765700	0.68230100	-0.18732300
H	-3.09046600	1.09375900	-1.17008600
C	-3.10049800	1.72627000	0.89883100
H	-2.46053100	2.59271800	0.72626100
H	-4.14232700	2.05039400	0.89063500
H	-2.87679400	1.31805600	1.88567200
C	-3.72963800	-0.53507700	0.00814800
O	-4.28791100	-0.83503800	1.03230700
O	-3.80253500	-1.28214200	-1.10186100
H	-4.34376700	-2.06345400	-0.91530800

O	1.46214700	2.04178400	-0.75203700
H	0.91217900	2.14643100	0.03946100

TS34

C	0.84820900	0.83623400	0.86718400
C	-0.48314100	0.53425600	1.23546200
C	-1.29931100	-0.19692100	0.39264900
C	-0.76605600	-0.67477500	-0.81589100
C	0.56281300	-0.43947300	-1.15869700
C	1.39965800	0.28620000	-0.31879300
H	1.51529400	1.26152700	1.60690800
H	-0.87024700	0.91744900	2.17325800
H	-1.39786400	-1.24261500	-1.49221300
H	0.95466100	-0.83648400	-2.08904600
C	2.85096500	0.50695300	-0.62782900
H	3.04701500	0.26686900	-1.67814400
H	3.08112400	1.56740800	-0.48107700
C	3.79120400	-0.33605600	0.25674900
H	3.57983800	-0.08875500	1.30410200
C	5.24441200	0.02789400	-0.04187000
H	5.43065500	1.09099200	0.12872300
H	5.92684600	-0.54541100	0.59003200
H	5.48485000	-0.19541400	-1.08636100
C	3.55314500	-1.83164600	0.05418600
H	2.53005800	-2.11699000	0.31064100
H	3.72778300	-2.10464600	-0.99223900
H	4.23444000	-2.41945400	0.67390100
C	-2.74145000	-0.50118700	0.76440800
H	-2.96418200	0.02002900	1.69847200
C	-2.99784900	-1.99845200	0.92068800
H	-2.34676600	-2.40055000	1.69775100
H	-4.03611000	-2.18537600	1.19888300

H	-2.79479700	-2.52657000	-0.01195300
C	-3.63951700	0.10012800	-0.29881200
O	-4.20768300	-0.51728300	-1.16290800
O	-3.71104000	1.43427800	-0.19511800
H	-4.25838500	1.77280400	-0.91885200
O	0.58868200	2.75014200	0.16212300
H	-0.14238100	2.54916900	-0.44217300

TS35

C	-0.56873400	0.57744800	1.53109100
C	0.79869500	0.77689500	1.43693500
C	1.49694900	0.36182600	0.30227200
C	0.79704600	-0.29129300	-0.72884500
C	-0.56052200	-0.49945900	-0.63792100
C	-1.31432600	-0.00270500	0.46710500
H	-1.10178000	0.89751600	2.41918400
H	1.33203500	1.25183300	2.25264500
H	1.33882200	-0.65830500	-1.59498200
H	-1.07170700	-1.04818900	-1.41890500
C	-2.71049200	-0.52862300	0.74434400
H	-2.65083000	-1.62394800	0.69720500
H	-2.96228400	-0.28084400	1.77949000
C	-3.88002800	-0.07851500	-0.14720400
H	-3.99425000	1.00062600	-0.02507400
C	-5.15512100	-0.76533900	0.34669100
H	-5.33730300	-0.55795800	1.40434000
H	-6.02374000	-0.42331700	-0.22097700
H	-5.07973600	-1.85072800	0.22349200
C	-3.66381400	-0.37025700	-1.63075000
H	-2.83000400	0.20785300	-2.02999000
H	-3.46714300	-1.43598000	-1.79338200
H	-4.55994600	-0.10827800	-2.19945400

C	2.98736500	0.60955600	0.17090100
H	3.35228500	0.99885800	1.12423700
C	3.30148200	1.59264000	-0.95683100
H	2.80014300	2.54176300	-0.76392000
H	4.37584300	1.76865900	-1.02497800
H	2.95538100	1.20296000	-1.91512400
C	3.68266300	-0.72033300	-0.05462500
O	4.15244200	-1.09400600	-1.09820100
O	3.69530700	-1.46820600	1.05673600
H	4.11660800	-2.31684100	0.85517300
O	-1.79389800	1.84752800	-0.26545800
H	-0.89018500	2.18074600	-0.37258200

TS36

C	-0.82408700	-0.57177400	1.29129600
C	0.48504300	-0.18322000	1.49980800
C	1.28277100	0.23554000	0.42779000
C	0.73597200	0.26008300	-0.86269900
C	-0.57054000	-0.13167000	-1.07773200
C	-1.38360600	-0.60273100	-0.01249900
H	-1.43901600	-0.88582500	2.12839800
H	0.90028300	-0.19612700	2.50137700
H	1.34299700	0.59114500	-1.69952200
H	-0.99025500	-0.10619200	-2.07759700
C	-2.87637900	-0.72009600	-0.17850300
H	-3.10282500	-0.95319800	-1.22435200
H	-3.22988800	-1.55880300	0.42691900
C	-3.63332200	0.55444500	0.23398600
H	-3.41666200	0.74482700	1.29237900
C	-5.13641100	0.32214500	0.08287600
H	-5.46574400	-0.53793000	0.67122500
H	-5.70250000	1.19769000	0.40928700

H	-5.38662900	0.13059600	-0.96558100
C	-3.19242000	1.77417000	-0.57506600
H	-2.13970200	2.01498900	-0.40821200
H	-3.33212800	1.59132500	-1.64607200
H	-3.78550400	2.65048500	-0.30254300
C	2.71170000	0.68973700	0.65758800
H	2.97419400	0.47232900	1.69606700
C	2.89094000	2.17990700	0.37019800
H	2.23007300	2.75925700	1.01591100
H	3.92161400	2.48488000	0.55664700
H	2.64898400	2.40465700	-0.66959900
C	3.63347200	-0.14831300	-0.20874300
O	4.22609100	0.24401100	-1.18018700
O	3.70073200	-1.41587700	0.22025900
H	4.27368400	-1.91649600	-0.37915400
O	-1.04703600	-2.60723400	-0.39574000
H	-0.07807600	-2.60415400	-0.37002100

TS37

C	0.73930300	1.00851700	1.17927200
C	-0.60169400	0.69931500	1.42281200
C	-1.38955100	0.08149300	0.44651600
C	-0.80693700	-0.24104200	-0.76981800
C	0.57081300	-0.01642500	-0.99371700
C	1.33989900	0.69366200	-0.02996300
H	1.31326700	1.52290300	1.94269500
H	-1.04444900	0.95786000	2.37888800
H	-1.39178600	-0.71585800	-1.55125100
H	0.96451000	-0.11962400	-1.99756000
C	2.76321500	1.07102300	-0.33187600
H	2.80255600	1.52840800	-1.32663000
H	3.09533200	1.82875900	0.38632600

C	3.75458300	-0.10796300	-0.29527300
H	3.40010100	-0.86481800	-1.00098900
C	3.80876400	-0.73570400	1.09547300
H	2.82885400	-1.10717200	1.40268000
H	4.51070800	-1.57317900	1.11528600
H	4.14308500	0.00186600	1.83363200
C	5.13808400	0.37341200	-0.72904600
H	5.11360800	0.80114400	-1.73455500
H	5.50889100	1.14194200	-0.04292900
H	5.85502000	-0.45132300	-0.72743000
C	-2.84525500	-0.26119400	0.72124200
H	-3.13010600	0.20658700	1.66672400
C	-3.06929700	-1.77083300	0.78876000
H	-2.44933400	-2.19628000	1.57911600
H	-4.11515600	-1.99997800	0.99908000
H	-2.79736400	-2.24141200	-0.15753900
C	-3.70247100	0.37105100	-0.35648000
O	-4.21135800	-0.21595700	-1.27697500
O	-3.81544600	1.69627300	-0.19224400
H	-4.33494900	2.05579000	-0.92630000
O	1.12671200	-1.94716500	-0.65044600
H	0.73122100	-2.03270000	0.23066200

TS38

C	-0.85448900	0.03791400	1.45502300
C	0.47692900	0.44301400	1.50778600
C	1.27761600	0.45365300	0.35534200
C	0.72444400	0.03445200	-0.84159500
C	-0.60415600	-0.44618300	-0.89420600
C	-1.42670400	-0.38426000	0.26059800
H	-1.45579100	0.05522800	2.35818100
H	0.90239700	0.76379200	2.45290000

H	1.31872400	0.02756000	-1.74976600
H	-1.07017300	-0.60174900	-1.85937000
C	-2.87702900	-0.76458400	0.18643100
H	-3.05833300	-1.34236000	-0.72573400
H	-3.12703900	-1.40690700	1.03684000
C	-3.81506700	0.45908100	0.19940800
H	-3.61582300	1.01940400	1.12070500
C	-5.27038600	-0.00416900	0.21637000
H	-5.47366100	-0.64497600	1.07793100
H	-5.95056200	0.84987200	0.25776100
H	-5.49904500	-0.57286400	-0.69058800
C	-3.55078700	1.37650400	-0.99382700
H	-2.52744000	1.76033400	-0.99138000
H	-3.70641300	0.83402900	-1.93255600
H	-4.23110100	2.23129300	-0.98273800
C	2.72127000	0.92772500	0.41602100
H	2.96153000	1.14431900	1.45969900
C	2.96581800	2.16309900	-0.44730100
H	2.31804500	2.97511700	-0.11516600
H	4.00459200	2.48775300	-0.37166900
H	2.74992400	1.95083100	-1.49535600
C	3.61291900	-0.22226100	-0.00952300
O	4.18610300	-0.30739200	-1.06515900
O	3.67280400	-1.17924700	0.92687600
H	4.21652000	-1.90727700	0.59189100
O	-0.26547000	-2.46185600	-0.84899900
H	0.21387700	-2.47934400	-0.00648400

TS39

C	-0.82946000	-1.03529700	1.10585000
C	0.50371200	-0.70855900	1.37740000
C	1.27006400	-0.03383200	0.44524900

C	0.66130300	0.36955200	-0.77456500
C	-0.65476400	-0.05669100	-1.06749300
C	-1.42298900	-0.72495400	-0.12279300
H	-1.41116100	-1.55803900	1.85826200
H	0.94318000	-1.00093000	2.32482300
H	1.28944100	0.73054100	-1.58033300
H	-1.07991600	0.19152200	-2.03472700
C	-2.86394400	-1.05965500	-0.41036000
H	-2.94460100	-1.46903600	-1.42225200
H	-3.20950600	-1.83520400	0.28179600
C	-3.79529600	0.16117000	-0.29432900
H	-3.41607800	0.93196000	-0.97701600
C	-3.80113200	0.72881000	1.12421000
H	-2.80420800	1.04188600	1.44402300
H	-4.46417600	1.59465300	1.19088900
H	-4.15906300	-0.02594500	1.83271100
C	-5.20989500	-0.21907100	-0.72839700
H	-5.22085600	-0.60736900	-1.74974400
H	-5.61449900	-0.99211100	-0.06720000
H	-5.87820300	0.64411200	-0.68390600
C	2.73640200	0.26439700	0.69759200
H	2.98938100	-0.12192500	1.68738300
C	3.08377800	1.74895500	0.60302800
H	2.50985000	2.30799800	1.34127500
H	4.14889400	1.89571100	0.78970000
H	2.84308900	2.14317600	-0.38364200
C	3.53968000	-0.54102400	-0.30874000
O	4.01740700	-0.10569500	-1.32493400
O	3.63388500	-1.83054000	0.04221900
H	4.11403400	-2.30636500	-0.65168700
O	0.18666600	2.30310300	-0.36559700
H	-0.64402100	2.13761800	0.10624600

TS40

C	-0.99622100	-0.20594400	1.39280100
C	0.32214400	0.23286100	1.52672300
C	1.13525300	0.37551900	0.41383500
C	0.62332800	0.00108600	-0.85563300
C	-0.73417700	-0.37418200	-0.97754600
C	-1.54623200	-0.50583200	0.13776400
H	-1.61380400	-0.30911100	2.27971500
H	0.70999300	0.47530100	2.50997500
H	1.18084800	0.25532300	-1.74856400
H	-1.12809800	-0.59620100	-1.96356800
C	-2.99368500	-0.90869100	0.02095000
H	-3.16997500	-1.35896800	-0.96194300
H	-3.21615500	-1.67399400	0.77164500
C	-3.96860900	0.26836000	0.20743900
H	-3.78055800	0.70727600	1.19516200
C	-5.40824100	-0.24204600	0.17094500
H	-5.58009600	-0.99984200	0.93941200
H	-6.11723500	0.57369700	0.33035400
H	-5.62641900	-0.69203600	-0.80302100
C	-3.74942200	1.34749800	-0.85207100
H	-2.74331800	1.76989300	-0.79846100
H	-3.88730000	0.92735100	-1.85428500
H	-4.46670000	2.16198700	-0.72635400
C	2.54380800	0.91940900	0.53339500
H	2.75780200	1.06219100	1.59504000
C	2.70967900	2.24306000	-0.21497400
H	2.00154100	2.97564300	0.17418000
H	3.72164600	2.63032000	-0.08715400
H	2.52823900	2.11220100	-1.28240100
C	3.53065700	-0.11636500	0.02275300
O	4.06947400	-0.08869900	-1.05307000

O	3.75592500	-1.07629100	0.92780700
H	4.32846600	-1.74608900	0.52657100
O	1.46932600	-1.85997500	-0.99340000
H	0.93364400	-2.28361900	-0.30527700

TS41

C	1.23207900	-0.91346500	-1.04487900
C	-0.09907500	-0.62308500	-1.32826100
C	-0.89851500	0.03128100	-0.39236100
C	-0.33757700	0.38045200	0.83672300
C	0.99173000	0.08256900	1.11889500
C	1.79930100	-0.56565700	0.18226200
H	1.83852500	-1.42367600	-1.78721200
H	-0.52088000	-0.90901400	-2.28635300
H	-0.94394400	0.88552600	1.58268100
H	1.41074500	0.36064700	2.08091000
C	3.25444600	-0.84800800	0.45755800
H	3.44462000	-0.78716000	1.53491100
H	3.49160300	-1.87027200	0.14526600
C	4.20797700	0.12125000	-0.26544700
H	4.00359100	0.04802800	-1.34070700
C	5.65767500	-0.29262300	-0.01830000
H	5.84020700	-1.31732100	-0.35167200
H	6.34901900	0.36718800	-0.54802000
H	5.89169200	-0.23742500	1.04983800
C	3.97432600	1.56574500	0.17433600
H	2.95579100	1.89466400	-0.04407600
H	4.13652400	1.66426900	1.25325000
H	4.66643800	2.24203000	-0.33327100
C	-2.34353500	0.37615100	-0.71312300
H	-2.59345400	-0.05561800	-1.68505000
C	-2.57024300	1.88696100	-0.73197100

H	-1.88818200	2.34281600	-1.45110300
H	-3.59488100	2.12603600	-1.01463100
H	-2.37129400	2.31665100	0.25139200
C	-3.23343500	-0.32122200	0.30456400
O	-3.55632500	0.19744100	1.40440400
O	-3.16677900	-1.65940400	0.18920100
H	-3.57198500	-2.06109400	0.97051800
O	-4.88428800	0.14323100	-0.31724200
H	-5.49593600	-0.31851500	0.28243500

·OH

O	0.00000000	0.00000000	0.10817500
H	0.00000000	0.00000000	-0.86540300

OH⁻

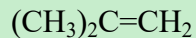
O	0.00000000	0.00000000	0.10678000
H	0.00000000	0.00000000	-0.85424300

H₂O

O	0.00000000	0.00000000	0.11762800
H	0.00000000	0.76018100	-0.47051000
H	0.00000000	-0.76018100	-0.47051000

HO₂

O	0.05492000	-0.59696800	0.00000000
H	-0.87871600	-0.88064600	0.00000000
O	0.05492000	0.70704800	0.00000000



C	0.00004100	1.45827700	-0.00000200
H	-0.92663900	2.02255300	-0.00011700
H	0.92675800	2.02249200	0.00015100
C	0.00000000	0.12539300	-0.00000800
C	1.27149500	-0.67887800	0.00001000
H	2.15495500	-0.03966700	0.00086600
H	1.30919400	-1.33116900	0.87792300
H	1.31004800	-1.32973400	-0.87896000
C	-1.27153500	-0.67881500	0.00000600
H	-2.15496500	-0.03956500	-0.00064200
H	-1.30942900	-1.33090000	-0.87806900
H	-1.30993200	-1.32987600	0.87881400



O	0.00000000	0.00000000	0.59418100
O	0.00000000	0.00000000	-0.59418100



C	0.00002700	0.00001400	0.00000000
H	0.97562200	0.46193100	0.00000000
H	-0.88802500	0.61381700	0.00000000
H	-0.08776000	-1.07583200	0.00000000



C	0.00231100	0.04123500	0.36652500
H	-0.00949000	0.09777700	1.46201200
C	1.34105000	-0.50713300	-0.08959600
H	2.15534200	0.13691200	0.24671900
H	1.49878500	-1.50826300	0.31585000

H	1.36818100	-0.56516800	-1.18088900
C	-1.16125800	-0.81953600	-0.10262600
H	-2.11593500	-0.39730700	0.22152400
H	-1.16144700	-0.88574200	-1.19369900
H	-1.08079700	-1.82812000	0.30889000
O	-0.09966600	1.36615400	-0.16517000
H	-0.94993000	1.73328700	0.09512900

CH₃CH=CH₂

C	0.13373300	0.45785000	-0.00002300
H	0.16809700	1.54536500	-0.00000200
C	1.27639800	-0.22213800	0.00001900
H	2.23615400	0.28158200	0.00003400
H	1.28552200	-1.30816600	-0.00007900
C	-1.23038000	-0.16388200	-0.00000800
H	-1.80089000	0.15249900	-0.87749300
H	-1.16718500	-1.25334600	-0.00084800
H	-1.80020500	0.15108700	0.87846500

(CH₃)₂C=CHOOH

C	0.30600000	-0.54769500	-0.19844400
H	0.52525600	-1.60931500	-0.25583200
C	-0.91097200	-0.04307700	-0.00827000
H	3.10832800	-0.46679400	-0.21241400
C	-2.09797700	-0.95910200	0.08421100
H	-1.80760000	-2.00911400	0.02983700
H	-2.62936000	-0.79031600	1.02523700
H	-2.80448600	-0.75255100	-0.72510400
C	-1.18470200	1.43036900	0.07918100
H	-0.26665400	2.01426400	0.11995800
H	-1.76774300	1.75840200	-0.78692000

H	-1.78540100	1.64364900	0.96766300
O	2.45530200	-0.16052100	0.43204500
O	1.38889400	0.27662200	-0.41985600

NH₃

N	0.00000000	0.00000000	0.11498400
H	0.00000000	0.93979500	-0.26829500
H	-0.81388600	-0.46989700	-0.26829500
H	0.81388600	-0.46989700	-0.26829500

CH₃OH

C	0.66679000	-0.01989400	0.00000400
H	1.08916800	0.98410500	-0.00123800
H	1.01679600	-0.54940000	-0.89037500
H	1.01700900	-0.54731900	0.89154000
O	-0.74778100	0.12312800	0.00000600
H	-1.14146200	-0.75304600	0.00000300

C₂H₅OH

C	-0.08202000	0.54878800	-0.00006100
H	-0.14502300	1.18897000	0.88644200
H	-0.14487900	1.18892500	-0.88661400
O	-1.15020400	-0.39633900	-0.00013500
H	-1.98424100	0.08123200	0.00097300
C	1.22063800	-0.22229600	0.00006400
H	2.06905500	0.46448400	-0.00003200
H	1.28749700	-0.85580900	0.88695000
H	1.28751500	-0.85604200	-0.88665700

HCOOH

C	-0.13051800	0.40010900	-0.00002200
O	-1.12869800	-0.26537800	0.00001300
O	1.10725600	-0.08928400	-0.00000200
H	-0.11040700	1.49481200	0.00006800
H	1.06504800	-1.05817500	-0.00001700

CH₃COOH

C	-0.08903200	0.12165400	0.00002900
O	-0.62678800	1.20012500	-0.00013000
O	-0.78674400	-1.02552700	0.00004500
H	-1.73077000	-0.81016000	-0.00001900
C	1.38904700	-0.12207300	0.00005300
H	1.66032700	-0.70506100	0.88123600
H	1.66031800	-0.70542100	-0.88089300
H	1.91828400	0.82636900	-0.00013600

Text S2.

The energy barrier of the single electron transfer process was calculated by

$$\Delta G = \frac{(\lambda + \Delta G_{\text{SET}})^2}{4\lambda} \quad (13)$$

$$\lambda = \Delta E_{\text{SET}} - \Delta G_{\text{SET}} \quad (14)$$

where ΔG_{SET} is the Gibbs free energy change for single electron transfer reaction, λ is the reorganization energy related to solute and solvent rearrangements, ΔE_{SET} is the nonadiabatic energy change between reactants and vertical products (i.e., the energies of products are calculated at the same geometries of reactants with a change of charge and spin multiplicity).

Text S3.

The free energies $\Delta G(T)$ and energy barrier $\Delta G^*(T)$ in solution phase were calculated by

$$G(\text{solv}) = G(\text{gas})(T) + G^{\text{solv}}(T) + \Delta G_{1M}(T) \quad (1)$$

$$G(\text{gas})(T) = E_0(\text{gas})(T) + G_{\text{corrected}}(T) \quad (2)$$

$$G^{\text{solv}}(T) = E_1(\text{solv})(T) - E_1(\text{gas})(T) \quad (3)$$

$$\Delta G(T) = \sum_{\text{Products}} G(\text{solv}) - \sum_{\text{reactants}} G(\text{solv}) \quad (4)$$

$$\Delta G^*(T) = (E_0 + G_{\text{corrected}})_{TS} - \sum_{\text{reactants}} G(\text{solv}) \quad (5)$$

where $G(\text{solv})(T)$ is the free energy in solution phase; $G(\text{gas})(T)$ is the free energy in gas phase; $G^{\text{solv}}(T)$ is the solvation free energy; $E_0(\text{gas})(T)$ is the total electronic energy in gas phase computed using CBS-QB3 method; $G_{\text{corrected}}(T)$ is the thermal correction to Gibbs free energy computed at M06-2X-D3/6-311+g(d,p) level; $E_1(\text{solv})(T)$ is the single point energy computed under the solvent model using CBS-QB3 method; $E_1(\text{gas})(T)$ is the single point energy computed in the gas phase using CBS-QB3 method.

Text S4.

Based on the transition state theory (TST), the rate constants were calculated by

$$K^{TST} = \sigma \kappa \frac{k_B T}{h} e^{-\frac{\Delta G^{0,\ddagger}}{RT}} \quad (6)$$

$$\Delta G^{0,\ddagger}(T) = G_{TS}^0(T) - G_{Reactant}^0(T) \quad (7)$$

$$\kappa = \frac{\frac{\pi\beta}{\alpha}}{\alpha \cdot \sin\left(\frac{\pi\beta}{\alpha}\right)} + \frac{\beta}{\alpha - \beta} e^{(\beta - \alpha)V_0} \quad (\beta < \alpha) \quad (8)$$

$$\kappa = \alpha V_0 = \beta V_0 \quad (\beta = \alpha) \quad (9)$$

$$\kappa = \frac{\beta}{\beta - \alpha} [e^{(\beta - \alpha)V_0} - 1] \quad (\beta > \alpha) \quad (10)$$

$$\alpha = \frac{2\pi}{h\nu^\ddagger} \quad (11)$$

$$\beta = \frac{1}{k_B T} \quad (12)$$

where k_B and h are the Boltzmann and Planck constants, respectively; σ is the reaction path degeneracy; R is the gas constant; T is the temperature; κ is Skodje-Truhlar tunneling factor; V_0 is the barrier height; ν^\ddagger is the imaginary frequency.

The one-dimensional Wigner function was used for curvature correction of tunneling effect. The resonance frequency correction coefficient was set as 0.967 at M06-2X-D3/6-311+g(d,p) level.