

Supporting Information

Mechanistic Investigation Inspired Activation Mode of DBU and the Function of α -Diazo Group for the Reaction of α -Amino Ketone Compound and EDA: [DBU-H]⁺-DMF-H₂O and α -Diazo as strong N-Terminal Nucleophile

Lihan Zhu, Haiyan Yuan*, Jingping Zhang*

Faculty of Chemistry, Northeast Normal University, Changchun 130024, China

*yuanhy034@nenu.edu.cn; jpzhang@nenu.edu.cn

Table of contents

Figure S1.	DFT computed energy surfaces for DBU-DMF co-assisted concerted H-shift pathway PA2, DBU-DMF-1H ₂ O co-assisted concerted H-shift pathway PA3, DBU-DMF-2H ₂ O co-assisted concerted H-shift pathway PA4, DBU-DMF-3H ₂ O co-assisted concerted H-shift pathway PA5 in the solvent phase, and free energies are given in kcal/mol.	S-2
Figure S2.	Orbital interactions in HOMOs of TS2w and TS2 .	S-3
Figure S3.	The charges of key H1, H2, O1, O2, O3, O4, C4, N1, N2, N3, and N4 atoms in Int1w and TS2w .	S-3
Table S1.	The total charges of substrates 1 , 2 , DMF, H ₂ O, and DBU-H ⁺ in Int1w and TS2w .	S-4
Scheme S1.	Optimized structure of TS4a' .	S-2
S1.	The B3LYP/6-31+G** optimized coordinates between benzaldehyde and 1-cinnamoylcyclopropanecarboxamides in gas phase.	S-4-S-72

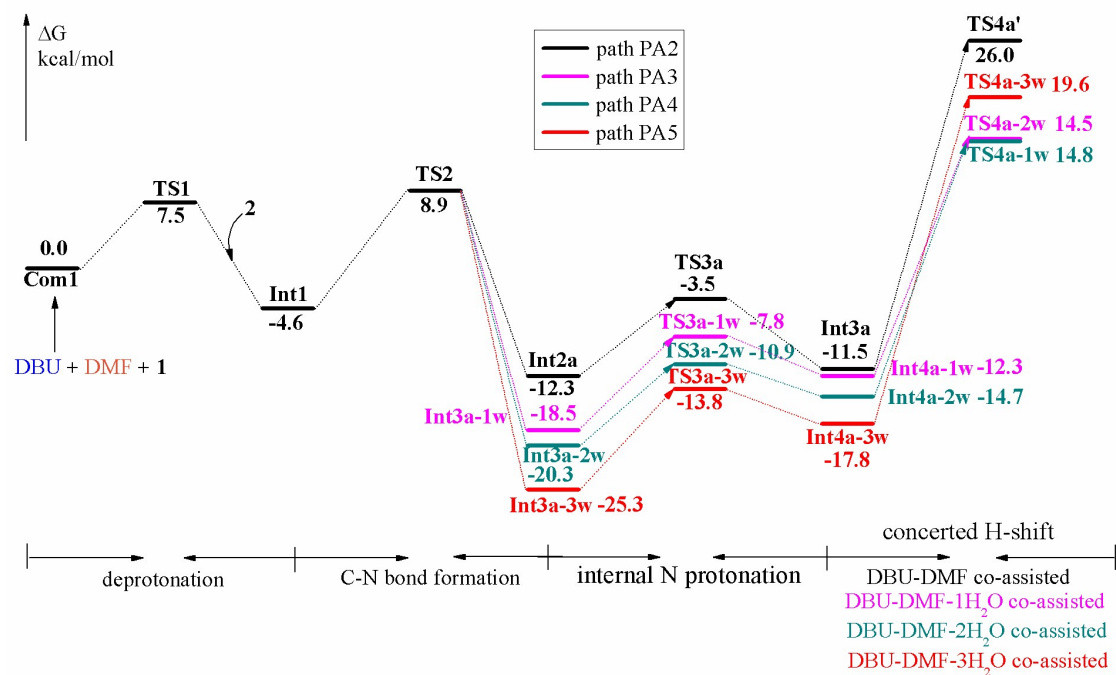
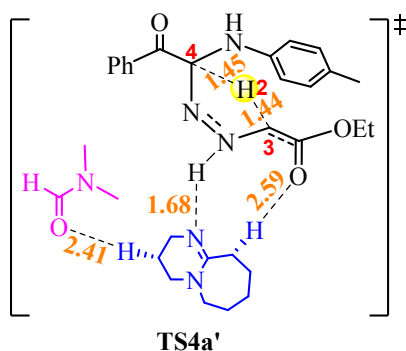


Figure S1. DFT computed energy surfaces for DBU-DMF co-assisted concerted H-shift pathway PA2, DBU-DMF-1H₂O co-assisted concerted H-shift pathway PA3, DBU-DMF-2H₂O co-assisted concerted H-shift pathway PA4, DBU-DMF-3H₂O co-assisted concerted H-shift pathway PA5 in the solvent phase, and free energies are given in kcal/mol.



Scheme S1. Optimized structure of TS4a'.

Distortion-interaction analyses

Both transition states were separated into two fragments (the substrates and catalyst) by single point energy calculations. The differences in energy between the distorted species and optimized ground state geometries are defined as the distortion energy of substrates ($\Delta E_{\text{sub}}^{\ddagger}$) and catalyst ($\Delta E_{\text{cat}}^{\ddagger}$), respectively. The interaction energy (ΔE_{int}) is the energy of interaction between distorted substrates and catalyst ($\Delta E_{\text{int}} = \Delta E_{\text{sub}}^{\ddagger} - \Delta E_{\text{cat}}^{\ddagger}$).

Non-covalent interaction (NCI) analysis

NCI is demonstrated to be capable of distinguishing strong attractive (blue regions), van der Waals interactions (green regions), and repulsive steric interactions (red regions) in a complex structure.

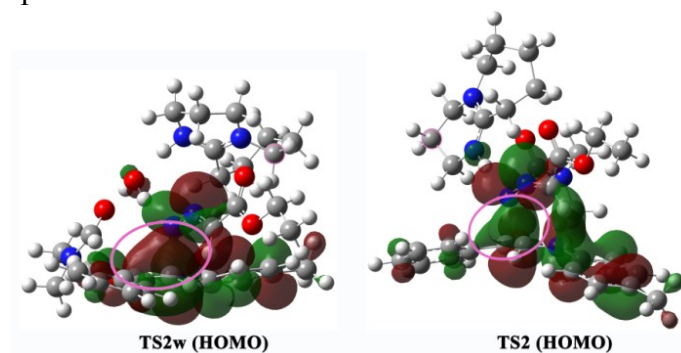


Figure S2. Orbital interactions in HOMOs of TS2w and TS2.

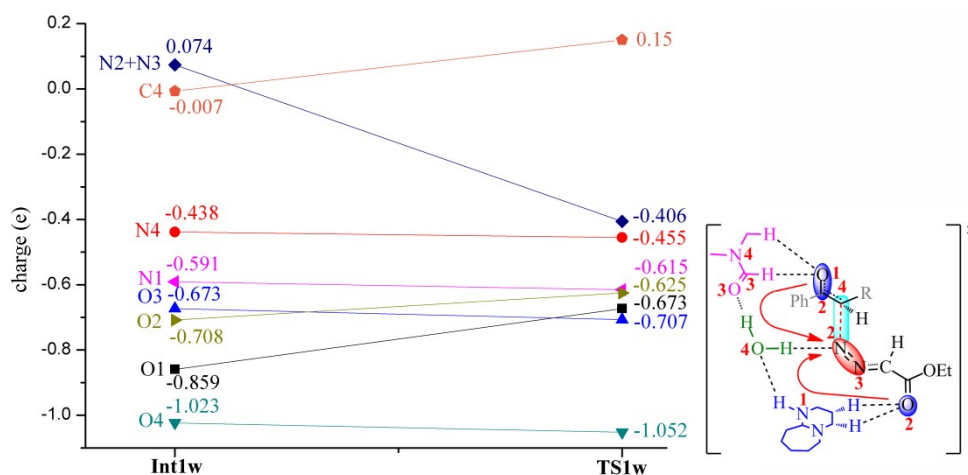


Figure S3. The charges of key H1, H2, O1, O2, O3, O4, C4, N1, N2, N3, and N4 atoms in Int1w and TS2w.

Table S1. The total charges of substrates **1**, **2**, DMF, H₂O, and DBU-H⁺ in **Int1w** and **TS2w**.

charge (e)	substrate 1	substrate 2	DMF	H ₂ O	DBU-H ⁺
Int1w	-0.123	-0.413	0.084	-0.062	0.514
TS2w	0.285	-0.72	0.031	-0.02	0.424

DBU regulate the charge of C4 by activating α -H of substrate **1**, and the negative charges of α -diazo group comes from two carbonyl oxygen atoms of substrates **1** and **2**. The negative charge transfer follows O1 (-0.370) $\rightarrow$ N4 (-0.017) $\rightarrow$ O3 (-0.034) $\rightarrow$ O4 (-0.029) $\rightarrow$ N2=N3 (-0.332) and O2 (-0.083) $\rightarrow$ N1 (-0.024) $\rightarrow$ O4 (-0.029) $\rightarrow$ N2=N3 (-0.332), respectively. Thus, DBU, DMF, and H₂O catalysts can regulate the negative charge migration by noncovalent interactions.

S1. The B3LYP/6-31+G optimized coordinates between benzaldehyde and 1-cinnamoylcyclopropanecarboxamides in gas phase.**

Com0

C	-3.36875900	-3.29641300	-0.05003300
C	-3.79297100	-2.80893100	-1.44079000
C	-1.02362200	-1.92338200	-1.39933600
C	-2.87009400	-3.26544500	-2.58302800
C	-1.37898100	-3.17760800	-2.21973500
H	-3.04020700	-4.34894300	-0.10222300
H	-1.61411300	-1.06646600	-1.75066700
H	-3.86895400	-1.71595300	-1.41475700
H	-3.07241900	-2.64716800	-3.46672300
H	-4.25211200	-3.28673500	0.59607700
H	-4.80760300	-3.17897500	-1.63071200
H	0.02419200	-1.66261300	-1.55496700
H	-3.11458000	-4.29698400	-2.86725100
H	-0.78217700	-3.18189100	-3.13887900
H	-1.07028000	-4.07120700	-1.66206200
C	-2.44974700	-2.62783700	2.11762400

C	-1.57588800	-1.59765100	2.82114500
C	-0.16204400	-1.68773000	2.25169700
H	-3.49944700	-2.50579900	2.40832800
H	-1.98199500	-0.59358700	2.64983800
H	0.45735900	-0.86388200	2.62617700
N	-2.36806700	-2.47901400	0.65821700
H	0.32488800	-2.61351800	2.59498800
H	-1.58383900	-1.77680300	3.90220800
H	-2.14932400	-3.64681900	2.41529400
C	-1.16326500	-2.04215600	0.11346300
N	-0.13163700	-1.64959200	0.79202500
C	3.13298300	1.51663600	-0.36698100
O	3.69842700	2.55885900	-0.67977600
C	3.89765600	0.25509300	-0.13285500
C	3.26655700	-0.96069700	0.18506400
C	5.29911100	0.30185800	-0.23570800
C	4.03602200	-2.10723300	0.39656900
H	2.18438100	-1.03667000	0.26955400
C	6.06012300	-0.84481700	-0.02310700
H	5.76852900	1.24842200	-0.48240000
C	5.42858700	-2.05341800	0.29374900
H	3.54223800	-3.04364000	0.63931100
H	7.14236700	-0.80004800	-0.10342000
H	6.02108900	-2.94907100	0.45896400
C	1.61878600	1.50044900	-0.18366200
H	1.41512700	1.27008700	0.87784800
H	1.19151600	0.66155200	-0.74848100
N	1.05508400	2.75720900	-0.59214100
H	1.74063000	3.49121000	-0.71989600
C	-0.25046100	3.12276800	-0.30734400
C	-0.66334100	4.45946400	-0.50076300
C	-1.20896800	2.19778000	0.14749100
C	-1.97529900	4.84321600	-0.25018500
H	0.05801000	5.19300700	-0.85333300
C	-2.52462400	2.60695500	0.39284500
H	-0.93671900	1.15882700	0.30348500
C	-2.94147600	3.92773200	0.20394300
H	-2.25646700	5.88237700	-0.40917500
H	-3.24171900	1.86728700	0.74323800
C	-4.36448900	4.36257400	0.47293200
H	-4.41100300	5.14520600	1.24044400
H	-4.84217200	4.76710400	-0.42815000
H	-4.97504200	3.52334100	0.82087600

TS1'

C	1. 86752500	3. 76009100	0. 38312600
C	2. 54336100	3. 55290700	-0. 97642600
C	0. 41631100	1. 58078500	-1. 17255400
C	1. 58219900	3. 64138300	-2. 17168000
C	0. 25032600	2. 92328300	-1. 90832400
H	1. 13462000	4. 57901200	0. 32738100
H	1. 32037000	1. 06374700	-1. 51929100
H	3. 06483800	2. 58926800	-0. 96330300
H	2. 07135300	3. 20484000	-3. 05099800
H	2. 62834000	4. 07493600	1. 10181400
H	3. 32291300	4. 31714900	-1. 07753200
H	-0. 41849200	0. 92764000	-1. 43086200
H	1. 38804100	4. 69334200	-2. 41613400
H	-0. 25949100	2. 72797100	-2. 85688600
H	-0. 42751900	3. 57104100	-1. 33794300
C	1. 25051100	2. 58563300	2. 47164300
C	1. 00377800	1. 19579100	3. 04633300
C	-0. 27307000	0. 63535300	2. 43514400
H	2. 23047700	2. 95731800	2. 78504800
H	1. 84751800	0. 54054400	2. 80350900
H	-0. 40134100	-0. 42501900	2. 67648900
N	1. 23390300	2. 56981300	0. 99585000
H	-1. 15651900	1. 16260700	2. 81969300
H	0. 92572600	1. 25701100	4. 13655000
H	0. 49722700	3. 29730500	2. 84106600
C	0. 47038500	1. 65084000	0. 34336900
N	-0. 24046600	0. 74899000	0. 98147500
C	-2. 17098800	-1. 01681900	-1. 03978900
O	-2. 02216800	-0. 54938500	-2. 20093700
C	-3. 52026900	-0. 89984500	-0. 37643300
C	-3. 80728100	-1. 38856900	0. 91054200
C	-4. 55120000	-0. 27194300	-1. 09464600
C	-5. 08178000	-1. 24769900	1. 46236000
H	-3. 03927300	-1. 89088600	1. 48975700
C	-5. 82671400	-0. 13198100	-0. 54569300
H	-4. 32261900	0. 09357400	-2. 09023800
C	-6. 09836200	-0. 61790700	0. 73666300
H	-5. 28370700	-1. 63584900	2. 45725500
H	-6. 61114400	0. 35362600	-1. 12023600
H	-7. 09146300	-0. 51333400	1. 16490600
C	-1. 05985200	-1. 54498000	-0. 30729400
H	-1. 27183700	-2. 28855300	0. 46130300
H	-0. 68044300	-0. 21937900	0. 40419100

N	0.06526200	-1.86306100	-1.13652800
H	-0.07894600	-1.63054900	-2.11286700
C	1.34114200	-2.12905900	-0.70970400
C	2.39908700	-2.22788700	-1.64906500
C	1.66472800	-2.34234600	0.64931000
C	3.69539700	-2.51904500	-1.24310600
H	2.18186900	-2.08475900	-2.70550600
C	2.97700600	-2.63525500	1.03304700
H	0.88469300	-2.29704700	1.40159200
C	4.02357700	-2.72963100	0.10930400
H	4.47595100	-2.58906200	-1.99873700
H	3.18456500	-2.80339300	2.08858200
C	5.43815600	-3.05595900	0.53186500
H	5.79676500	-3.98569400	0.07196800
H	6.14331400	-2.26470000	0.24594800
H	5.50682400	-3.18067200	1.61744200

Com1

C	0.12192000	-4.43767400	0.10796100
C	-1.02554200	-4.58244000	-0.89856800
C	-0.74039900	-1.69180800	-0.82436000
C	-0.79824900	-3.84404600	-2.22850100
C	-0.16952500	-2.45481100	-2.03533100
H	1.09603400	-4.50672300	-0.40142900
H	-1.81483500	-1.89577700	-0.72578200
H	-1.95160600	-4.24336800	-0.42002300
H	-1.75995100	-3.74711800	-2.74854100
H	0.07433400	-5.28566900	0.79814500
H	-1.16282300	-5.65162000	-1.10107600
H	-0.65562400	-0.61781800	-0.98957300
H	-0.15328200	-4.44649300	-2.88105200
H	-0.33170300	-1.85543400	-2.93853300
H	0.91758000	-2.54826400	-1.92410200
C	0.82981000	-3.44424900	2.22690400
C	0.54809200	-2.30856600	3.20083500
C	0.86517700	-0.98736100	2.50432900
H	0.51098000	-4.40253300	2.65202400
H	-0.50792800	-2.33119800	3.49682500
H	0.51387500	-0.14298800	3.11220000
N	0.08842900	-3.24265600	0.97323200
H	1.95677800	-0.87049400	2.41594200
H	1.14999400	-2.43295400	4.10838300
H	1.90745500	-3.51218600	2.01465100
C	-0.06375400	-1.94137400	0.51809500

N	0.26323900	-0.86971700	1.17798900
C	0.03444300	3.17453400	-0.61931200
O	-0.18206300	3.75932900	-1.67538900
C	1.31123200	3.39038100	0.13095700
C	1.71522100	2.55868400	1.18910700
C	2.12450300	4.47499100	-0.24120800
C	2.90872100	2.81782900	1.86724300
H	1.11946500	1.69614100	1.46837500
C	3.31209400	4.73261700	0.44009500
H	1.80193400	5.10613100	-1.06277000
C	3.70586600	3.90484000	1.49825200
H	3.21601200	2.16866200	2.68194800
H	3.92930800	5.57865500	0.15197600
H	4.63037200	4.10667800	2.03196000
C	-1.01894600	2.25619800	-0.01863700
H	-1.35433400	2.73287700	0.92298300
H	-0.56495500	1.29843800	0.27515500
N	-2.10262700	2.06579000	-0.95160300
H	-2.11394000	2.76486200	-1.68539900
C	-3.33863200	1.56966200	-0.54995900
C	-4.47516600	1.78185300	-1.35890100
C	-3.50099200	0.81999000	0.62902500
C	-5.71486600	1.26683300	-0.99597900
H	-4.37485600	2.35532600	-2.27767500
C	-4.75721500	0.31248500	0.97680000
H	-2.64673200	0.60924400	1.26380200
C	-5.88963000	0.52226100	0.18332700
H	-6.56983600	1.45221800	-1.64303300
H	-4.84876600	-0.26572000	1.89383900
C	-7.24871000	-0.01032600	0.57768600
H	-7.93060200	0.79794300	0.87210200
H	-7.72692700	-0.54995000	-0.24834600
H	-7.17323200	-0.69960800	1.42455300
C	3.49309400	-1.40315000	-0.43750000
O	3.50101100	-2.58580900	-0.09941600
H	2.69868800	-0.71088800	-0.10904900
N	4.41997500	-0.80740400	-1.23511000
C	5.53530400	-1.57002500	-1.77515700
H	5.46165300	-2.59525300	-1.41199500
H	5.50686800	-1.56808700	-2.87192800
H	6.48889000	-1.13498600	-1.45157700
C	4.32455500	0.59801000	-1.59671900
H	4.21164400	0.71537700	-2.68180900
H	3.46045900	1.04988400	-1.10503200

H	5.22448500	1.14043200	-1.28215900
---	------------	------------	-------------

TS1

C	-0.29715100	3.98679800	0.13027000
C	-1.02767900	4.11035500	1.47235300
C	-0.53092100	1.24607700	1.41309000
C	-0.27728600	3.47977000	2.65674400
C	0.36834100	2.13446900	2.29379200
H	0.78140700	4.16077300	0.25039900
H	-1.58344900	1.35965000	1.70256600
H	-2.02823800	3.67504600	1.36770900
H	-0.97898600	3.34477900	3.48945100
H	-0.67007300	4.76924400	-0.53594200
H	-1.18283900	5.17809600	1.66786200
H	-0.28208600	0.20005400	1.58990100
H	0.49811200	4.16927900	3.01404700
H	0.60694200	1.57994800	3.20714800
H	1.32256300	2.30040400	1.78080400
C	-0.34181800	2.89095400	-2.07468600
C	-0.88960900	1.68442100	-2.82705700
C	-0.22660100	0.42898200	-2.27519000
H	-0.88530200	3.79627300	-2.36217700
H	-1.97534000	1.62069800	-2.69277100
H	-0.71359800	-0.47754800	-2.65236400
N	-0.49976600	2.72559400	-0.61778400
H	0.82670400	0.38591400	-2.58328600
H	-0.68879900	1.79500900	-3.89779300
H	0.72193100	3.04297400	-2.30003200
C	-0.42429100	1.47798200	-0.08459100
N	-0.30395900	0.39565000	-0.81941600
C	0.36618200	-2.33565900	1.01392700
O	0.36693600	-2.06530500	2.24102100
C	1.64002100	-2.83351400	0.37929000
C	1.83114500	-2.94433300	-1.00962700
C	2.68915400	-3.22011600	1.23020900
C	3.03128300	-3.43296900	-1.53022400
H	1.04094800	-2.64974600	-1.69288300
C	3.88645100	-3.71705700	0.71183300
H	2.53224700	-3.12796100	2.29989000
C	4.06384000	-3.82596600	-0.67143500
H	3.15861700	-3.51293700	-2.60656400
H	4.67950400	-4.02704200	1.38751100
H	4.99251800	-4.21811900	-1.07698000
C	-0.79073300	-2.10482600	0.19288100

H	-0.90511600	-2.76598100	-0.66907800
H	-0.45398100	-0.75206800	-0.33805000
N	-1.99069100	-1.93895100	0.95973300
H	-1.83859300	-1.94811000	1.96167500
C	-3.21760200	-1.55173400	0.48231200
C	-4.27515900	-1.27732400	1.38531600
C	-3.49917200	-1.43026300	-0.89619400
C	-5.53179000	-0.90239000	0.92668300
H	-4.09433900	-1.36927700	2.45420400
C	-4.77202900	-1.05231600	-1.33373000
H	-2.72522700	-1.64170700	-1.62580400
C	-5.81763500	-0.77879400	-0.44551400
H	-6.31514600	-0.70134400	1.65537100
H	-4.95148400	-0.97604600	-2.40479800
C	-7.19703300	-0.39065400	-0.92803600
H	-7.94004300	-1.16858800	-0.70824000
H	-7.55007900	0.53298700	-0.45255700
H	-7.20559000	-0.22824400	-2.01078000
C	3.39001200	1.33781200	-0.49964600
O	2.77715100	2.36725200	-0.78947800
H	2.88252400	0.36170600	-0.41809200
N	4.72029800	1.25927500	-0.24776000
C	5.56016300	2.44672600	-0.30372600
H	4.93913800	3.29952700	-0.57772300
H	6.02615600	2.63178200	0.67179000
H	6.35402600	2.31756800	-1.04928900
C	5.35668800	-0.00324400	0.09914200
H	5.81315900	0.05611900	1.09464800
H	4.61784500	-0.80701900	0.10310700
H	6.13947800	-0.25176400	-0.62772800

Int1

C	5.04450700	2.20886000	0.04522200
C	4.87073900	3.56178400	-0.65128700
C	2.30678900	2.36943800	-1.26729500
C	3.60270000	4.32790300	-0.24094900
C	2.36584100	3.42182000	-0.14490200
H	4.77347400	2.26891300	1.10701600
H	2.69046700	2.78570100	-2.20742500
H	4.90427100	3.40947200	-1.73669700
H	3.42580400	5.12893700	-0.96959800
H	6.09915800	1.92670000	-0.00578100
H	5.75340900	4.16516600	-0.40903500
H	1.26447100	2.11633000	-1.47036200

H	3.76587700	4.81861700	0.72633900
H	1.45481200	4.02397400	-0.20825300
H	2.33879900	2.90945700	0.82289200
C	4.92454400	-0.24636100	-0.17418600
C	4.41702900	-1.37096600	-1.06857300
C	2.89700600	-1.39784800	-1.03992700
H	6.00768500	-0.13755600	-0.27522200
H	4.77508700	-1.22069200	-2.09379500
H	2.48743700	-2.02555900	-1.83398300
N	4.31930900	1.05362800	-0.54121200
H	2.50181700	-1.77712000	-0.09216000
H	4.81336600	-2.32741500	-0.71652600
H	4.69085900	-0.43739000	0.87985100
C	3.05449300	1.08635200	-0.98064900
N	2.39533900	-0.03509400	-1.24389200
C	-0.38873600	-2.67117000	0.07663100
O	0.17962800	-2.13654200	1.10689500
C	0.35078800	-3.71157500	-0.70462900
C	0.12960100	-3.95628700	-2.07375100
C	1.33061000	-4.47815200	-0.04634500
C	0.84641800	-4.94458800	-2.75189200
H	-0.59092700	-3.35142200	-2.61625300
C	2.04434200	-5.46891600	-0.72247000
H	1.50839600	-4.28157600	1.00639900
C	1.80769300	-5.70904600	-2.08082900
H	0.66100900	-5.11162700	-3.80995900
H	2.78382500	-6.06077600	-0.18818200
H	2.36470600	-6.47795600	-2.60907600
C	-1.69382900	-2.36112000	-0.29625900
H	-2.20995200	-2.84948100	-1.10750200
H	1.41162400	0.04360700	-1.49977200
N	-2.39641400	-1.45675900	0.48447700
H	-1.84656400	-1.13819100	1.27712300
C	-3.76014300	-1.21893600	0.50864000
C	-4.28906500	-0.34232000	1.48312500
C	-4.65761900	-1.78496900	-0.41875300
C	-5.64951200	-0.05299500	1.52298600
H	-3.62051000	0.10234200	2.21717400
C	-6.01809100	-1.47697300	-0.36217900
H	-4.30047000	-2.46680700	-1.18202600
C	-6.55056700	-0.61015700	0.60059200
H	-6.01840800	0.62327200	2.29162600
H	-6.68327000	-1.93312900	-1.09230800
C	-8.02639700	-0.28718800	0.65375700

H	-8.47248100	-0.58462000	1.61114700
H	-8.21110100	0.78761900	0.53256600
H	-8.57299600	-0.80673800	-0.13944100
C	2.04386300	-0.03008400	2.62700100
O	2.92098000	0.76575200	2.25119300
H	1.45531600	-0.64021800	1.92382500
N	1.70774500	-0.25242200	3.91991200
C	2.36408700	0.45807500	5.00503800
H	3.09502400	1.14686300	4.58087100
H	1.62894800	1.02122800	5.59329200
H	2.87277900	-0.24777700	5.67374100
C	0.67897800	-1.22873400	4.26483200
H	-0.14789600	-0.73986200	4.79573900
H	0.30129500	-1.69868300	3.35234700
H	1.09684700	-2.00272200	4.92089200
C	-1.79429200	2.87245000	-1.27452300
O	-0.78827200	3.15515700	-1.92369700
O	-2.71108800	3.80061400	-0.88914100
C	-2.45601000	5.16237200	-1.29418500
C	-3.62426200	6.00619800	-0.81789300
H	-2.34530600	5.19454200	-2.38267000
H	-1.50952300	5.49362500	-0.85325200
H	-3.46769700	7.05097600	-1.10720600
H	-4.56230400	5.66169200	-1.26352600
H	-3.72332400	5.96082700	0.27099400
N	-1.42200500	0.54046500	-1.17482200
N	-0.66723000	-0.20288900	-1.63343000
C	-2.16673300	1.55581000	-0.80335900
H	-3.03962700	1.37304400	-0.19100800

TS2

C	4.76123300	2.89993300	0.31137800
C	4.23857000	4.22539500	-0.25117700
C	1.95269600	2.52999700	-0.78620300
C	2.87308300	4.65792500	0.30791200
C	1.87546600	3.49358100	0.41056200
H	4.57588200	2.83116900	1.39183600
H	2.14611600	3.08621500	-1.71195500
H	4.21142100	4.15822100	-1.34512200
H	2.46127400	5.44196700	-0.33891900
H	5.84464000	2.86707200	0.17171100
H	4.98653000	4.99260400	-0.01860700
H	0.97910700	2.06362700	-0.93722800
H	3.00682600	5.11091000	1.29818600

H	0.85319100	3.87991900	0.44976100
H	2.03521000	2.92972100	1.33710800
C	5.18358400	0.50982400	-0.16003900
C	4.85824500	-0.60505400	-1.14718700
C	3.39511200	-0.99459100	-1.00046800
H	6.19757400	0.88295700	-0.32790500
H	5.05897100	-0.26846500	-2.17102000
H	3.05795900	-1.63196500	-1.82103600
N	4.26250400	1.65604000	-0.32557900
H	3.22128800	-1.53772100	-0.06616100
H	5.50040500	-1.46837000	-0.95001100
H	5.10354800	0.15465700	0.87399500
C	2.98609300	1.43078300	-0.67567500
N	2.57273800	0.21571000	-1.00931100
C	-0.17439800	-2.70906900	-0.19556300
O	0.27386700	-2.75564100	0.98257400
C	0.59428800	-3.35156400	-1.30361200
C	0.42579000	-3.01550900	-2.65955700
C	1.53623100	-4.34132500	-0.96796400
C	1.17359400	-3.65871900	-3.64858600
H	-0.26654700	-2.22932600	-2.93904300
C	2.27612000	-4.98843600	-1.95716100
H	1.66460600	-4.59167100	0.08006100
C	2.09895600	-4.64907400	-3.30352300
H	1.03542500	-3.38248700	-4.69038700
H	2.98810300	-5.76172800	-1.68085000
H	2.67446600	-5.15233100	-4.07552900
C	-1.38673700	-1.99912200	-0.49042700
H	-1.92292300	-2.20296900	-1.40698100
H	1.55996500	0.07020600	-1.16281100
N	-2.14883400	-1.64519300	0.61716700
H	-1.64117400	-1.74740400	1.48821700
C	-3.51808900	-1.44860000	0.69468900
C	-4.10579700	-1.23685500	1.96163100
C	-4.36362100	-1.43243800	-0.42988400
C	-5.47354200	-1.03436400	2.09058600
H	-3.47336000	-1.23790700	2.84663500
C	-5.73961700	-1.22827900	-0.27732300
H	-3.96301900	-1.58876200	-1.42532700
C	-6.32857800	-1.02598500	0.97325600
H	-5.88936900	-0.87968200	3.08420100
H	-6.36397300	-1.22449400	-1.16795500
C	-7.81441300	-0.79679600	1.12910300
H	-8.26670900	-1.52553900	1.81306300

H	-8.02981800	0.20085200	1.53240100
H	-8.33060000	-0.88104200	0.16774500
C	2.31350500	-0.64308200	2.69558900
O	3.17709300	0.18346500	2.37203500
H	1.73373800	-1.21373200	1.95283300
N	1.97274400	-0.95266700	3.96993300
C	2.61502800	-0.30091700	5.10016800
H	3.34310700	0.41685200	4.72192600
H	1.87065900	0.22191800	5.71318700
H	3.12478100	-1.04048400	5.73006700
C	0.95367000	-1.95692500	4.25141400
H	0.12305200	-1.51156800	4.81337100
H	0.57510400	-2.36828700	3.31303400
H	1.37721100	-2.77125600	4.85237000
C	-2.17257100	2.72432600	-1.24332300
O	-1.23138100	3.49203400	-1.44813500
O	-3.46386000	3.17126000	-1.15299500
C	-3.65972600	4.58843500	-1.30045400
C	-5.14828300	4.86089400	-1.17092700
H	-3.27237400	4.90644300	-2.27450000
H	-3.08354500	5.11378800	-0.53060000
H	-5.34108300	5.93412200	-1.27817100
H	-5.71150800	4.33007400	-1.94482800
H	-5.52172900	4.53851800	-0.19393000
N	-0.93132500	0.72149900	-1.19486700
N	-0.29396300	-0.30363900	-1.17733600
C	-2.11155900	1.29409500	-1.05105400
H	-3.00121900	0.72329300	-0.79778700

Int2

C	-5.71585700	-2.16819600	-0.95810300
C	-6.57113600	-1.02309700	-0.40602900
C	-3.94815900	0.18431200	-0.16934400
C	-6.33757900	0.33114100	-1.09479400
C	-4.84882200	0.62029200	-1.33763900
H	-5.68399400	-2.12585300	-2.05701000
H	-4.45108700	0.36782200	0.78964900
H	-6.40136900	-0.94837800	0.67433400
H	-6.77222400	1.12192700	-0.47106900
H	-6.19783700	-3.11417100	-0.69753000
H	-7.62079600	-1.31743900	-0.52447500
H	-3.04840800	0.80778200	-0.16355900
H	-6.87831600	0.35943000	-2.04919000
H	-4.68728900	1.69086800	-1.49550700

H	-4.51019800	0.12919700	-2.25900600
C	-3.79371100	-3.66533600	-0.51114000
C	-2.62560700	-3.85083600	0.45013700
C	-1.58016600	-2.78445400	0.16506800
H	-4.60866500	-4.35084500	-0.26313000
H	-2.98480600	-3.77326000	1.48319100
H	-0.82795100	-2.73442400	0.95688500
N	-4.33389400	-2.29110600	-0.43648700
H	-1.05232700	-3.00482500	-0.77015100
H	-2.19309500	-4.84630600	0.31609900
H	-3.48094700	-3.88189700	-1.54229900
C	-3.49111600	-1.25885600	-0.18816000
N	-2.21780100	-1.46695000	0.08388300
C	1.28305700	-0.42635300	1.58680500
O	1.70437900	-1.50534900	1.18256700
C	1.02666300	-0.20325100	3.04521600
C	0.25934000	0.87483600	3.52027000
C	1.57915300	-1.10963100	3.96654500
C	0.05186700	1.03839300	4.89094000
H	-0.20084500	1.56651800	2.82345300
C	1.37922900	-0.93817500	5.33497500
H	2.16769700	-1.93891800	3.58770800
C	0.61400900	0.13720100	5.79999700
H	-0.54975000	1.86900200	5.24815500
H	1.81905300	-1.63851800	6.03930600
H	0.45653000	0.27192700	6.86648000
C	0.97588500	0.71612600	0.59428900
H	1.21020400	1.67312800	1.08486600
H	-1.54211000	-0.63312200	0.22941300
N	1.73105800	0.64242800	-0.63750600
H	1.29445800	0.07628500	-1.35134500
C	3.09970500	0.84147200	-0.74663700
C	3.73986600	0.59804600	-1.98213000
C	3.89203900	1.31686100	0.31452300
C	5.10234800	0.82471600	-2.13987100
H	3.14990500	0.24071500	-2.82331600
C	5.25999500	1.54524400	0.13307300
H	3.45289800	1.50847700	1.28788400
C	5.89952100	1.30714400	-1.08710500
H	5.55722200	0.62861700	-3.10905400
H	5.83997700	1.91524900	0.97579400
C	7.37754000	1.56275800	-1.27718400
H	7.90198200	0.66738700	-1.63316900
H	7.56000000	2.35655600	-2.01257600

H	7.84898100	1.87025100	-0.33856900
C	1.61925600	-3.73978700	-1.43747500
O	0.58796900	-4.20630800	-1.93112400
H	1.59760200	-2.96855500	-0.65130500
N	2.88294400	-4.09684400	-1.78158900
C	3.12424800	-5.10090100	-2.80534700
H	2.16263400	-5.44578200	-3.18613900
H	3.71227300	-4.67554200	-3.62798600
H	3.67780600	-5.95078000	-2.38682300
C	4.03850000	-3.49208300	-1.13323300
H	4.67189200	-2.98130800	-1.86797700
H	3.70452200	-2.75939400	-0.39591400
H	4.63995700	-4.25757000	-0.62677200
C	-1.52305900	3.89720600	-0.77293100
O	-2.72593900	3.79991100	-0.98635900
O	-0.85033000	5.07989100	-0.94862300
C	-1.63467800	6.19652700	-1.40485100
C	-0.71052300	7.39753100	-1.50540100
H	-2.45427100	6.37182900	-0.69953500
H	-2.08320500	5.94785600	-2.37301800
H	-1.27196200	8.27110800	-1.85477800
H	-0.27179100	7.63675800	-0.53153200
H	0.10445700	7.20675100	-2.21068500
N	-1.10727000	1.66880300	-0.10077600
N	-0.46437800	0.60137000	0.32380300
C	-0.60339400	2.85855400	-0.32038800
H	0.44945200	3.11793800	-0.22523100

TS3a

C	-6.37437900	-0.93350700	-0.19831000
C	-6.68006200	-0.56924400	1.25952800
C	-4.08421500	0.70566200	0.93763300
C	-6.56616800	0.93203200	1.57065500
C	-5.34674400	1.58611200	0.90333600
H	-6.83200600	-0.19586700	-0.87753100
H	-4.02734900	0.15856900	1.88827400
H	-6.01797500	-1.15408500	1.90854800
H	-6.51068700	1.06295000	2.65901600
H	-6.85565700	-1.89066900	-0.41809000
H	-7.69888400	-0.90866700	1.48180900
H	-3.20981800	1.35167200	0.88169600
H	-7.47888200	1.44758400	1.24549900
H	-5.12092400	2.53554100	1.40002900
H	-5.56946200	1.84976900	-0.13716800

C	-4.76053700	-2.07554300	-1.66438600
C	-3.30121400	-2.49008900	-1.78656700
C	-2.43744500	-1.23994800	-1.85685400
H	-5.39412500	-2.94807400	-1.47130400
H	-3.00913900	-3.08877000	-0.91679700
H	-1.38011300	-1.50184000	-1.78521000
N	-4.95503800	-1.13199300	-0.54794100
H	-2.58164700	-0.72354500	-2.81713500
H	-3.15106400	-3.11414800	-2.67150400
H	-5.11282400	-1.61919900	-2.60310200
C	-3.92605600	-0.28664900	-0.20357300
N	-2.75312900	-0.31111600	-0.76882700
C	2.08933100	-0.92334600	1.30372200
O	2.70364800	-1.81607400	0.73563900
C	1.81883100	-0.98278100	2.77283900
C	0.89420300	-0.13400800	3.40454800
C	2.52394700	-1.92271200	3.54403600
C	0.68016600	-0.22741100	4.78082900
H	0.31909800	0.57694700	2.82216500
C	2.31582200	-2.00835100	4.91877200
H	3.23564100	-2.57221600	3.04512800
C	1.39230600	-1.16008200	5.54017100
H	-0.04332000	0.42608800	5.25935600
H	2.87165300	-2.73252700	5.50731300
H	1.22823800	-1.22660600	6.61203700
C	1.56865100	0.28766800	0.48250400
H	1.62859300	1.19864300	1.09857100
H	-1.68514500	0.49236200	-0.42244700
N	2.32740800	0.51648300	-0.73130600
H	2.16540700	-0.21050100	-1.41721100
C	3.63614600	1.01302400	-0.73031300
C	4.40047100	0.91685500	-1.91169300
C	4.22025800	1.65450300	0.37433700
C	5.68403200	1.44543300	-1.97980000
H	3.97110700	0.42637800	-2.78233200
C	5.51119500	2.18770700	0.28504800
H	3.68457400	1.74192100	1.31350200
C	6.27254100	2.09889500	-0.88316000
H	6.24223600	1.34949700	-2.90888800
H	5.93155600	2.67799800	1.16031000
C	7.66660600	2.67679800	-0.97319900
H	7.98029400	3.10388700	-0.01569500
H	8.40331200	1.91391600	-1.25311000
H	7.72569200	3.47343300	-1.72532200

C	0.78690300	-3.90190800	-1.76604200
O	-0.25026800	-3.87852100	-2.42863100
H	1.01884800	-3.13055000	-1.01305400
N	1.76007800	-4.84695300	-1.86514100
C	1.62961900	-5.94971300	-2.80390300
H	0.68684100	-5.83968800	-3.34020900
H	2.46060300	-5.94391600	-3.52040300
H	1.63784900	-6.90963900	-2.27215100
C	2.95834700	-4.79674900	-1.04030000
H	3.85588800	-4.74468600	-1.66963200
H	2.93203500	-3.91484200	-0.39753900
H	3.03124900	-5.69392700	-0.41195000
C	-1.28918900	3.17080300	-0.72966100
O	-2.49720100	2.95934800	-0.79559100
O	-0.74736800	4.39914800	-0.97618100
C	-1.67341400	5.44785900	-1.32601900
C	-0.86679400	6.71248800	-1.55920500
H	-2.39737700	5.56988000	-0.51311000
H	-2.22883600	5.14752200	-2.22064100
H	-1.53794900	7.53493800	-1.82939100
H	-0.31643400	6.99878700	-0.65761900
H	-0.14693700	6.57372800	-2.37162400
N	-0.57566200	0.94656500	-0.19173100
N	0.18041500	-0.05053000	0.18130800
C	-0.24986600	2.22084500	-0.38439800
H	0.77709900	2.55569500	-0.34293300

Int3a

C	-1.91078200	-0.07422800	4.61812100
C	-2.05524800	1.44004900	4.81469700
C	-0.62636500	1.35254600	2.27711100
C	-2.66656500	2.17942300	3.61259600
C	-2.13249000	1.67603900	2.26112700
H	-2.80288000	-0.47604700	4.10872200
H	-0.09214700	2.08295500	2.90073400
H	-1.06950600	1.84976300	5.06383400
H	-2.46005000	3.25243000	3.71976000
H	-1.88454400	-0.54405200	5.60621500
H	-2.68578400	1.60779000	5.69633600
H	-0.21510100	1.44824100	1.27132000
H	-3.75877800	2.07314800	3.63052000
H	-2.31706200	2.44350200	1.49955700
H	-2.68998200	0.79161600	1.93131100
C	-0.30326000	-1.89731300	4.32951900

C	1.07447200	-2.24990400	3.78481100
C	1.07896800	-1.99913100	2.27873600
H	-0.31272600	-1.95134100	5.42443100
H	1.83146600	-1.62218800	4.27086700
H	2.09381400	-2.09657300	1.87485300
N	-0.68164000	-0.53092100	3.94544300
H	0.47050900	-2.75992300	1.76928800
H	1.31282500	-3.29447700	4.01496500
H	-1.05100900	-2.62018900	3.96239000
C	-0.23173400	-0.05164100	2.71683000
N	0.57970900	-0.67282700	1.92113300
C	1.25602100	-2.49689300	-1.98256400
O	2.19645200	-3.01985900	-2.56253600
C	0.10844200	-3.29830100	-1.46621200
C	-0.98340400	-2.72015000	-0.79685700
C	0.12775300	-4.69022800	-1.67037500
C	-2.04004200	-3.51489100	-0.34880700
H	-1.02592000	-1.65333900	-0.61692500
C	-0.92239600	-5.48384300	-1.21637400
H	0.97564000	-5.12593600	-2.18846000
C	-2.01011800	-4.89630500	-0.55755800
H	-2.88112800	-3.04146200	0.14830200
H	-0.89876100	-6.55776000	-1.37805700
H	-2.83264800	-5.51563400	-0.21001700
C	1.25355900	-0.94861600	-1.80588300
H	1.04857600	-0.70477100	-0.75268300
H	-0.93749300	1.06552300	-3.08150000
N	2.51444100	-0.36533300	-2.20616100
H	2.86390200	-0.82364800	-3.04084400
C	3.54959500	-0.04841800	-1.30504600
C	4.86109200	0.05323200	-1.81089700
C	3.34232600	0.23745000	0.05405400
C	5.91814200	0.43178600	-0.99069200
H	5.04574800	-0.17114700	-2.85895600
C	4.42079900	0.61883700	0.86156100
H	2.36174500	0.14978100	0.51476800
C	5.72409500	0.72833500	0.36870700
H	6.91727100	0.49390400	-1.41697800
H	4.22680300	0.83134200	1.91070600
C	6.87902000	1.14527300	1.25083300
H	6.55686100	1.27527500	2.28861000
H	7.68244000	0.39871300	1.24368800
H	7.31830500	2.09462900	0.91968600
C	-3.91752400	0.32998000	-0.89558800

O	-3.95052400	-0.54477900	-0.03151100
H	-3.17805900	1.14955900	-0.86918600
N	-4.74904600	0.42021500	-1.96544800
C	-5.79968400	-0.56512000	-2.17421300
H	-5.76518700	-1.28732700	-1.35862000
H	-6.78221600	-0.07766100	-2.18993900
H	-5.65296100	-1.08494200	-3.12871400
C	-4.62700600	1.49785700	-2.93706200
H	-5.53820600	2.10911900	-2.95439500
H	-3.77678100	2.13638000	-2.68535000
H	-4.46915100	1.08928600	-3.94285900
C	-0.40524200	3.00667600	-1.87618600
O	-1.43511500	3.13506100	-2.54586600
O	0.14889400	4.00699000	-1.16221900
C	-0.51582400	5.29329900	-1.21811600
C	0.28766100	6.25718800	-0.36611700
H	-1.54011700	5.17474700	-0.85064200
H	-0.56902200	5.61395800	-2.26300000
H	-0.18444700	7.24504400	-0.38551200
H	0.33490700	5.91791100	0.67298200
H	1.30953200	6.35569700	-0.74404300
N	-0.14407700	0.76893800	-2.50301600
N	0.15011300	-0.47945400	-2.65689100
C	0.33813000	1.76976700	-1.76009100
H	1.22281400	1.65793800	-1.15592200

TS4a

C	2.76246300	-4.20433800	-0.50269100
C	1.62802800	-4.44261400	-1.50532600
C	1.52126400	-1.57082700	-1.35191300
C	1.76851000	-3.65741700	-2.81816500
C	2.19665100	-2.19930600	-2.58738300
H	3.73484900	-4.20288800	-1.02069500
H	0.49974000	-1.95777400	-1.25175200
H	0.67037000	-4.21735200	-1.02459700
H	0.80361200	-3.67913700	-3.33712600
H	2.78613600	-5.04818800	0.19252900
H	1.61247000	-5.51652700	-1.72733700
H	1.42177500	-0.49407400	-1.48628800
H	2.49475700	-4.15300000	-3.47549100
H	1.94137000	-1.60023400	-3.46820500
H	3.28780400	-2.13020600	-2.48770200
C	3.35497800	-3.16533300	1.65205300
C	2.95567500	-2.07526000	2.63795000

C	3.13743300	-0.71932900	1.96832100
H	3.08840900	-4.15157700	2.04556900
H	1.90797100	-2.20178000	2.93104200
H	2.72870100	0.08674500	2.58265900
N	2.66430100	-3.00497300	0.35928200
H	4.20330400	-0.49720100	1.81894600
H	3.56974900	-2.15339300	3.54114900
H	4.44408000	-3.16240200	1.49123900
C	2.26307600	-1.76282900	-0.04307200
N	2.45580700	-0.68200000	0.67354900
C	2.12002800	2.58209400	0.66325400
O	2.45345800	2.97784300	1.79371500
C	2.93121400	3.02875300	-0.52110600
C	2.87956500	2.44486100	-1.79853700
C	3.83206600	4.08737500	-0.30161600
C	3.71008100	2.90662700	-2.82215900
H	2.18207300	1.64159700	-1.99285300
C	4.64984800	4.55600200	-1.32810700
H	3.87462800	4.52707500	0.68875200
C	4.59352700	3.96471200	-2.59443000
H	3.66055300	2.44118700	-3.80275200
H	5.33197500	5.38066100	-1.14102400
H	5.23142200	4.32638600	-3.39626900
C	0.98588800	1.61728000	0.56427300
H	1.75640700	0.43215500	0.50234400
H	-1.36900400	1.64283100	-1.66516000
N	0.25294200	1.58635500	1.81046800
H	0.70727200	2.19426000	2.48791500
C	-0.33299900	0.44294900	2.35657000
C	-0.52686500	0.36562800	3.75168000
C	-0.79385300	-0.63047800	1.57310800
C	-1.15200700	-0.73754000	4.32813100
H	-0.18166100	1.18160800	4.38281800
C	-1.41332000	-1.73164600	2.16795500
H	-0.67336300	-0.61091100	0.49630200
C	-1.61152800	-1.81406600	3.55256200
H	-1.28170900	-0.76116900	5.40837700
H	-1.75238300	-2.54086100	1.52486200
C	-2.32119400	-2.99087100	4.18369600
H	-3.37719100	-2.76643500	4.38472700
H	-2.29462100	-3.86848600	3.52959700
H	-1.86466100	-3.27161200	5.13964400
C	-2.67542600	-1.81020100	-1.93663400
O	-1.75309600	-2.59327400	-1.69384900

H	-2.67279300	-0.76867900	-1.57706600
N	-3.78748400	-2.10421600	-2.65500100
C	-3.98878500	-3.43439500	-3.20794800
H	-3.13966900	-4.05966100	-2.93165900
H	-4.91181300	-3.87623500	-2.81274100
H	-4.06784000	-3.38688600	-4.30111500
C	-4.81652800	-1.10186000	-2.90199500
H	-5.77496500	-1.42379000	-2.47526900
H	-4.52570100	-0.14954700	-2.45214000
H	-4.95269100	-0.95446200	-3.98061100
C	-3.24874900	2.31454600	-0.44489200
O	-3.55765400	1.81597100	-1.54172100
O	-4.16239200	2.89447600	0.37740100
C	-5.52921900	2.91100600	-0.08112300
C	-6.35462100	3.62485500	0.97418200
H	-5.86866400	1.88023900	-0.23058400
H	-5.57535800	3.42107100	-1.04890200
H	-7.40462500	3.65722500	0.66388900
H	-6.29422700	3.10551200	1.93547500
H	-6.00485400	4.65206300	1.11528600
N	-0.97644700	1.85775100	-0.74487800
N	0.28544200	1.58160300	-0.67541200
C	-1.92287800	2.35454400	0.08919200
H	-1.67001900	2.71454900	1.06882400

Int4a

C	3.25228800	2.60200600	-2.48831400
C	3.58741100	1.32950000	-3.27039500
C	1.55672200	0.24049200	-1.54989400
C	2.37510200	0.66342000	-3.93760900
C	1.16143000	0.58664300	-2.99800300
H	2.55186600	3.23325500	-3.05455700
H	2.39393400	-0.47107500	-1.54955200
H	4.09821900	0.61826800	-2.61278200
H	2.66601100	-0.34610200	-4.24824400
H	4.16916000	3.18442600	-2.36447700
H	4.31576100	1.61140900	-4.03987100
H	0.72356100	-0.25021100	-1.04259300
H	2.09744600	1.20881900	-4.84845400
H	0.46387500	-0.17758100	-3.35534800
H	0.60116100	1.52989400	-3.01278700
C	2.94940200	3.58959600	-0.22502000
C	2.98515000	3.17223700	1.24244800
C	1.70967000	2.41232600	1.57732500

H	3.89901100	4.04522600	-0.51562100
H	3.86157600	2.53943800	1.42172300
H	1.78489400	1.88522700	2.53199500
N	2.72709700	2.42626600	-1.11036900
H	0.84397300	3.08311500	1.62600900
H	3.07914000	4.05997300	1.87468700
H	2.15678500	4.32991300	-0.39822200
C	1.94060300	1.41998500	-0.68522300
N	1.46472800	1.40429500	0.54710400
C	-4.51843200	-0.46218900	0.49145400
O	-5.28419700	0.44908900	0.85832900
C	-5.09357500	-1.59823700	-0.31442900
C	-4.68584900	-2.93866600	-0.21485800
C	-6.16393900	-1.28194700	-1.16935300
C	-5.32858700	-3.93128100	-0.95931800
H	-3.87384100	-3.20495200	0.44924500
C	-6.79010200	-2.26988900	-1.92849700
H	-6.49697200	-0.25042000	-1.21844700
C	-6.37472900	-3.60146800	-1.82491200
H	-5.01054600	-4.96574100	-0.86014900
H	-7.60752500	-2.00374600	-2.59329700
H	-6.86736000	-4.37545100	-2.40736600
C	-3.10571700	-0.38912700	0.86078400
H	0.85274000	0.60342700	0.84120800
H	-0.59384900	-2.29665800	0.39783200
N	-2.73741800	0.74307200	1.65799400
H	-3.45686400	0.93154600	2.34997500
C	-2.32604600	1.93581400	1.03678500
C	-2.26900400	3.12338100	1.79439200
C	-1.93264800	1.99700800	-0.30969800
C	-1.85859700	4.32197800	1.21719900
H	-2.56723800	3.10032100	2.83990000
C	-1.52070300	3.20788600	-0.87308700
H	-1.98397600	1.10237700	-0.92192700
C	-1.47555900	4.39627300	-0.13319900
H	-1.84845400	5.22312500	1.82739200
H	-1.25125400	3.22778100	-1.92768200
C	-1.09678800	5.71553200	-0.76938600
H	-1.98330900	6.32550900	-0.98608200
H	-0.45086900	6.31382300	-0.11582900
H	-0.56995400	5.56536700	-1.71773700
C	3.78714400	-2.68633900	-0.85059800
O	4.14827900	-1.82498800	-1.66466600
H	2.95487800	-2.52182100	-0.14821400

N	4.35023100	-3.91161700	-0.71435300
C	5.46217600	-4.32895400	-1.55335400
H	5.70901800	-3.51367400	-2.23378000
H	6.33789800	-4.56953600	-0.93789800
H	5.19129600	-5.21962700	-2.13375500
C	3.83902000	-4.85875800	0.26895800
H	4.63234700	-5.14821700	0.96942500
H	3.02099100	-4.39816800	0.82756200
H	3.46944000	-5.76555300	-0.22612000
C	0.98033000	-1.49355400	2.04151200
O	1.43880300	-2.48409300	1.42368000
O	1.69442800	-0.91652600	3.08418700
C	2.89153000	-1.59591700	3.48845800
C	3.43619000	-0.88058900	4.71386700
H	3.61840000	-1.58602400	2.66705000
H	2.65999700	-2.64355200	3.71003900
H	4.35143000	-1.37401100	5.05907200
H	3.67606300	0.16387000	4.48779300
H	2.70719800	-0.89501000	5.52996400
N	-1.03309700	-1.47248900	0.79730400
N	-2.28331400	-1.34325900	0.45696500
C	-0.21197700	-0.80825500	1.74707000
H	-0.69365900	-0.15417000	2.45451700

TS5a

C	3.33135200	2.77518000	-2.32961100
C	3.74815200	1.54082000	-3.13552500
C	1.67961400	0.34548100	-1.53418400
C	2.59064800	0.85209500	-3.87360200
C	1.33946500	0.71166800	-2.99244000
H	2.62674200	3.39097800	-2.91046700
H	2.54720500	-0.32637200	-1.51384700
H	4.25600500	0.82944500	-2.47594300
H	2.92846400	-0.13933300	-4.19579600
H	4.21855500	3.39334000	-2.16471500
H	4.49771500	1.86981100	-3.86518500
H	0.84416200	-0.19548400	-1.08898100
H	2.33679800	1.41204200	-4.78295300
H	0.68507600	-0.06446300	-3.40323600
H	0.75021900	1.63738600	-3.01138400
C	2.92870600	3.69386300	-0.07057800
C	2.79366900	3.27353100	1.38908400
C	1.48105700	2.52050100	1.56382600
H	3.91651300	4.12727100	-0.25328000

H	3.63671700	2.62912400	1.66411800
H	1.42318500	2.03426100	2.54299000
N	2.77414700	2.54148500	-0.97743300
H	0.62478700	3.20259600	1.48743700
H	2.82646500	4.15874700	2.03243200
H	2.18147700	4.46158700	-0.31948100
C	1.94571400	1.52234400	-0.61491300
N	1.34772900	1.47935300	0.55030100
C	-4.46596200	-0.64853400	0.45312100
O	-5.29776700	0.16550900	0.88371100
C	-4.95357600	-1.81217900	-0.36712200
C	-4.41885000	-3.10970800	-0.31167400
C	-6.07141600	-1.57615300	-1.18634600
C	-4.98654900	-4.14008900	-1.06530200
H	-3.56904000	-3.31480700	0.32626600
C	-6.62249100	-2.60032000	-1.95525700
H	-6.49959700	-0.57930400	-1.20295000
C	-6.08158500	-3.88876800	-1.89596000
H	-4.57141900	-5.14223000	-1.00110500
H	-7.47800600	-2.39652800	-2.59331700
H	-6.51494700	-4.69140800	-2.48647800
C	-3.04337000	-0.43364400	0.77085200
H	0.68322900	0.50205100	0.93381300
H	-0.41785900	-2.12434000	0.18264600
N	-2.76520600	0.71449700	1.57629300
H	-3.51890300	0.84643800	2.24480200
C	-2.44462600	1.94282300	0.95695700
C	-2.52421600	3.12895300	1.71123900
C	-2.01820400	2.03524400	-0.37584900
C	-2.20746900	4.35944600	1.14199500
H	-2.85014800	3.07977600	2.74753300
C	-1.69867400	3.27755800	-0.93078300
H	-1.95388400	1.13916100	-0.98429900
C	-1.78799800	4.46531400	-0.19471800
H	-2.29634000	5.25824500	1.74884900
H	-1.38741900	3.31877500	-1.97279000
C	-1.50021500	5.81142900	-0.82158500
H	-0.96600500	6.47448500	-0.13151600
H	-0.89315900	5.70897000	-1.72711000
H	-2.42637300	6.32610000	-1.10869300
C	3.89110100	-2.66753500	-0.86258800
O	4.30094200	-1.80556000	-1.64707600
H	3.04336300	-2.48961900	-0.18237600
N	4.41109300	-3.91434200	-0.73056400

C	5.53422100	-4.34922400	-1.54569000
H	5.83284600	-3.52427200	-2.19285700
H	6.37953400	-4.63979200	-0.90971200
H	5.25090900	-5.21190900	-2.16156500
C	3.84460800	-4.86444400	0.21709900
H	4.60808200	-5.19269500	0.93357700
H	3.02571600	-4.39154300	0.76380200
H	3.46073500	-5.74967000	-0.30567300
C	0.99435300	-1.45264400	2.03548100
O	1.44169100	-2.45067800	1.45091900
O	1.57769300	-0.96594000	3.17293100
C	2.73018000	-1.67671100	3.66668600
C	3.14697900	-1.02310100	4.97246000
H	3.53029800	-1.62950200	2.91931000
H	2.46812300	-2.73011200	3.80880000
H	4.02052900	-1.53988700	5.38441600
H	3.41060700	0.02837600	4.82060600
H	2.33881300	-1.07183000	5.70862500
N	-0.88080900	-1.31115300	0.57456700
N	-2.16350400	-1.29549200	0.31978100
C	-0.08436800	-0.61437800	1.56672600
H	-0.67588000	-0.12387000	2.33041300

TS3b

C	-5.37751000	-1.96749700	-1.75057400
C	-5.12859100	-3.44156300	-2.08824600
C	-2.69968800	-2.85421800	-0.61231900
C	-4.79176900	-4.31959900	-0.87217900
C	-3.81890700	-3.63524100	0.10014600
H	-5.98580700	-1.88532300	-0.83558100
H	-2.38917000	-3.38359700	-1.52286700
H	-4.33491900	-3.49667300	-2.84215700
H	-4.35908800	-5.26297900	-1.22828800
H	-5.97334900	-1.52830100	-2.55582000
H	-6.03323900	-3.82644700	-2.57395100
H	-1.81720500	-2.82375500	0.02630300
H	-5.71408000	-4.58527900	-0.34009800
H	-3.35637500	-4.38212200	0.75260000
H	-4.36100700	-2.95795700	0.77120600
C	-4.47687200	0.32156100	-1.91136700
C	-3.19455600	1.09835400	-2.18453900
C	-2.23741200	0.88694600	-1.01865000
H	-5.14455300	0.36273500	-2.77788700
H	-2.74347800	0.74210500	-3.11847400

H	-1.23672100	1.26176800	-1.25801300
N	-4.18755500	-1.09826400	-1.64044500
H	-2.58478600	1.43806800	-0.13593400
H	-3.42375700	2.16157700	-2.30774600
H	-5.01577000	0.76355200	-1.05966200
C	-3.02335000	-1.41610900	-0.98525300
N	-2.10824300	-0.53247600	-0.69113400
C	3.64650500	-1.54255800	-0.97697000
O	3.87540400	-1.52432800	-2.17760700
C	4.66465500	-2.03318200	0.00207600
C	4.37367200	-2.23973400	1.36103800
C	5.96419500	-2.29326400	-0.46702300
C	5.36494800	-2.69683700	2.23171000
H	3.37129300	-2.07918600	1.74103500
C	6.95355300	-2.74189100	0.40433600
H	6.17348600	-2.13532000	-1.51986400
C	6.65540400	-2.94451900	1.75710900
H	5.12658800	-2.86550000	3.27768400
H	7.95560000	-2.93603700	0.03278500
H	7.42560600	-3.29823100	2.43680800
C	2.27445600	-1.05049900	-0.46051400
H	2.41704300	-0.43312700	0.43265300
H	-1.05907700	-0.80139500	0.15376500
N	1.54697900	-0.29558000	-1.45140900
H	1.37452400	-0.85219500	-2.28085300
C	1.84510300	1.04089000	-1.74789800
C	1.36047000	1.59136000	-2.95309000
C	2.55490900	1.89176200	-0.88425900
C	1.57153300	2.92848100	-3.26896400
H	0.82091700	0.95156900	-3.64768400
C	2.75435300	3.23662200	-1.21652700
H	2.97730600	1.51744900	0.04205000
C	2.27131000	3.78916700	-2.40582900
H	1.18934300	3.31113300	-4.21310600
H	3.32076100	3.86178000	-0.52938500
C	2.49295900	5.24201500	-2.75996000
H	3.13581800	5.73518000	-2.02416000
H	2.97056800	5.34967700	-3.74105300
H	1.54749000	5.79784500	-2.79918500
C	-1.56058800	3.44758300	1.83571600
O	-2.70498000	3.36278400	1.39157500
H	-0.98387000	2.55414100	2.12984200
N	-0.87477000	4.60672000	2.02240900
C	-1.47061300	5.88803400	1.67577300

H	-2.48459900	5.71126800	1.31675200
H	-1.50257200	6.54524000	2.55331600
H	-0.88636400	6.38297500	0.89013200
C	0.48637400	4.60996000	2.53213500
H	0.55460100	5.20405000	3.45194700
H	0.79784000	3.58652800	2.75353800
H	1.17872400	5.03196400	1.79319900
C	-0.87668000	-1.14338300	2.30589500
O	-1.44098200	-2.14440300	2.70856500
O	-0.98217400	0.06854000	2.94073700
C	-1.84208500	0.11805800	4.10597300
C	-3.29851300	0.34709300	3.72507600
H	-1.44999300	0.95285900	4.69354100
H	-1.72030900	-0.80881500	4.67175200
H	-3.90074000	0.46662300	4.63345000
H	-3.40934800	1.24864500	3.11471200
H	-3.68839200	-0.50981200	3.16915600
N	0.48453400	-2.20724400	0.62025500
N	1.50953300	-2.30619100	-0.09961000
C	-0.08160300	-0.99681200	1.06225800
H	0.51560000	-0.08205800	1.03647100

Int3b

C	3.57346200	-3.84671700	1.80703300
C	3.51178100	-4.44116400	0.39545700
C	3.20702800	-1.65089700	-0.25683100
C	4.52248600	-3.82306100	-0.58117400
C	4.59138600	-2.29437700	-0.45350900
H	4.62383700	-3.70750600	2.11283500
H	2.45686400	-2.18629900	-0.85045100
H	2.49052600	-4.33518300	0.01495600
H	4.23666000	-4.09632200	-1.60372000
H	3.15313500	-4.58030300	2.50250500
H	3.69963600	-5.51807900	0.47866200
H	3.21987800	-0.62810000	-0.63338300
H	5.51816700	-4.25222500	-0.41099900
H	5.05129900	-1.87320500	-1.35383100
H	5.25112900	-2.01197500	0.37721900
C	2.38025100	-2.44740800	3.43324800
C	1.25831300	-1.42397600	3.54823900
C	1.69645300	-0.14652900	2.83917100
H	2.04507100	-3.42321000	3.80186900
H	0.35394200	-1.82253700	3.07347300
H	0.87079400	0.57364100	2.79488500

N	2. 80298700	-2. 61255600	2. 03754900
H	2. 48976600	0. 34768300	3. 42138000
H	1. 02488700	-1. 24108900	4. 60275600
H	3. 23495100	-2. 14691500	4. 06066400
C	2. 71062200	-1. 53104600	1. 17836900
N	2. 17881500	-0. 38219600	1. 48149400
C	1. 29337400	3. 17617900	-1. 45870400
O	0. 72890300	4. 06006600	-2. 08863200
C	2. 72451300	3. 28117600	-1. 07245900
C	3. 34533800	2. 37429200	-0. 19827600
C	3. 46659300	4. 35198300	-1. 60190000
C	4. 69064600	2. 54266100	0. 13251600
H	2. 80546500	1. 54057300	0. 24492100
C	4. 80701600	4. 50997100	-1. 27180800
H	2. 96634100	5. 04341800	-2. 27119000
C	5. 42237200	3. 60302200	-0. 40214800
H	5. 16293600	1. 83964800	0. 81212600
H	5. 37521900	5. 33630900	-1. 68852800
H	6. 47013400	3. 72632400	-0. 14258700
C	0. 48211100	1. 89750000	-1. 12096400
H	0. 73372000	1. 50329800	-0. 13438000
H	-1. 23520200	-0. 20317800	-1. 01141200
N	-0. 93434500	2. 16391100	-1. 24106400
H	-1. 05967500	2. 84659000	-1. 98482500
C	-1. 72336600	2. 48496300	-0. 11883400
C	-2. 76440700	3. 41961100	-0. 26261500
C	-1. 57098400	1. 86085700	1. 13026800
C	-3. 60436900	3. 72438500	0. 80364500
H	-2. 90309100	3. 91752500	-1. 21898300
C	-2. 41816700	2. 18284000	2. 19103600
H	-0. 79580900	1. 11850200	1. 28373700
C	-3. 44773700	3. 12035500	2. 05927200
H	-4. 39178200	4. 46039700	0. 65815700
H	-2. 26993100	1. 68512300	3. 14658400
C	-4. 33020800	3. 49398300	3. 22728200
H	-4. 38480400	2. 68550700	3. 96278000
H	-3. 95196300	4. 38191900	3. 74976500
H	-5. 35072500	3. 72354700	2. 90394800
C	-5. 11336200	-1. 77163500	-0. 44040200
O	-5. 35444000	-2. 96533500	-0. 58623800
H	-4. 10192700	-1. 35374000	-0. 58542600
N	-6. 02559500	-0. 82318700	-0. 09338900
C	-7. 41291200	-1. 19131100	0. 13076400
H	-7. 50825700	-2. 26422400	-0. 03501700

H	-7.71791800	-0.95037700	1.15664300
H	-8.07295400	-0.65330900	-0.56070100
C	-5.65474400	0.57091700	0.06356400
H	-5.86202900	0.92087300	1.08193300
H	-4.58760400	0.69857400	-0.12823400
H	-6.21130800	1.20640900	-0.63668300
C	-0.57545400	-2.25475200	-1.26946200
O	0.28913800	-3.10774600	-1.30434600
O	-1.88992100	-2.49746000	-1.40696600
C	-2.29402200	-3.88340100	-1.62585600
C	-2.19470800	-4.24651900	-3.09829900
H	-3.32331300	-3.91361300	-1.26528700
H	-1.65559700	-4.52570700	-1.01481600
H	-2.56375200	-5.26656900	-3.24817800
H	-2.80478000	-3.57208200	-3.70594000
H	-1.15947300	-4.20000700	-3.44497900
N	0.56471700	-0.28215600	-2.15152900
N	0.93229500	0.89885700	-2.18751700
C	-0.30934600	-0.77814700	-1.04694300
H	0.23623300	-0.66754000	-0.09969000

TS4b

C	-2.01510200	-4.12487200	1.67027300
C	-0.73703100	-4.01856300	2.50952800
C	-1.06720500	-1.24364100	1.79040400
C	-0.81956200	-2.98951200	3.64683900
C	-1.49348600	-1.68255800	3.20416800
H	-2.90282600	-4.10718000	2.32143300
H	-0.01351200	-1.49915800	1.62133200
H	0.10768700	-3.79101000	1.85215400
H	0.19775800	-2.77859900	3.99541700
H	-2.01992200	-5.10052900	1.17611700
H	-0.54088800	-5.01096600	2.93256500
H	-1.13942500	-0.15951600	1.70122900
H	-1.36415400	-3.41275200	4.50039900
H	-1.23946000	-0.88335500	3.90817300
H	-2.58566700	-1.77984100	3.24936200
C	-2.95191100	-3.65964700	-0.56545100
C	-2.75727400	-2.79864800	-1.80699300
C	-3.03107900	-1.34579500	-1.44108300
H	-2.61303200	-4.68290700	-0.75680000
H	-1.72861300	-2.89551200	-2.16878100
H	-2.76241100	-0.67111700	-2.25797600
N	-2.17878700	-3.14365800	0.57745700

H	-4.09997800	-1.19026300	-1.23864700
H	-3.42862900	-3.14121000	-2.60075900
H	-4.01783100	-3.71768100	-0.29796600
C	-1.88958500	-1.81162700	0.64927300
N	-2.25899800	-0.95057000	-0.26495300
C	-2.38980800	2.18833400	-0.98718200
O	-2.79257200	2.36526900	-2.14461900
C	-3.27572300	2.62831800	0.14957200
C	-2.97618300	2.51626300	1.51778100
C	-4.51823400	3.17518500	-0.22202400
C	-3.89722300	2.93634600	2.47801400
H	-2.01310300	2.12531300	1.81635300
C	-5.43348400	3.59324000	0.73820500
H	-4.74122200	3.26012500	-1.27930400
C	-5.12632400	3.47362300	2.09582400
H	-3.64704600	2.84710000	3.53149900
H	-6.38660500	4.01329800	0.42926800
H	-5.83843100	3.80074900	2.84861800
C	-1.09029600	1.45060600	-0.81540300
H	-1.65422900	0.23020000	-0.42684200
H	1.38306100	3.13629200	-1.30084800
N	-0.43786300	1.29918800	-2.10039800
H	-0.98667000	1.77771200	-2.81065300
C	0.12448000	0.09899700	-2.53907200
C	0.15286800	-0.19694700	-3.91715300
C	0.73287600	-0.81862100	-1.66233200
C	0.75565600	-1.35905700	-4.38599500
H	-0.30864100	0.49426400	-4.61854900
C	1.32720400	-1.98324000	-2.14921500
H	0.74287400	-0.63362700	-0.59470600
C	1.35681300	-2.28169100	-3.51618400
H	0.75347900	-1.55670000	-5.45601700
H	1.78103400	-2.66135600	-1.43076500
C	2.03699800	-3.52481900	-4.04067900
H	3.05328300	-3.31297200	-4.39832400
H	2.12195800	-4.29074700	-3.26356900
H	1.48786000	-3.96126000	-4.88219600
C	3.01259100	-1.40280900	1.45383900
O	2.09547900	-2.21516100	1.30478900
H	2.87783500	-0.32046000	1.30114000
N	4.27954800	-1.73051500	1.81286300
C	4.64215500	-3.11585000	2.05496700
H	3.75680600	-3.73152800	1.89898700
H	5.43522700	-3.43356400	1.36697100

H	5.00478500	-3.24721400	3.08187800
C	5.31373200	-0.71879900	1.95973700
H	6.15807800	-0.93580100	1.29329500
H	4.90969400	0.26172500	1.70365700
H	5.69120100	-0.69666100	2.99009100
C	3.11039600	2.65880600	-0.10719400
O	3.72120300	1.96747500	0.68582000
O	3.59012500	3.81205400	-0.61766500
C	4.90553700	4.22541100	-0.17648600
C	4.82557600	5.01758100	1.11931000
H	5.28829200	4.83654900	-0.99726100
H	5.53377100	3.33901600	-0.06028800
H	5.82086300	5.38133800	1.39589400
H	4.16287400	5.88020600	1.00635400
H	4.44999600	4.38883500	1.92999900
N	0.83975000	2.09912100	0.50498100
N	-0.37140400	1.81218900	0.35926800
C	1.74499400	2.32428900	-0.66756900
H	1.86007700	1.43158100	-1.28937600

Int4b

C	5.26080200	2.73566500	-0.23121400
C	4.97030100	3.63649300	-1.43525900
C	2.29592200	2.53232000	-1.00584400
C	3.79782800	4.60518000	-1.21804400
C	2.62354800	3.94036600	-0.49030500
H	5.19844600	3.30860500	0.70482600
H	2.35330200	2.49514300	-2.10286900
H	4.79643100	3.00125000	-2.31190200
H	3.46789600	4.98734300	-2.19223800
H	6.28926900	2.37387700	-0.30874200
H	5.88439900	4.20221100	-1.65062700
H	1.25799500	2.28488500	-0.73562200
H	4.13735900	5.47662900	-0.64407500
H	1.71879000	4.54585400	-0.58558100
H	2.81606300	3.89133300	0.58825100
C	5.08115400	0.39067000	0.60444800
C	4.61271900	-0.94928300	0.04785000
C	3.09651900	-1.02231600	0.13899700
H	6.16115200	0.50351000	0.48826100
H	4.94498900	-1.04853700	-0.99192800
H	2.69845900	-1.81593400	-0.49664500
N	4.43453900	1.51088700	-0.11398200
H	2.77300200	-1.22564200	1.16656100

H	5.05727400	-1.76685900	0.62215300
H	4.85084700	0.46566000	1.67568900
C	3.13431700	1.39782700	-0.45698100
N	2.50550400	0.24204300	-0.31777300
C	-0.86558400	-2.36786200	-0.71745800
O	-1.46623200	-3.36605800	-0.24719100
C	0.29178000	-2.62919700	-1.65159200
C	0.64252000	-1.77208700	-2.70816100
C	0.97483900	-3.85052300	-1.52451000
C	1.66434700	-2.11871000	-3.59566600
H	0.10508400	-0.84017500	-2.83558900
C	2.00732900	-4.19067000	-2.39993800
H	0.66870000	-4.53235300	-0.73804400
C	2.35800100	-3.32334900	-3.43989400
H	1.91133200	-1.45191700	-4.41771800
H	2.52871700	-5.13664500	-2.28029200
H	3.15133500	-3.59145200	-4.13252000
C	-1.28562100	-1.03547300	-0.34926600
H	-2.56063600	1.61017900	0.31639800
H	1.49138800	0.20455500	-0.52064900
N	-2.56301700	-0.95297500	0.29854700
H	-2.72520000	-1.80620800	0.82569200
C	-3.70556600	-0.59329900	-0.44308100
C	-4.98418500	-0.90484300	0.05954500
C	-3.62876300	0.11895500	-1.65093200
C	-6.13293100	-0.52429600	-0.62697500
H	-5.06838800	-1.45643800	0.99316200
C	-4.79398400	0.49817900	-2.32514400
H	-2.65876200	0.36542100	-2.07015100
C	-6.06741000	0.19069900	-1.83497400
H	-7.10426000	-0.79103500	-0.21507700
H	-4.70008000	1.04408400	-3.26163000
C	-7.32357500	0.61852500	-2.55975400
H	-7.09793700	0.96242400	-3.57418100
H	-8.04245900	-0.20523800	-2.63977200
H	-7.83194000	1.44118400	-2.03985900
C	1.08527600	-3.09791600	2.63798400
O	2.15294500	-2.56400500	2.95129400
H	0.57093500	-2.86414500	1.69244000
N	0.41458000	-4.01372700	3.37885300
C	0.92535400	-4.44325500	4.67118900
H	1.85757100	-3.91465700	4.87119600
H	0.19989800	-4.21737200	5.46245900
H	1.11051300	-5.52455000	4.66923800

C	-0.83988400	-4.59500600	2.91456700
H	-1.65426100	-4.35311700	3.60924500
H	-1.09085800	-4.20987100	1.92242300
H	-0.75291700	-5.68696900	2.85487100
C	-1.33255400	3.11089100	1.17540200
O	-0.40275400	3.82361900	0.85220900
O	-2.34031100	3.53846300	1.97598900
C	-2.27040600	4.90752700	2.43548700
C	-3.50507300	5.17206100	3.27725300
H	-2.21878200	5.56926600	1.56496700
H	-1.34732300	5.03982800	3.00954300
H	-3.48739900	6.20340500	3.64580700
H	-4.41706200	5.03146500	2.68927300
H	-3.54431200	4.49876900	4.13903500
N	-0.47620400	1.20345500	-0.07349200
N	-0.41630700	-0.01872000	-0.49079200
C	-1.56890000	1.66265100	0.78469100
H	-1.65014600	1.07979400	1.71176300

TS5b

C	-5.93954700	-0.40744000	-0.85257800
C	-5.95027500	-1.30537800	-2.09433900
C	-3.16672100	-1.58321700	-1.30536400
C	-5.40123500	-2.72170200	-1.85492700
C	-4.14069100	-2.72800000	-0.97715800
H	-6.27386300	-0.97649200	0.02991900
H	-3.15110600	-1.39648200	-2.38773000
H	-5.39432600	-0.80020400	-2.89265600
H	-5.18100700	-3.18231200	-2.82636900
H	-6.67515100	0.38832800	-1.00106900
H	-6.98696700	-1.37307300	-2.44507200
H	-2.15762500	-1.87669900	-1.02008400
H	-6.17471500	-3.34451500	-1.38773800
H	-3.61164200	-3.67901400	-1.09648200
H	-4.40915700	-2.67633900	0.08452000
C	-4.85976700	1.52501100	0.23647700
C	-3.63451300	2.42422600	0.12999100
C	-2.39969100	1.63418600	0.54257000
H	-5.74714900	2.03565300	-0.14989800
H	-3.53202700	2.77576500	-0.90348300
H	-1.48564700	2.15557100	0.24408300
N	-4.67541600	0.29350000	-0.55131500
H	-2.34714100	1.51776200	1.63171500
H	-3.75968400	3.30369400	0.76940200

H	-5.05969800	1.27068000	1.28890800
C	-3.42149200	-0.26322400	-0.59741300
N	-2.36702000	0.31502100	-0.09290900
C	2.53367800	1.92656100	-1.04842200
O	3.69892000	2.25699100	-0.75837600
C	1.66603800	2.91059400	-1.78575100
C	0.62187900	2.53821700	-2.64848700
C	1.99340800	4.27166700	-1.66797900
C	-0.07944400	3.50852600	-3.36670000
H	0.36398000	1.49226200	-2.75343900
C	1.27852300	5.24227800	-2.37003900
H	2.82411400	4.54970300	-1.02771000
C	0.23848900	4.86272100	-3.22387700
H	-0.87510900	3.20558000	-4.04203000
H	1.53831200	6.29145200	-2.25940800
H	-0.31412200	5.61502400	-3.78019400
C	2.04663200	0.61557200	-0.59590300
H	1.51269200	-1.97239400	0.72783600
H	-1.18542700	-0.24219100	-0.02274900
N	3.06020800	-0.25651600	-0.10283500
H	3.87891200	0.29742800	0.13709900
C	3.40637600	-1.43434000	-0.79862300
C	4.62463100	-2.07282100	-0.49367700
C	2.57031500	-2.02600500	-1.75841700
C	4.98998700	-3.25206700	-1.13446800
H	5.28572600	-1.63114300	0.24824000
C	2.95131300	-3.21705100	-2.38623600
H	1.62783000	-1.55814400	-2.02056700
C	4.16022700	-3.85618300	-2.09475100
H	5.94259000	-3.71368600	-0.88285800
H	2.28419300	-3.65065400	-3.12811600
C	4.56447600	-5.14408800	-2.77570700
H	4.62330500	-5.97719500	-2.06392200
H	3.84511100	-5.42364700	-3.55152900
H	5.54873400	-5.05652000	-3.25126800
C	0.48176700	2.61069000	2.89587500
O	-0.63233900	2.47170300	3.39829300
H	0.68496400	2.34728500	1.84333400
N	1.58284400	3.08722000	3.53458400
C	1.51244000	3.48859300	4.93104300
H	0.49631200	3.32083700	5.28845400
H	2.21473400	2.90019200	5.53442600
H	1.76734900	4.55030100	5.03867100
C	2.86241100	3.22087500	2.85408000

H	3.63114200	2.62040700	3.35569500
H	2.77540700	2.87817300	1.82106900
H	3.19062300	4.26764100	2.84710000
C	-0.34105900	-2.31875100	1.67005300
O	-1.39131500	-2.65635200	1.15955700
O	0.09671200	-2.79825600	2.85348600
C	-0.73812200	-3.78675300	3.50642500
C	-0.05586600	-4.17428700	4.80470800
H	-0.85839900	-4.64176200	2.83364700
H	-1.72713200	-3.35016200	3.67605300
H	-0.65912800	-4.92348000	5.32834200
H	0.93411400	-4.60010400	4.61564000
H	0.06023200	-3.30604700	5.46028000
N	0.07892700	-0.53317900	0.04470700
N	0.74371500	0.42995800	-0.54950000
C	0.67798800	-1.35935300	1.08954600
H	1.08430300	-0.75051800	1.90743300

TS3c

C	-5.33822000	-2.87742900	-0.97969400
C	-6.31635500	-2.04992000	-0.13885000
C	-3.98408900	-0.33028500	-0.01762700
C	-6.47041800	-0.59350500	-0.60499300
C	-5.12646700	0.04855100	-0.97801700
H	-5.48063600	-2.66119800	-2.04987900
H	-4.36025900	-0.40132100	1.01179800
H	-5.99950200	-2.09424100	0.90943900
H	-6.94951700	-0.01566400	0.19535300
H	-5.57966700	-3.93521300	-0.84420900
H	-7.29057800	-2.55163200	-0.18032500
H	-3.24222800	0.46979400	-0.02955700
H	-7.15002100	-0.54924900	-1.46554400
H	-5.21501800	1.13920500	-0.98432500
H	-4.84275400	-0.22625600	-2.00189800
C	-3.12883500	-3.97402800	-1.00813400
C	-1.77719500	-4.00257900	-0.30790400
C	-1.06054500	-2.68912400	-0.57304900
H	-3.72660800	-4.84581900	-0.72481000
H	-1.92526500	-4.13981600	0.77004600
H	-0.17032400	-2.59038300	0.05141100
N	-3.90179200	-2.76962900	-0.64121700
H	-0.72226200	-2.64557400	-1.61598500
H	-1.17173400	-4.83432000	-0.67730400
H	-2.99808200	-4.00880600	-2.10004500

C	-3.24027600	-1.61281300	-0.34515800
N	-1.93095600	-1.54516600	-0.29245300
C	1.14198100	-0.23377000	1.42872900
O	1.72477300	-1.23182300	1.01865600
C	0.76921200	-0.09696500	2.87098900
C	-0.11077400	0.89758400	3.33328100
C	1.32718600	-1.00018800	3.79230800
C	-0.42146300	0.98401500	4.69121600
H	-0.57684300	1.58520900	2.63625400
C	1.02183900	-0.90664800	5.14839600
H	2.00205900	-1.76556400	3.42337400
C	0.14642000	0.08704500	5.60072500
H	-1.10828600	1.75044700	5.03784200
H	1.46461300	-1.60444500	5.85324900
H	-0.09296900	0.16105400	6.65780200
C	0.76187700	0.89995500	0.44570000
H	0.85870900	1.85752100	0.97622900
H	-1.32677700	-0.51627000	-0.05868300
N	1.59794700	0.95529000	-0.73560500
H	1.32072300	0.29750000	-1.45140800
C	2.94850300	1.29487600	-0.72124500
C	3.72357600	1.08858300	-1.88226700
C	3.58144500	1.88107900	0.38948600
C	5.06224300	1.46255100	-1.92596300
H	3.25914200	0.63935600	-2.75733700
C	4.92733200	2.25554000	0.32428500
H	3.03714700	2.04750300	1.31306700
C	5.69919500	2.06051200	-0.82519900
H	5.62542500	1.28872000	-2.84076200
H	5.38299900	2.70716900	1.20278200
C	7.14642700	2.49225000	-0.89516500
H	7.54727800	2.69847400	0.10223700
H	7.77632100	1.72166800	-1.35453000
H	7.26699200	3.40566300	-1.49206000
C	2.34873900	-3.90623300	-1.13972500
O	1.46327800	-4.64272000	-1.57829400
H	2.12460500	-3.00073900	-0.55405800
N	3.68438100	-4.09522300	-1.30753300
C	4.18998000	-5.24039800	-2.04717500
H	3.34100200	-5.82340800	-2.40509100
H	4.79268500	-4.90911800	-2.90184700
H	4.81795500	-5.86814700	-1.40241300
C	4.65268600	-3.16775200	-0.74063100
H	5.28001200	-2.73283900	-1.52814800

H	4.13033200	-2.35816600	-0.22642000
H	5.30497700	-3.68023800	-0.02206300
C	-2.01628400	3.88917800	-0.85458300
O	-3.20335100	3.69943000	-1.07467500
O	-1.43953700	5.12574000	-0.97246800
C	-2.31055500	6.19791500	-1.38083500
C	-1.47549600	7.46360000	-1.46124500
H	-3.12522300	6.29260500	-0.65470900
H	-2.75950700	5.94439700	-2.34708100
H	-2.10488800	8.30476100	-1.77185500
H	-1.03358300	7.70454800	-0.48928800
H	-0.66524800	7.35230300	-2.18853200
N	-1.39367200	1.66921000	-0.31055600
N	-0.63623400	0.66258900	0.08584400
C	-1.00915800	2.90883800	-0.44026200
H	0.01073000	3.26343000	-0.30019300

Int3c

C	-1.81481600	0.26465300	4.59722200
C	-2.01820200	1.78453500	4.63094200
C	-0.61272700	1.48653300	2.10353300
C	-2.67360300	2.36658900	3.36728900
C	-2.13061800	1.74944100	2.06782400
H	-2.69843400	-0.22576100	4.15518800
H	-0.10488600	2.29088600	2.65364700
H	-1.04717200	2.25694900	4.82018800
H	-2.51453900	3.45289000	3.36032600
H	-1.75149300	-0.09155000	5.63020900
H	-2.64451100	2.02030800	5.49999000
H	-0.20704800	1.50296800	1.09143600
H	-3.75962600	2.21538900	3.41183000
H	-2.35047600	2.42518300	1.23316900
H	-2.65559900	0.81585000	1.83451000
C	-0.14963000	-1.52416200	4.46772100
C	1.22595800	-1.89179500	3.92839000
C	1.18783700	-1.80188900	2.40477200
H	-0.13303200	-1.46129100	5.56210400
H	1.97338600	-1.19386300	4.32518000
H	2.19459700	-1.91787800	1.98577900
N	-0.58112600	-0.21907400	3.95065700
H	0.58735900	-2.62772400	1.99619400
H	1.50278400	-2.89841100	4.26164300
H	-0.88138500	-2.30479600	4.19968400
C	-0.16785400	0.14571200	2.67154700

N	0.64568000	-0.53232800	1.92408800
C	1.24536600	-2.52439500	-1.79405400
O	2.18611700	-3.05844700	-2.36179800
C	0.12829700	-3.31945400	-1.20488800
C	-0.94791700	-2.72942200	-0.51786800
C	0.15493800	-4.71801300	-1.36902200
C	-1.98571200	-3.51940300	-0.01949500
H	-0.99081400	-1.65898400	-0.35469600
C	-0.87341000	-5.50503800	-0.85947400
H	0.99096300	-5.16204600	-1.89908300
C	-1.94794300	-4.90568900	-0.18855900
H	-2.81939900	-3.03537800	0.47882900
H	-0.84494700	-6.58309200	-0.98869900
H	-2.75580100	-5.52080500	0.19819600
C	1.20712000	-0.96212800	-1.73021600
H	1.04216200	-0.65224200	-0.68868600
N	2.42440000	-0.36848500	-2.22282400
H	2.71161200	-0.80234300	-3.09321700
C	3.52454600	-0.07182700	-1.39221100
C	4.80674100	-0.03453400	-1.97305300
C	3.40354700	0.26233300	-0.03403300
C	5.92179100	0.32953700	-1.22536100
H	4.92449900	-0.29626300	-3.02215400
C	4.53856500	0.62394100	0.70045500
H	2.44412100	0.23947600	0.47578900
C	5.81567000	0.66925200	0.13295600
H	6.89629700	0.34409200	-1.70897000
H	4.41196100	0.87826200	1.75057700
C	7.03393000	1.05750100	0.93974500
H	6.75998700	1.32695100	1.96443700
H	7.75935800	0.23639100	0.99598300
H	7.55328800	1.91678800	0.49833500
C	-3.86819300	0.08926500	-0.96974000
O	-3.89895600	-0.70713400	-0.02801100
H	-3.07520800	0.84570200	-1.07427900
N	-4.76946400	0.14608900	-1.98290400
C	-5.89866400	-0.76847000	-2.02955400
H	-5.85981000	-1.41508700	-1.15264000
H	-6.84291800	-0.20987500	-2.03050100
H	-5.85941900	-1.38244400	-2.93816200
C	-4.63420600	1.12016300	-3.05882600
H	-5.51339800	1.77595300	-3.09414300
H	-3.74092300	1.72806300	-2.89953500
H	-4.54593000	0.61005400	-4.02631500

C	-0.71697200	2.93527900	-1.88248300
O	-1.86821500	3.11866100	-2.24416400
O	0.06644600	3.91716300	-1.37401200
C	-0.52260100	5.23604600	-1.28992800
C	0.52420900	6.16959900	-0.71177800
H	-1.41753600	5.18083600	-0.66177500
H	-0.83813900	5.54250500	-2.29219800
H	0.11215500	7.18133400	-0.63445700
H	0.83163000	5.84521400	0.28697200
H	1.41179400	6.20671600	-1.35038600
N	-0.53810900	0.65252600	-2.47955600
N	0.05995100	-0.53607600	-2.54557100
C	0.02955100	1.65991100	-1.90207700
H	1.02365800	1.64565500	-1.46336400
H	-0.56162000	-1.24949400	-2.89895700

TS4c

C	0.33091800	-1.80711200	4.51051100
C	-0.15132500	-0.42157700	4.95267700
C	-0.46477700	-0.15856400	2.08820700
C	-1.53637500	-0.03444600	4.40792400
C	-1.72498900	-0.42484800	2.93532600
H	-0.49315300	-2.53416700	4.57148300
H	0.04707500	0.74514900	2.44229100
H	0.60517400	0.31921900	4.66856100
H	-1.67319900	1.04768500	4.52482300
H	1.09594900	-2.14580600	5.21427800
H	-0.17566300	-0.41899400	6.04885600
H	-0.74776200	0.05018600	1.05701800
H	-2.31878200	-0.51027700	5.01188200
H	-2.56513500	0.12096800	2.49538900
H	-1.99312300	-1.48649600	2.85716200
C	1.93823300	-3.01782700	3.08367400
C	2.82427800	-2.88596500	1.85193400
C	1.94323400	-2.70472100	0.62499600
H	2.54445100	-3.00316400	3.99476000
H	3.48923900	-2.02180400	1.95991100
H	2.53077500	-2.43718400	-0.25609200
N	0.97261900	-1.90494600	3.17830300
H	1.40543800	-3.63136400	0.38547000
H	3.45165800	-3.77717200	1.75270800
H	1.39464600	-3.97416600	3.06820700
C	0.53649500	-1.29699800	2.03814600
N	0.97137000	-1.63059000	0.84716100

C	0.08081300	-2.05301300	-2.14411400
O	0.92932500	-2.70724500	-2.76708100
C	-1.23722600	-2.72460400	-1.82249800
C	-2.13158700	-2.30236100	-0.82266700
C	-1.56471700	-3.87025800	-2.57167200
C	-3.31806100	-3.00060400	-0.58281900
H	-1.91791500	-1.42724300	-0.22262400
C	-2.75092700	-4.56324600	-2.33777700
H	-0.86558800	-4.20054200	-3.33245600
C	-3.63305800	-4.13023900	-1.34127600
H	-3.99480000	-2.64656800	0.18921600
H	-2.98969700	-5.44042600	-2.93275000
H	-4.55983800	-4.66777400	-1.16067400
C	0.39509400	-0.67384300	-1.68309600
H	0.66745300	-1.06447000	-0.21674000
N	1.53066100	-0.13284500	-2.39839000
H	1.55540200	-0.45583600	-3.36115300
C	2.82209300	0.06886200	-1.90902300
C	3.89816400	0.04957400	-2.82513000
C	3.12958200	0.36530100	-0.56896600
C	5.19962200	0.32115100	-2.42082500
H	3.69811300	-0.18593300	-3.86790100
C	4.44668600	0.63262400	-0.17775400
H	2.34636300	0.39213100	0.17714600
C	5.51081700	0.62150800	-1.08346400
H	5.99493700	0.29396500	-3.16306500
H	4.63971800	0.86830900	0.86724800
C	6.92964300	0.92149100	-0.65621900
H	6.98349000	1.13125700	0.41680800
H	7.60286500	0.08018800	-0.86348000
H	7.33442700	1.79433200	-1.18333700
C	-4.03250900	1.68805600	0.14954500
O	-4.19562400	0.73681000	0.92182000
H	-3.11414500	2.29185500	0.13976600
N	-4.93495200	2.10610800	-0.77386300
C	-6.21696100	1.43847500	-0.92451300
H	-6.29064900	0.65232100	-0.17258800
H	-7.03799800	2.15341400	-0.78826900
H	-6.30705800	0.99549500	-1.92474900
C	-4.63401300	3.21946400	-1.66438000
H	-5.36087200	4.03009300	-1.52513100
H	-3.62987700	3.59401500	-1.45526800
H	-4.67802100	2.89290800	-2.71121300
C	-0.36554100	3.48421700	-0.40837400

O	-1.45354700	4.04253000	-0.48301600
O	0.72795500	4.09226900	0.13443100
C	0.54647700	5.44930000	0.58952500
C	1.88029200	5.93570900	1.12671900
H	-0.23477100	5.46587200	1.35698000
H	0.19763900	6.06024300	-0.24936400
H	1.78297800	6.96837300	1.47877000
H	2.21634900	5.31669600	1.96456600
H	2.64928300	5.90708200	0.34885400
N	-0.96752500	1.42860200	-1.40595300
N	-0.78584700	0.19193600	-1.80956500
C	-0.02407700	2.12737800	-0.83999100
H	0.99591500	1.79055400	-0.69572100
H	-1.60825300	-0.17298600	-2.27040900

Int4c

C	3.58242600	-0.28228300	-3.37164000
C	3.16209000	1.13035200	-3.78840200
C	1.69943100	0.88530500	-1.27424300
C	3.38246400	2.19681500	-2.70519500
C	3.00464000	1.69869100	-1.30458000
H	4.51557500	-0.27338700	-2.79468300
H	0.94649400	1.32701400	-1.93841200
H	2.11225400	1.10241700	-4.10196200
H	2.79267600	3.08556600	-2.95857600
H	3.77059400	-0.86861000	-4.27448400
H	3.73413800	1.39516400	-4.68457700
H	1.28508800	0.92649000	-0.26686300
H	4.43274200	2.51195700	-2.70433000
H	2.88463800	2.55071700	-0.62887200
H	3.81209100	1.08914800	-0.88516800
C	2.74529900	-2.52503300	-2.76774900
C	1.49884000	-3.28091300	-2.32125600
C	1.14209700	-2.85437700	-0.90464800
H	2.94839800	-2.72198800	-3.82374700
H	0.66644100	-3.06417500	-2.99969800
H	0.15230300	-3.21239400	-0.60724000
N	2.57608100	-1.06452600	-2.61631400
H	1.86747200	-3.25184900	-0.18497200
H	1.68875900	-4.35701600	-2.36259800
H	3.62053600	-2.82428000	-2.18034400
C	1.83973300	-0.58923800	-1.59979500
N	1.13759000	-1.39721700	-0.82157700
C	-4.50882800	-0.61248600	0.47099100

O	-5.55271100	-0.01827200	0.84396500
C	-4.58321000	-2.08754800	0.16318100
C	-4.02637100	-2.64999900	-0.99520700
C	-5.30869800	-2.92023100	1.02668000
C	-4.15240400	-4.01528200	-1.26300900
H	-3.54095300	-2.00160900	-1.72303600
C	-5.42805900	-4.28387800	0.76809600
H	-5.78033500	-2.47192500	1.89512600
C	-4.84449600	-4.83896500	-0.37484900
H	-3.72920700	-4.43069800	-2.17418700
H	-5.98385600	-4.91737500	1.45424600
H	-4.94537500	-5.90116000	-0.57953200
C	-3.27142000	0.07299900	0.37846800
N	-3.27139100	1.43639500	0.73111900
H	-4.13761900	1.64974300	1.21942300
C	-2.79052100	2.45700900	-0.09134700
C	-2.98859300	3.79831700	0.29457100
C	-2.08981000	2.21552600	-1.28602500
C	-2.50972200	4.84336100	-0.48328100
H	-3.52883600	4.00699500	1.21468600
C	-1.61119800	3.28035900	-2.05162000
H	-1.95324200	1.19611200	-1.62700400
C	-1.80110800	4.61265600	-1.67393200
H	-2.69090700	5.86628300	-0.15953500
H	-1.09132100	3.06435100	-2.98410100
C	-1.26430900	5.75801800	-2.49970200
H	-0.91920200	5.41370700	-3.47980700
H	-2.02664200	6.52699400	-2.67027700
H	-0.41603800	6.25548900	-2.01092200
C	4.23739500	-1.33974700	0.87385600
O	4.57305300	-1.59023500	-0.28926700
H	3.26987000	-0.88087200	1.12662500
N	4.99595700	-1.58869400	1.96933900
C	6.31011100	-2.19489100	1.84443800
H	6.49821900	-2.38353800	0.78766900
H	7.08395800	-1.52613400	2.24026800
H	6.35429300	-3.13915700	2.40037200
C	4.51673000	-1.24329900	3.29904200
H	5.20854100	-0.54614400	3.78794000
H	3.53585300	-0.76925900	3.21597700
H	4.43398900	-2.13860300	3.92790000
C	0.51057900	0.66186500	2.44845700
O	1.60683100	0.26997400	2.01373100
O	0.42308100	1.41902100	3.58451200

C	1. 65492400	1. 76464800	4. 22724500
C	1. 34029700	2. 80040900	5. 29226800
H	2. 36261800	2. 14687300	3. 48386300
H	2. 10225300	0. 86580400	4. 67123600
H	2. 25490100	3. 08725500	5. 82134700
H	0. 90433100	3. 69713900	4. 84303600
H	0. 62884300	2. 40435100	6. 02246700
N	-0. 87768300	-0. 38681000	0. 84081100
N	-2. 03710900	-0. 57424000	0. 22580400
H	-2. 01366700	-1. 35498700	-0. 41157800
C	-0. 78846800	0. 42721700	1. 89082700
H	-1. 64984400	0. 90299800	2. 33608500
H	0. 51396900	-0. 96791800	-0. 08939500

TS5c

C	3. 36363400	-2. 78599500	2. 26652100
C	2. 92888600	-4. 12980100	1. 67285700
C	1. 61568300	-2. 34129400	-0. 19499500
C	3. 24498500	-4. 28872100	0. 17792300
C	2. 92729900	-3. 01965000	-0. 62680000
H	4. 36271800	-2. 50873600	1. 89534200
H	0. 85368500	-3. 09294100	0. 04723800
H	1. 85760000	-4. 26492600	1. 86043400
H	2. 66728100	-5. 13316300	-0. 21792200
H	3. 46149500	-2. 90655000	3. 34902700
H	3. 43703100	-4. 92091000	2. 23678600
H	1. 21096900	-1. 77041700	-1. 03075400
H	4. 30299900	-4. 54868400	0. 04712800
H	2. 85524900	-3. 27015100	-1. 69063800
H	3. 75198600	-2. 30026000	-0. 54539400
C	2. 58461400	-0. 59336900	3. 11123500
C	1. 30013000	0. 21881800	3. 23009000
C	0. 95443000	0. 77570700	1. 85452800
H	2. 81959300	-1. 08285500	4. 06068000
H	0. 48967800	-0. 41935100	3. 60255200
H	-0. 05738100	1. 19353000	1. 83284100
N	2. 43318900	-1. 65222500	2. 09126600
H	1. 64503700	1. 58588000	1. 59895300
H	1. 44402200	1. 03330800	3. 94702500
H	3. 42073400	0. 06565300	2. 84311900
C	1. 71299300	-1. 36482300	0. 96753500
N	1. 02924100	-0. 25853300	0. 82380000
C	-4. 35290000	0. 72457900	-0. 59213100
O	-5. 24516500	-0. 05174300	-0. 98185500

C	-4.75729800	1.93670700	0.21862300
C	-4.12518400	2.29116300	1.42197900
C	-5.86572700	2.68552900	-0.20932800
C	-4.58142000	3.37971100	2.17249100
H	-3.29635400	1.69390000	1.79307100
C	-6.31057400	3.78045400	0.53042700
H	-6.37504100	2.38591600	-1.11977400
C	-5.66887600	4.13184200	1.72389800
H	-4.09235200	3.63235900	3.10912000
H	-7.16305100	4.35690900	0.18221700
H	-6.02142600	4.98014400	2.30359200
C	-2.96980000	0.48344500	-0.92100900
N	-2.61930500	-0.68822000	-1.62701500
H	-3.10566900	-0.76330200	-2.51568000
C	-2.54214600	-1.93626800	-0.97468700
C	-2.62528000	-3.11656600	-1.73473600
C	-2.32189500	-2.05186000	0.40432100
C	-2.50563400	-4.36426300	-1.12864000
H	-2.79612200	-3.05091000	-2.80697300
C	-2.20599600	-3.31107100	0.99887200
H	-2.25580600	-1.15596500	1.01242900
C	-2.29689100	-4.49345100	0.25416900
H	-2.58608100	-5.25774900	-1.74428500
H	-2.05125000	-3.36879500	2.07446500
C	-2.21928900	-5.85368700	0.91049200
H	-3.21198100	-6.31366000	0.99887700
H	-1.59418700	-6.54631600	0.33514200
H	-1.80175100	-5.78557200	1.92030100
C	3.95727500	2.83429900	0.66330400
O	4.20852100	2.15895400	1.66641000
H	3.16476500	2.55934100	-0.05025400
N	4.59962100	3.97596600	0.30738000
C	5.67717000	4.51432100	1.12204500
H	5.83199300	3.85248300	1.97445000
H	6.60332700	4.58109800	0.53768400
H	5.42136100	5.51887500	1.48161300
C	4.21470200	4.71131000	-0.88994900
H	5.06573800	4.79674100	-1.57739100
H	3.40058300	4.18854600	-1.39634300
H	3.88016300	5.72327900	-0.62906500
C	1.24412000	1.22348100	-2.12375600
O	1.80511200	2.29465600	-1.93328400
O	1.79155300	0.25607500	-2.92458100
C	3.05839000	0.56997100	-3.53861000

C	3.42808900	-0.58662000	-4.45006100
H	3.80791600	0.72351200	-2.75420200
H	2.96174700	1.50849700	-4.09343300
H	4.38647900	-0.38173000	-4.93927600
H	3.52394600	-1.51910800	-3.88506400
H	2.66961700	-0.73107400	-5.22553700
N	-0.82296300	1.75013500	-1.02559000
N	-2.06772200	1.52809900	-0.78878700
H	-2.51020300	2.36018000	-0.40203500
C	0.00710000	0.72032900	-1.50037000
H	-0.45919400	-0.09621100	-2.04625700
H	0.51201700	0.13373300	-0.35214700

Int5c

C	-6.28779100	-0.09989300	-1.05302000
C	-6.72247400	0.93395000	-0.00721600
C	-3.83932900	1.02274400	0.33619500
C	-6.02171100	2.29667500	-0.13581900
C	-4.52161800	2.16616000	-0.43890700
H	-6.20288200	0.37827300	-2.04349000
H	-4.27529700	0.93492800	1.34078400
H	-6.56380000	0.50513700	0.98904000
H	-6.16538400	2.85573900	0.79776700
H	-7.08362200	-0.84578800	-1.14287200
H	-7.80594800	1.07259000	-0.10776700
H	-2.78672500	1.27287700	0.45917100
H	-6.50464000	2.88809300	-0.92451500
H	-4.00594900	3.10107000	-0.19860700
H	-4.36181600	2.01399600	-1.51373500
C	-5.06408000	-2.18255600	-1.43497600
C	-3.92478600	-3.05785700	-0.93251100
C	-2.62359600	-2.27011000	-1.04146800
H	-6.03103000	-2.66218700	-1.24389700
H	-4.10294600	-3.33163200	0.11411800
H	-1.80384400	-2.81566100	-0.56325700
N	-5.06950900	-0.87805500	-0.75767000
H	-2.34266200	-2.14458600	-2.09825300
H	-3.88118600	-3.98410900	-1.51633500
H	-4.98342300	-2.04347600	-2.52598400
C	-3.86172900	-0.34268800	-0.33339900
N	-2.71650600	-0.95323600	-0.41380500
C	0.90115300	-1.67482200	0.93129600
O	1.83888000	-2.47502600	0.76660400
C	-0.21850600	-2.06406700	1.86018900

C	-0.89545200	-1.13972300	2.67161800
C	-0.51931100	-3.43046100	1.99474100
C	-1.86022600	-1.57075500	3.58589200
H	-0.65444100	-0.08367100	2.61188800
C	-1.49366300	-3.85902000	2.89365900
H	0.03535700	-4.14318800	1.39295900
C	-2.16783300	-2.92832300	3.69368700
H	-2.36593600	-0.84496600	4.21631200
H	-1.72117400	-4.91781400	2.98172900
H	-2.91947800	-3.26241300	4.40350600
C	0.93404300	-0.36206400	0.29117500
H	1.17483000	2.44570300	0.51364600
H	-1.14001300	-0.27377700	0.06349700
N	2.12858100	0.13058200	-0.25717000
H	2.33829900	-0.19541300	-1.20500000
C	3.25299500	0.43458900	0.52006800
C	4.51042800	0.55708500	-0.10424000
C	3.17222300	0.68741500	1.89814800
C	5.63665300	0.90810300	0.63349600
H	4.59160400	0.37177800	-1.17173100
C	4.31594500	1.03469900	2.62345200
H	2.21878000	0.60135200	2.40993800
C	5.56982000	1.15370000	2.01543100
H	6.59298500	0.99277700	0.12096500
H	4.22100500	1.21665600	3.69176900
C	6.80528100	1.52349300	2.80489900
H	7.54326400	0.71136100	2.80466200
H	7.30094900	2.40935100	2.38931500
H	6.55708700	1.74210900	3.84819200
C	3.18174700	-2.40888000	-2.22768100
O	2.92963700	-1.30705500	-2.73192200
H	2.94990200	-2.62353100	-1.17246100
N	3.74840900	-3.44759100	-2.88987300
C	4.12098600	-3.33210700	-4.29162300
H	3.85317000	-2.33430300	-4.63941300
H	5.20024400	-3.48486900	-4.41507300
H	3.59242900	-4.08292200	-4.89178500
C	4.02419100	-4.70602000	-2.21461600
H	5.09913500	-4.92565300	-2.22639700
H	3.69101000	-4.64450200	-1.17633700
H	3.49695600	-5.53333200	-2.70597700
C	-0.06992700	3.85738000	-0.47488100
O	-1.18980700	4.17839300	-0.13916100
O	0.84937300	4.72975800	-0.94753900

C	0.45129600	6.12149000	-1.00486200
C	1.63546600	6.91575600	-1.52276500
H	0.14845100	6.43992300	-0.00236900
H	-0.42071500	6.20780700	-1.66058900
H	1.37052600	7.97692900	-1.57946600
H	2.49873100	6.81090000	-0.85872300
H	1.92657800	6.57959700	-2.52254700
N	-0.52506300	1.48831300	-0.34261500
N	-0.23730100	0.29248400	0.04975400
C	0.54137900	2.46501100	-0.38868500
H	1.22723600	2.31938500	-1.23053700

TS6c

C	-6.19681000	-0.20886200	-0.84441000
C	-6.56232600	0.59099900	0.41074800
C	-3.67678500	0.99235500	0.36208700
C	-6.02750500	2.03226300	0.40931300
C	-4.59455400	2.12445300	-0.13305200
H	-6.30163200	0.42005300	-1.74203200
H	-3.90079200	0.75007400	1.40969700
H	-6.20241800	0.04137300	1.28824900
H	-6.06461700	2.42523200	1.43316000
H	-6.91758000	-1.02365600	-0.95421300
H	-7.65589100	0.60578500	0.48988200
H	-2.64711700	1.35121500	0.32266400
H	-6.68733600	2.67252400	-0.18998600
H	-4.14147100	3.07696000	0.15820200
H	-4.60023900	2.13008900	-1.23017300
C	-4.84222300	-2.10269300	-1.65190200
C	-3.61193300	-2.94251600	-1.33459300
C	-2.37518500	-2.06323600	-1.45624300
H	-5.75482700	-2.66534800	-1.43031200
H	-3.68370400	-3.33733400	-0.31494700
H	-1.48518800	-2.58229000	-1.08991900
N	-4.87364800	-0.86876200	-0.84644800
H	-2.18491800	-1.80416000	-2.50753000
H	-3.55903100	-3.79421400	-2.02065000
H	-4.86914700	-1.84786500	-2.72250000
C	-3.69666000	-0.29735700	-0.44180400
N	-2.52668100	-0.83385700	-0.68043100
C	0.81646500	-1.66000600	0.84775600
O	1.78569400	-2.44401600	0.79314500
C	-0.39066600	-2.10011600	1.64209200
C	-1.14458700	-1.22239700	2.43697900

C	-0.69689200	-3.47115400	1.67632600
C	-2.18729300	-1.70228900	3.23482100
H	-0.90101000	-0.16550700	2.45162400
C	-1.75056900	-3.94859500	2.45486200
H	-0.08078900	-4.15190000	1.09718700
C	-2.50010600	-3.06368800	3.23935600
H	-2.74699100	-1.01294500	3.86135900
H	-1.97753200	-5.01137700	2.46624400
H	-3.30985900	-3.43628500	3.86085000
C	0.87293300	-0.34487600	0.23375600
H	1.13922400	2.45940100	0.42963000
H	-1.40417700	-0.32177900	-0.25608700
N	2.11454500	0.15652500	-0.21721300
H	2.41045100	-0.17919500	-1.13611900
C	3.16059900	0.49393900	0.64460800
C	4.46483800	0.64178400	0.12843100
C	2.96026000	0.75705900	2.00973800
C	5.51605000	1.02869900	0.95371800
H	4.64112100	0.44595400	-0.92581700
C	4.02972500	1.14181000	2.82360200
H	1.96995800	0.64537900	2.43968100
C	5.32707700	1.28893800	2.32167900
H	6.51039900	1.13049000	0.52277500
H	3.84125200	1.33020900	3.87852500
C	6.47898400	1.71504500	3.20391000
H	6.88178000	2.69069100	2.90287500
H	6.16643000	1.79713500	4.24973100
H	7.30801800	0.99789600	3.16176200
C	3.40223000	-2.40246700	-2.01982600
O	3.15669700	-1.34583300	-2.61462300
H	3.07754300	-2.56545500	-0.97969500
N	4.06955800	-3.45381800	-2.56053500
C	4.56833400	-3.40582300	-3.92585300
H	4.27773000	-2.45172800	-4.36609200
H	5.66184700	-3.49614800	-3.94039000
H	4.14434300	-4.22661200	-4.51764400
C	4.33531800	-4.65195200	-1.78048500
H	5.41524700	-4.81809600	-1.67781600
H	3.90164000	-4.54228500	-0.78410200
H	3.89508900	-5.53437500	-2.26205700
C	-0.08825700	3.85884600	-0.58553400
O	-1.18071300	4.18503400	-0.16856200
O	0.77537700	4.72556500	-1.16474000
C	0.35580900	6.10917200	-1.23364900

C	1.47220600	6.89374600	-1.89727300
H	0.15093700	6.46426700	-0.21856800
H	-0.57859000	6.16346300	-1.80107100
H	1.19004800	7.94975200	-1.96738000
H	2.39877700	6.82187900	-1.31978100
H	1.66626800	6.52108700	-2.90766000
N	-0.53002900	1.48719800	-0.48242000
N	-0.29243100	0.28912700	-0.07331300
C	0.53736600	2.47495800	-0.49316200
H	1.24605100	2.34050100	-1.31677300

Pr

C	-5.72088200	-0.31366900	-0.56815900
C	-5.31503900	0.61279900	-1.72075200
C	-3.27081800	-1.40947900	-1.98924600
C	-5.18370000	-0.09433700	-3.07817700
C	-4.45542900	-1.44265900	-2.97261300
H	-6.51048400	-1.00907500	-0.90211200
H	-2.76893400	-0.43610700	-2.03895800
H	-4.37697300	1.10830800	-1.45039700
H	-4.64093300	0.56592700	-3.76579000
H	-6.17662400	0.30171900	0.21489100
H	-6.07355100	1.40116500	-1.79953800
H	-2.53423400	-2.16594300	-2.26383600
H	-6.17757000	-0.24794100	-3.51792600
H	-4.09125200	-1.73737100	-3.96313100
H	-5.15694200	-2.22995000	-2.66879400
C	-4.94131700	-1.38578900	1.49259400
C	-3.69268400	-1.85229500	2.23090100
C	-3.03586300	-2.96432200	1.41626700
H	-5.36032500	-0.49372700	1.97379300
H	-2.99306000	-1.01506200	2.33536800
H	-2.06681400	-3.24048000	1.84923000
N	-4.63337700	-1.04376100	0.10027400
H	-3.65358400	-3.87514300	1.45520700
H	-3.96107000	-2.19081100	3.23816500
H	-5.72052100	-2.16521100	1.53694700
C	-3.59865000	-1.72125100	-0.53468500
N	-2.82037100	-2.59265900	0.02294600
C	3.20027200	1.82577800	0.50384500
O	4.18329100	1.70550400	1.24001300
C	2.73951100	3.19680100	0.10544900
C	1.99937000	3.47766600	-1.05385800
C	3.15982600	4.26187000	0.91918900

C	1. 68320300	4. 79638400	-1. 38094300
H	1. 67139200	2. 66633300	-1. 68931600
C	2. 82650500	5. 57549800	0. 60059900
H	3. 75426100	4. 03442800	1. 79730900
C	2. 08718200	5. 84689500	-0. 55384600
H	1. 12519400	5. 00293900	-2. 28979200
H	3. 15176100	6. 38796800	1. 24401300
H	1. 83694900	6. 87208500	-0. 81268800
C	2. 48537800	0. 57667600	0. 10252300
H	-0. 52939900	-2. 07253800	-0. 07396600
H	-0. 47896800	0. 06831300	-0. 80530500
N	3. 17417900	-0. 60184000	0. 44861300
H	3. 91300200	-0. 36183100	1. 10552700
C	3. 57540100	-1. 56867200	-0. 50102000
C	4. 47456900	-2. 56853300	-0. 09243200
C	3. 11372900	-1. 58357800	-1. 82480900
C	4. 89923700	-3. 54596100	-0. 98410400
H	4. 83987400	-2. 56957500	0. 93141200
C	3. 54328900	-2. 58110300	-2. 70196000
H	2. 42378800	-0. 82271600	-2. 16939300
C	4. 43936100	-3. 57910700	-2. 30901000
H	5. 60311600	-4. 30132700	-0. 64237800
H	3. 17234100	-2. 57118100	-3. 72411600
C	4. 88092300	-4. 66498100	-3. 26169700
H	4. 34410200	-5. 60488800	-3. 08008500
H	4. 69678500	-4. 38132700	-4. 30211500
H	5. 94965600	-4. 88088900	-3. 15790700
C	-1. 53711600	2. 14891600	0. 18713700
O	-1. 85762500	1. 55594100	-0. 84841400
H	-1. 06790300	1. 62617900	1. 03366100
N	-1. 71165000	3. 47455300	0. 40167500
C	-2. 25772400	4. 32971300	-0. 63829100
H	-2. 53545800	3. 70132000	-1. 48394600
H	-3. 14048400	4. 86727400	-0. 27227600
H	-1. 50973300	5. 06422800	-0. 95999300
C	-1. 23600600	4. 10789100	1. 61969800
H	-2. 05084000	4. 64370400	2. 12164400
H	-0. 84813400	3. 34639600	2. 29944800
H	-0. 43218100	4. 82043700	1. 39970600
C	0. 23353000	-1. 24821200	1. 72852400
O	-0. 17035200	-0. 21381500	2. 22418600
O	0. 58237600	-2. 33111600	2. 44858800
C	0. 46488000	-2. 21022800	3. 88603400
C	0. 96714900	-3. 50551800	4. 49335500

H	-0.58215600	-2.01601900	4.13994800
H	1.05056000	-1.34610700	4.21366400
H	0.89599400	-3.45630600	5.58439700
H	0.37379000	-4.35648800	4.14717100
H	2.01188400	-3.68283700	4.22357900
N	0.43477200	-0.32445800	-0.57928200
N	1.28042000	0.69939000	-0.35949000
C	0.37530200	-1.53004100	0.23795200
H	1.23403900	-2.18145500	0.07974700

Com2

C	0.60276100	3.24856200	1.76831300
C	1.89317100	3.27853200	0.94091200
C	0.26722600	1.50189500	-0.68112500
C	1.67995500	3.63565300	-0.53835400
C	0.42922400	2.96751000	-1.12502100
H	-0.06297400	4.07641400	1.48275100
H	1.25245800	1.02221800	-0.60976800
H	2.39098600	2.30735700	1.03778900
H	2.56898500	3.33234700	-1.10514400
H	0.86919200	3.41062700	2.81769300
H	2.56957600	4.01138900	1.39634500
H	-0.29578900	0.94598100	-1.43110300
H	1.59561600	4.72390300	-0.64975700
H	0.47954900	3.00139400	-2.21945000
H	-0.46975500	3.52442200	-0.84075600
C	-1.00129000	1.81732400	2.93927100
C	-1.48404600	0.37760300	3.05917900
C	-2.16893500	-0.01514900	1.75324200
H	-0.41507500	2.10031900	3.82040600
H	-0.62416900	-0.27769000	3.24220100
H	-2.36106400	-1.09445600	1.72471000
N	-0.14457600	1.97629500	1.75815700
H	-3.15551600	0.46914500	1.69022200
H	-2.16351400	0.27594000	3.91256000
H	-1.85474300	2.50930700	2.87647800
C	-0.48936200	1.27027100	0.62135700
N	-1.39342600	0.33738200	0.56895200
C	0.00370800	-2.78384700	-0.97973300
O	-0.29767300	-2.14857000	-1.98379400
C	-0.98337700	-3.64472300	-0.26864200
C	-0.58858000	-4.68932200	0.58331500
C	-2.35384700	-3.39820600	-0.46680400
C	-1.54430700	-5.48312800	1.21421300

H	0.46287500	-4.90324800	0.74311500
C	-3.30338900	-4.18646300	0.17770800
H	-2.65854100	-2.56259400	-1.08919200
C	-2.90269400	-5.23279700	1.01260200
H	-1.22912800	-6.29718500	1.85981200
H	-4.35968200	-3.98332800	0.02934600
H	-3.64714900	-5.85010600	1.50707800
C	1.41403700	-2.65381300	-0.40844800
H	1.84076600	-3.65428500	-0.24477200
H	1.30435300	-2.20189700	0.59357100
N	2.23272000	-1.86582800	-1.28641900
H	1.69073200	-1.41584800	-2.01444100
C	3.37003600	-1.20167600	-0.84829500
C	3.92486000	-0.17453300	-1.64072700
C	4.02300100	-1.52843900	0.35224300
C	5.07649900	0.48969700	-1.24079100
H	3.44326200	0.09057100	-2.57882300
C	5.18065100	-0.84809400	0.73615000
H	3.63941800	-2.32121900	0.98592900
C	5.73395200	0.17182200	-0.04110600
H	5.47669700	1.27586400	-1.87739000
H	5.66321200	-1.12626800	1.67033700
C	6.98414800	0.90653200	0.38193500
H	6.79312200	1.97471800	0.54239100
H	7.38640600	0.50115800	1.31496400
H	7.77277000	0.83430500	-0.37646300
C	-3.68488700	3.07231500	0.14019800
O	-2.72043300	3.80796600	0.33538600
H	-4.32930000	2.72334100	0.97095400
N	-4.11077800	2.60307800	-1.05603200
C	-3.37993700	2.90376800	-2.28017000
H	-2.65828700	3.69097000	-2.06536500
H	-2.86897100	2.00146100	-2.63276500
H	-4.07769500	3.25096500	-3.05125900
C	-5.17238200	1.61313600	-1.15378800
H	-4.76590000	0.66359600	-1.51854500
H	-5.62170600	1.45914100	-0.16891900
H	-5.95573800	1.95803500	-1.83981900
O	-2.57878500	-0.31867700	-1.91242600
H	-1.92970600	-0.91014600	-2.32009700
H	-2.16519800	-0.10544600	-1.03655000

TS1w

C	1.18452800	3.76964400	0.37258800
---	------------	------------	------------

C	1. 87491200	3. 84068300	-0. 99394200
C	0. 71470700	1. 18238500	-1. 13321200
C	0. 95289300	3. 50730500	-2. 17751800
C	0. 00853400	2. 34202300	-1. 86219000
H	0. 17497500	4. 19959600	0. 32964700
H	1. 74859800	1. 07470400	-1. 48495900
H	2. 74797100	3. 17861400	-0. 97680400
H	1. 56777000	3. 26717000	-3. 05344400
H	1. 75738300	4. 37979200	1. 07617600
H	2. 27096000	4. 85574200	-1. 11287100
H	0. 21692700	0. 24507600	-1. 37953500
H	0. 36145500	4. 39067700	-2. 44769900
H	-0. 45045000	1. 95299100	-2. 77490300
H	-0. 82182000	2. 69644400	-1. 24158800
C	1. 02595000	2. 50019400	2. 47478300
C	1. 34575000	1. 14796500	3. 09816600
C	0. 41815200	0. 10619000	2. 48797800
H	1. 74308600	3. 25390000	2. 81315900
H	2. 38762600	0. 88078800	2. 89062700
H	0. 73100900	-0. 90924500	2. 75792300
N	1. 11058200	2. 43349100	1. 00514400
H	-0. 60526400	0. 23819100	2. 86476900
H	1. 22014400	1. 19905100	4. 18426000
H	0. 01846800	2. 83472400	2. 75421700
C	0. 73620500	1. 28620400	0. 38216400
N	0. 41069600	0. 19288800	1. 03312700
C	-0. 85420400	-2. 23112000	-0. 87857800
O	-0. 91703800	-1. 84550800	-2. 07944900
C	-2. 12109200	-2. 57823500	-0. 15366800
C	-2. 21197400	-2. 66800100	1. 24574100
C	-3. 27291100	-2. 82438300	-0. 91733300
C	-3. 41942900	-2. 99515300	1. 86120600
H	-1. 33795800	-2. 47429700	1. 85917900
C	-4. 47765100	-3. 16175800	-0. 30318400
H	-3. 19837400	-2. 74954100	-1. 99627500
C	-4. 55709100	-3. 24666000	1. 08865900
H	-3. 47287800	-3. 05815500	2. 94458900
H	-5. 35574600	-3. 36069200	-0. 91118500
H	-5. 49525400	-3. 50996000	1. 56882300
C	0. 39753100	-2. 25464700	-0. 17989600
H	0. 48185000	-2. 99580200	0. 61747000
H	0. 32213100	-0. 94484100	0. 45418900
N	1. 53085500	-2. 20075000	-1. 05567800
H	1. 26995900	-2. 05736700	-2. 02386500

C	2.81968100	-1.89725900	-0.68297800
C	3.78453900	-1.58494500	-1.66862200
C	3.24772200	-1.91208200	0.66080100
C	5.09894200	-1.30579900	-1.32018800
H	3.48543600	-1.57059400	-2.71435900
C	4.57348300	-1.62744900	0.98725800
H	2.54332900	-2.15900900	1.44777100
C	5.53104000	-1.31884900	0.01589200
H	5.81065200	-1.06908100	-2.10872900
H	4.86971500	-1.65286500	2.03430500
C	6.97004600	-1.03536900	0.37766300
H	7.34696800	-0.13794900	-0.12688800
H	7.08610100	-0.88187700	1.45507700
H	7.63470300	-1.86196600	0.09433700
C	-2.90033900	1.87248700	1.04154700
O	-2.07763900	2.77626500	1.18264600
H	-2.91250800	0.98109900	1.69499700
N	-3.86992900	1.82086700	0.09543900
C	-4.04689200	2.91394300	-0.85342500
H	-3.34032100	3.70403000	-0.60118800
H	-3.86698600	2.56128400	-1.87428800
H	-5.06894400	3.30470200	-0.78813700
C	-4.77564000	0.68368700	-0.01772400
H	-4.66177500	0.21827800	-1.00122800
H	-4.53528600	-0.05891500	0.74622100
H	-5.81496700	1.00657500	0.11706000
O	-2.61545000	0.32968100	-2.50373300
H	-2.10330900	-0.50695900	-2.52485700
H	-2.43414400	0.66069400	-1.61586200

Int1w

C	2.95022400	-2.40464100	1.13049200
C	4.28318700	-3.04378400	0.69428300
C	3.51330200	-0.22005600	-0.54526800
C	5.28416500	-2.04300100	0.09734800
C	4.71579300	-1.10787800	-0.98222900
H	2.45659000	-3.03070300	1.87557600
H	2.56854200	-0.64637200	-0.89306500
H	4.04691300	-3.82714300	-0.03529300
H	6.13012400	-2.59667100	-0.32469200
H	2.26242400	-2.33140800	0.28393600
H	4.75448200	-3.54283900	1.54897700
H	3.59417600	0.76824800	-1.00136600
H	5.70235500	-1.43314300	0.90796700

H	4.40110800	-1.69326400	-1.85323500
H	5.52654700	-0.45572200	-1.32276600
C	2.79483900	-0.88339700	3.15871500
C	2.32004100	0.54100100	3.43330500
C	3.30164800	1.53912300	2.82777300
H	1.99920400	-1.58749500	3.41292800
H	1.33980300	0.67269600	2.96920600
H	2.90784100	2.55795100	2.85908200
N	3.11116800	-1.06693300	1.72836800
H	4.25798300	1.53702300	3.36725300
H	2.22944100	0.69441600	4.51185100
H	3.67820300	-1.13692800	3.75987700
C	3.36950700	-0.02006900	0.94089200
N	3.53302700	1.20000300	1.42344000
C	-1.72585200	1.64443500	-0.92660800
O	-0.53438900	2.15892300	-0.68993600
C	-2.91849800	2.38163600	-0.42054000
C	-4.21981000	2.19004500	-0.91936800
C	-2.73673900	3.32910200	0.60133500
C	-5.29936300	2.89591900	-0.39263600
H	-4.38234400	1.50167100	-1.74296100
C	-3.81562200	4.03800100	1.12552500
H	-1.72787900	3.48673500	0.96722200
C	-5.10526000	3.82321100	0.63469700
H	-6.29554600	2.73403700	-0.79654900
H	-3.65117200	4.76140800	1.92044100
H	-5.94738800	4.37822500	1.03869600
C	-1.86100600	0.45267700	-1.59859300
H	-2.80725500	-0.03199700	-1.79955100
H	3.58405400	1.98108100	0.73548300
N	-0.71237700	-0.07795400	-2.21992800
H	0.02911200	0.61241200	-2.26605800
C	-0.32222700	-1.39936300	-2.25899800
C	0.90818100	-1.74891800	-2.86506900
C	-1.10593300	-2.44513600	-1.72218400
C	1.32735200	-3.07372100	-2.92284000
H	1.51621300	-0.96543800	-3.31230900
C	-0.66561400	-3.76506000	-1.79867200
H	-2.04581000	-2.21637700	-1.23173300
C	0.55189600	-4.11833400	-2.39538500
H	2.27516500	-3.30455200	-3.40632900
H	-1.29051600	-4.54613800	-1.36994800
C	0.98923500	-5.56010300	-2.50671700
H	2.08061700	-5.65403400	-2.48803400

H	0.58894800	-6.16519900	-1.68655300
H	0.64600900	-6.02186700	-3.44221200
C	2.29944600	3.55132000	-0.75987700
O	3.45123900	3.27704200	-0.36030700
H	1.43502300	2.89552800	-0.58753400
N	1.99153200	4.66285800	-1.44850200
C	3.01052200	5.64629200	-1.78069500
H	3.96614400	5.30644800	-1.38332800
H	3.08508200	5.76432500	-2.86794300
H	2.75558500	6.61963900	-1.34578100
C	0.61950200	4.91825500	-1.88115400
H	0.57936300	5.00141400	-2.97381600
H	-0.02295000	4.09546300	-1.54972800
H	0.26110000	5.86153900	-1.45242600
C	-3.39520700	-2.05279300	1.74633800
O	-3.64267500	-2.83703900	2.64517500
O	-4.10431200	-1.97004600	0.59043400
C	-5.23503600	-2.86236900	0.49253300
C	-5.91143200	-2.59312100	-0.83791100
H	-5.90565400	-2.67812000	1.33775300
H	-4.88319200	-3.89598600	0.57343400
H	-6.78439900	-3.24399500	-0.94893700
H	-6.24506900	-1.55359200	-0.90066300
H	-5.22977000	-2.78694200	-1.67111400
N	-1.51078000	-1.05261000	2.75496700
N	-0.81653000	-1.04094400	3.65786100
C	-2.31210600	-1.07791300	1.72868300
H	-2.12014000	-0.38134200	0.91681300
O	0.52371700	0.18452400	0.73111200
H	0.16553100	0.98377500	0.23900000
H	0.13966800	-0.55310700	0.24009300

TS2w

C	3.99573900	-1.41564000	-0.61292600
C	4.40582600	-2.89979900	-0.53271400
C	1.31753200	-2.24008400	-0.78341800
C	3.34912700	-3.86868300	-1.08708600
C	1.91639200	-3.66166300	-0.56969100
H	4.87110000	-0.76603700	-0.60989000
H	1.41528100	-1.64304200	0.12643300
H	4.61737800	-3.12852200	0.51894500
H	3.65984100	-4.89600700	-0.86547200
H	3.40521500	-1.12618300	0.25862900
H	5.34304500	-3.05790400	-1.08065100

H	0.24690700	-2.30297100	-0.97864600
H	3.34289100	-3.79088100	-2.18163000
H	1.86245900	-3.88391000	0.50115300
H	1.27141500	-4.39154200	-1.06918000
C	3.84220800	-0.23619500	-2.85671000
C	2.77735100	0.57885700	-3.58338000
C	1.65799800	-0.33526300	-4.06924500
H	4.52516700	0.44041700	-2.34356300
H	2.38359700	1.31314800	-2.87662400
H	0.79363700	0.23622200	-4.41647500
N	3.22435000	-1.08987500	-1.82412100
H	1.99428400	-0.96724900	-4.90195300
H	3.23152800	1.10886300	-4.42554100
H	4.41211700	-0.86769300	-3.55187300
C	1.94452200	-1.45934400	-1.91030500
N	1.20073100	-1.18623500	-2.97024500
C	-2.66179000	1.56634500	0.76401700
O	-3.61671500	0.85918500	0.37669700
C	-2.65017500	3.03110400	0.47091400
C	-1.86353100	3.95322400	1.17802500
C	-3.50590200	3.50681900	-0.53527600
C	-1.92089300	5.31289300	0.87629200
H	-1.21882900	3.61907700	1.98406900
C	-3.55766400	4.86307300	-0.84222600
H	-4.12131500	2.78815300	-1.06486500
C	-2.76364700	5.77154900	-0.13759500
H	-1.30896600	6.01432900	1.43573000
H	-4.21750200	5.21470900	-1.63038500
H	-2.80475900	6.83099400	-0.37399300
C	-1.52653300	0.93263600	1.41874200
H	-0.86299800	1.53156500	2.03044600
H	0.16385600	-1.28760700	-2.84723900
N	-1.80203400	-0.34670900	1.90494700
H	-2.66553400	-0.72390200	1.53322700
C	-0.88009000	-1.23643100	2.42892000
C	-1.28381800	-2.55141000	2.73358900
C	0.45370400	-0.87651600	2.71247600
C	-0.39603800	-3.45876000	3.30098900
H	-2.30731900	-2.85413300	2.52561000
C	1.32377700	-1.80017700	3.29067400
H	0.81717300	0.11776800	2.47767700
C	0.92855300	-3.10869000	3.59921000
H	-0.74522000	-4.46434300	3.52601000
H	2.34180000	-1.48471400	3.51084300

C	1. 89053700	-4. 09841600	4. 21471500
H	1. 35874100	-4. 96043500	4. 63344200
H	2. 60868600	-4. 48463700	3. 48238200
H	2. 47461500	-3. 64240900	5. 02444900
C	-4. 31628500	-1. 74226400	-1. 31851100
O	-3. 56409600	-2. 56065400	-1. 86301600
H	-4. 00341300	-0. 71221000	-1. 09993400
N	-5. 57874400	-2. 01018400	-0. 91454700
C	-6. 16361400	-3. 32374200	-1. 12505700
H	-5. 42700700	-3. 94879500	-1. 62900400
H	-6. 43923000	-3. 78144600	-0. 16728800
H	-7. 06600500	-3. 24852100	-1. 74362200
C	-6. 38759000	-0. 99279800	-0. 25950200
H	-6. 73094400	-1. 35168500	0. 71838000
H	-5. 79042100	-0. 09181800	-0. 10771200
H	-7. 27143100	-0. 74932100	-0. 86263500
C	2. 67758400	2. 30857000	0. 18215400
O	3. 41505300	1. 78603400	-0. 65797500
O	3. 14525300	3. 29151600	1. 02142700
C	4. 51852400	3. 66013600	0. 84610300
C	4. 82541900	4. 76484400	1. 84168800
H	4. 68231700	3. 99049300	-0. 18591200
H	5. 15907900	2. 78476600	1. 00670600
H	5. 86925800	5. 08092300	1. 74550900
H	4. 18464100	5. 63411400	1. 66720500
H	4. 66219300	4. 42167600	2. 86758400
N	0. 64989800	1. 12446000	-0. 26990800
N	-0. 47315600	0. 62440200	-0. 21237600
C	1. 30086900	2. 02614100	0. 46597600
H	0. 79982600	2. 58443800	1. 25015300
O	-1. 40202300	-0. 96249200	-2. 44323700
H	-2. 09683200	-1. 63115000	-2. 24647100
H	-1. 27595800	-0. 41419200	-1. 63650300

Int2w

C	6. 12948200	0. 75224000	-0. 40740700
C	5. 88652000	-0. 75856200	-0. 38608000
C	3. 46204600	0. 09069200	-1. 73664100
C	5. 56534300	-1. 37037700	-1. 75684100
C	4. 60771000	-0. 49754100	-2. 57953500
H	6. 74525400	1. 04004900	-1. 27160800
H	3. 12047700	-0. 63219000	-0. 98119400
H	5. 08191300	-0. 99102800	0. 31696400
H	5. 10712400	-2. 34829600	-1. 58296400

H	6.69992200	1.02567400	0.48390700
H	6.79360200	-1.22408100	0.01699700
H	2.59513300	0.29478800	-2.36797100
H	6.48783400	-1.53507800	-2.32807200
H	4.16594600	-1.09632200	-3.38230000
H	5.15614800	0.31056000	-3.08175800
C	5.12649600	2.90734400	0.32290000
C	3.80625900	3.50410300	0.79948500
C	2.84780200	3.58547200	-0.37899400
H	5.78735900	2.72333600	1.17396100
H	3.37942600	2.87095600	1.58432600
H	1.82448200	3.82269100	-0.07701600
N	4.92365800	1.61695200	-0.36510800
H	3.16549700	4.36437900	-1.08489900
H	3.98485400	4.49483000	1.22697100
H	5.64707300	3.60412200	-0.34915800
C	3.77137500	1.38595600	-1.02460000
N	2.81392500	2.29562400	-1.06476000
C	-2.37436300	0.04215800	0.95643700
O	-2.99639400	1.03469700	0.58756700
C	-2.37149600	-0.35395000	2.40043000
C	-1.40962300	-1.21226200	2.95602200
C	-3.38027800	0.16742600	3.22727900
C	-1.46065900	-1.53663700	4.31168300
H	-0.60527900	-1.61225000	2.34824000
C	-3.43712600	-0.17003900	4.57582800
H	-4.11826200	0.82846800	2.78552700
C	-2.47438700	-1.02338800	5.12214300
H	-0.70550500	-2.19315700	4.73386900
H	-4.23004700	0.22869000	5.20228500
H	-2.51586500	-1.28784200	6.17507200
C	-1.57542800	-0.79529000	-0.06330300
H	-1.61273000	-1.84756900	0.23630100
H	1.87033300	2.01672000	-1.46686000
N	-2.06025200	-0.66881100	-1.41787100
H	-1.63406300	0.09514600	-1.92659300
C	-3.31903300	-1.06968100	-1.83671300
C	-3.78003800	-0.68172500	-3.11253500
C	-4.15572900	-1.89581300	-1.06528100
C	-5.01271400	-1.10757000	-3.58675100
H	-3.15235500	-0.04204400	-3.72847900
C	-5.38981900	-2.31710100	-1.56258600
H	-3.85171900	-2.21124200	-0.07266000
C	-5.85025800	-1.93886100	-2.82595500

H	-5.33434300	-0.78577700	-4.57536900
H	-6.01184800	-2.95575400	-0.93901300
C	-7.18757900	-2.39925400	-3.35714800
H	-7.83084900	-1.55373800	-3.63025600
H	-7.07829000	-3.01903100	-4.25607000
H	-7.72561300	-2.99443900	-2.61315000
C	-1.62158700	3.87165500	-0.11861200
O	-0.57767900	4.14594200	-0.72888300
H	-2.05986200	2.86398300	-0.13169500
N	-2.33170800	4.75274700	0.61829600
C	-1.91254000	6.13977300	0.72940500
H	-1.01589100	6.27605300	0.12563400
H	-2.70252300	6.80859800	0.36806200
H	-1.69502700	6.39501700	1.77361200
C	-3.53991600	4.34164400	1.31927800
H	-4.41667200	4.87136500	0.92685200
H	-3.68183700	3.26596000	1.19899800
H	-3.45251900	4.56846000	2.38868800
C	2.12667600	-2.93604700	0.50110400
O	3.25321800	-2.46481200	0.33893700
O	1.95310300	-4.25860800	0.82085200
C	3.14977600	-5.03957300	0.93407600
C	2.73997600	-6.44997000	1.31909700
H	3.81147200	-4.59096500	1.68360300
H	3.68958400	-5.02387900	-0.02000500
H	3.62512600	-7.08719200	1.41517100
H	2.20725900	-6.45357400	2.27461700
H	2.08236600	-6.88505300	0.56092600
N	0.83642000	-0.97947600	0.12013000
N	-0.20429300	-0.21643700	-0.04212800
C	0.84792900	-2.27221300	0.39655900
H	-0.03613000	-2.89598900	0.51993000
O	0.32676800	1.72499000	-1.81807000
H	-0.06944400	2.58474500	-1.56135800
H	0.10321100	1.07438500	-1.07167200

TS3w

C	-5.60140600	-1.44576700	-1.16248300
C	-5.45683800	-2.72575400	-1.99146900
C	-2.73756900	-2.48699000	-0.96849300
C	-4.86236200	-3.90610500	-1.20985200
C	-3.70231100	-3.47766900	-0.30367000
H	-5.96721300	-1.68155900	-0.15332300
H	-2.54905700	-2.75397200	-2.01729400

H	-4.85314300	-2.49833000	-2.87759500
H	-4.52237800	-4.66667400	-1.92294100
H	-6.36309000	-0.81510200	-1.62849900
H	-6.45179100	-2.99272800	-2.36550100
H	-1.76878800	-2.56047200	-0.46952900
H	-5.64411000	-4.37984100	-0.60347400
H	-3.12440500	-4.35522200	0.00063700
H	-4.06868400	-3.04022400	0.63088100
C	-4.69186000	0.85134600	-0.89498800
C	-3.55344500	1.70643900	-1.43770600
C	-2.25930300	1.27305000	-0.76748700
H	-5.62336100	1.06503900	-1.42556900
H	-3.49212400	1.58350100	-2.52572500
H	-1.38606600	1.71933300	-1.25451700
N	-4.39940400	-0.58690200	-1.06680300
H	-2.24970800	1.61391100	0.27267100
H	-3.74983600	2.76197900	-1.22948400
H	-4.85997100	1.06855600	0.16827500
C	-3.12100400	-1.01780000	-0.93220200
N	-2.09661600	-0.18625000	-0.80932400
C	3.55143700	-1.59061900	-0.86052700
O	3.90105100	-1.33551000	-2.00065600
C	4.42740300	-2.38953500	0.05552400
C	4.01720500	-2.83039300	1.32334100
C	5.72402200	-2.69643700	-0.38827200
C	4.89191700	-3.55818700	2.13009500
H	3.00862100	-2.63867500	1.66978200
C	6.59573600	-3.41928500	0.41911900
H	6.02030500	-2.35272900	-1.37356800
C	6.18092700	-3.85070200	1.68264400
H	4.56303800	-3.90272400	3.10607900
H	7.59737100	-3.64898700	0.06715700
H	6.85989600	-4.41686300	2.31416900
C	2.19816000	-1.05458800	-0.33297300
H	2.37132200	-0.55402200	0.63167300
H	-1.15360700	-0.55036900	-0.02658700
N	1.56500400	-0.13608000	-1.24070700
H	1.15068500	-0.58103100	-2.05674700
C	1.99980300	1.16685400	-1.44157200
C	1.41206000	1.92669700	-2.47714000
C	2.95962200	1.80556900	-0.63556900
C	1.76466200	3.25301500	-2.68546300
H	0.68013000	1.44428000	-3.11829900
C	3.29972600	3.14155700	-0.85991900

H	3.46856000	1.25946000	0.15110900
C	2.71752000	3.89870700	-1.88131200
H	1.29367300	3.80108500	-3.49907400
H	4.06247500	3.59663700	-0.23093600
C	3.13278700	5.32702300	-2.14810400
H	3.64246000	5.76313700	-1.28330900
H	3.82262600	5.39734900	-2.99904600
H	2.27203200	5.96313900	-2.38343800
C	-1.00024400	3.31822600	2.17776500
O	-2.14273300	3.42562800	1.73243900
H	-0.69244400	2.45894500	2.79646700
N	0.00774400	4.20088500	1.96696700
C	-0.19142700	5.35692200	1.10768000
H	-1.24295400	5.38991100	0.82371300
H	0.07488800	6.27875500	1.63781700
H	0.43074100	5.27689900	0.20824200
C	1.34503400	3.96476800	2.48274100
H	1.67927700	4.81245600	3.09320000
H	1.34332300	3.06797200	3.10668700
H	2.05750300	3.81757200	1.66313400
C	-1.23628400	-1.09713100	2.10935600
O	-2.03379900	-2.01179900	2.23231600
O	-1.23480500	-0.00945400	2.94793300
C	-2.25748200	0.00884800	3.96869600
C	-3.56191800	0.59401300	3.44462800
H	-1.83908100	0.62912900	4.76617800
H	-2.40200900	-1.00768600	4.34161300
H	-4.28665000	0.68274100	4.26163700
H	-3.39772400	1.58472900	3.00989000
H	-3.98727300	-0.06685500	2.68408300
N	0.24398800	-2.12561000	0.51539300
N	1.31688200	-2.26198700	-0.13211600
C	-0.24629700	-0.91842700	1.02954600
H	0.42482200	-0.06851500	1.16613600
O	-0.51928500	-1.00418800	-3.24015900
H	-0.76828000	-0.42623900	-3.97176300
H	-1.03625900	-0.68937300	-2.47545700

Int3w

C	-5.95413700	-2.64427300	-0.64060300
C	-4.93936300	-3.64657700	-0.07824000
C	-3.44241000	-1.17739800	0.23547900
C	-4.41134500	-3.29163100	1.32042100
C	-4.10248300	-1.79568600	1.47870800

H	-6.65313800	-2.33134100	0.15297100
H	-2.72470500	-1.88748600	-0.19431600
H	-4.11429100	-3.73508100	-0.79353600
H	-3.50401400	-3.87647000	1.51292900
H	-6.56171900	-3.15938800	-1.39177900
H	-5.42035400	-4.63148400	-0.04610400
H	-2.85515900	-0.30803900	0.52652400
H	-5.14235400	-3.59729300	2.07992700
H	-3.42653100	-1.64924200	2.32593300
H	-5.02026800	-1.24186300	1.71695900
C	-6.30526400	-0.91075800	-2.34060300
C	-5.56833000	0.05672300	-3.25856500
C	-4.85799800	1.09929900	-2.39925500
H	-6.72509200	-1.74222400	-2.91809800
H	-4.83237800	-0.49778900	-3.85226500
H	-4.18165600	1.70837700	-3.01051300
N	-5.39643400	-1.47289900	-1.33582100
H	-5.59263500	1.79833200	-1.97089900
H	-6.27298800	0.52278700	-3.95589800
H	-7.15269300	-0.39986100	-1.85397900
C	-4.36969200	-0.66981200	-0.85931200
N	-4.07845500	0.50683100	-1.31941600
C	3.02016600	-2.65908500	-1.06722900
O	3.15356000	-2.57460100	-2.27891800
C	3.51832500	-3.83983900	-0.30730500
C	3.25635500	-4.03622500	1.05774300
C	4.28843600	-4.78788200	-1.00164400
C	3.75981600	-5.15853100	1.71370500
H	2.63602200	-3.33707300	1.60636700
C	4.79472300	-5.90301600	-0.34348000
H	4.47620700	-4.62315300	-2.05708900
C	4.53143300	-6.08969200	1.01693200
H	3.54515200	-5.30802800	2.76739300
H	5.39292200	-6.62842900	-0.88672400
H	4.92468900	-6.96155800	1.53174300
C	2.31258600	-1.50192400	-0.31815900
H	2.86958100	-1.25707600	0.58931300
H	-0.21464100	0.58404600	0.32233400
N	2.18235200	-0.35075900	-1.16642500
H	2.01342900	-0.65057000	-2.12145700
C	3.06802600	0.73817200	-1.11179800
C	3.22429900	1.53153300	-2.26471800
C	3.77097900	1.12126500	0.04194000
C	4.06004500	2.64016700	-2.26444900

H	2.68245300	1.26364600	-3.16811100
C	4.60764900	2.24054900	0.02537200
H	3.68902700	0.55238000	0.96213700
C	4.77992500	3.02047300	-1.12074700
H	4.16341700	3.21948200	-3.17917900
H	5.14522500	2.50109900	0.93414900
C	5.72543800	4.19863600	-1.14443500
H	5.95709000	4.54581600	-0.13301900
H	6.67766100	3.94163700	-1.62562600
H	5.30547600	5.04355800	-1.70086200
C	-0.36225400	4.35363000	0.64918600
O	-1.57756300	4.41915200	0.83473000
H	0.22378400	3.45969200	0.91511100
N	0.39438200	5.34346800	0.11380300
C	-0.22103400	6.58762400	-0.31713100
H	-1.28617700	6.53355000	-0.09391900
H	0.22287900	7.44089400	0.20965600
H	-0.07982100	6.73434400	-1.39482000
C	1.81848600	5.17339900	-0.10954200
H	2.39122300	5.94302700	0.42284400
H	2.13734300	4.19143400	0.24479400
H	2.05840300	5.24207800	-1.17730500
C	-0.40310900	0.25766300	2.39115500
O	-1.15546200	-0.48088800	2.98567300
O	-0.07696400	1.50391300	2.80415700
C	-0.72704900	1.97531200	4.01480300
C	-2.12968200	2.49259000	3.73800500
H	-0.06929200	2.77058900	4.37381300
H	-0.73719800	1.15937700	4.74192400
H	-2.54122400	2.93671100	4.65118500
H	-2.11703200	3.25108400	2.95086000
H	-2.78435400	1.67365400	3.43151100
N	0.12250100	-1.43167700	0.71067600
N	0.96101100	-2.10310200	0.09675800
C	0.31232700	-0.02717100	1.08133400
H	1.34534800	0.32469100	1.14363000
O	-1.71108000	1.76480800	-0.41089100
H	-2.53684600	1.35742100	-0.77103200
H	-1.99736100	2.53642000	0.10209700

TS4w

C	1.13534200	-5.14811000	0.59663000
C	1.81797400	-4.84692000	-0.73947200
C	2.37548400	-2.34285000	0.58160300

C	3.28402700	-4.41339600	-0.60750000
C	3.48525800	-3.40108100	0.52791400
H	1.79390600	-5.73987100	1.24903500
H	2.08294400	-2.01508900	-0.42492300
H	1.22655600	-4.08861700	-1.26136600
H	3.60623200	-3.97086700	-1.55691900
H	0.25634400	-5.76703600	0.39787600
H	1.75925200	-5.75837100	-1.34578400
H	2.73132900	-1.43775400	1.07798100
H	3.92339600	-5.28866200	-0.43701800
H	4.44333800	-2.88784700	0.39773400
H	3.55202400	-3.91908000	1.49351900
C	-0.55172100	-4.24965800	2.20658800
C	-1.53515100	-3.08624700	2.14374000
C	-0.82010900	-1.81093600	2.56198900
H	-1.01841800	-5.17132000	1.85346500
H	-1.91065000	-2.97299900	1.12464000
H	-1.39615800	-0.93886400	2.24168200
N	0.61999800	-3.98220300	1.35068200
H	-0.70116400	-1.75880100	3.65257800
H	-2.38975900	-3.27488500	2.79948100
H	-0.21642900	-4.42674900	3.23831100
C	1.10718900	-2.72832200	1.31007900
N	0.50214000	-1.73611900	1.93831400
C	2.68843900	2.88619100	-0.70611900
O	2.46646600	4.04451400	-1.05931300
C	4.10578400	2.45670000	-0.46536400
C	4.46054800	1.39833200	0.38405900
C	5.11830200	3.19984600	-1.09241800
C	5.80577600	1.09248700	0.59307100
H	3.68466600	0.84629400	0.90306300
C	6.45856200	2.87857400	-0.89735600
H	4.82861100	4.02852000	-1.72954400
C	6.80601600	1.82167100	-0.05207300
H	6.07464000	0.28091000	1.26420200
H	7.23274000	3.45340600	-1.39797600
H	7.85179000	1.57237700	0.10693800
C	1.52709600	1.92023800	-0.53448100
H	1.55243700	1.39368300	0.69678800
H	-0.78318100	0.69861700	-2.22340200
N	0.29846100	2.60140800	-0.90544800
H	0.51930100	3.33315400	-1.57557500
C	-0.71192100	3.02165500	-0.04009900
C	-1.59082400	4.03421000	-0.48582200

C	-0.96530700	2.45704500	1.22457900
C	-2.64699400	4.47342900	0.30307600
H	-1.42484500	4.48426400	-1.46197900
C	-2.03344400	2.91333200	2.00171600
H	-0.30641000	1.68722200	1.61038900
C	-2.89547300	3.92676600	1.57267200
H	-3.28730100	5.26979100	-0.07167900
H	-2.19049300	2.46421400	2.98073500
C	-4.01484400	4.44316400	2.44649000
H	-4.28766200	3.71575900	3.21752800
H	-3.73307600	5.37050400	2.96217000
H	-4.91583900	4.66595600	1.86375700
C	-3.83721900	0.13450800	0.15970100
O	-3.45164000	-0.97166300	0.53579400
H	-3.15422900	0.99147700	0.04970800
N	-5.12182800	0.44658600	-0.15519300
C	-6.16930600	-0.55461200	-0.05551300
H	-5.72119600	-1.47732800	0.31238800
H	-6.95292300	-0.22566200	0.63772500
H	-6.63038300	-0.73589200	-1.03441400
C	-5.49226000	1.78001900	-0.59581500
H	-6.24869900	2.21195900	0.07107600
H	-4.61386700	2.42895200	-0.58716400
H	-5.90559200	1.75639600	-1.61204400
C	-1.04608200	-1.37819300	-1.73977000
O	-0.64814600	-2.44376400	-1.30893800
O	-2.17908000	-1.24931200	-2.46137900
C	-2.97511100	-2.44508000	-2.61765200
C	-4.09735100	-2.12051300	-3.58505600
H	-3.35479000	-2.73098700	-1.63190900
H	-2.33591300	-3.25295700	-2.98543000
H	-4.73449100	-2.99928200	-3.72646200
H	-4.71661700	-1.30357200	-3.20302900
H	-3.70055900	-1.82266800	-4.55979800
N	1.08572900	-0.18766700	-1.62809900
N	1.87132000	0.69170400	-1.21764800
C	-0.39410700	-0.03099600	-1.51291600
H	-0.69232200	0.29791500	-0.50960900
O	1.60058800	0.63004600	1.75582600
H	0.95849500	-0.76097700	1.90012100
H	1.75730000	1.17272300	2.54007000

Int4w

C	4.18854100	-2.96791100	0.43463300
---	------------	-------------	------------

C	3. 51534600	-3. 09607200	-0. 93605200
C	3. 63922100	-0. 19951600	-0. 69498300
C	4. 20784400	-2. 30074500	-2. 05271200
C	4. 66413600	-0. 90786300	-1. 59505200
H	5. 28270500	-2. 99661900	0. 33973300
H	2. 60541300	-0. 39672700	-1. 00868500
H	2. 46934300	-2. 80028000	-0. 82095200
H	3. 51407000	-2. 20298300	-2. 89575800
H	3. 90545900	-3. 82891200	1. 04152700
H	3. 50632500	-4. 15938900	-1. 20101700
H	3. 76219400	0. 88263000	-0. 76004400
H	5. 07474500	-2. 85738800	-2. 42886500
H	4. 84712500	-0. 27727000	-2. 47117300
H	5. 62740700	-0. 97335300	-1. 07380900
C	3. 54978300	-2. 08079000	2. 67308600
C	2. 71311300	-0. 99187600	3. 33153300
C	3. 33491300	0. 36542400	3. 03722600
H	3. 00344200	-3. 02561800	2. 70534400
H	1. 70525600	-1. 02413700	2. 91019400
H	2. 68837100	1. 18811400	3. 35070300
N	3. 80460400	-1. 78783200	1. 24462800
H	4. 29913000	0. 48307100	3. 54940300
H	2. 65692700	-1. 17531800	4. 40821300
H	4. 50977600	-2. 21823800	3. 18920800
C	3. 67117400	-0. 54238900	0. 77794000
N	3. 52441500	0. 48975900	1. 59453100
C	-1. 00484100	3. 09772200	-1. 21651400
O	-2. 07868800	3. 69778700	-1. 42593800
C	0. 25421900	3. 68763400	-1. 79569800
C	1. 25564700	2. 93800300	-2. 43227900
C	0. 38267600	5. 08529900	-1. 75820400
C	2. 37181800	3. 57065500	-2. 98644600
H	1. 15259300	1. 86143600	-2. 49862700
C	1. 50502200	5. 71444400	-2. 29168100
H	-0. 41537500	5. 66214300	-1. 30289700
C	2. 50725500	4. 95815300	-2. 90666500
H	3. 13164800	2. 97897200	-3. 49073200
H	1. 59627000	6. 79566200	-2. 23706700
H	3. 37838100	5. 44795400	-3. 33289100
C	-1. 00065000	1. 85345600	-0. 47303700
H	1. 51843500	2. 22270400	0. 22924100
H	-1. 19278600	-0. 97926400	-0. 73150100
N	-2. 30727600	1. 41671200	-0. 08507700
H	-2. 96832800	1. 91026800	-0. 68302000

C	-2.71692700	1.50789200	1.26406800
C	-4.09187000	1.44700000	1.56078900
C	-1.81499300	1.61403200	2.33387200
C	-4.54129000	1.49674800	2.87366700
H	-4.80667500	1.36714300	0.74512800
C	-2.28551800	1.65290400	3.64843200
H	-0.75086000	1.67388900	2.13835400
C	-3.64785700	1.59622500	3.95207900
H	-5.61130400	1.45850000	3.06695800
H	-1.56473500	1.74084300	4.45878400
C	-4.14663700	1.63265600	5.37757400
H	-3.33111400	1.83584600	6.07806800
H	-4.90716400	2.40919900	5.52049900
H	-4.60422200	0.68019300	5.67390900
C	-3.37959700	-3.08216700	-2.29786100
O	-3.19453700	-4.24654000	-2.63724000
H	-2.91927600	-2.65398900	-1.39130600
N	-4.15247700	-2.18305900	-2.96709300
C	-4.84980400	-2.57800300	-4.17859200
H	-4.62070500	-3.62562900	-4.37312300
H	-5.93351300	-2.45526600	-4.06006700
H	-4.52562700	-1.96699800	-5.03002600
C	-4.31239800	-0.81597000	-2.50461100
H	-5.36064800	-0.60475400	-2.25638600
H	-3.70176300	-0.64244200	-1.61512400
H	-3.99680100	-0.10491300	-3.27811300
C	-0.25717300	-2.29977400	0.64149100
O	0.82890000	-2.63432100	1.07857600
O	-1.27973400	-3.16475400	0.45246600
C	-1.05916900	-4.56517300	0.75492600
C	-0.65317900	-5.32764200	-0.49603000
H	-2.01979700	-4.91746800	1.13834200
H	-0.30561800	-4.63709800	1.54217900
H	-0.57396400	-6.39611700	-0.26667100
H	-1.39668000	-5.19162000	-1.28709700
H	0.32172300	-4.98529900	-0.85683200
N	0.39969900	0.04029100	0.24806800
N	0.16311400	1.24227000	-0.19709600
C	-0.71246900	-0.90546900	0.25592900
H	-1.52735700	-0.64947800	0.94763600
O	2.33925800	2.67108700	0.60223200
H	3.20829300	1.38823500	1.16154800
H	2.60512800	3.30537100	-0.07468700

TS5w

C	-5.81552200	1.38949600	0.44096300
C	-5.73710600	2.22007900	1.72688700
C	-2.98876200	2.47227200	0.79158100
C	-5.16171300	3.63121800	1.52674900
C	-3.95864000	3.64621100	0.57254200
H	-6.16687000	2.01161400	-0.39644800
H	-2.87273700	2.26326000	1.86224800
H	-5.15261700	1.66135100	2.46677200
H	-4.86551500	4.03423200	2.50294400
H	-6.56864500	0.60996200	0.58088500
H	-6.75134100	2.29497300	2.13648000
H	-1.99908500	2.75867200	0.43753700
H	-5.94205400	4.29893900	1.14003900
H	-3.39973400	4.57886700	0.70141100
H	-4.29891300	3.64873400	-0.47103900
C	-4.84563500	-0.60104600	-0.67000800
C	-3.61875000	-1.50281300	-0.66587800
C	-2.42853100	-0.71409800	-1.18604100
H	-5.68481500	-1.09357600	-0.16953400
H	-3.41701900	-1.84866400	0.35429000
H	-1.49733900	-1.26143000	-1.03882800
N	-4.58759000	0.66669300	0.04628900
H	-2.52791800	-0.53141500	-2.26390700
H	-3.78755700	-2.38326200	-1.29090200
H	-5.16264800	-0.38047900	-1.70011500
C	-3.32448500	1.17549600	0.07636800
N	-2.30714700	0.56592300	-0.48343200
C	1.59109100	-2.29991100	0.90388500
O	2.42174200	-3.12497400	0.47925500
C	0.55124900	-2.75260400	1.89034400
C	-0.03634800	-1.89770400	2.83815100
C	0.23298700	-4.12061700	1.92258600
C	-0.92808200	-2.40367300	3.78570200
H	0.20874500	-0.84330000	2.83650900
C	-0.67334700	-4.62169400	2.85662500
H	0.71675000	-4.78338300	1.21285000
C	-1.25684000	-3.76266700	3.79322700
H	-1.36331900	-1.73367800	4.52196900
H	-0.91687100	-5.68053800	2.86096700
H	-1.95473200	-4.15135500	4.52999500
C	1.64331400	-0.91966500	0.38849900
H	-1.16396300	0.88932600	-0.29455600
N	2.85838800	-0.57059700	-0.27559400

H	3.29686400	-1.42178100	-0.61784900
C	3.80212600	0.28205900	0.34305800
C	5.12329500	0.30009800	-0.14372400
C	3.46898700	1.15064800	1.39325800
C	6.07380900	1.15225900	0.40996000
H	5.39992000	-0.36458300	-0.95894600
C	4.43681200	2.00489300	1.93285500
H	2.46466300	1.16599600	1.80263200
C	5.75285500	2.02883300	1.46033200
H	7.08842500	1.13444800	0.01725300
H	4.14773800	2.66199800	2.74978400
C	6.79028100	2.96155600	2.04348600
H	7.70507800	2.42418300	2.32011700
H	7.07883800	3.74327600	1.32906600
H	6.41315100	3.45989500	2.94177500
C	-0.38583900	-3.91880500	-2.26868400
O	-1.52029000	-3.60418700	-2.62906600
H	0.12668300	-3.40677600	-1.43742200
N	0.37456500	-4.90177700	-2.81607900
C	-0.12528000	-5.69269100	-3.92970900
H	-1.12928500	-5.34798000	-4.17788000
H	0.52715700	-5.57811800	-4.80426600
H	-0.15961900	-6.75534600	-3.65939300
C	1.71319200	-5.19475800	-2.32130100
H	2.45755600	-5.04090500	-3.11280800
H	1.95601500	-4.54309800	-1.47827800
H	1.77805000	-6.23776300	-1.98715800
C	0.54987800	2.91885400	-1.48956400
O	-0.16604600	3.61120200	-0.78770200
O	1.03155400	3.32838800	-2.68074200
C	0.70630900	4.68126500	-3.08836100
C	1.38398700	4.93223000	-4.42203200
H	1.05409200	5.37147200	-2.31362800
H	-0.38217700	4.77314300	-3.15600900
H	1.16075000	5.94891900	-4.76229400
H	2.46964000	4.82848800	-4.33539200
H	1.02912800	4.22910600	-5.18162900
N	0.21789900	0.92712200	-0.11750000
N	0.52779100	-0.23151300	0.43866700
C	1.06229900	1.53238200	-1.15351400
H	1.09427200	0.93462500	-2.07406100
H	2.10521500	1.65926100	-0.84052200
O	0.15163000	2.63337100	2.32248700
H	0.12505300	2.07182200	1.52033600

H	0.23938500	3.52687800	1.96725600
---	------------	------------	------------