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Supporting Information for

Theoretical study on mechanism of NHC-catalyzed oxidative *N* vs *O* chemoselective acylation of aldehydes with alkanolamines.

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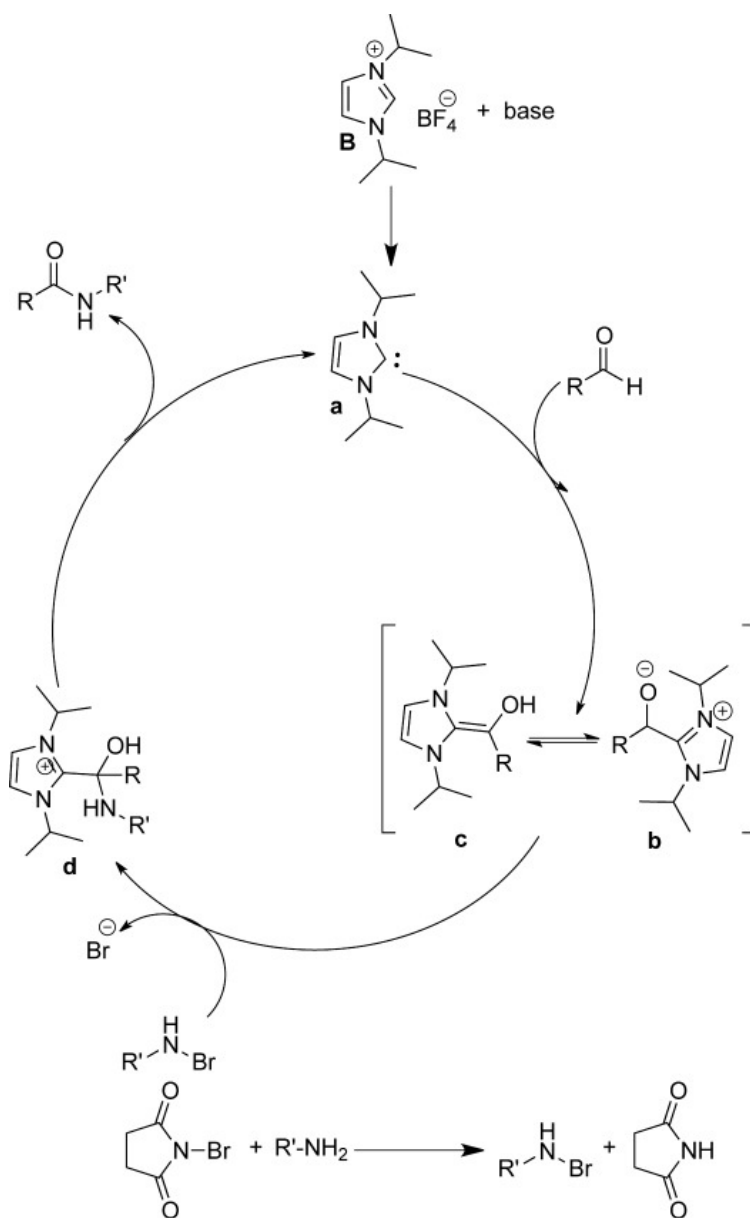
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Table of Content

Part 1: A plausible mechanism proposed Maheswari and coworkers.....	S2
Part 2: Deprotonation pathways of precursor NHC·H⁺	S3
Part 3: The possible channels for the formation of bromoamine intermediates.....	S5
Part 4: Another path of generating PR1 from intermediates M1 and M2	S14
Part 5: The two paths of generating PR2 from intermediates M1 and M2'	S15
Part 6: The AIM analysis details of TS3b and TS3b'	S17
Part 7: The AIM analysis details of TS5 and TS5'	S18
Part 8: List of Cartesian coordinates of all structures involved in this work.....	S19

Part 1. Plausible mechanism



Scheme S1 A plausible mechanism proposed Maheswari and coworkers.

Part 2: Deprotonation pathways of precursor NHC·H⁺

We have calculated Et₃N-assisted directly deprotonation process of the pre catalyst, and found that the generation of active NHC is impossible. We also considered 3Et₃N-, 2Et₃N-, CH₃CN-, BF₄⁻-H₂O-, BF₄⁻-, 2H₂O-, and H₂O-CH₃CN-assisted deprotonation, whereas the relative Gibbs energies of product NHC are higher than those of the corresponding transition states in the range of 2.4-6.5 kcal/mol except the H₂O-CH₃CN-assisted case with lower of 0.2 kcal/mol (Figure S2). Moreover, the above reactions are all endothermic processes.

Thereby, we considered one molecule of Et₃N and one molecule of water assisted deprotonation of the pre catalyst. Although the reverse energy barrier of this process is smaller than the forward energy barrier, considering reversible reaction equilibrium and the relative Gibbs energy of the formation of NHC is 1 kcal/mol lower than that of the **TS0**, there may be activated catalysts exist in the system for subsequent reactions.

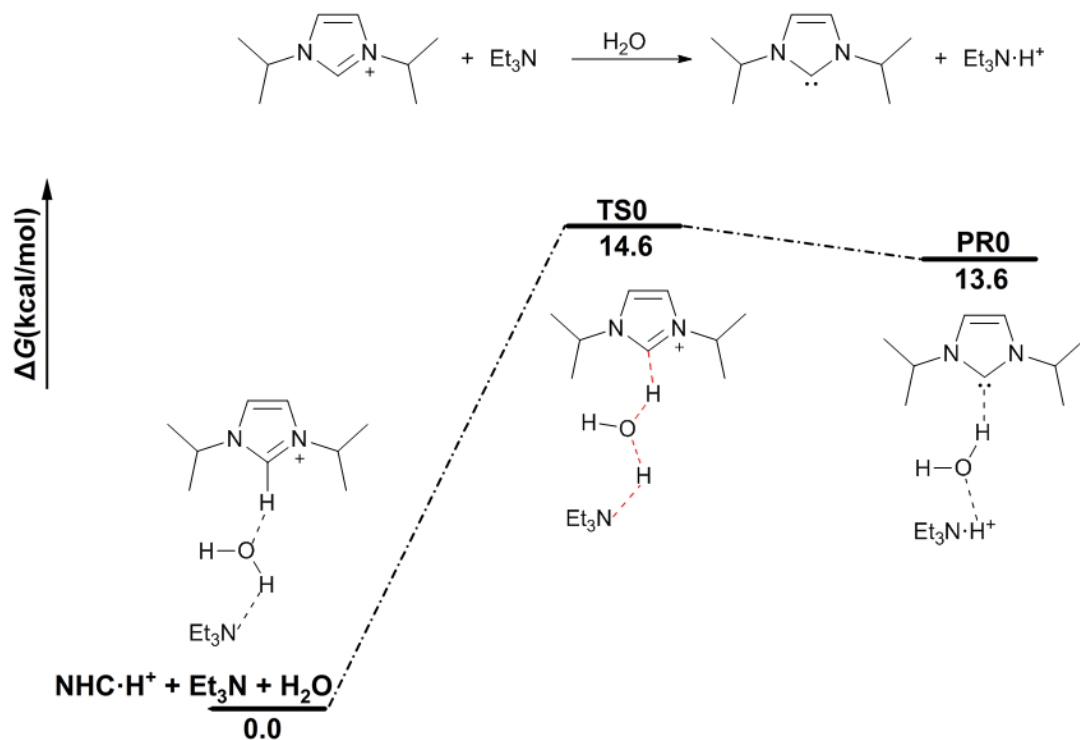


Figure S1 Free energy profile for Et₃N and H₂O assisted deprotonation pathways of precursor NHC·H⁺, relative free energies are in kcal/mol.

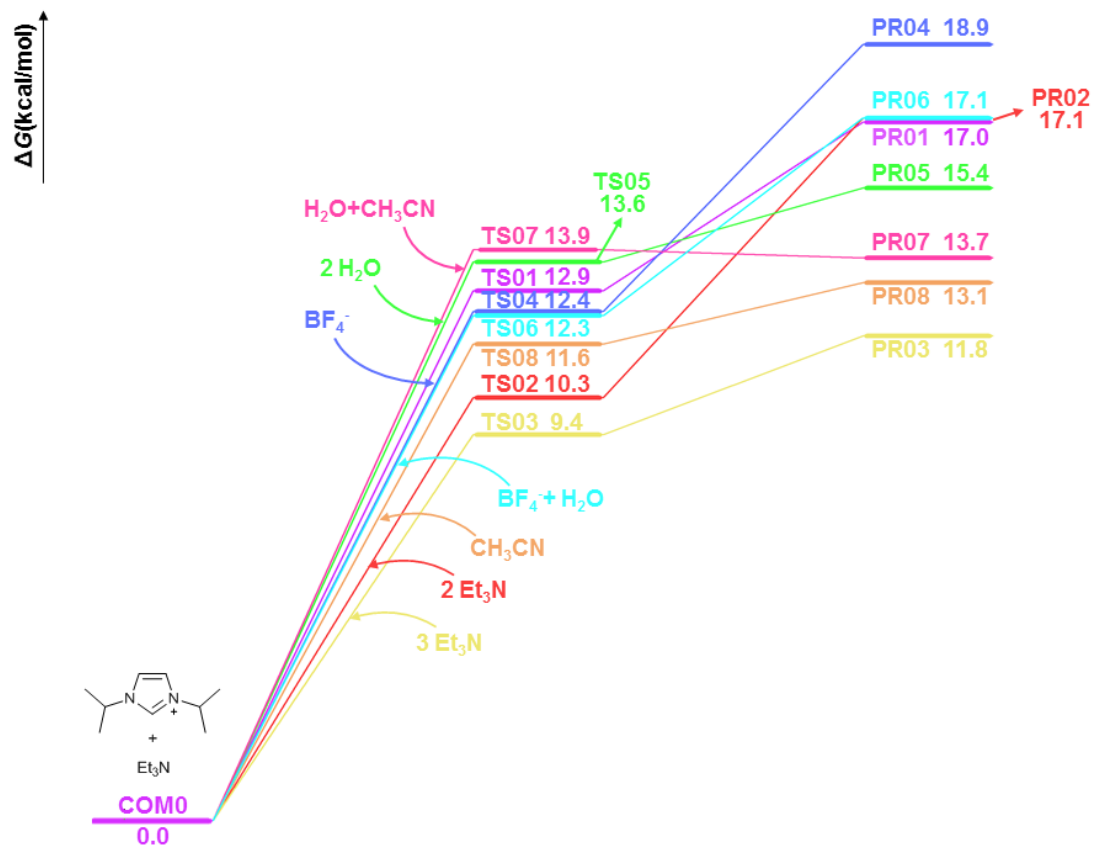


Figure S2 Free energy profile for different pathways for deprotonation of precursor NHC·H⁺.

Part 3: Formation of bromoamine intermediate

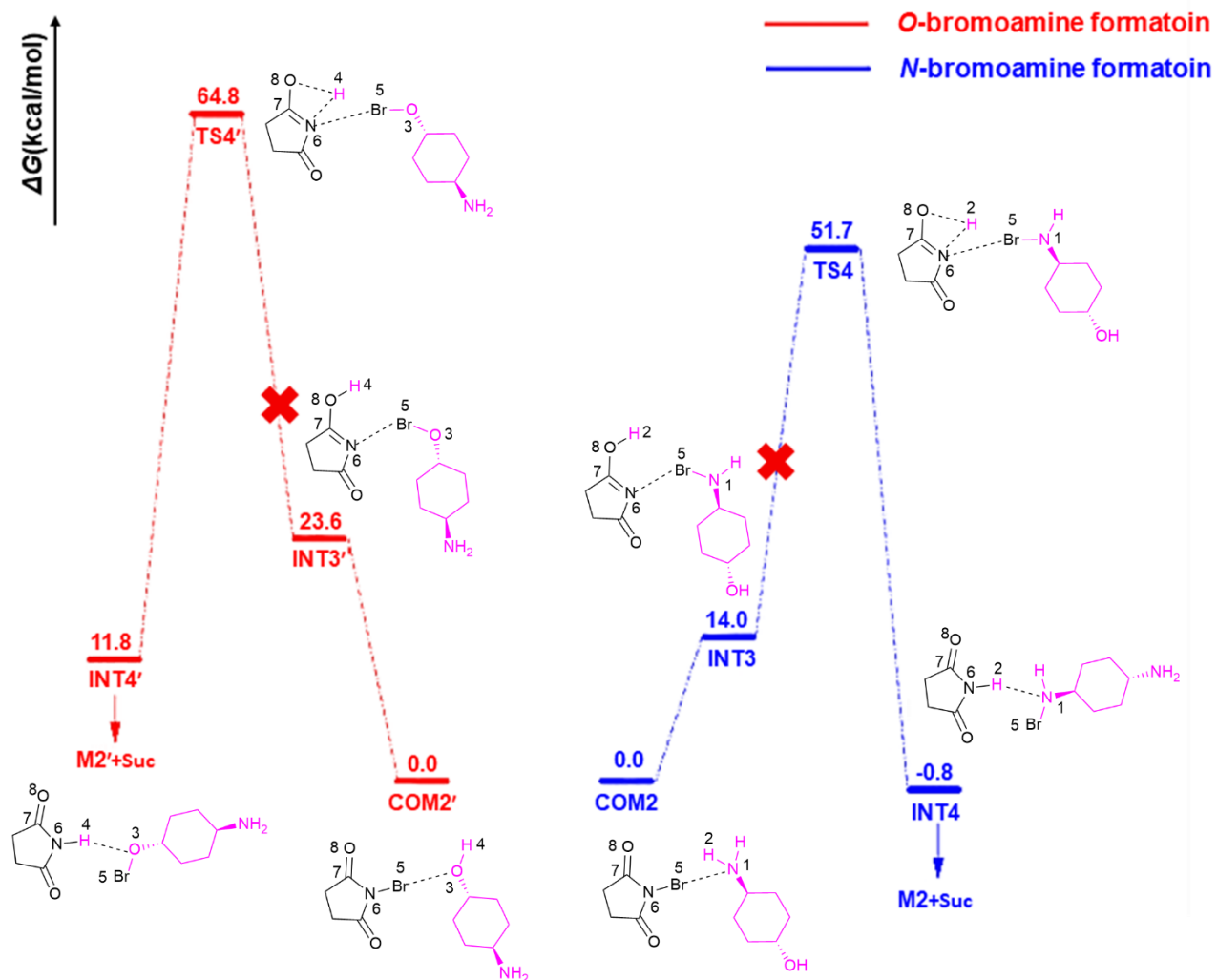
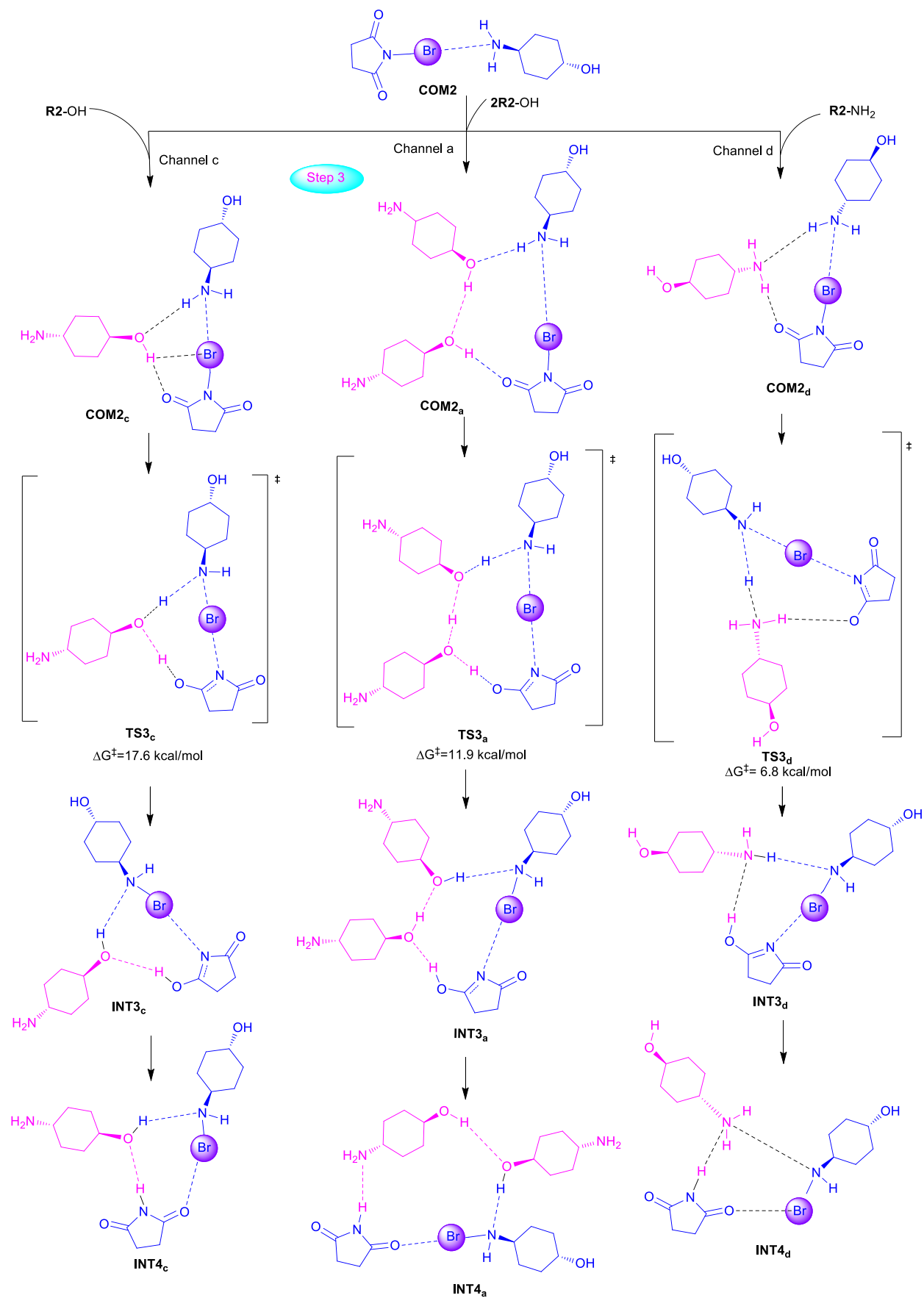
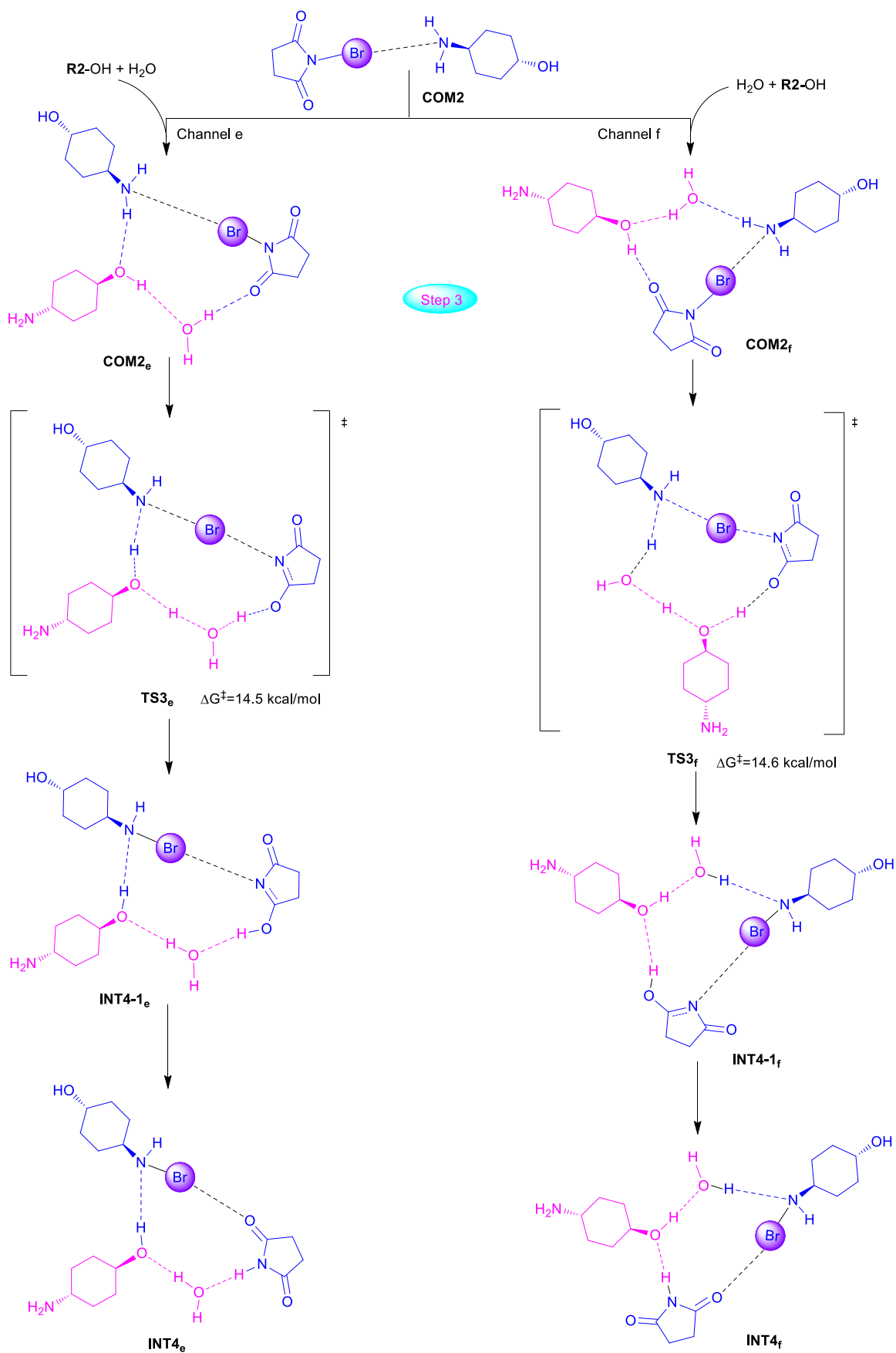


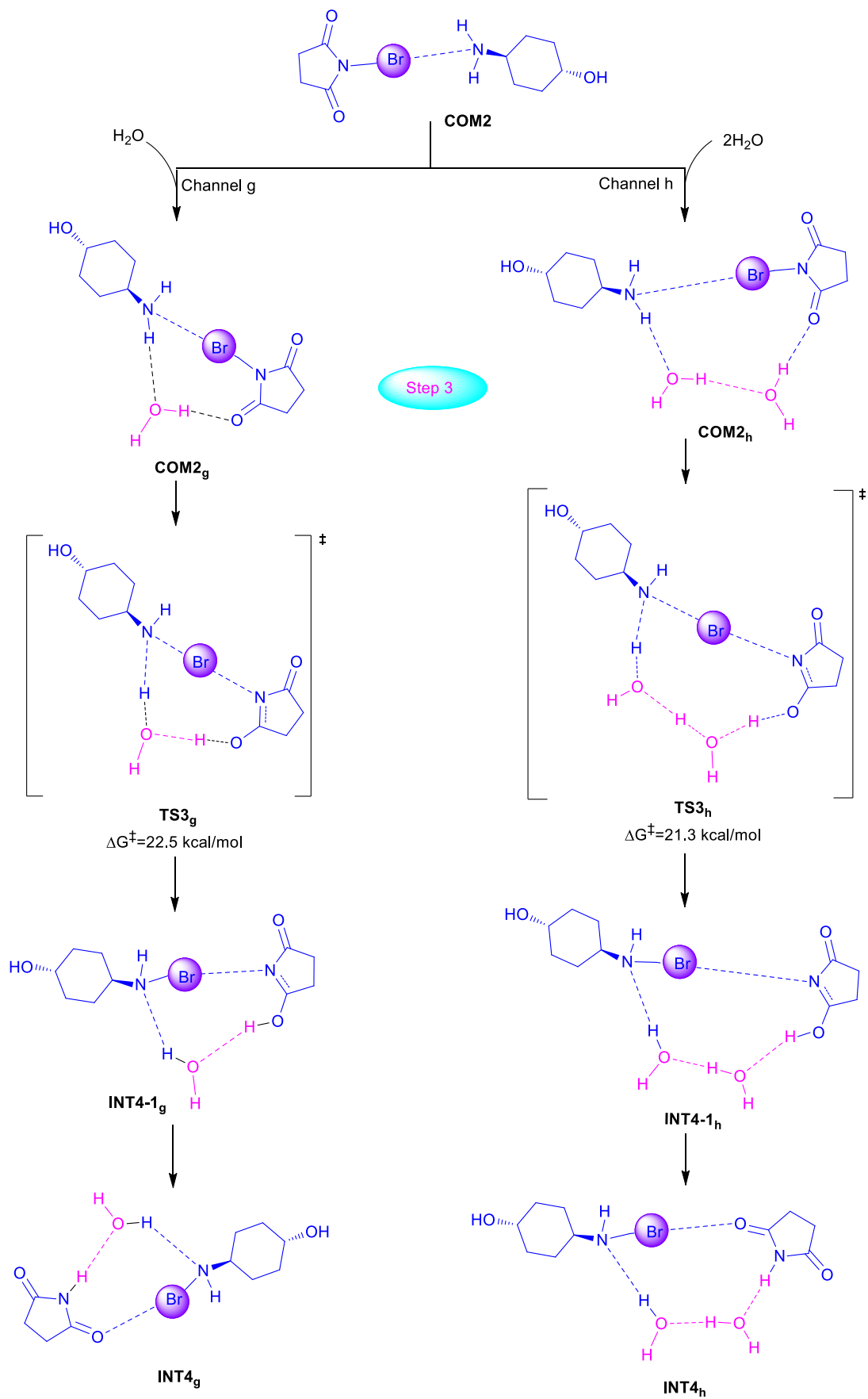
Figure S3 Free energy profile for unassisted bromoamine intermediate formation, relative free energies are in kcal/mol.



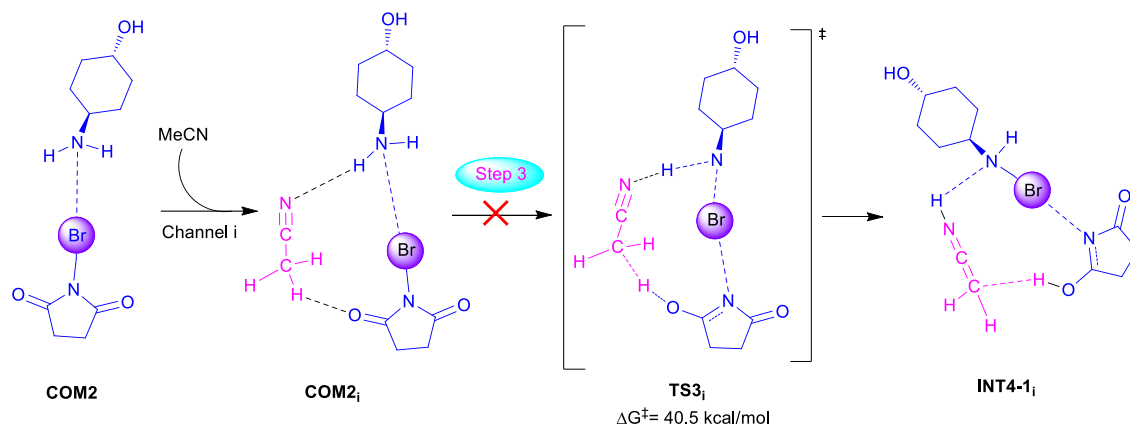
Scheme S2 The possible reaction channels a, c and d for *N*-Bromoamine intermediate formation.



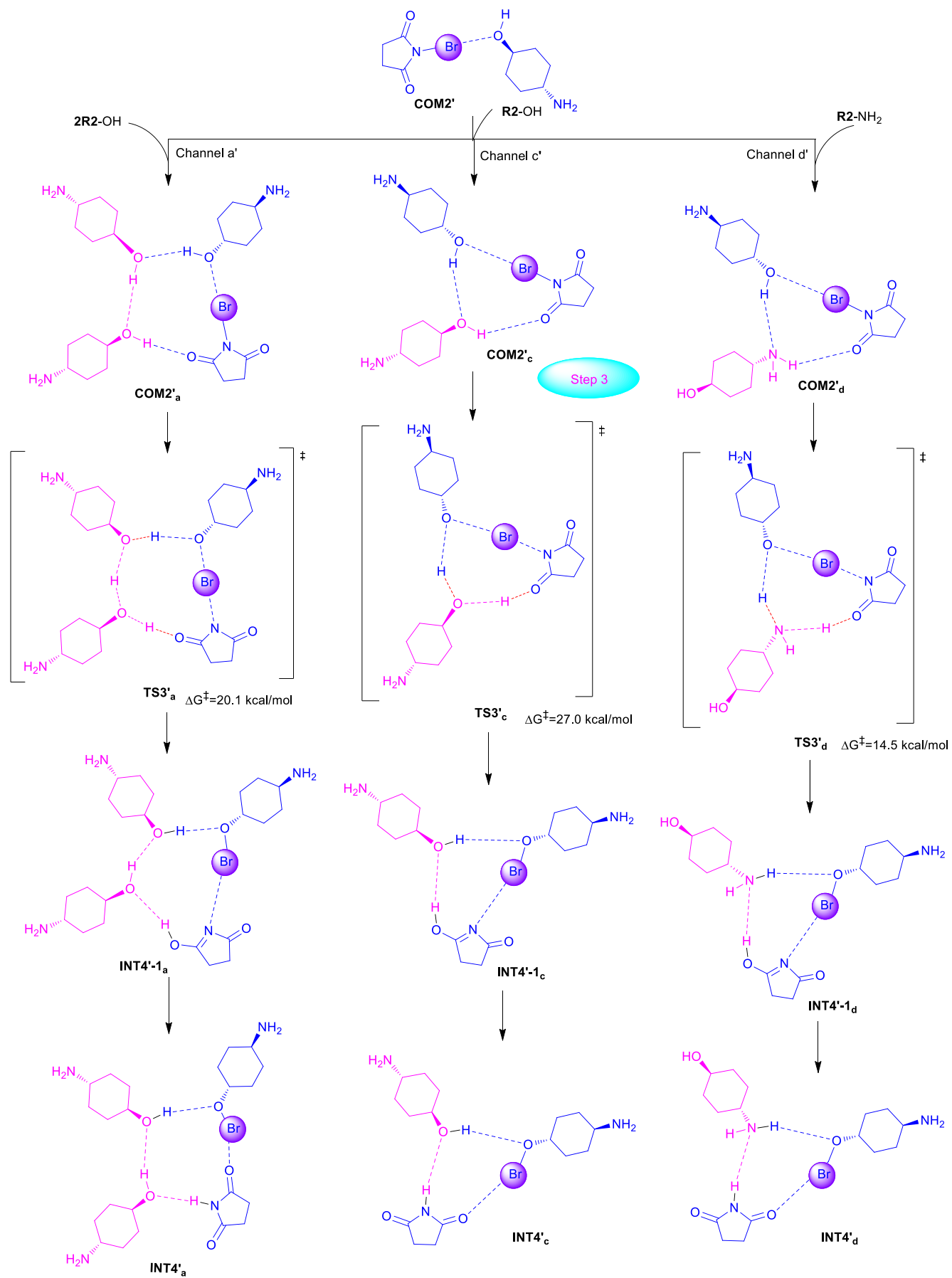
Scheme S3 The possible reaction channels e and f for *N*-Bromoamine intermediate formation.



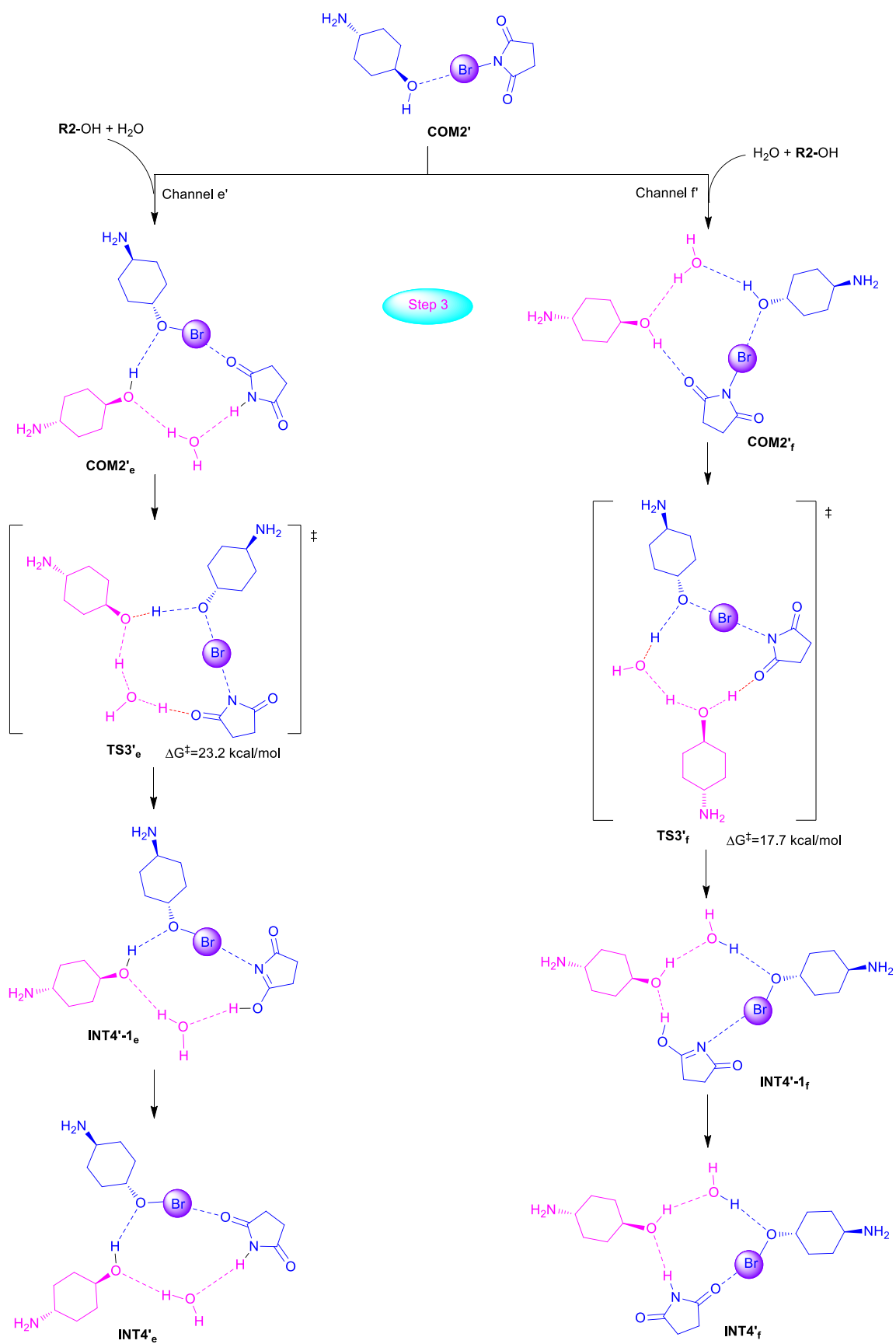
Scheme S4 The possible reaction channels g and h for *N*-Bromoamine intermediate formation.



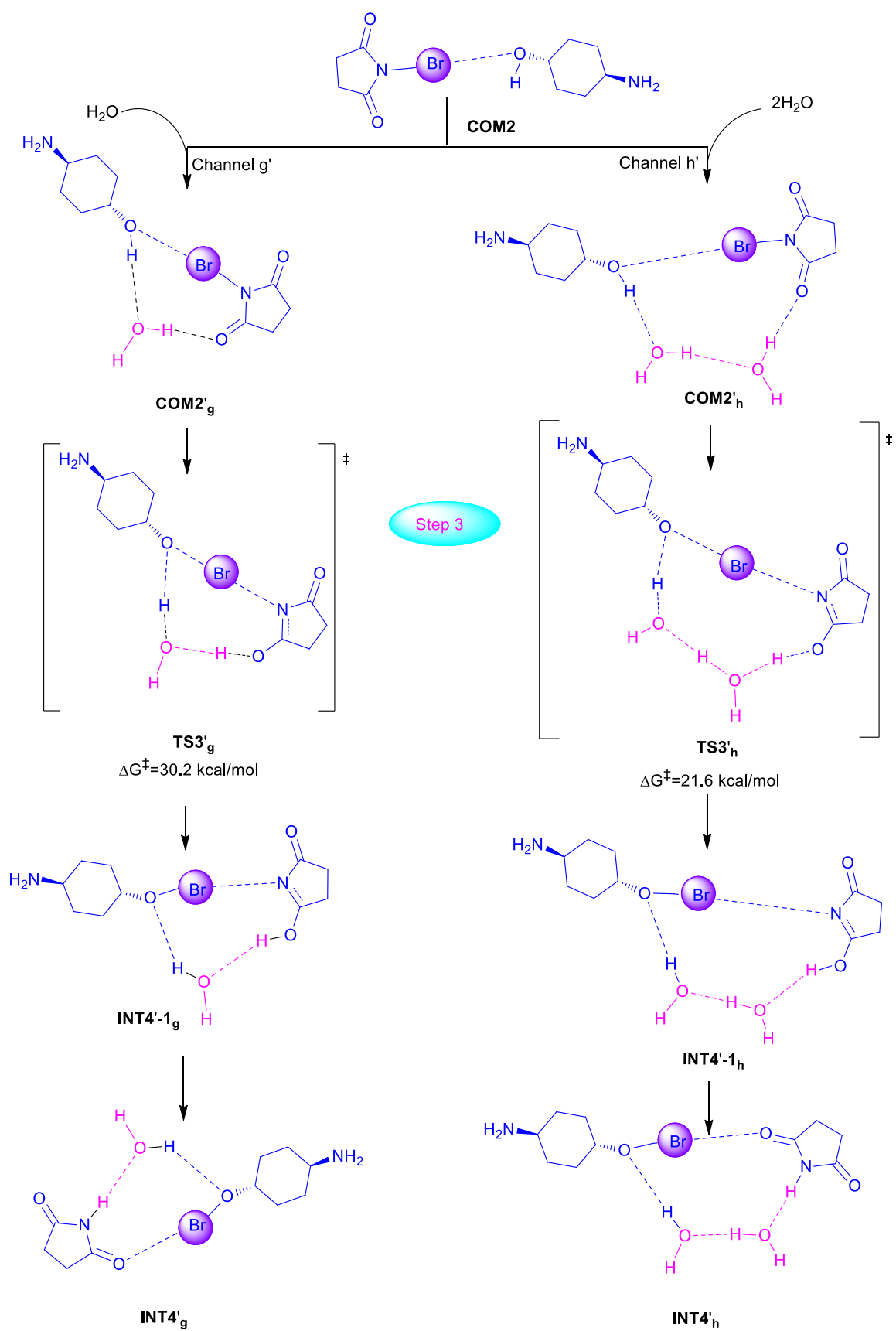
Scheme S5 The possible reaction channel i for *N*-Bromoamine intermediate formation.



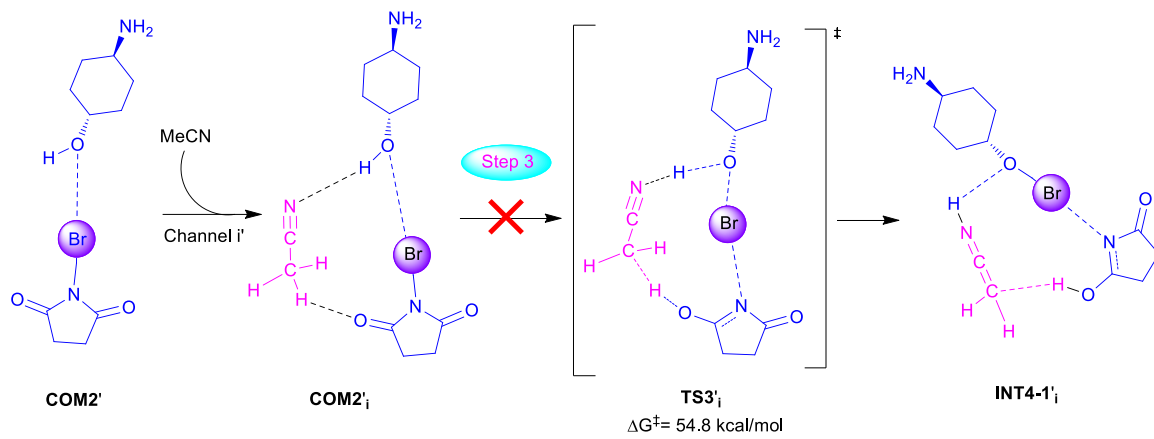
Scheme S6 The possible reaction channel a' and c' for *O*-Bromoamine intermediate formation.



Scheme S7 The possible reaction channel e' and f' for *O*-Bromoamine intermediate formation.

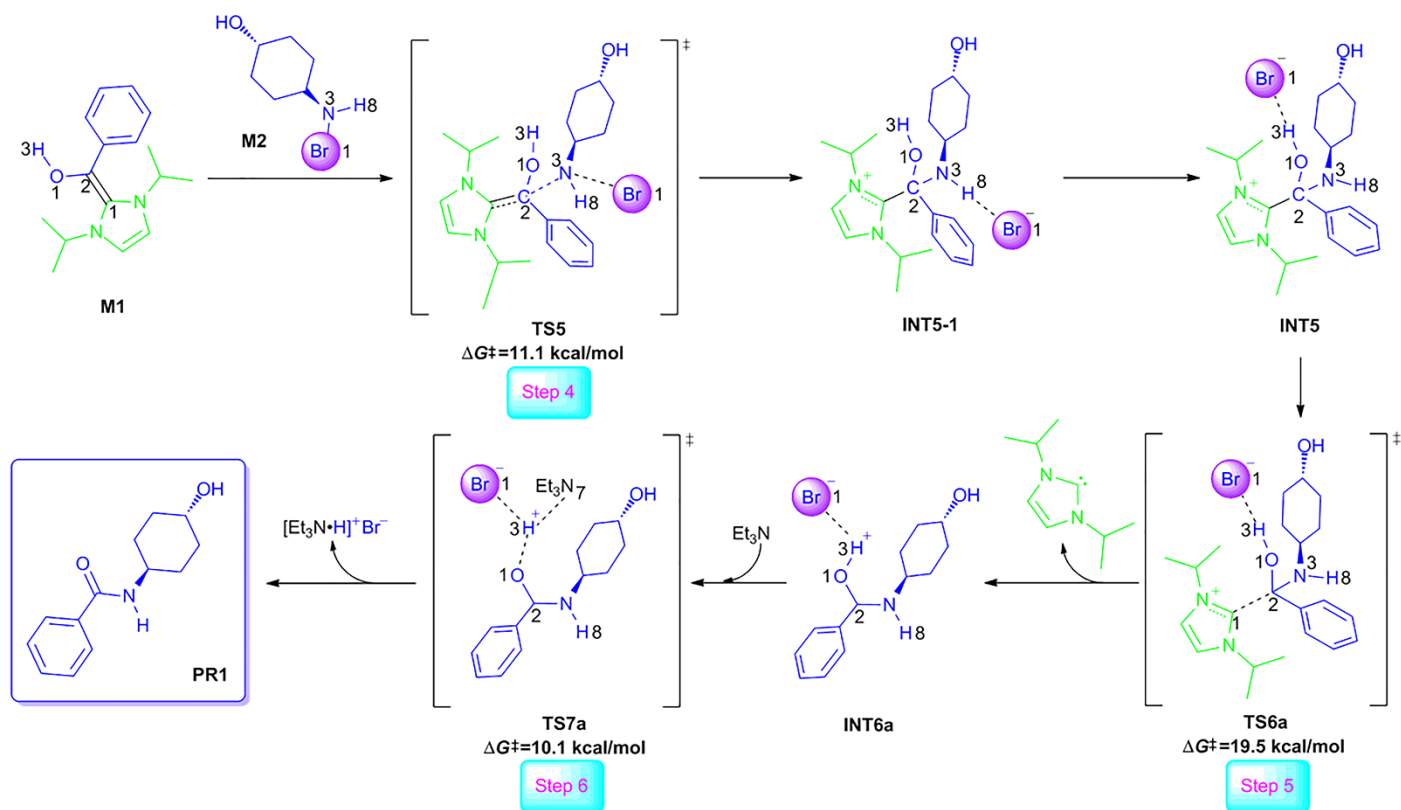


Scheme S8 The possible reaction channels g' and h' for *O*-Bromoamine intermediate formation.



Scheme S9 The possible reaction channel *i'* for *O*-Bromoamine intermediate formation.

Part 4: Another process of generating PR1 from intermediates M1 and M2



Scheme S10 The process of first removing NHC and then removing HBr to generate the main product.

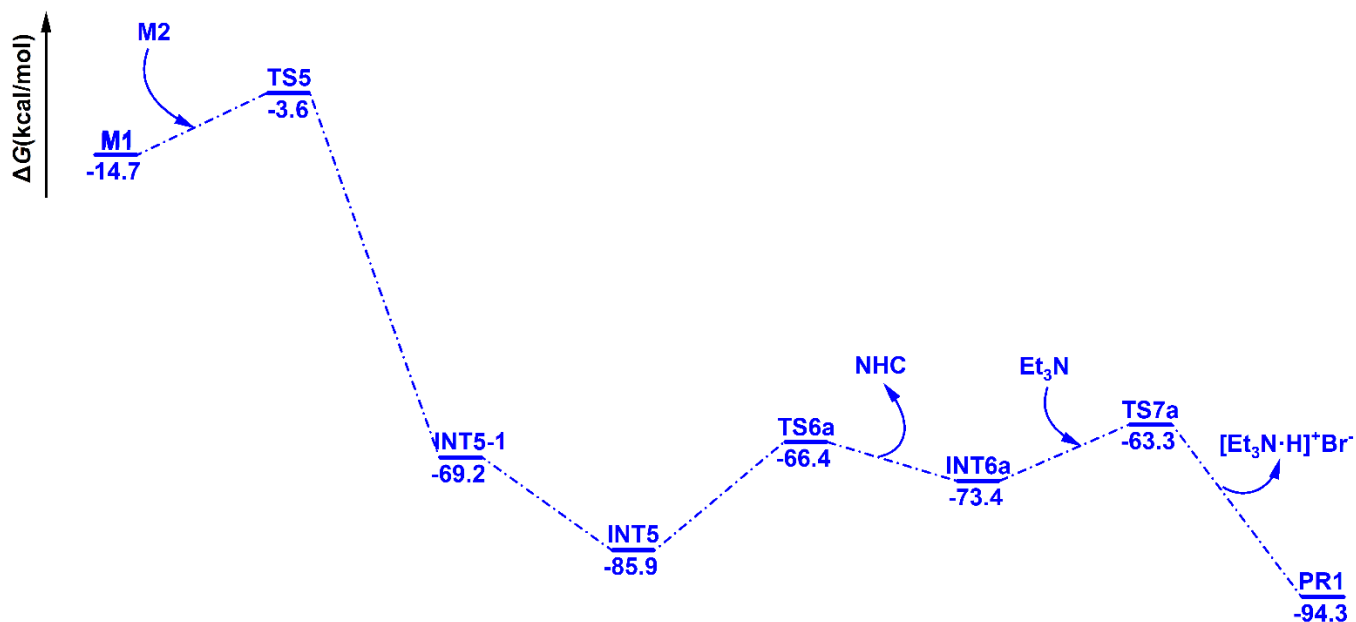
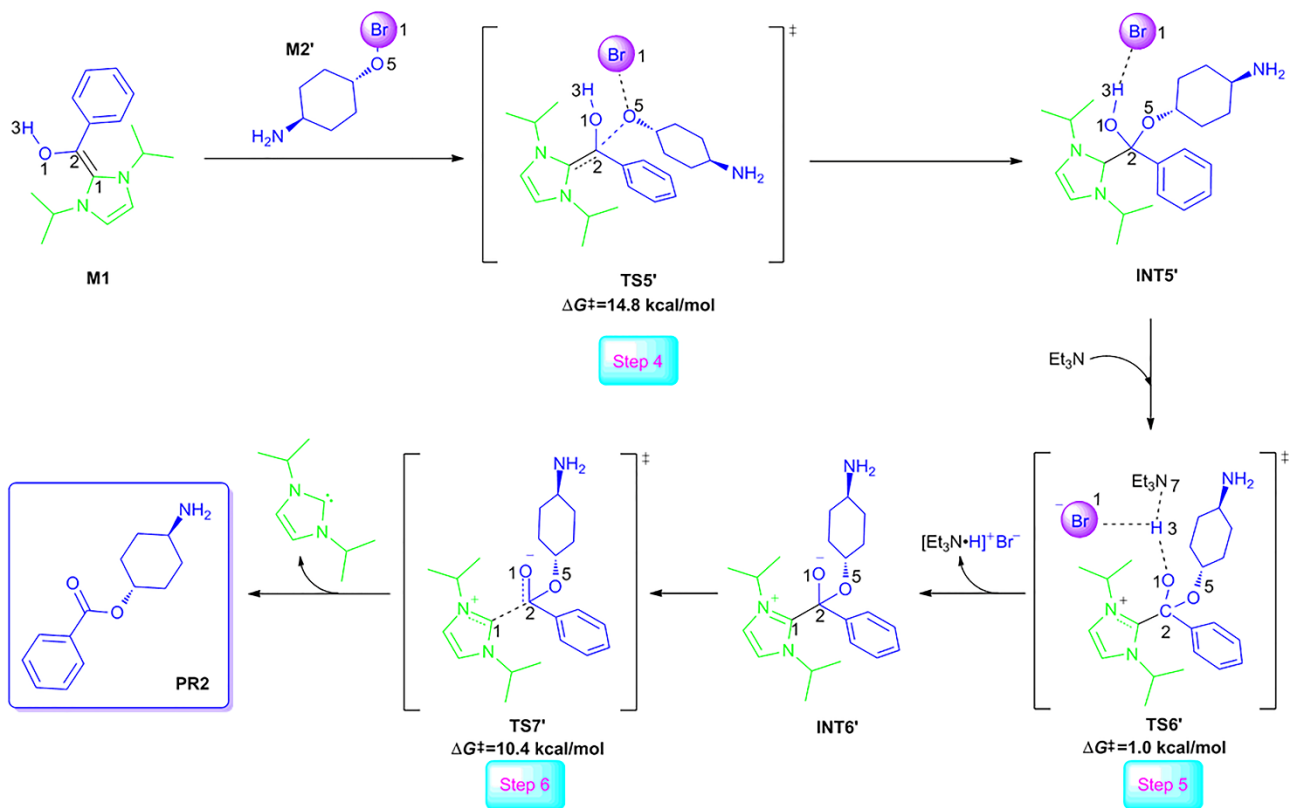


Fig. S4 Free energy profile for the PR1 formation. The relative free energies are in kcal/mol.

Part 5: The process of generating PR2 from intermediates M1 and M2'



Scheme S11 The process of removing HBr and then removing NHC to generate PR2.

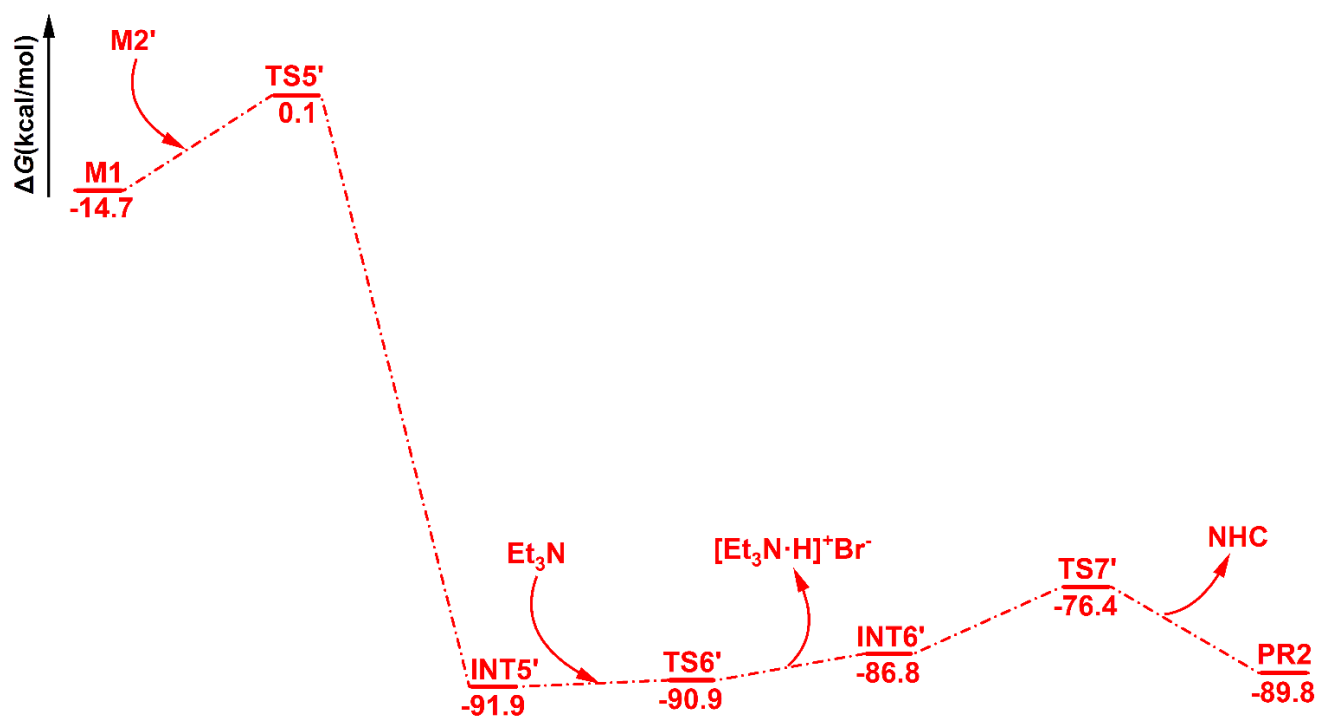
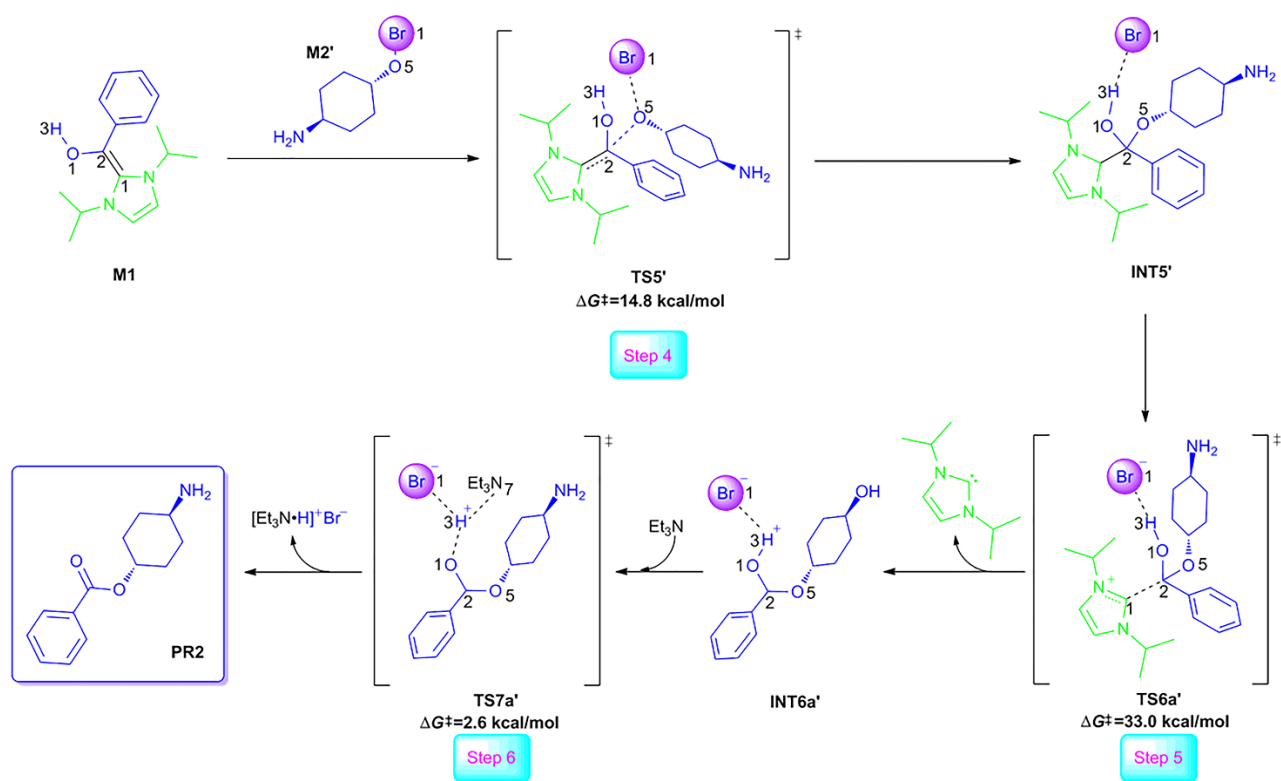


Fig. S5 Free energy profile for removing HBr and then removing NHC to generate PR2. The relative free energies are in kcal/mol.



Scheme S12 The process of removing NHC and then removing HBr to generate **PR2**.

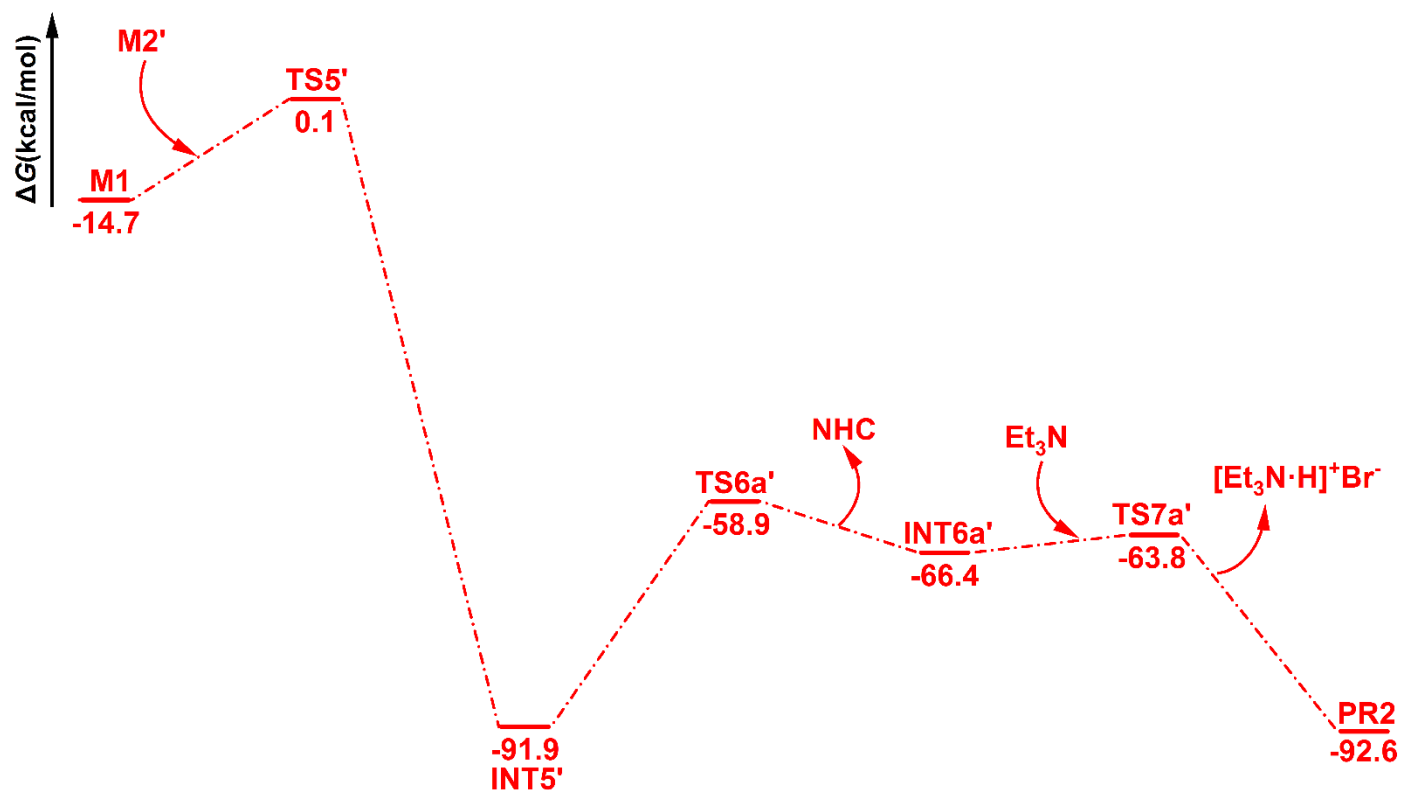


Fig. S6 Free energy profile for removing NHC and then removing HBr to generate **PR2**. The relative free energies are in kcal/mol.

Part 6: The AIM analysis details of TS3_b and TS3'_b

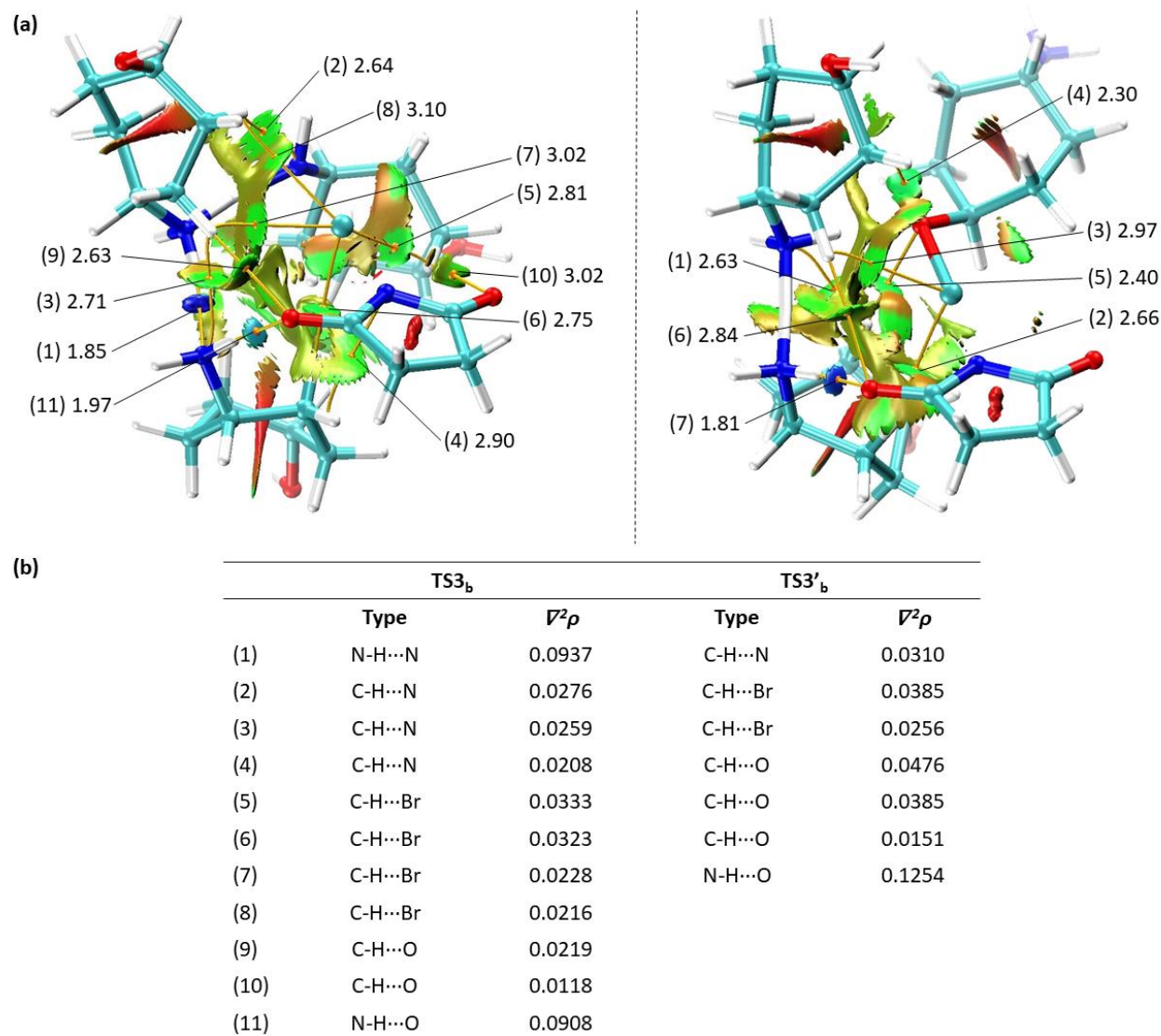


Fig. S7 (a) AIM analyses of the transition states TS3_b and TS3'_b (distance in Å); (b) summary of the Laplacian electron density values.

Part 7: The NCI analysis details of TS5 and TS5'

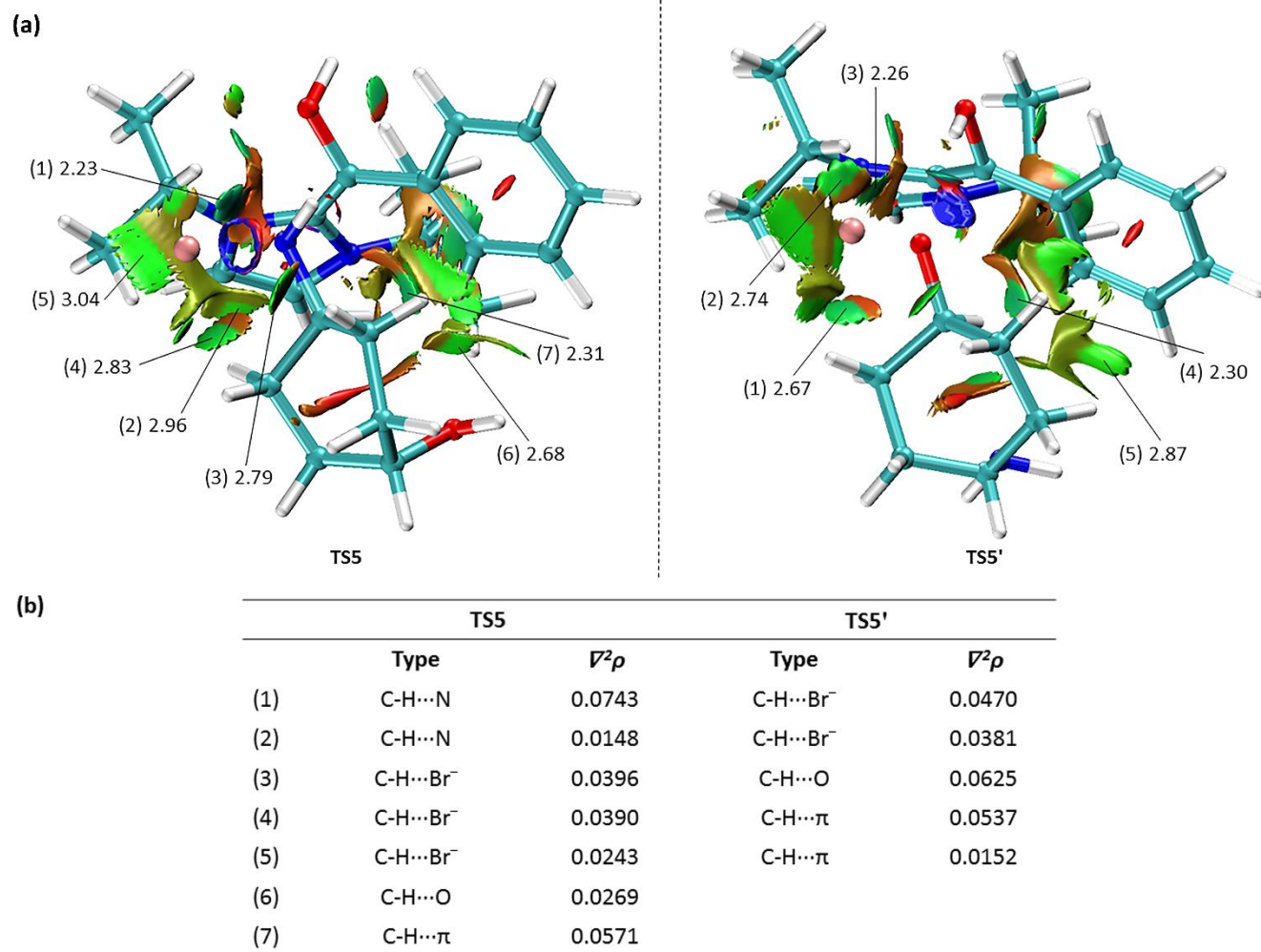


Fig. S8 (a) NCI analyses of the transition states **TS5** and **TS5'** (distance in Å); (b) summary of the Laplacian electron density ($\nabla^2\rho$, a.u.) values from AIM analyses.

Part 8: List of Cartesian coordinates of all structures involved in this work

R1

C	-1.99092200	0.46985100	0.00024800
O	-2.83531200	-0.39652000	-0.00037500
H	-2.28105800	1.54096300	0.00083800
C	-0.52986100	0.21204700	0.00013400
C	-0.04670700	-1.10062900	0.00019100
C	0.35738500	1.28947600	-0.00006400
C	1.32389300	-1.32833600	0.00001500
H	-0.76064300	-1.91891500	0.00022900
C	1.73156400	1.05999600	-0.00008000
H	-0.03064300	2.30570800	0.00005700
C	2.21162000	-0.24850600	-0.00006800
H	1.70676000	-2.34386700	0.00013600
H	2.42425200	1.89525600	-0.00028200
H	3.28200100	-0.43038600	-0.00023400\

R2

C	0.73299600	1.29958300	0.15398700
C	1.43476700	0.08614100	-0.48412600
C	-0.76059100	1.30212100	-0.17017600
C	0.47397200	-1.11452900	-0.58209700
C	-1.45784000	0.09830000	0.47479500
C	-0.50122600	-1.10037600	0.59150900
H	0.87405200	1.24372600	1.24178900
H	-0.09138300	-1.06851800	-1.52028600
H	-0.90747900	1.22556000	-1.25470500
H	1.20575500	2.22887100	-0.18150300
H	1.74084900	0.36550000	-1.50592700
H	-1.24078300	2.23120900	0.14907500
H	1.05599000	-2.04254900	-0.60269500
H	-1.81161700	0.37555800	1.47953700
H	-1.08684500	-2.02620200	0.63977300
H	0.06974000	-1.03415200	1.52546400
N	2.57918100	-0.28420800	0.35402400
H	3.15535400	-0.98151900	-0.10874800
H	3.17056800	0.52292200	0.53348100
O	-2.57808400	-0.19750200	-0.35418500
H	-3.09625500	-0.89836600	0.05669600

Et₃N

N	-0.00034500	-0.00037500	-0.00517400
C	-1.39223500	-0.07325000	0.43861400
C	-2.23898500	-0.99956700	-0.42661300
H	-1.81879500	0.93287100	0.38716600

H	-1.44573600	-0.38019200	1.50149700
H	-3.27407100	-1.01160900	-0.07229800
H	-2.22530300	-0.65455100	-1.46367500
H	-1.87154900	-2.02939800	-0.40896900
C	0.75858400	-1.17046600	0.43615300
C	1.98768300	-1.43488200	-0.42556900
H	0.10164500	-2.04327600	0.37737000
H	1.04689800	-1.06847700	1.50093800
H	1.68650200	-1.58402700	-1.46576500
H	2.69839500	-0.60425900	-0.39554200
H	2.51124700	-2.33048900	-0.07781400
C	0.63328200	1.24108300	0.43829100
C	0.25192200	2.43732900	-0.42586400
H	1.71783400	1.10764000	0.38428200
H	0.39668900	1.44060300	1.50183000
H	0.76416700	3.33902700	-0.07705500
H	0.53596000	2.24985100	-1.46464000
H	-0.82296800	2.63743100	-0.40117200

NHC H⁺

C	0.54982700	-1.31413700	-0.83760200
C	-0.79687900	-1.21469900	-0.65833700
C	0.14028300	0.59125900	0.17604800
N	1.11706600	-0.17487000	-0.31243000
H	1.14524000	-2.08885800	-1.29609500
H	-1.59390900	-1.88713400	-0.93415800
N	-1.02974200	-0.01675700	-0.02154600
C	2.58179400	0.08902400	-0.25415700
C	3.13088376	0.18617666	-1.67406810
C	3.28661993	-0.97263395	0.57665982
H	2.66606631	1.05724525	0.24904650
H	2.61987414	0.95835139	-2.25422031
H	4.19281760	0.43893178	-1.63476651
H	3.02361569	-0.77165860	-2.19186315
H	2.85190707	-1.06715566	1.57533549
H	3.27756525	-1.94660855	0.07662011
H	4.33257779	-0.68289031	0.69367413
C	-2.36021600	0.52689600	0.36049600
C	-3.06009600	-0.44501300	1.30267700
C	-3.16786700	0.83256500	-0.89550600
H	-2.13609300	1.45701700	0.89197800
H	-2.44111600	-0.67717600	2.17239800
H	-3.99260500	0.00366000	1.65188700
H	-3.31426400	-1.37748700	0.78973700
H	-2.63507100	1.52063600	-1.55610900
H	-3.39381400	-0.08412400	-1.44847200
H	-4.11666000	1.29204000	-0.60955600

TS0

C	3.60633600	0.54093400	0.26904400
C	2.87012900	1.68478600	0.32662000
C	1.46973900	0.00194000	-0.21423500
N	2.72365400	-0.47412300	-0.06226800
H	4.65875200	0.37409700	0.43414200
H	3.16954000	2.69938600	0.54829000
N	1.57337100	1.33004500	0.03223400
C	3.08641400	-1.88982700	-0.21786700
C	3.59817900	-2.45272600	1.11011700
C	4.09259000	-2.06214200	-1.35435400
H	2.14273500	-2.38523700	-0.48425600
H	2.85433400	-2.31484200	1.90247600
H	3.80475500	-3.51693900	1.00195200
H	4.52591500	-1.95333800	1.41162600
H	3.70670200	-1.63089100	-2.28339900
H	5.04167800	-1.57409400	-1.10582600
H	4.29442100	-3.11754100	-1.51257400
C	0.42445500	2.24036900	-0.05878200
C	0.52709300	3.09671300	-1.31745200
C	0.29977700	3.08137900	1.20733600
H	-0.43796800	1.57812600	-0.14861100
H	0.59632400	2.47031700	-2.21119200
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H	1.41065900	3.74498000	-1.27747000
H	0.30724400	2.44620700	2.10343500
H	1.12061700	3.79830700	1.29210400
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H	-2.65471000	1.53153400	0.49981300
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H	-3.92752000	0.87186000	-2.23907800
C	-3.99602100	-1.42601500	-0.44035600
C	-3.57868400	-2.89022500	-0.35992300
H	-4.09520400	-1.13375700	-1.48377400
H	-4.95712300	-1.24414400	0.05278000
H	-2.53203800	-3.01005900	-0.65429200
H	-3.71476400	-3.31317900	0.64037100
H	-4.19763400	-3.47479600	-1.04486200
C	-2.79174900	-0.76005400	1.61799300
C	-1.59143500	-0.03206100	2.19843200

H	-2.63778900	-1.83688900	1.72596400
H	-3.71982400	-0.49880300	2.14032300
H	-1.40679100	-0.40504200	3.21240500
H	-0.68848800	-0.21982000	1.59606300
H	-1.74598700	1.05169400	2.28649700
H	0.25918400	-0.63872600	-0.59820600
O	-0.77452800	-1.09411400	-0.90867600
H	-0.77545100	-1.27786000	-1.85560200
H	-1.98394100	-0.74026400	-0.34918500

PRO

C	3.35574700	-0.26854900	0.60183600
C	3.08880800	1.05866800	0.63708600
C	1.36288600	0.04869100	-0.43458700
N	2.29099000	-0.86163400	-0.05156200
H	4.19962100	-0.82100300	0.97999500
H	3.65568900	1.87455600	1.05336100
N	1.87090900	1.22638200	0.00324800
C	2.18135900	-2.30138900	-0.32833300
C	2.23686800	-3.10018200	0.96945600
C	3.25624900	-2.73429700	-1.31943400
H	1.19837200	-2.41895600	-0.78968300
H	1.49123300	-2.74076400	1.68097900
H	2.04316400	-4.15373900	0.76138600
H	3.22401400	-3.02431600	1.43245800
H	3.19414500	-2.14773700	-2.23762000
H	4.25271900	-2.60624400	-0.88869100
H	3.12679900	-3.78917200	-1.56742200
C	1.20822900	2.52298500	-0.19138500
C	2.05613500	3.42729900	-1.07944400
C	0.89421800	3.16901500	1.15405500
H	0.27891100	2.27865400	-0.71096200
H	2.27406500	2.93870200	-2.03046300
H	1.52104100	4.35753100	-1.27739200
H	3.00043100	3.67705000	-0.58911100
H	0.29028900	2.50768000	1.77970800
H	1.81398900	3.40639200	1.69428100
H	0.34921100	4.10206900	0.99885700
N	-2.84661000	-0.23590800	0.14389800
C	-2.22121800	0.98921500	0.74548500
C	-2.45564300	2.24630500	-0.07421000
H	-1.15198900	0.77672000	0.79907600
H	-2.61178500	1.08716800	1.76085700
H	-1.82191500	3.03873000	0.32625100
H	-2.18374700	2.08927800	-1.12124300
H	-3.48691900	2.59310000	-0.02187100
C	-4.27647000	-0.01638900	-0.24961600

C	-4.92549200	-1.24991000	-0.85473800
H	-4.27477000	0.79063000	-0.97897400
H	-4.80491200	0.32441100	0.64390200
H	-4.30147500	-1.67358100	-1.64514000
H	-5.13421200	-2.02045500	-0.11381100
H	-5.87396400	-0.95017100	-1.30089900
C	-2.69377500	-1.42897100	1.04192900
C	-1.25740800	-1.67582400	1.47118200
H	-3.05827400	-2.28577200	0.47885300
H	-3.35442100	-1.26691900	1.89670800
H	-1.21316700	-2.64981900	1.96009300
H	-0.59226700	-1.69784600	0.60510600
H	-0.89247100	-0.92941200	2.17711700
H	-0.10291500	-0.31609900	-1.33849100
O	-0.98258500	-0.59061500	-1.77913500
H	-0.98302300	-0.22219200	-2.66743400
H	-2.28078200	-0.42542900	-0.72148300

TS0-1

C	0.40785600	-2.88090700	-0.08951000
C	-0.93822000	-2.71355100	-0.11650300
C	-0.01303000	-0.66168300	-0.01887400
N	0.94817200	-1.61175200	-0.02521900
H	1.00855800	-3.76983700	-0.10986600
H	-1.73366900	-3.44495200	-0.16153500
N	-1.16853100	-1.35944700	-0.07111100
C	2.39949300	-1.33086600	0.02750000
C	3.03053800	-1.57708200	-1.33854300
C	3.06097500	-2.14652400	1.13904900
H	2.46505000	-0.26990300	0.28483300
H	2.51480900	-0.99549100	-2.11585900
H	4.07963200	-1.28881200	-1.31854200
H	2.97005600	-2.63828700	-1.60435400
H	2.56560000	-1.99562100	2.10116700
H	3.05651700	-3.21536200	0.90457400
H	4.10864000	-1.84301900	1.23383000
C	-2.51037800	-0.74847100	-0.00252400
C	-3.20224600	-1.14210700	1.30537200
C	-3.33362200	-1.12454400	-1.23043000
H	-2.33043600	0.33120600	-0.00205700
H	-2.59022800	-0.86914800	2.17147800
H	-4.16005100	-0.62977300	1.38305900
H	-3.39127100	-2.22147900	1.33961600
H	-2.81091800	-0.86833300	-2.15224100
H	-3.55044100	-2.19253200	-1.24508500
H	-4.28829600	-0.59258300	-1.20738600
N	0.15407500	2.08479600	0.05475400

C	-0.82689300	2.51259000	1.08953000
C	-0.70016100	1.73322100	2.40204600
H	-1.83403900	2.35772500	0.66799800
H	-0.70794800	3.60193300	1.24552100
H	-1.53752600	2.02830200	3.05177400
H	-0.76897500	0.64073700	2.23283600
H	0.24253100	1.96018700	2.94962100
C	1.54388200	2.38206800	0.53161600
C	2.62192100	2.27185500	-0.54182700
H	1.74392500	1.67918600	1.34076700
H	1.54934700	3.39517500	0.96465700
H	2.52270400	1.35538300	-1.12733700
H	2.61787200	3.12020100	-1.21826800
H	3.59763700	2.24193500	-0.04656000
C	-0.14419600	2.70953600	-1.26139500
C	-1.44123600	2.19735100	-1.89478300
H	0.68303600	2.46289500	-1.93538400
H	-0.16021300	3.79596100	-1.14374300
H	-1.52163900	2.61663300	-2.89465000

PR0-1

C	-3.04264800	0.90204600	0.46790400
C	-2.30029800	2.01734600	0.29029900
C	-0.92220800	0.22421200	-0.00601800
N	-2.19120800	-0.17250300	0.28876700
H	-4.08750500	0.77801400	0.70032000
H	-2.57208900	3.05718500	0.35159700
N	-1.02252300	1.58096500	-0.00477200
C	-2.72546500	-1.54634000	0.26505300
C	-1.68846900	-2.57592100	0.67231900
C	-3.30237000	-1.84613700	-1.11600100
H	-3.53376300	-1.55100000	1.00086500
H	-1.19896200	-2.30545200	1.60848000
H	-2.18017900	-3.54136800	0.80254100
H	-0.93909400	-2.68523300	-0.11064800
H	-4.06846600	-1.11796600	-1.38855000
H	-2.50675400	-1.81234500	-1.86505100
H	-3.74952300	-2.84187700	-1.12686000
C	0.11331000	2.48103300	-0.23832700
C	0.65883600	2.99844700	1.08880500
C	-0.26343800	3.61310800	-1.18631700
H	0.85820800	1.85649900	-0.73227600
H	0.93685900	2.16958500	1.74447300
H	1.53609100	3.62679200	0.91993800
H	-0.09805200	3.60052900	1.59823700
H	-0.70566600	3.22286500	-2.10439700
H	-0.96805100	4.30612500	-0.72104600

H	0.63415500	4.17734200	-1.44438900
N	1.91403100	-0.89576400	-0.04978700
C	2.74432500	-0.15955500	-1.07415800
C	3.48916500	1.06589200	-0.56975800
H	2.05893600	0.10327900	-1.88120200
H	3.46236600	-0.88109700	-1.46778800
H	3.92824800	1.55864600	-1.43820900
H	2.84419500	1.78716100	-0.06860300
H	4.30030000	0.79618500	0.10592300
C	2.47987800	-0.82056900	1.33678900
C	1.55213000	-1.40503700	2.38841600
H	2.64452300	0.23281700	1.55169400
H	3.45019400	-1.32247900	1.31720500
H	0.56403900	-0.94395700	2.32505500
H	1.45125100	-2.48750800	2.31603400
H	1.96851600	-1.17750500	3.37032300
C	1.72384200	-2.31902200	-0.48629600
C	1.08156200	-2.42093800	-1.86075400
H	1.09771900	-2.79476300	0.26378900
H	2.70810400	-2.79147600	-0.45884700

TS0-2

C	0.70759900	1.51546400	-1.17143400
C	1.07190100	0.23146200	-1.39523800
C	-1.02214600	0.20628300	-0.56237800
N	-0.57137700	1.47597300	-0.65364600
H	1.25214300	2.43087400	-1.32599200
H	2.01132400	-0.18135000	-1.72315400
N	-0.00007900	-0.55034900	-1.02423700
C	-1.31001000	2.67238700	-0.22396800
C	-1.69802400	3.52977500	-1.43321100
C	-0.50063000	3.44847000	0.81732400
H	-2.21733100	2.27956600	0.25230600
H	-2.25966100	2.94283800	-2.16857200
H	-2.31017900	4.36833100	-1.10913700
H	-0.80073000	3.93707200	-1.92030500
H	-0.21189500	2.79443400	1.64838200
H	0.40814400	3.87912300	0.37572000
H	-1.10507900	4.27177000	1.20648500
C	0.04418500	-2.02393500	-0.99937800
C	0.88583100	-2.48447100	0.18794800
C	0.55500300	-2.56883700	-2.32741900
H	-0.99062200	-2.33947000	-0.86436500
H	0.42379200	-2.18538500	1.13203000
H	0.99613000	-3.56941600	0.17283200
H	1.87496000	-2.02633600	0.13627300
H	-0.01161300	-2.16036500	-3.16696800

H	1.61319200	-2.33548600	-2.47025200
H	0.45974100	-3.65476200	-2.33657600
N	-3.36322100	-0.72124100	0.47082200
C	-2.87258600	-1.74099200	1.43943400
C	-2.00948900	-1.16367700	2.55367600
H	-2.28581800	-2.46155200	0.86757600
H	-3.73667500	-2.27330400	1.84690900
H	-1.53361600	-1.98915800	3.08900200
H	-1.21585500	-0.51849600	2.15651300
H	-2.59338300	-0.60199300	3.27981000
C	-4.00776200	0.41534900	1.18114900
C	-4.70421900	1.40955500	0.26112600
H	-3.22126400	0.91708000	1.74488100
H	-4.72026300	0.00458400	1.91040400
H	-4.09358900	1.65682200	-0.60745500
H	-5.67049900	1.04079800	-0.09212800
H	-4.88940900	2.33073600	0.81770600
C	-4.27439500	-1.32611600	-0.53729000
C	-3.65410500	-2.42071500	-1.38409800
H	-4.60135100	-0.52009500	-1.19469000
H	-5.16470300	-1.69760300	-0.00833000

PR0-2

C	1.09284300	0.10448000	-2.17844200
C	0.76610800	1.37644400	-1.86026800
C	-0.74702100	0.00889500	-0.84725100
N	0.16454600	-0.70891200	-1.55803800
H	1.89865100	-0.28743300	-2.77995800
H	1.23230700	2.30782800	-2.13465300
N	-0.34699900	1.29321800	-1.04543300
C	0.30320900	-2.17792300	-1.57548900
C	-0.95192700	-2.86230400	-2.09174000
C	0.72177900	-2.68329600	-0.20103700
H	1.11826600	-2.36789500	-2.28000000
H	-1.27660700	-2.43085700	-3.04114300
H	-0.74564500	-3.92517100	-2.24093500
H	-1.76167600	-2.77760700	-1.36837700
H	1.60462200	-2.15009300	0.15409400
H	-0.08499400	-2.52839900	0.52006900
H	0.94582100	-3.75010700	-0.24801500
C	-1.00202500	2.45920200	-0.44176700
C	-1.90931000	3.14496900	-1.45577400
C	0.02496100	3.41384200	0.15888700
H	-1.60202900	2.04967500	0.37190200
H	-2.64983000	2.44651900	-1.85152900
H	-2.43279400	3.98352300	-0.99019800
H	-1.32242300	3.53148500	-2.29508000

H	0.70632200	2.87634600	0.82302500
H	0.60600300	3.91399100	-0.61970000
H	-0.49021700	4.18133800	0.73301500
N	-3.24457600	-0.42431500	0.76766400
C	-3.45534000	0.65312800	1.79640100
C	-4.18023600	1.88996000	1.29041600
H	-2.46799200	0.91144600	2.17285500
H	-4.01641900	0.19543000	2.61402400
H	-4.08218900	2.66622500	2.05266500
H	-3.75826600	2.27640900	0.36260100
H	-5.24418600	1.70667100	1.13672400
C	-4.45129300	-0.59671600	-0.11007800
C	-4.27862900	-1.63969300	-1.19509500
H	-4.64048400	0.37236800	-0.57025100
H	-5.29076100	-0.83141400	0.55118300
H	-3.41802500	-1.40073100	-1.82378600
H	-4.17170100	-2.65256900	-0.80003900
H	-5.16980000	-1.62284200	-1.82354300
C	-2.84726500	-1.71492800	1.42376100
C	-1.72770600	-1.54040200	2.43738400
H	-2.52587000	-2.37936700	0.62422300
H	-3.74887000	-2.13335700	1.88300900

TS0-3

C	1.31342100	-1.61480400	-0.34279400
C	0.84072600	-1.81207000	0.91104900
C	-0.02322200	0.12887600	0.15857200
N	0.77314800	-0.42664800	-0.78366500
H	2.00455700	-2.19514600	-0.92793600
H	1.02076400	-2.61379000	1.60631500
N	0.03242700	-0.73209900	1.19787100
C	0.94465500	0.12737200	-2.14113900
C	-0.25788300	-0.25904700	-2.99666800
C	2.26165700	-0.32839600	-2.75566200
H	0.97487900	1.21121700	-2.00507600
H	-1.19274700	0.02724400	-2.50997600
H	-0.19956000	0.22549000	-3.97366900
H	-0.27422900	-1.34184800	-3.14809600
H	3.08361500	-0.23653300	-2.04285400
H	2.20097300	-1.37015000	-3.08158000
H	2.47513700	0.27687100	-3.63757400
C	-0.74720100	-0.58780600	2.43823500
C	0.14543300	-0.75634300	3.66187700
C	-1.92501700	-1.55561800	2.41795000
H	-1.12870000	0.43372400	2.40723500
H	1.00673500	-0.08628200	3.62234200
H	-0.42649400	-0.53464500	4.56417100

H	0.50774400	-1.78315200	3.74854700
H	-2.52315900	-1.40466600	1.51597500
H	-1.57186000	-2.59052900	2.43324800
H	-2.55419000	-1.39757900	3.29649100
N	-1.01163200	2.65764300	0.44859600
C	-0.61510200	3.06292100	1.82693900
C	0.84742500	2.80072800	2.15704200
H	-1.25516700	2.52295600	2.52376800
H	-0.84860100	4.12744400	1.93962600
H	1.00896900	3.00461300	3.21673600
H	1.12603500	1.76289200	1.96251600
H	1.52130900	3.44648900	1.59336900
C	-0.21908300	3.43053900	-0.54943700
C	-0.72593300	3.32264100	-1.98202500
H	0.80052300	3.03862900	-0.48789600
H	-0.18607800	4.47959200	-0.23557900
H	-0.97979600	2.29378900	-2.24748000
H	-1.60059400	3.94817500	-2.15893500
H	0.05988700	3.66129800	-2.65923500
C	-2.48409000	2.80285200	0.28543000
C	-3.27071200	1.70173700	0.98483300
H	-2.70985800	2.76180100	-0.77703600
H	-2.77413000	3.79726600	0.64411100

PR0-3

C	1.27663700	-1.78204000	-0.40479400
C	0.84136500	-1.91987300	0.87022100
C	0.02081000	0.04529100	0.08181600
N	0.76944100	-0.58223500	-0.86210400
H	1.90667300	-2.42143500	-0.99868200
H	1.01151000	-2.70583500	1.58687500
N	0.08803100	-0.79521700	1.14480600
C	0.92201500	-0.06759000	-2.23341500
C	-0.27873300	-0.49146000	-3.07331700
C	2.24274300	-0.51106200	-2.84949600
H	0.93106900	1.01989500	-2.12903500
H	-1.21042800	-0.16865600	-2.60334600
H	-0.21473600	-0.05456700	-4.07224500
H	-0.30388600	-1.58096000	-3.16910500
H	3.07725700	-0.32505800	-2.16984800
H	2.22463300	-1.57561100	-3.09716700
H	2.40402300	0.04018500	-3.77713900
C	-0.62226900	-0.57076600	2.41078700
C	0.32729900	-0.70086700	3.59572100
C	-1.82280700	-1.50657500	2.50359700
H	-0.98065200	0.45827100	2.35021900
H	1.19555200	-0.04901800	3.47488600

H	-0.19386900	-0.42229900	4.51301000
H	0.67733600	-1.72963700	3.70884300
H	-2.46165300	-1.38770500	1.62478800
H	-1.49349100	-2.54836800	2.55555800
H	-2.40303200	-1.28301400	3.40150300
N	-1.05892000	2.73123700	0.38799200
C	-0.62276700	3.15615800	1.75807700
C	0.84465100	2.88254300	2.04161000
H	-1.25041500	2.62294400	2.46977300
H	-0.85413900	4.22006200	1.84546100
H	1.02899400	3.05845800	3.10221100
H	1.10536600	1.84618300	1.81499800
H	1.50285000	3.54110500	1.47499000
C	-0.28900600	3.46882100	-0.66526100
C	-0.78988200	3.21728200	-2.07969800
H	0.74101800	3.12049000	-0.56889200
H	-0.31475700	4.53178000	-0.41505500
H	-1.00315700	2.15876900	-2.24754900
H	-1.68421000	3.79412600	-2.31325800
H	-0.00912600	3.51695300	-2.78015000
C	-2.54513500	2.85899400	0.25845900
C	-3.28598400	1.75541100	0.99825000
H	-2.79091000	2.80585100	-0.79862300
H	-2.81841300	3.85405700	0.61741100

TS0-4

C	2.58631600	1.05698200	-1.09618600
C	1.70572900	2.07510800	-1.23491000
C	0.51737100	0.21181700	-0.76507600
N	1.83809400	-0.06991000	-0.81732600
H	3.66269300	1.04582300	-1.15477900
H	1.86536100	3.12142000	-1.43766300
N	0.45450400	1.53428200	-1.03411600
C	2.42382400	-1.37100000	-0.48360100
C	3.26735300	-1.25401300	0.78156800
C	3.19839700	-1.93107700	-1.67213600
H	1.56833700	-2.01786200	-0.27685500
H	2.67344600	-0.78161700	1.56457100
H	3.58622700	-2.24773300	1.10833100
H	4.16500100	-0.65517200	0.59531900
H	2.56166000	-1.99739900	-2.55878700
H	4.05890500	-1.29938500	-1.91388700
H	3.57518000	-2.92932200	-1.43515800
C	-0.79346100	2.30257000	-0.97986700
C	-1.28629400	2.62332100	-2.38750100
C	-0.61798100	3.54044200	-0.10600400
H	-1.49430700	1.63914200	-0.47207200

H	-1.40508400	1.71160600	-2.98123700
H	-2.24867400	3.14091400	-2.34129100
H	-0.57565500	3.27720600	-2.90402900
H	-0.08880700	3.25873200	0.80602100
H	-0.07631300	4.33138600	-0.63642700
H	-1.60071800	3.93853800	0.15968800
N	-1.65701900	-1.42311900	-0.33840100
C	-2.42488600	-1.08432700	-1.56476200
C	-1.66770000	-1.32534400	-2.86446700
H	-2.68482300	-0.02523500	-1.48284600
H	-3.35809800	-1.66170500	-1.55059500
H	-2.24608700	-0.89890100	-3.68771500
H	-0.68841700	-0.84134600	-2.84463900
H	-1.52977600	-2.38805900	-3.07376800
C	-1.09723600	-2.80249100	-0.42044900
C	-0.45654700	-3.27956100	0.87427200
H	-0.34832800	-2.78840100	-1.21905400
H	-1.91029900	-3.46945500	-0.73734800
H	0.18071100	-2.49399200	1.28217300
H	-1.20143800	-3.54646000	1.62576600
H	0.14502300	-4.16817800	0.66606500
C	-2.47529500	-1.28378700	0.91167300
C	-3.45352500	-0.12364000	0.95036700
H	-1.75313900	-1.18120700	1.72259000
H	-3.02611700	-2.22698200	1.02885100
H	-3.91591600	-0.12500700	1.94042300
H	-2.94362500	0.82981900	0.84847000

PR0-4

C	-3.17768600	0.19339300	0.37628800
C	-2.88830500	-1.12434400	0.30095400
C	-1.15072000	-0.00174200	-0.67216100
N	-2.11364700	0.85391600	-0.22562100
H	-4.01675300	0.70800800	0.81406600
H	-3.43587400	-1.98304900	0.65453000
N	-1.66688100	-1.21811800	-0.33885100
C	-2.00904000	2.30836700	-0.30386000
C	-1.78609200	2.90887200	1.08017700
C	-3.22942200	2.90475800	-1.00822700
H	-1.12553400	2.48253300	-0.92362500
H	-0.92310800	2.44144700	1.56649400
H	-1.62908600	3.99124000	1.00825500
H	-2.66620200	2.73803200	1.71435200
H	-3.38018300	2.44311800	-1.98418900
H	-4.13591700	2.76371400	-0.40981900
H	-3.08829800	3.98440500	-1.14272500
C	-1.00152500	-2.48971600	-0.62958600

C	-1.61459500	-3.13405100	-1.86631000
C	-1.03462000	-3.41185000	0.58526600
H	0.03831800	-2.21671100	-0.82564700
H	-1.55309600	-2.46351100	-2.73139500
H	-1.09394400	-4.06825300	-2.10910000
H	-2.67275300	-3.37366900	-1.69205300
H	-0.73396400	-2.85777100	1.48070500
H	-2.03467500	-3.83172300	0.73833800
H	-0.34671500	-4.24657000	0.43090500
N	2.08411400	0.51175500	-0.88253100
C	2.37629600	-0.66291100	-1.76862600
C	1.37271400	-0.85194100	-2.89692500
H	2.37241900	-1.51949800	-1.09134500
H	3.38742900	-0.52407600	-2.15332900
H	1.51112100	-1.85071500	-3.31424900
H	0.35309400	-0.75701900	-2.51745400
H	1.52252400	-0.13040900	-3.70178800
C	1.64915800	1.72177000	-1.66118600
C	1.48156100	2.95247300	-0.78373000
H	0.69562600	1.44390800	-2.10680100
H	2.39401600	1.87953700	-2.45011300
H	0.90289500	2.69687700	0.11145400
H	2.43861400	3.37589700	-0.47129200
H	0.94508700	3.71541700	-1.35023300
C	3.24868500	0.83545700	0.01229200
C	3.92786600	-0.35340600	0.67111500
H	2.85423400	1.49840200	0.77807000
H	3.95667900	1.39043700	-0.62105700
H	4.74211200	0.04774000	1.28771900

TS0-5

C	-3.44322300	-0.13697800	-0.61970300
C	-3.02644900	1.13458500	-0.83887200
C	-1.39863400	0.07182400	0.28977400
N	-2.42763500	-0.76937900	0.07071500
H	-4.35990300	-0.63049400	-0.89535700
H	-3.51486900	1.95345800	-1.33946100
N	-1.76920700	1.23628200	-0.27667600
C	-2.46563200	-2.16647200	0.53676700
C	-2.66083400	-3.11397500	-0.64099200
C	-3.54321700	-2.33433800	1.60196900
H	-1.48423000	-2.33579400	0.98528200
H	-1.90209600	-2.95105200	-1.40821200
H	-2.59019500	-4.14558200	-0.29275200
H	-3.64716300	-2.97758500	-1.09109400
H	-3.38256400	-1.64018400	2.42818600
H	-4.53460700	-2.15410700	1.17873200

H	-3.51959700	-3.35397900	1.98941400
C	-0.94611700	2.45758900	-0.23638900
C	-1.55341100	3.46740900	0.72998300
C	-0.76594800	3.02639600	-1.63823600
H	0.01881300	2.13030100	0.15747900
H	-1.67871000	3.02464800	1.71985700
H	-0.89586300	4.33437300	0.81440100
H	-2.52825900	3.80909800	0.37241300
H	-0.36686300	2.27410200	-2.32199300
H	-1.71415900	3.39181300	-2.03992100
H	-0.07436900	3.86979400	-1.60112900
N	2.65072800	-0.68880200	-0.37605000
C	2.22756700	0.37472600	-1.34488500
C	2.61183300	1.78018300	-0.91181700
H	1.14111600	0.29270200	-1.42160000
H	2.66024100	0.12275200	-2.31615200
H	2.09902000	2.48835700	-1.56436200
H	2.30576200	1.98380800	0.11759300
H	3.68212100	1.96226400	-1.00644000
C	4.06572600	-0.52015500	0.08051700
C	4.50232100	-1.58650500	1.07154500
H	4.12312400	0.45919800	0.55145300
H	4.69712800	-0.51318200	-0.81152900
H	3.77206700	-1.69516600	1.87723100
H	4.66037400	-2.55648200	0.60175400
H	5.44723100	-1.27282300	1.51583200
C	2.40392800	-2.06004500	-0.92624500
C	0.97565500	-2.26276100	-1.40423100
H	2.61832200	-2.75971000	-0.12064100
H	3.12925200	-2.22129400	-1.72774200

PR0-5

C	-3.45966500	-0.17870800	-0.63390200
C	-3.05145900	1.09177000	-0.86899500
C	-1.41041100	0.05685900	0.29710000
N	-2.44218500	-0.78991700	0.07506300
H	-4.37033000	-0.68353600	-0.90994200
H	-3.54328800	1.89895000	-1.38550900
N	-1.79831900	1.20895200	-0.29721900
C	-2.47955500	-2.17936900	0.55580500
C	-2.64351300	-3.14460100	-0.61306700
C	-3.57607600	-2.34788800	1.60195100
H	-1.50620400	-2.33545100	1.02604000
H	-1.87123700	-2.98326300	-1.36721900
H	-2.57153300	-4.17208900	-0.25263600
H	-3.62154800	-3.02099900	-1.08486100
H	-3.43871700	-1.64196500	2.42257100

H	-4.56137400	-2.18270900	1.15850600
H	-3.55024600	-3.36248700	2.00277900
C	-0.99448700	2.44039100	-0.27262000
C	-1.61804200	3.45961500	0.67399400
C	-0.81175200	2.99221200	-1.68146200
H	-0.02691800	2.13339700	0.13121700
H	-1.74204200	3.03094200	1.67037500
H	-0.97388300	4.33785000	0.74708400
H	-2.59657000	3.78122100	0.30765900
H	-0.40062100	2.23419400	-2.35188400
H	-1.76175500	3.34003800	-2.09472400
H	-0.13063900	3.84472000	-1.65444800
N	2.69064200	-0.68966300	-0.37195800
C	2.20386000	0.36700900	-1.32311200
C	2.57884300	1.77870100	-0.90502500
H	1.11751100	0.26211800	-1.35226200
H	2.60291900	0.11868000	-2.30913800
H	2.02570300	2.47511700	-1.53692400
H	2.30658000	1.97843700	0.13457400
H	3.64036200	1.98261900	-1.04203100
C	4.12855600	-0.50326200	0.01045400
C	4.62485200	-1.56078500	0.98222900
H	4.19947000	0.47970000	0.47120300
H	4.70730200	-0.49637900	-0.91583000
H	3.93876900	-1.67053800	1.82565700
H	4.76721200	-2.53166300	0.50962700
H	5.58829400	-1.23545200	1.37514500
C	2.43125800	-2.06973900	-0.90283600
C	0.98642600	-2.28867800	-1.31767900
H	2.69038900	-2.76035100	-0.10300800
H	3.12421100	-2.22379000	-1.73320800

TS0-6

C	-3.36583000	-1.52496000	-0.00970100
C	-2.55390500	-2.19745700	-0.86321000
C	-1.27069200	-0.79097300	0.33278200
N	-2.55601000	-0.66686300	0.70940700
H	-4.43052100	-1.58937600	0.13685800
H	-2.77981500	-2.94986700	-1.60001600
N	-1.27454700	-1.73087100	-0.63074600
C	-3.00254000	0.24204800	1.77878800
C	-3.25948400	-0.54730200	3.05786100
C	-4.22067500	1.03799500	1.32998600
H	-2.16383100	0.92454600	1.92099200
H	-2.36483100	-1.09428200	3.36099100
H	-3.54252200	0.13355400	3.86261100
H	-4.07371900	-1.26219300	2.91215400

H	-4.01727500	1.54589000	0.38738700
H	-5.09607400	0.39386300	1.21468200
H	-4.45713200	1.78731300	2.08738800
C	-0.06288600	-2.15677300	-1.34581900
C	-0.13223000	-1.74420700	-2.81094500
C	0.16340900	-3.65279200	-1.16451500
H	0.73947300	-1.60126000	-0.85469900
H	-0.29693400	-0.66918100	-2.89230700
H	0.80615500	-2.00045200	-3.30752400
H	-0.94147100	-2.27150500	-3.32325000
H	0.18615100	-3.91959900	-0.10611800
H	-0.62871000	-4.22656300	-1.65232000
H	1.11307400	-3.93950800	-1.62111800
N	3.17595000	-0.10525800	0.58653800
C	3.34597300	-0.52147900	-0.83751400
C	2.63828400	0.40694500	-1.81421300
H	2.94589500	-1.52955500	-0.93512200
H	4.41972000	-0.57809800	-1.03882300
H	2.71162900	-0.02191400	-2.81523400
H	1.58010600	0.52007000	-1.56595000
H	3.09012000	1.39864400	-1.84892800
C	4.02868000	1.08496200	0.88285400
C	3.73626500	1.72181100	2.23351600
H	3.83612100	1.80877900	0.09180800
H	5.07345700	0.77014900	0.80539700
H	2.66595600	1.89548100	2.35542700
H	4.09442400	1.12022600	3.06851400
H	4.24815700	2.68382000	2.27917800
C	3.45264100	-1.22825900	1.52662600
C	2.39709800	-2.32361700	1.45998900
H	3.46434000	-0.80589800	2.52958000
H	4.45293600	-1.61429800	1.30822500
H	2.55702700	-3.01503700	2.28813500

PR0-6

C	4.26572300	0.22761700	-1.33955800
C	3.18969500	-0.31606100	-1.95767800
C	2.63391500	-0.01028400	0.22647300
N	3.90347200	0.40239800	-0.01536500
H	5.23109300	0.50340500	-1.73036800
H	3.04948400	-0.60643500	-2.98501900
N	2.20946800	-0.44176800	-0.98948200
C	4.77956500	0.97714100	1.01335000
C	5.11438100	2.42702100	0.67871400
C	6.02984000	0.12283000	1.19076300
H	4.18402100	0.94385300	1.92724700
H	4.20278800	3.01415300	0.55381800

H	5.70604600	2.86642900	1.48377400
H	5.69855900	2.48788400	-0.24335400
H	5.76338200	-0.91001300	1.42208300
H	6.64058200	0.13133600	0.28416000
H	6.63472500	0.51909200	2.00821600
C	0.88978100	-1.06049100	-1.18996700
C	0.97294800	-2.56845800	-0.98349000
C	0.31555100	-0.70373900	-2.55514800
H	0.25530600	-0.63755200	-0.40943600
H	1.35463700	-2.79455600	0.01403900
H	-0.02171400	-3.00731500	-1.08141100
H	1.63520900	-3.01880100	-1.72858900
H	0.36511900	0.37238800	-2.73968300
H	0.85020400	-1.21626600	-3.35903700
H	-0.72804400	-1.02136100	-2.59055200
N	-3.05043000	1.41739100	-0.12864900
C	-2.23069200	1.57953400	-1.37764400
C	-2.90864000	1.02837300	-2.61827900
H	-1.30483100	1.03853300	-1.19570500
H	-2.00756200	2.64492900	-1.46763700
H	-2.17484600	1.01490500	-3.42527600
H	-3.24482900	0.00238600	-2.45286800
H	-3.74953400	1.63914600	-2.94470700
C	-4.44060300	1.96647700	-0.28291500
C	-5.28235100	1.81031700	0.97188900
H	-4.89721200	1.42016500	-1.10528800
H	-4.33132700	3.01190100	-0.57839200
H	-5.23136700	0.78726100	1.35164500
H	-4.98681300	2.49927400	1.76176900
H	-6.31975000	2.02350200	0.71338100
C	-2.35304800	1.99677800	1.07236300
C	-0.93942500	1.47555000	1.25572200
H	-2.95740300	1.72299700	1.93413800
H	-2.38119000	3.08159500	0.95053800

TS0-7

C	3.30693600	0.17405600	-1.14868000
C	2.77331600	-1.06145500	-1.32463900
C	1.21662900	0.21692000	-0.33389100
N	2.33036400	0.94119800	-0.54354100
H	4.28089100	0.55479100	-1.40395700
H	3.19550500	-1.94735000	-1.76787300
N	1.49287600	-1.01193800	-0.80902700
C	2.47716100	2.33847700	-0.08975200
C	3.22518000	3.16561300	-1.12580100
C	3.14783700	2.36452900	1.27866600
H	1.45380500	2.70746300	-0.00087900

H	2.76834500	3.06749900	-2.11186000
H	3.19511400	4.21529800	-0.83109600
H	4.27473300	2.86925700	-1.18930500
H	2.55501000	1.80678000	2.00698500
H	4.14783100	1.92557800	1.22283200
H	3.24222700	3.39454000	1.62645200
C	0.50911000	-2.10960100	-0.82504100
C	1.11198000	-3.38767500	-0.25776800
C	-0.03038400	-2.30276700	-2.23828400
H	-0.28819700	-1.76313500	-0.16214600
H	1.52365700	-3.22234400	0.73877900
H	0.33344300	-4.14886300	-0.18584700
H	1.90050100	-3.77512100	-0.90702800
H	-0.42202900	-1.36525400	-2.63840600
H	0.75920300	-2.65824400	-2.90493300
H	-0.82997900	-3.04633700	-2.23189200
N	-3.18213900	0.42900000	-0.08352900
C	-3.14476300	-0.99396500	-0.52464400
C	-2.96921200	-1.97397300	0.62677300
H	-2.30016600	-1.08380500	-1.20678300
H	-4.05775000	-1.19857100	-1.09214100
H	-2.71101200	-2.95176900	0.21559400
H	-2.15728700	-1.66122300	1.28975800
H	-3.87851400	-2.09286300	1.21523900
C	-4.24635100	0.66224000	0.93448100
C	-4.30407700	2.10172500	1.42216900
H	-4.01936500	0.00796600	1.77531900
H	-5.20006600	0.34433400	0.50202500
H	-3.30843900	2.45359400	1.70187300
H	-4.72513000	2.77941900	0.68005100
H	-4.93905500	2.14134900	2.30783600
C	-3.30036400	1.36682900	-1.23774300
C	-2.22161700	1.15424100	-2.29002300
H	-3.20796900	2.37183700	-0.82950600
H	-4.30355100	1.25847900	-1.66134900

PR0-7

C	3.40465100	-0.09679600	1.09499800
C	2.81567300	1.10904300	1.28811000
C	1.27011800	-0.25899700	0.34473900
N	2.44258800	-0.91229000	0.52603100
H	4.40599500	-0.42610800	1.31520500
H	3.20812400	2.01633700	1.71604300
N	1.52156500	0.98773700	0.81516900
C	2.66206500	-2.29385000	0.06715400
C	3.46528000	-3.08758700	1.08914200
C	3.31833100	-2.28346500	-1.30920900

H	1.65980200	-2.71833100	-0.01381200
H	3.01496000	-3.01842200	2.08082200
H	3.48984100	-4.13646400	0.79005400
H	4.49775500	-2.73461700	1.14507000
H	2.68642000	-1.75738200	-2.02835400
H	4.29189300	-1.78688600	-1.26454400
H	3.46846900	-3.30543700	-1.66197200
C	0.49470600	2.03818000	0.87204300
C	1.02414500	3.36070100	0.33191400
C	-0.03607100	2.17362900	2.29579400
H	-0.29523700	1.67360400	0.20988900
H	1.43520900	3.24270300	-0.67185000
H	0.20695900	4.08265300	0.28591900
H	1.79812300	3.77349800	0.98323200
H	-0.39072200	1.21103500	2.67038000
H	0.75168100	2.53169100	2.96375200
H	-0.85841300	2.89190000	2.32629500
N	-3.26590600	-0.45503200	0.11140100
C	-3.17673400	0.95731100	0.59997600
C	-3.01805300	1.96710800	-0.52621000
H	-2.30753500	0.99897200	1.25403700
H	-4.06677500	1.15136300	1.20322600
H	-2.72392400	2.92371400	-0.09097600
H	-2.23320200	1.66046400	-1.22374700
H	-3.94266300	2.12592600	-1.07957700
C	-4.39287900	-0.63980700	-0.85806700
C	-4.48293500	-2.05632400	-1.40121300
H	-4.21066200	0.05489700	-1.67601800
H	-5.31002500	-0.33862500	-0.34659700
H	-3.50809600	-2.39955300	-1.75527600
H	-4.86516800	-2.76327200	-0.66578100
H	-5.16769100	-2.05459800	-2.24949300
C	-3.32784400	-1.43985600	1.24015300
C	-2.19354600	-1.26992700	2.23858200
H	-3.26881600	-2.42686500	0.78551100
H	-4.30777300	-1.33196500	1.71140600

TS0-8

C	-2.27740600	-0.88131100	-1.11556000
C	-2.39986200	0.46753600	-1.13354400
C	-0.25184600	-0.00979400	-0.64208900
N	-0.95564000	-1.14910600	-0.82025600
H	-3.00739800	-1.65262800	-1.29561300
H	-3.25656900	1.08991200	-1.33157900
N	-1.14870800	0.97879100	-0.85234100
C	-0.39349700	-2.50652300	-0.73882900
C	-0.44044300	-3.17993500	-2.10546100

C	-1.11102100	-3.31219700	0.33815400
H	0.64803200	-2.36163300	-0.45257300
H	0.09251700	-2.58299800	-2.84775800
H	0.02774300	-4.16372900	-2.04429700
H	-1.47274000	-3.31486900	-2.43743800
H	-1.11646500	-2.77449100	1.28865200
H	-2.14492000	-3.51689000	0.04838200
H	-0.60582600	-4.26912600	0.47926500
C	-0.85573800	2.42014200	-0.79387800
C	-1.61340900	3.06584500	0.36047600
C	-1.16299300	3.07664500	-2.13513500
H	0.21574700	2.48278200	-0.60991600
H	-1.39584400	2.55727700	1.30136000
H	-1.32324500	4.11417100	0.44998700
H	-2.69164400	3.02605700	0.18379900
H	-0.62194400	2.58022600	-2.94250100
H	-2.23268000	3.04018300	-2.35474800
H	-0.86149500	4.12486200	-2.10375200
N	2.30148000	0.16432700	0.33378200
C	2.65191100	1.60836400	0.26689100
C	1.97032800	2.44785600	1.34195000
H	2.35019400	1.95609400	-0.72244400
H	3.74142400	1.70521200	0.32827000
H	1.98554400	3.49575000	1.03763000
H	0.92920000	2.14559400	1.48311700
H	2.47739900	2.37034600	2.30346400
C	2.45863000	-0.36047700	1.71839000
C	2.01490100	-1.80236000	1.89741700
H	1.84410300	0.25995900	2.36598500
H	3.50871400	-0.23092000	2.00574700
H	0.95823100	-1.90641200	1.64882300
H	2.60376100	-2.51516400	1.31925100
H	2.12726500	-2.06196800	2.95143200
C	3.11097800	-0.62447200	-0.63457200
C	3.03800700	-0.10226200	-2.06358200
H	2.73329000	-1.64625900	-0.60928600
H	4.14615100	-0.64638100	-0.27620800

PR0-8

C	-2.56855600	-0.96645700	-0.88218700
C	-2.72150300	0.37841400	-0.89977400
C	-0.52479300	-0.04753400	-0.50719200
N	-1.22631700	-1.20148200	-0.64418000
H	-3.29199100	-1.75289300	-1.01785500
H	-3.60315700	0.97807100	-1.05277800
N	-1.46706100	0.91612200	-0.67147200
C	-0.61878300	-2.53988700	-0.58965100

C	-0.92660200	-3.32183300	-1.86147500
C	-1.05561500	-3.27734500	0.67042600
H	0.45447700	-2.35202300	-0.54422500
H	-0.63072800	-2.75326900	-2.74501000
H	-0.37628100	-4.26385500	-1.85136400
H	-1.99135400	-3.55564800	-1.93439600
H	-0.78748400	-2.71081900	1.56553800
H	-2.13667400	-3.44275400	0.66807000
H	-0.56418100	-4.25064200	0.72063000
C	-1.18319100	2.35917100	-0.63143400
C	-1.72998700	2.97790700	0.64988300
C	-1.71252100	3.04763200	-1.88408600
H	-0.09546400	2.42557500	-0.62746900
H	-1.29296100	2.49991600	1.52977100
H	-1.48750800	4.04171500	0.68119800
H	-2.81808700	2.87629100	0.69526200
H	-1.33046100	2.56173800	-2.78352100
H	-2.80442700	3.03406000	-1.91414100
H	-1.39157200	4.09049700	-1.88701400
N	2.34482100	0.22003000	-0.09292800
C	2.59285400	1.68890100	-0.22812200
C	2.10337300	2.48535800	0.97353000
H	2.06365800	2.00357200	-1.12701400
H	3.66285700	1.82948900	-0.40033100
H	2.00278500	3.53190100	0.68260900
H	1.12787200	2.12712900	1.31365500
H	2.79693300	2.43451500	1.81217800
C	2.87754500	-0.31583400	1.19920800
C	2.49539400	-1.76331800	1.45323600
H	2.45603000	0.29671000	1.99106700
H	3.96153600	-0.17602100	1.17838000
H	1.41028800	-1.87912700	1.42434200
H	2.95954000	-2.46195500	0.75700900
H	2.82408200	-2.02868400	2.45896800
C	2.88525500	-0.54433400	-1.26274400
C	2.42951200	-0.00553200	-2.61003800
H	2.54252900	-1.57126700	-1.14464000
H	3.97455400	-0.53904800	-1.17469300

[Et₃N·H]⁺

H	-0.00073700	0.00074800	1.21092000
N	0.00003100	0.00079000	0.18345800
C	0.73015000	-1.24837700	-0.25719900
C	0.04444400	-2.53437200	0.17264700
H	1.72701100	-1.18761300	0.17967100
H	0.82357500	-1.17438400	-1.34490900

H	0.73199900	-3.36238700	-0.01181200
H	-0.18238000	-2.53444900	1.24389000
H	-0.86889400	-2.73801500	-0.38767400
C	-1.44598400	-0.00701600	-0.25861800
C	-2.21937100	1.22751500	0.17316300
H	-1.89025900	-0.90254900	0.17575900
H	-1.42718200	-0.12265900	-1.34653900
H	-2.10814300	1.42180200	1.24498200
H	-1.94066900	2.12245200	-0.38457100
H	-3.27956400	1.04399500	-0.01299300
C	0.71721000	1.25687200	-0.25755700
C	2.17372700	1.30516900	0.17273500
H	0.16615700	2.09017500	0.17847300
H	0.60691400	1.29975700	-1.34536400
H	2.54800800	2.31402500	-0.01257200
H	2.28685500	1.11005700	1.24426200
H	2.80606200	0.61476800	-0.38675000

COM1

C	-2.54348700	1.39246200	-0.68312300
C	-1.42500600	2.15567000	-0.75736100
C	-0.91426900	0.32265400	0.51177500
N	-2.20732000	0.29147700	0.08636100
H	-3.52226600	1.54066300	-1.11322300
H	-1.25238800	3.09537400	-1.25891600
N	-0.45277500	1.48330100	-0.03438600
C	-3.11513000	-0.81975300	0.38123100
C	-3.56030300	-1.50592100	-0.90684300
C	-4.29168300	-0.34041900	1.22745800
H	-2.50569500	-1.51620000	0.96394000
H	-2.68981900	-1.83333500	-1.47977500
H	-4.17034300	-2.38231500	-0.66959100
H	-4.16557400	-0.83093200	-1.52237900
H	-3.93734400	0.14761200	2.13920100
H	-4.90919200	0.37261900	0.67000300
H	-4.92535900	-1.18769400	1.50462800
C	0.91991000	1.95751300	0.15747200
C	0.95397400	3.09905000	1.17043700
C	1.55296800	2.35064100	-1.17416700
H	1.45288800	1.09389100	0.56593300
H	0.51406300	2.77922500	2.11851000
H	1.98575400	3.41649300	1.34942000
H	0.39042600	3.96278300	0.79996500
H	1.44710200	1.54377100	-1.90410700
H	1.09806100	3.25973600	-1.58313600
H	2.61940800	2.54696500	-1.02939800
C	0.23783300	-2.32761400	0.22903900

O	-0.39105000	-2.70645100	-0.73533000
H	-0.14150100	-2.48193600	1.25707700
C	1.57383200	-1.67783300	0.15036000
C	2.11726500	-1.32537600	-1.08632900
C	2.27222600	-1.40961300	1.32772100
C	3.35566600	-0.69326500	-1.13993000
H	1.54893200	-1.54446600	-1.98583200
C	3.51604400	-0.78502500	1.27432000
H	1.82557300	-1.67067900	2.28422500
C	4.05449300	-0.42241700	0.03919200
H	3.77896300	-0.40588800	-2.09791700
H	4.06045900	-0.57308500	2.18918100
H	5.02091800	0.07103400	-0.00649800

TS1

C	-2.26849600	1.25090600	-1.08105700
C	-1.25893500	2.14063600	-0.91010800
C	-0.80088000	0.33285200	0.36426400
N	-1.96396900	0.14901400	-0.30016700
H	-3.15427100	1.31293500	-1.69139000
H	-1.10468700	3.11686300	-1.34192700
N	-0.37700200	1.55843900	-0.01762500
C	-2.82630600	-1.04324600	-0.12282600
C	-3.76939300	-1.20788200	-1.30693400
C	-3.57032700	-0.93513400	1.20300000
H	-2.14202200	-1.89140600	-0.06304200
H	-3.22996900	-1.20172200	-2.25884000
H	-4.28137700	-2.16845300	-1.21360000
H	-4.53873600	-0.42807900	-1.32819100
H	-2.85119900	-0.88906000	2.02372700
H	-4.21014400	-0.04516600	1.21593400
H	-4.19652600	-1.82002700	1.34944300
C	0.89153700	2.15806700	0.41671900
C	0.66147500	3.56131900	0.96936100
C	1.90250100	2.13039100	-0.72555500
H	1.24248700	1.51099500	1.22388100
H	-0.08811400	3.54985000	1.76485300
H	1.59776100	3.95199600	1.37636600
H	0.32860500	4.25040900	0.18626100
H	2.02453200	1.11286900	-1.10802000
H	1.57507000	2.78005100	-1.54500400
H	2.87474700	2.48629800	-0.37286700
C	0.12913900	-1.16643000	1.39176200
O	-0.62430400	-2.15935900	1.41839100
H	0.27603800	-0.55308400	2.30606500
C	1.38690300	-1.20878000	0.54056100
C	1.34413800	-1.75066000	-0.74586700

C	2.60417000	-0.76695500	1.05461700
C	2.49795900	-1.81763400	-1.51989000
H	0.39366500	-2.12099100	-1.12266800
C	3.76791800	-0.83974300	0.28540800
H	2.64453000	-0.37166600	2.06852800
C	3.71459800	-1.35762600	-1.00614300
H	2.45569700	-2.23163200	-2.52310600
H	4.71315800	-0.49685600	0.69613400
H	4.61596800	-1.41190500	-1.60898900

INT1

C	-2.30266900	1.12279000	-0.99961400
C	-1.32979400	2.06273800	-0.91083300
C	-0.73174700	0.32757100	0.35979000
N	-1.91378200	0.05254200	-0.21696900
H	-3.22750500	1.12605800	-1.55177400
H	-1.24535300	3.03400200	-1.37062800
N	-0.36611500	1.55516000	-0.06243700
C	-2.73407900	-1.17919600	-0.02994600
C	-3.35646400	-1.59216400	-1.35752500
C	-3.76239000	-0.92585800	1.06418500
H	-2.02218600	-1.92173600	0.33639800
H	-2.60388000	-1.66663900	-2.14819000
H	-3.81435000	-2.57635700	-1.23184900
H	-4.14658800	-0.90696800	-1.68503800
H	-3.24178100	-0.72181900	2.00251600
H	-4.42216400	-0.08848100	0.80684700
H	-4.37739600	-1.82008400	1.19933800
C	0.91214000	2.22176900	0.25218100
C	0.66187900	3.66369600	0.68095000
C	1.86258200	2.11164100	-0.93645000
H	1.32675400	1.66756400	1.09603900
H	-0.06233900	3.71187400	1.49812300
H	1.60167200	4.10418300	1.02297900
H	0.29636300	4.27428900	-0.15095300
H	2.02997300	1.06485300	-1.20532700
H	1.45707000	2.64447100	-1.80371200
H	2.82581500	2.55987500	-0.67729400
C	0.06149300	-0.61207400	1.33760200
O	-0.65814900	-1.63516800	1.74875100
H	0.39077000	0.10203400	2.14386400
C	1.34864100	-0.98528800	0.56817100
C	1.25258500	-1.64630400	-0.65946700
C	2.61279500	-0.71032600	1.08548600
C	2.39577600	-1.99419200	-1.37298200
H	0.26541500	-1.89241800	-1.04846500
C	3.76565300	-1.06056500	0.37930100

H	2.69557100	-0.22118500	2.05493200
C	3.65925800	-1.69398000	-0.85697500
H	2.30685300	-2.50031000	-2.33005900
H	4.74501400	-0.84317100	0.79617700
H	4.55279500	-1.96415400	-1.41134200

INT1w

C	-2.08225100	1.06745700	-1.38627900
C	-1.14351000	2.03316200	-1.24145500
C	-0.61476400	0.34540200	0.11636800
N	-1.73881200	0.02779700	-0.54520600
H	-2.96427400	1.03481700	-2.00448400
H	-1.04674200	2.99800400	-1.71177100
N	-0.24149700	1.57082200	-0.30463200
C	-2.53954100	-1.22591900	-0.45305100
C	-2.54558300	-1.91505400	-1.81391700
C	-3.94114400	-0.89538400	0.04675300
H	-2.00646300	-1.82835100	0.28591000
H	-1.53068900	-2.10631100	-2.17324600
H	-3.06096400	-2.87472400	-1.72258100
H	-3.07524100	-1.32335700	-2.56937500
H	-3.88030700	-0.38673600	1.01220900
H	-4.49120100	-0.27746600	-0.67341900
H	-4.49683400	-1.82882500	0.17464300
C	0.98290300	2.28770200	0.09982500
C	0.64817800	3.72660600	0.47833800
C	2.03028300	2.18725100	-1.00547200
H	1.34861700	1.76632700	0.98556700
H	-0.14696400	3.75880400	1.22727600
H	1.53912400	4.20489900	0.89263300
H	0.33746900	4.31031400	-0.39391700
H	2.25060300	1.14151700	-1.23787900
H	1.68045000	2.68932200	-1.91409700
H	2.95487800	2.67178800	-0.67979300
C	0.13707700	-0.50096300	1.17905000
O	-0.59474400	-1.52471700	1.64180200
H	0.38003400	0.25482400	1.96427800
C	1.47153600	-0.91936800	0.55033500
C	1.48754800	-1.64255600	-0.64498200
C	2.68310800	-0.61513600	1.16865600
C	2.69119500	-2.02997600	-1.22636400
H	0.54244000	-1.90787000	-1.11418000
C	3.89457400	-1.00316500	0.59414400
H	2.67757800	-0.07362300	2.11288700
C	3.90114300	-1.70378800	-0.60996300
H	2.68978400	-2.58898300	-2.15744000
H	4.83101900	-0.76108100	1.08809000

H	4.84144700	-2.00470700	-1.06163500
O	-2.37054300	-0.02520000	2.67167300
H	-1.69517400	-0.73400200	2.37425500
H	-2.45863900	-0.10321200	3.62520300

INT1E13NH

C	-3.41147800	1.75829600	0.29237000
C	-3.87654300	0.65821900	-0.34982600
C	-1.66372900	0.53363200	-0.28902800
N	-2.03443900	1.66377300	0.33560600
H	-3.94246300	2.59141400	0.72147500
H	-4.88467900	0.35410200	-0.58003800
N	-2.77832700	-0.09335200	-0.70476000
C	-1.16388300	2.71325300	0.95365000
C	-1.83771800	3.28019500	2.19727000
C	-0.84866700	3.77832300	-0.08911700
H	-0.24821400	2.19674200	1.23372200
H	-2.15660500	2.49032300	2.88312000
H	-1.11452300	3.91077600	2.71921200
H	-2.69717300	3.91180300	1.95448800
H	-0.32954400	3.33473400	-0.94118200
H	-1.76504900	4.26935900	-0.43302300
H	-0.20152400	4.53946600	0.35482000
C	-2.85907200	-1.43616600	-1.33419800
C	-3.76563300	-1.38602700	-2.55870900
C	-3.30989800	-2.45828500	-0.29491600
H	-1.84317200	-1.67551700	-1.65428400
H	-3.45156800	-0.60580900	-3.25631700
H	-3.72012400	-2.34888100	-3.07233300
H	-4.80959000	-1.21382100	-2.28115700
H	-2.63374300	-2.47405300	0.56432000
H	-4.32280200	-2.23330000	0.05356500
H	-3.31983900	-3.45327900	-0.74675500
C	-0.26997000	-0.02733700	-0.49070900
O	0.65851200	0.99214000	-0.31288500
H	-0.24586400	-0.40071700	-1.52888700
C	-0.05317300	-1.21528800	0.43665600
C	-0.30107800	-1.09399500	1.80709000
C	0.43416400	-2.41881500	-0.07198600
C	-0.05945500	-2.16661400	2.66034500
H	-0.67722100	-0.15506400	2.20980600
C	0.68007700	-3.49493900	0.78188000
H	0.62948200	-2.51538300	-1.13917600
C	0.43295300	-3.36872000	2.14716100
H	-0.25157300	-2.06778200	3.72382400
H	1.06331400	-4.42811600	0.38171900

H	0.62264900	-4.20441400	2.81281000
H	1.62579900	0.62830500	-0.37823100
N	3.19419500	0.33937600	-0.54098200
C	3.86001600	0.27547600	0.77713400
C	3.51792900	-0.96604900	1.59213600
H	3.54538000	1.15794400	1.33925500
H	4.95247100	0.34770500	0.63780500
H	3.88318800	-0.83191200	2.61334200
H	2.43518400	-1.12065300	1.63800200
H	3.98250200	-1.87239400	1.19735700
C	3.45913000	-0.88250500	-1.32217100
C	2.78388300	-0.89205500	-2.68942300
H	3.08510700	-1.72754600	-0.73879300
H	4.54777500	-1.02156200	-1.43819500
H	1.73510100	-0.58127200	-2.61006700
H	3.27470500	-0.23351600	-3.40872300
H	2.80995800	-1.90385300	-3.10234000
C	3.63284600	1.53937000	-1.28638400
C	3.40300100	2.84708400	-0.53613500
H	3.05921500	1.56950500	-2.21605100
H	4.69765500	1.43585900	-1.55610400
H	3.54716200	3.68345000	-1.22432700
H	2.37880400	2.89702000	-0.15090200
H	4.09949700	2.98233100	0.29373400

INT1E3N

C	0.66828100	2.00649100	1.94930800
C	-0.04975400	1.02914400	2.55657700
C	0.62992400	0.25385000	0.58089000
N	1.07946600	1.51017200	0.73198700
H	0.91191100	3.00365600	2.27777000
H	-0.55754000	1.01654900	3.50732700
N	-0.05894700	-0.05431000	1.69622500
C	1.93897000	2.22459100	-0.24258500
C	3.38488900	2.19880400	0.24192600
C	1.40692600	3.63534000	-0.45999100
H	1.81388800	1.65593200	-1.16863800
H	3.73468000	1.17098100	0.37685100
H	4.02443100	2.68154000	-0.50238100
H	3.49327300	2.74052500	1.18907000
H	0.35581300	3.60752900	-0.75730200
H	1.51336700	4.26009100	0.43408200
H	1.97871500	4.10906500	-1.26182600
C	-0.74177200	-1.32913000	1.99902500
C	-2.24910500	-1.11067200	2.06598200
C	-0.16959700	-1.93004400	3.28015700
H	-0.50852900	-1.98946200	1.16142300

H	-2.63198800	-0.69324200	1.12696700
H	-2.74417900	-2.06988100	2.24703800
H	-2.50774700	-0.43853800	2.89247800
H	0.91695300	-2.03569500	3.22207400
H	-0.41268300	-1.31213300	4.15056000
H	-0.60742000	-2.91825000	3.44160900
C	0.82050800	-0.55756800	-0.72718200
O	0.43688100	0.16872800	-1.77505100
H	0.22976100	-1.49253700	-0.56887500
C	2.30221700	-1.00787600	-0.74181600
C	3.05865000	-0.74313300	-1.88019100
C	2.90036700	-1.65543200	0.34198900
C	4.40510300	-1.10690800	-1.92972600
H	2.55506600	-0.24498100	-2.70448800
C	4.24491300	-2.01910600	0.29843000
H	2.31300100	-1.87169300	1.23487300
C	5.00300000	-1.73954500	-0.84017000
H	4.99032800	-0.89454800	-2.82007700
H	4.70322400	-2.51630100	1.14854600
H	6.05186900	-2.01826300	-0.87667400
N	-3.53153500	-0.07197600	-0.98546900
C	-2.65755000	-0.72530300	-1.96847300
C	-2.41627500	-2.20108400	-1.66514600
H	-1.68322600	-0.22352800	-1.96770600
H	-3.08079600	-0.61521700	-2.98660700
H	-1.63051900	-2.58357900	-2.32333300
H	-2.08063500	-2.32207600	-0.62898000
H	-3.30395500	-2.82630400	-1.80416700
C	-4.92291400	-0.49664700	-1.13205800
C	-5.73487200	-0.31428300	0.14663800
H	-4.93042200	-1.55799200	-1.39514300
H	-5.40598500	0.03676100	-1.97399200
H	-5.29380300	-0.90273900	0.95696300
H	-5.76795600	0.73044700	0.46893500
H	-6.76630200	-0.64797300	-0.00285000
C	-3.42278700	1.38481500	-1.08893700
C	-2.12840500	1.93180500	-0.49576900
H	-4.27294100	1.82730600	-0.55964300
H	-3.51391300	1.69855800	-2.14719200
H	-2.11837700	3.02466800	-0.57594200
H	-2.06392400	1.67132700	0.56840700
H	-1.24567100	1.53431100	-1.01120600

TS2_{DPT}

C	-2.83758300	0.29485800	-0.68251700
C	-2.26726400	1.52411700	-0.69513300
C	-0.82203100	0.10898700	0.25988200

N	-1.93603400	-0.57559500	-0.09395100
H	-3.79808200	-0.02727900	-1.04657100
H	-2.64439100	2.46462000	-1.06241300
N	-1.01779400	1.40152800	-0.11625000
C	-2.05410800	-2.04982800	-0.00441000
C	-1.00959700	-2.69557400	-0.90902900
C	-3.46950100	-2.49141000	-0.34477500
H	-1.79939700	-2.29124500	1.03133400
H	-0.00135900	-2.43212100	-0.57887100
H	-1.10608800	-3.78354700	-0.85226800
H	-1.14964300	-2.38414600	-1.95066900
H	-4.21557700	-1.99404200	0.28233700
H	-3.71081300	-2.31612700	-1.39938000
H	-3.54664900	-3.56586100	-0.16421300
C	-0.17153800	2.52829700	0.31373300
C	-0.78927600	3.18324300	1.54709000
C	0.03452800	3.51068000	-0.83289700
H	0.78823600	2.08483900	0.58587100
H	-0.92008900	2.44678600	2.34433400
H	-0.13529100	3.97957000	1.91239800
H	-1.76444900	3.62045000	1.30750900
H	0.43795000	3.01031800	-1.71704800
H	-0.90078500	4.00944200	-1.10816600
H	0.74142600	4.28396000	-0.52248900
C	0.31417000	-0.41160800	0.99674400
O	-0.00135900	-1.54272200	1.85877300
H	0.22373900	-0.30942100	2.18409800
C	1.64261400	-0.43587600	0.34363200
C	1.94835900	0.23979700	-0.85090700
C	2.65129500	-1.21344000	0.93726700
C	3.22545900	0.17859800	-1.40334200
H	1.17519500	0.79411600	-1.37809500
C	3.92410400	-1.27482200	0.37908500
H	2.39845600	-1.77386600	1.83095600
C	4.22609100	-0.57229000	-0.78837000
H	3.43317300	0.70681100	-2.32985700
H	4.68747100	-1.88249500	0.85702700
H	5.22030600	-0.62289300	-1.22091100

TS2_{E13N}

C	-3.49234800	0.19479800	0.45569200
C	-2.88858400	0.92359600	1.41685200
C	-1.29035700	0.24519100	-0.03461100
N	-2.51478600	-0.22667000	-0.43281200
H	-4.53175400	-0.05672100	0.33122200
H	-3.30070700	1.40443100	2.28935400
N	-1.53268400	0.96599200	1.12222400

C	-2.79023100	-0.74626100	-1.79265200
C	-2.57064900	0.37079500	-2.80846500
C	-4.19356100	-1.33163000	-1.86997300
H	-2.02382200	-1.50572700	-1.96340300
H	-1.52796500	0.69849600	-2.77505600
H	-2.77606300	-0.00312400	-3.81629800
H	-3.23502200	1.22026600	-2.60737000
H	-4.36877400	-2.07527600	-1.08597000
H	-4.97038700	-0.56024200	-1.81046200
H	-4.30455100	-1.83095100	-2.83559300
C	-0.54432900	1.41400000	2.11077500
C	-0.70432200	0.62347000	3.41478200
C	-0.67273500	2.90885800	2.40843600
H	0.43137900	1.20481800	1.66422400
H	-0.84113500	-0.44068200	3.22077200
H	0.17849400	0.76293600	4.04684100
H	-1.57455400	0.97578300	3.97843600
H	-0.50745700	3.53034800	1.52871700
H	-1.66697500	3.13265200	2.81007900
H	0.06300800	3.19002400	3.16763300
C	-0.03828400	-0.10811400	-0.69078700
O	-0.08747700	-1.15608000	-1.54467000
H	0.83100500	-0.91676500	0.19992900
C	0.86686000	1.01867400	-1.05805700
C	1.99604100	0.72161600	-1.84833300
C	0.69481100	2.36389400	-0.68312300
C	2.95164100	1.68982300	-2.13998100
H	2.08451600	-0.28529000	-2.24092800
C	1.64961200	3.33426600	-0.97517000
H	-0.22992500	2.66446300	-0.20453600
C	2.80529300	3.00155100	-1.68301400
H	3.81544700	1.42229400	-2.74362500
H	1.47645400	4.36354900	-0.66949400
H	3.55277100	3.75545400	-1.90875500
N	1.60248700	-1.82143600	0.65548500
C	1.53572100	-3.08731600	-0.13817400
C	2.23155400	-3.07013000	-1.48771800
H	0.47736500	-3.27180900	-0.31476400
H	1.95422400	-3.88490200	0.50078700
H	2.04609600	-4.03744600	-1.96431300
H	1.77626000	-2.29295200	-2.10393000
H	3.31546900	-2.94616100	-1.41761400
C	2.98642500	-1.28685400	0.71437700
C	3.12273700	0.03663400	1.45619400
H	3.30670300	-1.13534700	-0.31597500
H	3.62932100	-2.05908000	1.16617600
H	2.48347300	0.80090600	1.00332600

H	2.90327500	-0.04386700	2.52447000
H	4.15581500	0.38028200	1.35787100
C	1.07722600	-2.07295000	2.01663100
C	-0.33081500	-2.65737900	2.01346200
H	1.07418600	-1.11230400	2.53558400
H	1.77799400	-2.73659600	2.54494000
H	-0.73401800	-2.63511400	3.02968400
H	-0.99118400	-2.07603600	1.35906500
H	-0.34450100	-3.69605700	1.67919100

TS2w

C	1.40465600	2.18163800	-0.93731100
C	2.31707200	1.19539700	-1.13908300
C	0.68206900	0.35656000	0.10943000
N	0.39900900	1.64407700	-0.16626500
H	1.39123600	3.20536100	-1.27555600
H	3.24858200	1.20209600	-1.68081300
N	1.85299300	0.07205400	-0.48687600
C	-0.83258900	2.34539000	0.25664300
C	-1.72172300	2.59803400	-0.95581800
C	-0.46413300	3.61401800	1.01632600
H	-1.32817400	1.65814600	0.94317400
H	-1.97928100	1.65503000	-1.44691300
H	-2.64700200	3.08143900	-0.63124000
H	-1.22961400	3.25701300	-1.67976600
H	0.18315400	3.37596600	1.86374200
H	0.04088700	4.34077300	0.37067800
H	-1.37500300	4.08303600	1.39647200
C	2.58427900	-1.21781600	-0.41849900
C	3.77977000	-1.07297200	0.51342100
C	2.95807200	-1.66752600	-1.82654300
H	1.89082700	-1.92477800	0.03922800
H	3.42471800	-0.86140600	1.52457200
H	4.32052100	-2.02269200	0.54623600
H	4.46620100	-0.29399000	0.16100600
H	2.08311600	-1.70076400	-2.48209400
H	3.71070100	-1.01225600	-2.27821000
H	3.38614500	-2.67139200	-1.77389900
C	-0.14977100	-0.55260500	0.95119300
O	-0.37513100	0.09101800	2.20258400
H	0.57359500	-1.50075500	1.39647600
C	-1.41782500	-0.92846300	0.25375200
C	-2.62844500	-0.99227000	0.95430300
C	-1.42017300	-1.25704700	-1.11150900
C	-3.80396300	-1.36984700	0.30599500
H	-2.63014800	-0.73594800	2.00858400
C	-2.59429400	-1.63408500	-1.75610500

H	-0.48975500	-1.21932800	-1.67707500
C	-3.79688100	-1.69054700	-1.05046400
H	-4.73324100	-1.41128300	0.86716900
H	-2.57112000	-1.88518200	-2.81274200
H	-4.71373800	-1.98356800	-1.55197700
O	1.43123800	-1.95517800	2.32054000
H	1.17327400	-2.76932300	2.76480900
H	0.21452300	-0.41298400	2.80076000

TS2_{E13N-H}

C	3.29991500	-0.69197800	0.66500900
C	2.53264200	-1.10448700	1.69510900
C	1.15699400	-0.50348000	0.02152500
N	2.44933300	-0.34598900	-0.37518400
H	4.37144300	-0.63593200	0.57414400
H	2.80942800	-1.47403200	2.66925100
N	1.21287700	-0.98282300	1.29888100
C	2.95768800	0.10725900	-1.69525600
C	4.22158900	-0.66025300	-2.07379400
C	3.18135800	1.61495800	-1.66918300
H	2.18212100	-0.14111100	-2.41458200
H	4.08223300	-1.73960400	-1.97217200
H	4.45807000	-0.44257800	-3.11782000
H	5.08636500	-0.35395500	-1.47830900
H	2.24313900	2.13439900	-1.46232500
H	3.91842600	1.87713500	-0.90244100
H	3.56115700	1.95372800	-2.63657500
C	0.08203200	-1.21816900	2.21803800
C	0.30549000	-0.44656800	3.52218400
C	-0.10115500	-2.70607000	2.51088800
H	-0.79633300	-0.82865500	1.69630500
H	0.67708900	0.56465100	3.34168300
H	-0.63518900	-0.38721900	4.07689100
H	1.02757000	-0.96074500	4.16380500
H	-0.35662900	-3.27436000	1.61753200
H	0.81318300	-3.12093000	2.94774500
H	-0.90671000	-2.83331500	3.23886400
C	-0.07682400	-0.11794200	-0.65858200
O	0.14799300	0.70771100	-1.80980300
H	-0.82397800	1.13717100	0.04434400
C	-1.05071100	-1.21233900	-0.94908900
C	-2.31666200	-0.88005300	-1.46256600
C	-0.74326200	-2.57315400	-0.81141500
C	-3.24850500	-1.86129400	-1.78275000
H	-2.56266700	0.16659500	-1.62523300
C	-1.68098000	-3.55982900	-1.11505500
H	0.25098800	-2.86905600	-0.48544300

C	-2.94002100	-3.20936000	-1.59490400
H	-4.21796300	-1.57512600	-2.17884800
H	-1.41627600	-4.60647500	-0.99789000
H	-3.66726200	-3.97684200	-1.83769900
N	-1.28762100	2.17467700	0.37775600
C	-0.61956400	2.47895000	1.67695300
C	0.88674600	2.67618800	1.57302000
H	-0.83773100	1.64087400	2.33991800
H	-1.10117900	3.37128500	2.09628000
H	1.29677600	2.76583200	2.58235400
H	1.37397800	1.82527900	1.08581200
H	1.15379800	3.58669500	1.03326200
C	-0.95289400	3.23211700	-0.63175000
C	-1.77592500	3.19031800	-1.90859700
H	0.10014000	3.08976500	-0.87759000
H	-1.06815400	4.20307700	-0.13178000
H	-1.74975000	2.19501600	-2.35687900
H	-2.81020600	3.50550900	-1.75678400
H	-1.32586000	3.88488600	-2.62187600
C	-2.76131500	2.03626100	0.57571300
C	-3.15596500	0.89194300	1.49842300
H	-3.20149200	1.86797600	-0.40644400
H	-3.13652000	2.99839300	0.94801800
H	-4.24495700	0.80481800	1.49243700
H	-2.75211400	-0.05756400	1.13342600
H	-2.84845000	1.04901500	2.53472700
H	0.04344300	0.17455100	-2.61137900

M1

C	-2.70001700	1.07925900	-0.43631600
C	-1.75091400	2.02786600	-0.50644200
C	-0.72862200	0.08867100	0.05917600
N	-2.08672700	-0.12728000	-0.10085500
H	-3.75987300	1.14537000	-0.62268900
H	-1.83729400	3.07672300	-0.74081900
N	-0.51442400	1.43749300	-0.21250400
C	-2.70247400	-1.44334700	-0.31948900
C	-3.46543000	-1.47514100	-1.64383100
C	-3.59132600	-1.82048700	0.86196200
H	-1.87126500	-2.14609200	-0.37804700
H	-2.83379400	-1.12912500	-2.46652500
H	-3.77730200	-2.50160600	-1.85539100
H	-4.36828000	-0.85649400	-1.61206400
H	-3.00540600	-1.84887000	1.78333800
H	-4.40072800	-1.09139900	0.98308900
H	-4.04023300	-2.80527600	0.70279500
C	0.53321100	2.21406600	0.47412700

C	0.03081000	2.69258700	1.83632200
C	1.01115600	3.36004700	-0.40935800
H	1.36707300	1.53085800	0.63204800
H	-0.33135400	1.84507900	2.42614900
H	0.84125700	3.17744800	2.38807000
H	-0.78779900	3.41124900	1.72274200
H	1.36096000	2.98653100	-1.37541000
H	0.21690900	4.09344200	-0.58492300
H	1.83809100	3.88058000	0.08083200
C	0.20961900	-0.85229100	0.45184800
O	-0.28099300	-1.97476200	1.14590300
H	-0.28177700	-1.77278100	2.08918900
C	1.61297700	-0.88210400	0.08168700
C	2.14673800	-0.09608300	-0.96492200
C	2.49663300	-1.76797800	0.73202500
C	3.49167900	-0.16220200	-1.30473200
H	1.48616200	0.55310700	-1.53387400
C	3.84171100	-1.83190100	0.38245900
H	2.10994900	-2.42163100	1.50639000
C	4.35839100	-1.02393500	-0.62979700
H	3.86389300	0.45548200	-2.11777400
H	4.49331300	-2.52422300	0.90861700
H	5.40864900	-1.07392300	-0.89777700

COM2_b

C	-1.88699500	-1.16398500	1.80521300
C	-0.98684700	-0.60874700	2.91432700
C	-3.34598000	-0.84250000	2.12284400
C	-1.47230100	0.77971300	3.39034800
C	-3.61371600	0.66695700	2.06047300
C	-2.33172200	1.46830700	2.32796800
H	-1.58542500	-0.72396900	0.84321900
H	-2.07241100	0.66338700	4.30009800
H	-3.57750800	-1.16973100	3.14494800
H	-1.73844400	-2.24568600	1.71323300
H	-1.03311700	-1.30348000	3.76655100
H	-4.02983500	-1.38195900	1.46127100
H	-0.60613400	1.39715000	3.65362300
H	-4.00047500	0.93510300	1.06485400
H	-2.59970100	2.48319400	2.64517500
H	-1.76337500	1.57330100	1.39665600
N	0.39643800	-0.54636800	2.41538100
H	1.06395900	-0.44372700	3.17596100
H	0.62966000	-1.38128200	1.85585500
O	-4.61591300	0.92765300	3.03937400
H	-4.90299600	1.84408400	2.95902400
C	1.96939200	3.87523500	-2.18831800

C	3.23943800	3.96566500	-1.33805500
N	1.76193300	2.41365800	-0.35298200
H	2.14659500	3.55894000	-3.21862900
H	3.42222600	4.95881000	-0.92159500
C	3.01290300	2.99497300	-0.18282200
O	3.77833300	2.75714200	0.72049800
C	1.11379400	2.82163400	-1.49719400
O	0.04013200	2.40415600	-1.88273400
Br	1.04615900	1.10330700	0.89300900
H	1.39914900	4.80681800	-2.22256700
H	4.14350900	3.66006600	-1.86994700
C	2.70129300	-3.86003600	0.18567500
C	1.83317600	-2.86135900	-0.60535800
C	4.18610100	-3.67912600	-0.13467300
C	2.61626100	-1.56564900	-0.88512100
C	4.68256500	-2.30197900	0.32613200
C	3.55153000	-1.26303900	0.28173100
H	2.53365500	-3.68611700	1.25759800
H	3.21381900	-1.68083100	-1.79767100
H	4.34349400	-3.74027800	-1.21851000
H	2.38193000	-4.88742300	-0.02025100
H	1.57067300	-3.32067300	-1.57284500
H	4.79214400	-4.46978600	0.31645700
H	1.91416700	-0.74392500	-1.05795200
H	5.06631400	-2.37553600	1.35510000
H	3.97048500	-0.25135600	0.22072000
H	2.98403500	-1.30030900	1.22061000
N	0.62549400	-2.54604700	0.17517700
H	-0.00234900	-1.96171900	-0.38915000
H	0.12223300	-3.40898800	0.37603400
O	5.75018600	-1.95332300	-0.55012800
H	6.13296000	-1.11875300	-0.25623100
C	-2.72868900	0.70207200	-1.76051600
C	-1.94896700	-0.30875700	-2.61997600
C	-4.23479800	0.53991500	-1.95605800
C	-2.74783500	-1.61203000	-2.81008200
C	-4.71510500	-0.82884900	-1.46041400
C	-3.60136200	-1.88292800	-1.57435200
H	-2.46610900	0.52827200	-0.70688600
H	-3.40402300	-1.53130400	-3.68487600
H	-4.47885900	0.60600800	-3.02392700
H	-2.40000600	1.71807900	-1.99239800
H	-1.78087400	0.14629900	-3.60856100
H	-4.79369100	1.33857200	-1.45854400
H	-2.05210900	-2.43676400	-3.00302000
H	-5.03224000	-0.74733000	-0.40935700
H	-4.05163100	-2.88281800	-1.60167400

H	-2.95852000	-1.84568000	-0.68460600
N	-0.67336000	-0.60662200	-1.94934900
H	-0.03633700	-1.04262000	-2.61487200
H	-0.24351600	0.27839700	-1.67642000
O	-5.84252700	-1.16966400	-2.26267800
H	-6.24492400	-1.97317100	-1.91469100

TS3_b

C	1.30275200	-2.52634700	-0.10515000
C	0.40966600	-2.58100600	-1.34952600
C	2.66041200	-3.16240700	-0.39866900
C	1.22837800	-2.28029600	-2.63291100
C	3.45185900	-2.34586700	-1.43086300
C	2.52400800	-1.52245700	-2.33340700
H	1.43490000	-1.47610500	0.18929300
H	1.48667300	-3.22732400	-3.12177900
H	2.51021700	-4.16390900	-0.82217600
H	0.81030700	-3.03793300	0.73162600
H	0.01826400	-3.60661200	-1.43032200
H	3.24760900	-3.29404300	0.51592200
H	0.61021100	-1.71170500	-3.33606800
H	4.13688600	-1.65954000	-0.90941800
H	3.04826000	-1.28117000	-3.26563900
H	2.29969200	-0.55969100	-1.86208900
N	-0.76178800	-1.70914100	-1.14486700
H	-1.42924400	-1.86675600	-1.89919800
H	-1.24527800	-1.58114500	0.24304200
O	4.21342400	-3.29706900	-2.17009800
H	4.77595600	-2.82603800	-2.79520500
C	0.19351600	4.74027200	-0.83175800
C	1.26281300	4.45247900	-1.88632200
N	0.17055500	2.41838200	-1.31384600
H	-0.60347100	5.40526000	-1.17443000
H	2.27671600	4.71345600	-1.57298800
C	1.18395700	2.93371700	-2.08905400
O	1.91545500	2.28587400	-2.81373000
C	-0.40635000	3.36361600	-0.53462500
O	-1.27128600	3.15850600	0.31777800
Br	-0.31949300	0.28365100	-1.27131000
H	0.58860900	5.15652700	0.09906600
H	1.08006800	4.94123400	-2.84660100
C	-3.77220800	-2.30704500	1.08156900
C	-2.97696600	-1.06782600	1.51982700
C	-5.21101200	-1.91189200	0.74769300
C	-3.40126600	0.18945600	0.73578700
C	-5.26521300	-0.98880800	-0.47949300
C	-3.96316700	-0.18739100	-0.63217900

H	-3.29553600	-2.74711000	0.19447600
H	-4.18869600	0.70091500	1.30102600
H	-5.64685300	-1.36011400	1.58991100
H	-3.74753100	-3.07135000	1.86591400
H	-3.14351700	-0.89041500	2.58934800
H	-5.83779600	-2.79318100	0.58929400
H	-2.57108600	0.89614000	0.64124400
H	-5.42613200	-1.59186300	-1.38589100
H	-4.14613500	0.71131700	-1.23141300
H	-3.22919400	-0.77962600	-1.19103500
N	-1.51794700	-1.32661400	1.34460200
H	-0.98921600	-0.47291400	1.67763400
H	-1.23075600	-2.11651300	1.92441200
O	-6.38629800	-0.13911900	-0.27104600
H	-6.50904800	0.41990200	-1.04661600
C	1.73662900	1.53743600	1.61659900
C	0.83073400	1.46995900	2.85962700
C	3.16927000	1.13281900	1.95446900
C	1.32649000	0.40058100	3.85023000
C	3.23173600	-0.34012900	2.36798600
C	1.94338600	-0.77335700	3.09479300
H	1.33311200	0.87137800	0.84334400
H	2.08047500	0.82946300	4.52022000
H	3.54534700	1.72863300	2.79576100
H	1.70828400	2.54529000	1.18930200
H	0.85941500	2.44733000	3.36406600
H	3.84181700	1.31199500	1.11122900
H	0.49133200	0.07473000	4.48212400
H	3.36077400	-0.96280800	1.46849300
H	2.17281500	-1.61018100	3.76532700
H	1.22041800	-1.14656300	2.35831800
N	-0.54559500	1.15529800	2.42802300
H	-1.18581200	1.34221500	3.19899000
H	-0.81884400	1.80475300	1.68004200
O	4.37540200	-0.47149800	3.20455500
H	4.54156700	-1.40576900	3.37253500

INT3-1_b

C	1.45013300	-2.49587300	-0.18403500
C	0.56525900	-2.54816200	-1.43376400
C	2.83593500	-3.05865000	-0.49507600
C	1.37676000	-2.18085800	-2.70421500
C	3.59276500	-2.16236400	-1.48534200
C	2.63223100	-1.36759200	-2.38043200
H	1.53721400	-1.45124500	0.14514000
H	1.68276100	-3.10392700	-3.21130900
H	2.73319500	-4.04696700	-0.96177200

H	0.97636600	-3.05620900	0.63228800
H	0.21324600	-3.58496900	-1.54566200
H	3.42653800	-3.20308900	0.41522700
H	0.73530500	-1.62903800	-3.40030900
H	4.22304800	-1.45232900	-0.92763000
H	3.15228300	-1.08679200	-3.30396600
H	2.35973200	-0.42420600	-1.89529300
N	-0.65098400	-1.74492100	-1.20962100
H	-1.28606700	-1.89892800	-1.99250900
H	-1.19849700	-1.57349500	0.35166300
O	4.42576600	-3.04134100	-2.23636600
H	4.96721500	-2.51805900	-2.83825400
C	-0.21898800	4.80838300	-0.85453300
C	1.00002500	4.60488300	-1.75397500
N	0.09147800	2.47460800	-1.18627700
H	-1.04340000	5.34076500	-1.33656100
H	1.93068400	4.99495200	-1.33383900
C	1.11412300	3.07775300	-1.87692500
O	1.99658100	2.49476900	-2.48226300
C	-0.67401700	3.38043800	-0.53860500
O	-1.59747200	3.10966600	0.23587600
Br	-0.30175000	0.23129500	-1.25817500
H	-0.00103100	5.32537800	0.08386600
H	0.88964700	5.02952000	-2.75490500
C	-3.66311500	-2.40528700	1.11786400
C	-2.94108000	-1.10973300	1.51558200
C	-5.11520300	-2.10075700	0.74742100
C	-3.41545900	0.09376000	0.67950300
C	-5.19873600	-1.22360400	-0.51180000
C	-3.93465200	-0.36704200	-0.67982700
H	-3.14941800	-2.85261000	0.25554500
H	-4.23779000	0.58174500	1.21492100
H	-5.59586000	-1.54645400	1.56289900
H	-3.61145900	-3.13579200	1.93247800
H	-3.11802200	-0.90047500	2.57701700
H	-5.68827000	-3.02126200	0.61065300
H	-2.62600900	0.84407500	0.56930200
H	-5.32145200	-1.86390200	-1.39834700
H	-4.14914200	0.49687200	-1.31836500
H	-3.16258900	-0.94625400	-1.20013800
N	-1.46476000	-1.30053600	1.36970100
H	-0.97380900	-0.38845200	1.66696200
H	-1.14276000	-2.05261200	1.98095000
O	-6.36006200	-0.42115200	-0.34153500
H	-6.49473200	0.11389900	-1.13195400
C	1.76678000	1.50975400	1.58378500
C	0.79176100	1.48005400	2.77445800

C	3.17072700	1.09231600	2.01486900
C	1.20847200	0.41404400	3.80534100
C	3.18940000	-0.37320200	2.45922200
C	1.84689800	-0.77846500	3.09760600
H	1.39948700	0.83756700	0.79860800
H	1.93264200	0.83525200	4.51188800
H	3.50455900	1.69935000	2.86583900
H	1.77876700	2.50805700	1.13537400
H	0.81070700	2.46357600	3.26612200
H	3.89348900	1.24776100	1.20963000
H	0.33315700	0.11199100	4.39356300
H	3.37774700	-1.01505900	1.58457300
H	2.01123000	-1.61776200	3.78392400
H	1.17122700	-1.13670800	2.30975300
N	-0.57101900	1.18506000	2.28363800
H	-1.24229600	1.41860600	3.01520600
H	-0.81176000	1.80715200	1.50051400
O	4.26525800	-0.49844600	3.38214300
H	4.42167800	-1.43148000	3.56537300

INT3_b

C	2.32068700	-1.99790100	0.23012100
C	1.68797200	-2.58532200	-1.03527700
C	3.84348200	-2.08539800	0.13597200
C	2.49502900	-2.19872300	-2.30031400
C	4.39348800	-1.18804500	-0.98197000
C	3.33998600	-0.94405700	-2.07135800
H	2.00279800	-0.95204400	0.34047200
H	3.16973800	-3.02333400	-2.55854900
H	4.13422200	-3.11602100	-0.10506900
H	1.94926800	-2.53616100	1.10888400
H	1.70979400	-3.68048100	-0.93580500
H	4.32115300	-1.84402500	1.09040300
H	1.81535200	-2.06287700	-3.14798700
H	4.70028200	-0.21775200	-0.56103800
H	3.84112500	-0.64267200	-2.99890000
H	2.69674400	-0.10509700	-1.78101900
N	0.24310500	-2.28965100	-1.05512600
H	-0.19255000	-2.87415500	-1.76784400
H	-0.39854700	-1.78104000	0.91278800
O	5.53943400	-1.86242400	-1.49098700
H	5.98046400	-1.29463100	-2.13287700
C	-3.11027200	4.26623100	-1.34608600
C	-2.45871400	3.72850700	-2.61993500
N	-1.66300300	2.45321500	-0.76636200
H	-4.19718800	4.15150200	-1.32219700
H	-1.83094200	4.45877200	-3.13720600

C	-1.57036000	2.58257600	-2.11983100
O	-0.87361300	1.88673000	-2.85121500
C	-2.49914900	3.39739900	-0.24428600
O	-2.72039500	3.53444700	0.95784800
Br	-0.17539700	-0.52001800	-1.67497500
H	-2.88789800	5.31553500	-1.13671600
H	-3.16748900	3.33194800	-3.35104900
C	-2.49305000	-2.95533300	2.25638300
C	-2.11593800	-1.47998300	2.00497700
C	-3.96095500	-3.21319000	1.91536300
C	-2.91797800	-0.91057100	0.81605300
C	-4.21001800	-3.03147100	0.41149200
C	-3.22842500	-2.01435900	-0.19355200
H	-1.85356900	-3.59205800	1.62849300
H	-3.86584700	-0.49710500	1.17959900
H	-4.59684400	-2.49130400	2.44288700
H	-2.27742800	-3.22559200	3.29607100
H	-2.36916000	-0.89951100	2.90261300
H	-4.28109000	-4.20872700	2.23483100
H	-2.37800300	-0.08642700	0.33935100
H	-4.08716200	-3.99922100	-0.09896600
H	-3.64688800	-1.59537500	-1.11618600
H	-2.29976600	-2.52582400	-0.47878200
N	-0.66659200	-1.30187300	1.77928400
H	-0.47444500	0.52717500	1.58810000
H	-0.15210400	-1.75913900	2.53098600
O	-5.56045400	-2.60071500	0.28733600
H	-5.78218200	-2.51986700	-0.64709400
C	1.57289200	2.07108900	0.46802400
C	0.61218800	2.36759600	1.63287300
C	3.02074500	2.30003000	0.89270300
C	1.26080100	2.07129400	2.99469900
C	3.43488600	1.30273400	1.98101700
C	2.23877700	0.90462800	2.86511800
H	1.44103600	1.02615300	0.16087700
H	1.80656000	2.95643600	3.33992900
H	3.14182000	3.30915600	1.30546100
H	1.30014000	2.66969300	-0.40594500
H	0.28752300	3.41276600	1.59222100
H	3.69947100	2.22706800	0.03785500
H	0.48402600	1.86885300	3.74056500
H	3.84217200	0.39581800	1.50864700
H	2.60673100	0.58350400	3.84618800
H	1.72441900	0.04070000	2.42200500
N	-0.61591300	1.55642100	1.43406700
H	-1.38133800	1.90276400	2.01990900
H	-0.99174600	1.75755700	0.39855000

O	4.45528300	1.94586400	2.73488800
H	4.85458600	1.31130900	3.34054700

TS4_b

C	2.36960000	-1.95084500	0.26329000
C	1.76505300	-2.56628500	-1.00248100
C	3.89512500	-2.01303000	0.19143100
C	2.57926200	-2.17807700	-2.26251200
C	4.44816200	-1.12784200	-0.93528000
C	3.40233200	-0.90834100	-2.03667600
H	2.03168100	-0.90958500	0.35687800
H	3.26989300	-2.99405300	-2.50582300
H	4.20773300	-3.04275400	-0.02498700
H	1.99645100	-2.48438600	1.14402500
H	1.80711200	-3.65958400	-0.88957500
H	4.35310500	-1.74494400	1.14844100
H	1.90654600	-2.06133800	-3.11868800
H	4.74486700	-0.14914900	-0.52714700
H	3.90813400	-0.60731900	-2.96182600
H	2.74407000	-0.07679800	-1.75887500
N	0.31450200	-2.30218300	-1.04548600
H	-0.09637600	-2.89105000	-1.76936600
H	-0.35456300	-1.81353200	0.93428800
O	5.60299000	-1.80144800	-1.42566300
H	6.04935700	-1.23640200	-2.06625300
C	-3.40497900	4.00936800	-1.42027100
C	-2.61701700	3.54769200	-2.64675000
N	-1.76571000	2.41758600	-0.73356200
H	-4.46360100	3.73799700	-1.44947800
H	-2.05907500	4.34922600	-3.13780000
C	-1.61779900	2.53071300	-2.08555500
O	-0.80604100	1.91514000	-2.76489300
C	-2.74068900	3.25876900	-0.26522800
O	-3.02625000	3.38577600	0.91887300
Br	-0.12118900	-0.53792900	-1.66090400
H	-3.34767400	5.08326900	-1.22747200
H	-3.22489200	3.05819900	-3.41138600
C	-2.44995800	-2.96293300	2.28819900
C	-2.07241700	-1.49024400	2.01682900
C	-3.91370600	-3.23101300	1.93736900
C	-2.87560100	-0.93899900	0.82066700
C	-4.14817500	-3.07366100	0.42859600
C	-3.17021200	-2.05487900	-0.18030400
H	-1.80333500	-3.60785000	1.67606500
H	-3.82886300	-0.53082700	1.17615300
H	-4.55722100	-2.50322800	2.44716900
H	-2.24303700	-3.21710700	3.33365300

H	-2.32611100	-0.89684900	2.90563700
H	-4.23412300	-4.22268200	2.26855900
H	-2.33918600	-0.11402800	0.34247700
H	-4.01013400	-4.04743500	-0.06630400
H	-3.58650200	-1.64923500	-1.11006400
H	-2.23545300	-2.56164300	-0.45454600
N	-0.62501700	-1.31312800	1.78684200
H	-0.44641300	0.57836600	1.52806000
H	-0.10911800	-1.74724500	2.55101800
O	-5.50162100	-2.65861900	0.28324100
H	-5.71373200	-2.59484800	-0.65472000
C	1.54278000	2.14221500	0.41352100
C	0.57968400	2.43257400	1.57923900
C	2.99015900	2.39623900	0.82601800
C	1.24897200	2.17828600	2.94100100
C	3.42320700	1.41648400	1.92256500
C	2.24079300	1.02217100	2.82646400
H	1.42587200	1.09244700	0.11695200
H	1.78635200	3.07790100	3.26198900
H	3.10092500	3.41158300	1.22622700
H	1.25915600	2.72771400	-0.46632400
H	0.23839800	3.47272900	1.52625300
H	3.66501700	2.32113700	-0.03194300
H	0.48218400	1.98040800	3.69817000
H	3.83015900	0.50598900	1.45676200
H	2.62270100	0.72580700	3.81020200
H	1.73265300	0.14249400	2.40757600
N	-0.62730600	1.59582800	1.39255800
H	-1.37856500	1.88902400	2.02223100
H	-1.08822400	1.83971100	0.29768300
O	4.45011900	2.07494000	2.65466900
H	4.84912000	1.45419600	3.27468700

INT4_b

C	2.39514100	-1.93808300	0.18416900
C	1.75037500	-2.49157700	-1.09021700
C	3.91674600	-2.04125700	0.07630300
C	2.54624500	-2.07954700	-2.35389700
C	4.47571300	-1.14008800	-1.03520800
C	3.41145000	-0.84379000	-2.09995900
H	2.08748800	-0.89295400	0.32742600
H	3.20621100	-2.90502100	-2.64495200
H	4.19436300	-3.07278100	-0.17639600
H	2.02701300	-2.49545100	1.05176300
H	1.76213400	-3.58922200	-1.01733300
H	4.40037900	-1.81500400	1.03122400
H	1.85697000	-1.91081200	-3.18826600

H	4.82270700	-0.18877500	-0.60472900
H	3.90407000	-0.52168100	-3.02510800
H	2.78622700	-0.00495000	-1.77170900
N	0.30422200	-2.19665600	-1.09683800
H	-0.12876100	-2.73150600	-1.84963400
H	-0.27643800	-1.74573800	0.98940900
O	5.58847000	-1.84249000	-1.58146700
H	6.05358100	-1.26475500	-2.19685200
C	-4.09794400	2.87761800	-1.73478200
C	-2.98714700	2.82683400	-2.78802100
N	-2.04501200	2.40403000	-0.67117000
H	-4.86937100	2.11645500	-1.87454400
H	-2.82827100	3.77711200	-3.30365200
C	-1.72441800	2.48776200	-2.00386300
O	-0.61515500	2.31047300	-2.47114500
C	-3.38851400	2.60514200	-0.41088900
O	-3.89563300	2.56355300	0.68772300
Br	-0.08488000	-0.39086600	-1.60786900
H	-4.60106500	3.84491300	-1.66794800
H	-3.13583600	2.06024300	-3.55201300
C	-2.36428200	-2.82312100	2.41880100
C	-1.92861700	-1.36536800	2.14612500
C	-3.84631600	-3.02562300	2.10210600
C	-2.74983200	-0.76624400	0.98819300
C	-4.10293800	-2.85733000	0.59947300
C	-3.11555400	-1.85282900	-0.02141000
H	-1.76145700	-3.49143500	1.78679400
H	-3.67121000	-0.31578900	1.37391200
H	-4.44484900	-2.26958500	2.62528000
H	-2.14292100	-3.09449400	3.45695500
H	-2.12108500	-0.76886800	3.04779200
H	-4.20472500	-4.00261100	2.43831400
H	-2.17984200	0.03945900	0.51863300
H	-3.98756300	-3.83190400	0.09956500
H	-3.55398800	-1.41853500	-0.92918000
H	-2.20626400	-2.38124800	-0.33872100
N	-0.48896100	-1.24451700	1.85588000
H	-0.29652700	0.83272300	1.61703800
H	0.04191300	-1.70546500	2.59339900
O	-5.45244000	-2.42243900	0.47568100
H	-5.67783600	-2.35567900	-0.45875500
C	1.67635800	2.19607500	0.41771700
C	0.80857100	2.58583000	1.62902600
C	3.16316000	2.37135800	0.71770400
C	1.57016000	2.33673200	2.94970700
C	3.60972000	1.39803300	1.81417200
C	2.47149100	1.11226400	2.80937800

H	1.47529600	1.14357000	0.18073200
H	2.19047900	3.20650800	3.19823100
H	3.36338200	3.38917100	1.07509600
H	1.36814500	2.75853900	-0.46908000
H	0.56320300	3.65370900	1.56530200
H	3.77161000	2.22846300	-0.18136200
H	0.84993200	2.21425900	3.76640900
H	3.92170200	0.44839700	1.35268400
H	2.90155000	0.81522700	3.77362300
H	1.87480100	0.25951000	2.45515400
N	-0.45757100	1.84579200	1.53175200
H	-1.08829800	2.10974000	2.28790000
H	-1.35624400	2.17641200	0.11231500
O	4.73172800	2.00258700	2.44913600
H	5.09828700	1.38941700	3.09616600

M2

C	0.65810200	1.38200900	-0.57628200
C	0.07408100	0.93363600	0.76359500
C	2.15921600	1.09366500	-0.59553000
C	0.67779000	-0.41297500	1.23019700
C	2.44214600	-0.41356200	-0.57774600
C	1.29224300	-1.19538800	0.06950200
H	0.16317000	0.84884600	-1.39520600
H	1.45865900	-0.21355600	1.96959800
H	2.61738000	1.52605700	0.30096600
H	0.46032400	2.44535200	-0.72086200
H	0.32564400	1.69844200	1.50986000
H	2.64049600	1.55998800	-1.45642500
H	-0.09005600	-1.00366500	1.73689500
H	2.58205300	-0.77646900	-1.60237500
H	1.66572800	-2.16489600	0.41150100
H	0.53017300	-1.40183100	-0.68650400
N	-1.39646900	1.02636400	0.74280400
H	-1.74286100	0.82830200	1.68033100
O	3.66421200	-0.58553200	0.14460400
H	3.92329700	-1.51022700	0.08546300
Br	-2.22554000	-0.36174100	-0.28777500

COM2'b

C	-3.58466600	0.15261100	-2.74906100
C	-4.38204500	1.44692500	-2.50148300
C	-2.09336900	0.36483000	-2.49299500
C	-3.68702800	2.32524800	-1.44499300
C	-1.85093100	0.65132000	-1.00767900
C	-3.01908100	1.44594000	-0.39231600
H	-3.96319300	-0.61685500	-2.06114600

H	-2.92909400	2.95729300	-1.92243000
H	-1.72712600	1.22532100	-3.06683600
H	-3.76246600	-0.21445600	-3.76528200
H	-4.42357500	2.01310900	-3.44649900
H	-1.50452000	-0.50089700	-2.81028300
H	-4.42436700	2.99686900	-0.99063000
H	-1.76393800	-0.31221000	-0.47627200
H	-2.64582800	2.03858500	0.45031500
H	-3.76928800	0.75219300	0.00992400
N	-5.71916200	1.08708000	-2.01582200
H	-6.32579300	1.90216400	-1.99339300
H	-6.15478600	0.40754600	-2.63388700
O	-0.61891100	1.35158900	-0.90224500
H	-0.44036600	1.55291100	0.06938000
C	3.78565200	-3.66901100	-0.51379900
C	3.44699700	-3.84784100	-1.99782300
N	2.24631000	-2.01461400	-1.14600900
H	4.84027000	-3.45520800	-0.32620700
H	2.98353100	-4.80985700	-2.22776800
C	2.44655900	-2.74796800	-2.32200500
O	1.91234700	-2.52643700	-3.37589300
C	2.96794700	-2.47150900	-0.05690800
O	2.93807200	-1.99551300	1.05549500
Br	1.09615100	-0.55041600	-1.05990700
H	3.50786900	-4.52577700	0.10439500
H	4.30794100	-3.73062400	-2.65985100
C	0.82132400	4.08307400	1.38004200
C	1.12231900	2.67462800	1.92279600
C	2.11477000	4.79471700	0.98167500
C	2.34644800	2.06259000	1.21502900
C	2.78577100	4.08683000	-0.20312600
C	2.45141100	2.58720200	-0.21645400
H	0.16698900	3.98656200	0.50238100
H	3.25801400	2.34177700	1.75668300
H	2.82236900	4.77408200	1.82011000
H	0.26860000	4.66584800	2.12528700
H	1.35297100	2.75715200	2.99660100
H	1.93789600	5.84710800	0.74321600
H	2.28165400	0.96912400	1.24688500
H	2.44018800	4.53977200	-1.14445600
H	3.21978100	2.04534600	-0.78154400
H	1.50638000	2.42917900	-0.74930100
N	-0.05342400	1.80836200	1.71687400
H	0.12284500	0.88401900	2.13679000
H	-0.85761200	2.20806900	2.19988400
O	4.18524300	4.31636200	-0.05584300
H	4.64211500	3.95139000	-0.82174900

C	-0.61808700	-2.57951100	1.66902800
C	-0.36300300	-1.92343900	3.03702000
C	-2.05127000	-3.09847200	1.56881700
C	-1.64969500	-1.26544500	3.57611700
C	-3.05183800	-1.93670800	1.59667800
C	-2.50584400	-0.75571700	2.41819100
H	-0.43898800	-1.83321600	0.88516300
H	-2.23242000	-1.99177100	4.15523000
H	-2.27723900	-3.74728500	2.42440600
H	0.10626700	-3.38528300	1.50381700
H	-0.05749400	-2.71166300	3.74321600
H	-2.20047400	-3.69923000	0.66724100
H	-1.37763600	-0.45322200	4.26022000
H	-3.24963700	-1.59829400	0.56783200
H	-3.34487800	-0.14374800	2.77102300
H	-1.89588600	-0.11139800	1.77104400
N	0.68795600	-0.90627700	2.88545200
H	1.10584900	-0.69633700	3.78883000
H	1.43724400	-1.24951600	2.28420400
O	-4.25164600	-2.45757200	2.15945900
H	-4.95410300	-1.80508700	2.05844100

TS3'b

C	3.29519100	-2.44119200	2.32419200
C	4.54690600	-2.01888500	1.53389100
C	2.09696100	-1.56279800	1.96813700
C	4.15903400	-1.45402200	0.15341500
C	1.68999500	-1.75404400	0.49225600
C	2.90413400	-2.14977700	-0.36538900
H	3.07027400	-3.48710800	2.07488800
H	3.96352800	-0.37679700	0.23468200
H	2.35723400	-0.50315000	2.09805300
H	3.49948100	-2.40800500	3.39999000
H	5.05714800	-1.22163800	2.10001100
H	1.24761100	-1.75765000	2.62886400
H	5.00066300	-1.57741800	-0.53809600
H	0.92760400	-2.55302300	0.42782200
H	2.69042600	-1.88491400	-1.40772100
H	3.06188800	-3.23479700	-0.32889900
N	5.40265100	-3.19529800	1.34690900
H	6.30955600	-2.92796200	0.97454000
H	5.56877200	-3.66161300	2.23488800
O	1.16047200	-0.56022800	-0.03249700
H	0.88335300	0.24204800	-1.53889400
C	-4.27477800	1.94990900	2.18812000
C	-3.97276600	1.10011900	3.42241700
N	-2.32807700	0.67365800	1.75939700

H	-4.21875700	3.02657300	2.36931600
H	-4.74944000	0.36502400	3.64773600
C	-2.68834600	0.35004800	3.05910900
O	-2.08558000	-0.40735700	3.78541700
C	-3.17493600	1.57048100	1.20086500
O	-3.09066100	2.02571400	0.05808300
Br	-0.53778800	0.01673100	0.88096000
H	-5.24533100	1.74544600	1.72919800
H	-3.79429100	1.67999600	4.33068400
C	2.64273500	2.15145800	-2.29704500
C	1.10243600	2.18129500	-2.26088500
C	3.22022600	3.40995700	-1.64670800
C	0.59577700	2.88553200	-0.98708100
C	2.88868000	3.45597300	-0.14734300
C	1.59325200	2.69172100	0.15534400
H	2.98809200	1.26283200	-1.74935500
H	0.49586000	3.95843300	-1.18817800
H	2.77877200	4.30244700	-2.10785300
H	2.99519800	2.04506900	-3.32900900
H	0.73319000	2.72701700	-3.13945000
H	4.30048600	3.47715700	-1.80113700
H	-0.39976300	2.51907300	-0.71482000
H	3.71392300	3.00502300	0.42440500
H	1.16998200	3.04067800	1.10472800
H	1.81034500	1.62526200	0.28694800
N	0.54393300	0.80812100	-2.34435400
H	-0.82270100	0.79197500	-2.31568600
H	0.89771300	0.34726400	-3.18380800
O	2.78262700	4.83732800	0.18569900
H	2.61891400	4.91796700	1.13213500
C	-3.34831600	-1.01473300	-1.29566700
C	-2.76032800	-0.44800200	-2.60224400
C	-3.34970900	-2.54160200	-1.31080000
C	-1.78555700	-1.44275400	-3.25551200
C	-1.91515600	-3.07497200	-1.32588900
C	-0.98788100	-2.18982000	-2.18676600
H	-2.73859600	-0.67901400	-0.45107800
H	-2.35696400	-2.16435000	-3.84989600
H	-3.86553600	-2.92550200	-2.20013200
H	-4.35391700	-0.61344400	-1.13728900
H	-3.57590800	-0.24176800	-3.30405000
H	-3.87978600	-2.93876600	-0.44139200
H	-1.13190000	-0.91420600	-3.96030300
H	-1.52874500	-3.08745000	-0.29618400
H	-0.22203500	-2.82563300	-2.64680700
H	-0.45828800	-1.48128600	-1.53955500
N	-2.06814500	0.85496800	-2.32391300

H	-2.30994500	1.53819100	-3.04068000
H	-2.38266900	1.25767500	-1.42028300
O	-1.99752200	-4.40297500	-1.83167300
H	-1.15542100	-4.84860300	-1.68696100

INT3'-1b

C	3.36358200	-2.16107900	2.47437100
C	4.56513300	-1.87155500	1.55730200
C	2.13521300	-1.36160800	2.04106700
C	4.09401300	-1.54884800	0.12628100
C	1.65350100	-1.81589800	0.64816400
C	2.82708200	-2.33450100	-0.19947100
H	3.13947900	-3.23500700	2.41708700
H	3.88263400	-0.47520100	0.03706300
H	2.38921400	-0.29470500	1.97227400
H	3.62290400	-1.94560500	3.51663100
H	5.09406200	-0.98840100	1.95352000
H	1.32780200	-1.44386800	2.77373800
H	4.89961400	-1.77811100	-0.58076800
H	0.90553800	-2.61940600	0.76905800
H	2.55222300	-2.24697400	-1.25665300
H	3.00756200	-3.39620700	0.00811300
N	5.42499300	-3.05901100	1.52138700
H	6.31077900	-2.85144800	1.06889000
H	5.63669800	-3.37699200	2.46348100
O	1.07243100	-0.74511400	-0.06692000
H	0.86652900	0.15018100	-1.69325500
C	-4.13881300	2.24360400	2.24307900
C	-3.74171800	1.51851400	3.52763700
N	-2.28417300	0.84639900	1.76175300
H	-4.02029900	3.32939900	2.29453400
H	-4.51218000	0.84017200	3.90258500
C	-2.52046700	0.68709300	3.12177100
O	-1.86580500	-0.00627100	3.86724500
C	-3.16054000	1.70071500	1.20681400
O	-3.20109500	2.02602000	0.00883900
Br	-0.51185400	-0.00149100	0.82504100
H	-5.15905700	2.04135100	1.90770500
H	-3.45933100	2.18199700	4.34789100
C	2.65484100	1.96376300	-2.57769800
C	1.11593800	2.04022100	-2.46580600
C	3.31693600	3.18928200	-1.94586200
C	0.70566700	2.79329300	-1.18556200
C	3.05576100	3.23176700	-0.43308700
C	1.73209000	2.53818100	-0.08200600
H	2.99546000	1.05722500	-2.05684500
H	0.66925700	3.87005500	-1.38894400

H	2.89573200	4.10556200	-2.37799200
H	2.95222700	1.85281100	-3.62643100
H	0.72346500	2.58446100	-3.33541100
H	4.39155400	3.21122300	-2.14713600
H	-0.30064900	2.49207800	-0.87471600
H	3.87814600	2.72547500	0.09527200
H	1.36805000	2.89661100	0.88832200
H	1.89529500	1.45922000	0.03108200
N	0.49648600	0.69794500	-2.48150300
H	-1.19248500	0.67496600	-2.21327400
H	0.79092100	0.20285700	-3.32324600
O	3.04430100	4.61122900	-0.07655700
H	2.92512000	4.68546800	0.87704900
C	-3.47661400	-1.08504700	-1.04699200
C	-3.00628800	-0.50969900	-2.39787700
C	-3.44075400	-2.61203300	-1.05919700
C	-2.10566100	-1.49348700	-3.15821800
C	-2.00477100	-3.11701000	-1.21514900
C	-1.19004500	-2.23187700	-2.18231600
H	-2.81794100	-0.73092000	-0.24886300
H	-2.73744400	-2.21501300	-3.68743000
H	-4.03416600	-3.01346100	-1.89033100
H	-4.47861100	-0.71238400	-0.81511000
H	-3.87757300	-0.26374100	-3.01249900
H	-3.87296100	-3.01360300	-0.13925000
H	-1.53310000	-0.95791600	-3.92517300
H	-1.51269700	-3.10264400	-0.23169100
H	-0.47821200	-2.86336800	-2.72656300
H	-0.59327000	-1.51634000	-1.60517800
N	-2.26882600	0.78583700	-2.17379700
H	-2.49331400	1.45285900	-2.91210600
H	-2.54491900	1.24070800	-1.25475100
O	-2.11487800	-4.45616000	-1.68501000
H	-1.25067000	-4.87973900	-1.63623000

INT3'b

C	-4.37026900	-1.07209700	-2.30462600
C	-5.32259400	-0.37351300	-1.31672200
C	-2.93540800	-0.56932600	-2.14723400
C	-4.58050400	0.02273800	-0.02661200
C	-2.38343100	-0.94947300	-0.76330300
C	-3.49746800	-1.00347900	0.29197700
H	-4.40140400	-2.15143000	-2.10258200
H	-4.11813000	1.00993500	-0.14652500
H	-2.90737100	0.52534000	-2.22817000
H	-4.72013800	-0.93079200	-3.33250100
H	-5.70030400	0.54635800	-1.79261700

H	-2.29083900	-0.96115500	-2.93825500
H	-5.30076700	0.10349500	0.79498000
H	-1.87371100	-1.92422800	-0.81956800
H	-3.05215400	-0.83562800	1.27899300
H	-3.94744000	-2.00389300	0.30139900
N	-6.40295700	-1.30408300	-0.97564800
H	-7.13497700	-0.83269500	-0.45167800
H	-6.83263800	-1.68094900	-1.81632000
O	-1.45204200	0.02315300	-0.29376900
H	-0.74006500	0.64727100	1.43151400
C	5.53679300	0.17732800	-1.69117500
C	4.51891200	0.34465300	-2.81995800
N	3.32807700	0.00271700	-0.78222400
H	6.16107400	1.05868100	-1.52344800
H	4.58510900	-0.42262700	-3.59557300
C	3.17322800	0.21012900	-2.10441400
O	2.08725400	0.28588800	-2.69579400
C	4.65847700	-0.04904500	-0.45754800
O	5.07714100	-0.25391000	0.67666900
Br	0.11441600	0.10607900	-1.33593900
H	6.20471200	-0.67853700	-1.81614600
H	4.55981100	1.31713300	-3.31695700
C	-1.23243800	3.10282700	2.53009900
C	0.08112800	2.32816600	2.29093000
C	-1.11959700	4.54171700	2.02449200
C	0.77016000	2.81852300	1.00158300
C	-0.94923800	4.57398500	0.49846000
C	-0.27300600	3.29191200	-0.01001900
H	-2.04557600	2.58923500	1.99697200
H	1.42994200	3.66152700	1.23706800
H	-0.23438300	5.01910700	2.46303400
H	-1.49398100	3.07982000	3.59392500
H	0.75548100	2.51106100	3.13747600
H	-1.98309800	5.14229500	2.32338200
H	1.40202300	2.02586600	0.58594400
H	-1.93572500	4.67510000	0.02094200
H	0.18191300	3.47020800	-0.99143300
H	-1.03174800	2.51413000	-0.16418800
N	-0.13080500	0.86890800	2.22499700
H	1.35263100	-0.07565700	1.82075000
H	-0.62936000	0.56095100	3.05925500
O	-0.16852500	5.73149100	0.21761100
H	-0.07022700	5.81912900	-0.73729100
C	1.91326900	-2.75764800	0.38396700
C	2.11764700	-2.07275700	1.74780800
C	1.16365100	-4.07666200	0.56244600
C	0.95788000	-2.38577500	2.70954400

C	-0.26473500	-3.82782000	1.06562400
C	-0.33866100	-2.54592400	1.91531600
H	1.33937200	-2.09497400	-0.27275200
H	1.16502900	-3.32205500	3.23929800
H	1.67046800	-4.70797800	1.30294000
H	2.88034200	-2.90833000	-0.10378500
H	3.06348700	-2.40884300	2.18220800
H	1.14009400	-4.64364500	-0.37147200
H	0.88108100	-1.60195200	3.47094200
H	-0.94614700	-3.73223400	0.20727600
H	-1.20955900	-2.60315700	2.57979900
H	-0.49569900	-1.67401400	1.26338100
N	2.23769200	-0.59032200	1.55597200
H	3.01833900	-0.22042400	2.10213300
H	2.51544300	-0.34155800	0.52824300
O	-0.62199200	-4.97634400	1.82727400
H	-1.55698500	-4.92616100	2.05586000

TS4'b

C	-4.40514800	-1.15505400	-2.25022100
C	-5.29112700	-0.67276200	-1.08744900
C	-2.93832600	-0.79033100	-2.01924800
C	-4.50291400	-0.67482400	0.23617400
C	-2.38824200	-1.54477600	-0.79775500
C	-3.48545700	-1.81219600	0.24047400
H	-4.50214700	-2.24648400	-2.32496600
H	-3.97914200	0.28185000	0.36015500
H	-2.84789500	0.28665100	-1.82155700
H	-4.76276700	-0.73860700	-3.19761300
H	-5.60411500	0.36306700	-1.29992400
H	-2.33564000	-1.00042000	-2.90638600
H	-5.20116700	-0.76756600	1.07515100
H	-1.92134600	-2.48994500	-1.11214800
H	-3.01272000	-1.93757900	1.22040000
H	-3.99925400	-2.75045600	0.00083100
N	-6.43256100	-1.58310000	-0.96279200
H	-7.11971400	-1.21622800	-0.31030100
H	-6.90091900	-1.70030900	-1.85735200
O	-1.41111600	-0.77139200	-0.09495000
H	-0.85286200	0.17510300	1.61354300
C	5.19818800	1.98884900	-1.82451600
C	4.21113600	1.45070900	-2.86091800
N	3.35611100	0.97637700	-0.69706100
H	5.30340400	3.07660000	-1.84362800
H	4.62608400	0.66393100	-3.49639500
C	3.08615200	0.84706400	-2.02147700
O	2.08659900	0.31914300	-2.50608900

C	4.57727700	1.58241400	-0.48825300
O	5.07391700	1.75416100	0.61073300
Br	0.07174700	-0.31939300	-1.12291100
H	6.20038600	1.56038900	-1.89620000
H	3.79015800	2.21417200	-3.51921300
C	-1.97565100	2.40552500	2.65872100
C	-0.50275600	2.06297700	2.33499400
C	-2.38385800	3.74854500	2.05123300
C	-0.09315700	2.67694000	0.98289600
C	-2.34632500	3.68518100	0.51829500
C	-1.29008800	2.67976900	0.03225400
H	-2.61645400	1.61241700	2.24581100
H	0.23864400	3.71137500	1.12950200
H	-1.68062700	4.52955600	2.36562300
H	-2.13571100	2.39927600	3.74238000
H	0.14041400	2.48500100	3.11740500
H	-3.37472200	4.06085100	2.39275800
H	0.75805500	2.12568000	0.56910600
H	-3.33486200	3.37869700	0.14019100
H	-0.98712600	2.91971200	-0.99419800
H	-1.73395100	1.67583900	-0.00745700
N	-0.25222800	0.61051500	2.31718000
H	1.55780300	0.08159100	1.71913400
H	-0.52851200	0.20694400	3.21122900
O	-2.06237300	5.00834500	0.07671500
H	-2.06652100	5.02533000	-0.88692300
C	3.00761800	-2.12709700	0.21655100
C	2.97753600	-1.48225600	1.62174800
C	2.55916900	-3.58687100	0.25210900
C	2.03973200	-2.24871400	2.56850300
C	1.10185300	-3.69072800	0.70329800
C	0.77835100	-2.67324700	1.81743800
H	2.33661800	-1.57487500	-0.44837200
H	2.55168900	-3.13640400	2.95686200
H	3.17132700	-4.16893800	0.95221800
H	4.00894200	-2.03583100	-0.21530500
H	3.98989500	-1.48397400	2.03780700
H	2.67330200	-4.05228000	-0.73059700
H	1.79685100	-1.61882300	3.43218700
H	0.44425700	-3.48922700	-0.15677400
H	0.04595400	-3.11565900	2.50374100
H	0.29759500	-1.79192800	1.37736100
N	2.56565900	-0.05294700	1.50979200
H	3.08033200	0.51888200	2.17948200
H	2.85227000	0.44414600	0.36411900
O	0.92166300	-5.03466700	1.13846700
H	-0.00911100	-5.17807800	1.34227100

INT4'b

C	-4.37804000	-1.04906700	-2.39008900
C	-5.29583900	-0.64911100	-1.22041400
C	-2.91564900	-0.72094500	-2.08525800
C	-4.54834900	-0.76095100	0.12188400
C	-2.41495600	-1.57937400	-0.91279000
C	-3.54497400	-1.90946800	0.07004500
H	-4.48332400	-2.12975400	-2.55457900
H	-4.01829900	0.17658700	0.33481500
H	-2.82421300	0.33561500	-1.79884900
H	-4.70019300	-0.55393000	-3.31196900
H	-5.59508900	0.40297200	-1.36168100
H	-2.28567900	-0.86597400	-2.96648700
H	-5.27295100	-0.90799700	0.93005900
H	-1.94884200	-2.50257800	-1.28626500
H	-3.10186900	-2.11345500	1.05031400
H	-4.06054400	-2.82065600	-0.25423200
N	-6.44598800	-1.55619000	-1.20001500
H	-7.14973000	-1.23558400	-0.54094800
H	-6.88866900	-1.60101100	-2.11397000
O	-1.45275500	-0.88170800	-0.11071400
H	-0.98780500	0.11542900	1.66636500
C	5.46493000	2.01893600	-1.94470700
C	4.35289600	1.52851200	-2.87502400
N	3.72713300	1.07368500	-0.64982300
H	5.61284600	3.10114800	-1.97577400
H	4.66896100	0.73125200	-3.55247800
C	3.28944400	0.96313000	-1.94097700
O	2.22419800	0.48746300	-2.29853400
C	4.98895900	1.64034600	-0.54524400
O	5.59022200	1.80037000	0.49157400
Br	0.04717700	-0.33420000	-1.04002900
H	6.43437800	1.54938200	-2.12417100
H	3.90092200	2.31502900	-3.48348600
C	-2.21853500	2.29147000	2.71078200
C	-0.72699200	2.01017500	2.40470600
C	-2.67861500	3.61318700	2.09387700
C	-0.32538200	2.65520000	1.06510900
C	-2.61796400	3.54765500	0.56198200
C	-1.50401200	2.59714200	0.09424900
H	-2.82018800	1.46989400	2.29467900
H	-0.05127700	3.70525400	1.21980600
H	-2.01490800	4.42547200	2.41458600
H	-2.39101600	2.28169800	3.79246000
H	-0.11274100	2.45136800	3.19952400
H	-3.68712600	3.88225700	2.42057200

H	0.55940800	2.14452300	0.67182900
H	-3.58438800	3.18932900	0.17187300
H	-1.19962500	2.84932900	-0.92909700
H	-1.89628000	1.57175900	0.05316200
N	-0.40772500	0.57486300	2.37056900
H	1.58786600	0.06348000	1.64990500
H	-0.65093300	0.14604300	3.26171600
O	-2.39650200	4.88231400	0.11863400
H	-2.39094600	4.89589400	-0.84500600
C	3.05662400	-2.04710600	0.26982300
C	3.01576800	-1.44746400	1.69591700
C	2.59646100	-3.50358900	0.23603500
C	2.09085700	-2.27030100	2.61298600
C	1.14111300	-3.62595100	0.68838100
C	0.82548700	-2.66587300	1.85331400
H	2.40117100	-1.45762500	-0.37892300
H	2.60819000	-3.17342300	2.95872600
H	3.20781900	-4.11973700	0.90697000
H	4.06517000	-1.95188600	-0.14629000
H	4.02870900	-1.46143500	2.11369100
H	2.70487300	-3.92599500	-0.76706200
H	1.84786200	-1.67888700	3.50345500
H	0.47780800	-3.38394000	-0.15710600
H	0.09749800	-3.14252200	2.52180300
H	0.34048900	-1.76400200	1.46277700
N	2.61094200	-0.02618600	1.61696800
H	2.94694400	0.47154700	2.43900300
H	3.22264700	0.68507500	0.21541400
O	0.96056100	-4.99117000	1.05613600
H	0.03616500	-5.13358500	1.28770600

M2'

C	-1.24700400	-0.96685000	0.88730800
C	-2.04615100	-0.55968300	-0.37301800
C	-0.42446900	0.19075000	1.48433900
C	-2.42155700	0.91832800	-0.28292200
C	0.03634200	1.15160200	0.39766700
C	-1.16860600	1.81023900	-0.29196700
H	-1.95330900	-1.32866900	1.64540600
H	-3.08161800	1.17634100	-1.11517600
H	0.42659700	-0.18741700	2.05829900
H	-0.58880000	-1.80855000	0.64360500
H	-1.40050500	-0.68402800	-1.25031200
H	-1.03684800	0.77556000	2.18195000
H	-2.99492300	1.07875600	0.64241400
H	0.71614800	1.91114900	0.80378500
H	-0.87503600	2.04563400	-1.32057800

H	-1.37326700	2.76317400	0.20703400
N	-3.24130900	-1.36437400	-0.61570800
H	-2.99549200	-2.34166900	-0.74573300
H	-3.86863500	-1.31805600	0.18427900
O	0.71597500	0.46745500	-0.67179700
Br	2.27473500	-0.32964500	-0.14797400

TS5

C	0.12449300	2.93328100	-1.57648500
C	1.36854300	2.49401600	-1.86581600
C	0.74129900	1.55840200	0.07380600
N	-0.26789800	2.35599900	-0.38574400
H	-0.52627300	3.58994400	-2.12974800
H	2.01049300	2.71020900	-2.70375000
N	1.76428300	1.65846700	-0.83151600
C	-1.56134700	2.69262400	0.27088700
C	-2.69727200	2.66952600	-0.74264200
C	-1.42119500	4.04250400	0.96795200
H	-1.74323000	1.90825100	0.99741600
H	-2.73969600	1.70299800	-1.24855800
H	-3.63973100	2.78545400	-0.20218000
H	-2.62399700	3.48044500	-1.47662300
H	-0.61951200	4.01165300	1.71097300
H	-1.20679400	4.84281400	0.25002400
H	-2.35647700	4.28427400	1.47992700
C	3.20128600	1.46100800	-0.53616800
C	3.83464100	2.80210000	-0.16716200
C	3.89975000	0.79246600	-1.71541900
H	3.25126500	0.80820400	0.33259100
H	3.29268500	3.27166700	0.65887800
H	4.87092300	2.64412300	0.14438900
H	3.83422500	3.49018500	-1.01835800
H	3.39182300	-0.12851400	-2.01376100
H	3.94220800	1.45940500	-2.58276700
H	4.92816100	0.54866400	-1.43706100
C	0.62563000	0.69728300	1.22118800
O	-0.04515600	1.29457200	2.29716000
C	1.46054600	-0.45391500	1.55250900
C	1.43928100	-0.94721100	2.87782300
C	2.17741600	-1.21758900	0.60229300
C	2.10062300	-2.11953600	3.22593300
H	0.86231400	-0.42495800	3.63259700
C	2.83802700	-2.38620700	0.96128300
H	2.19147800	-0.93073700	-0.44249800
C	2.81165200	-2.85159900	2.27557500
H	2.05263300	-2.46652200	4.25392700
H	3.37591400	-2.93866900	0.19489600

H	3.32889600	-3.76441400	2.55148700
H	0.60300400	1.71010800	2.88166900
C	-1.47083100	-0.87653000	-1.84828100
C	-0.81668900	-1.16909600	-0.49967400
C	-0.73305200	-1.65172600	-2.95563100
C	-0.99080100	-2.64079400	-0.09856500
C	-0.18915100	-3.00902300	-2.48251200
C	-1.02697500	-3.56330400	-1.33195700
H	-2.52943200	-1.15239700	-1.80467700
H	-0.16394100	-2.91835500	0.56851400
H	0.12414100	-1.07583700	-3.32434300
H	-1.42613600	0.19919100	-2.05091200
H	0.25430500	-1.01917600	-0.67106100
H	-1.40462800	-1.80909300	-3.80588900
H	-1.92397900	-2.74676100	0.46231900
H	-0.19462300	-3.71698900	-3.32311700
H	-0.69342100	-4.57530200	-1.06965400
H	-2.05779000	-3.66440500	-1.69388400
N	-1.17988000	-0.19828900	0.54651800
H	-1.14368200	-0.66784900	1.45657400
O	1.16936100	-2.80030300	-2.07271800
H	1.47058800	-3.58529400	-1.59961700
Br	-3.49417500	-0.45913700	0.76195100

INT5-1

C	1.60025000	-2.71610000	1.62136300
C	2.84781100	-2.27173900	1.33797700
C	1.39725500	-1.10651100	0.10610600
N	0.71821400	-1.99581300	0.84813900
H	1.26095000	-3.48669300	2.29382400
H	3.80765300	-2.57748200	1.72104600
N	2.71422200	-1.28020000	0.39099400
C	-0.70651800	-2.42683000	0.70708300
C	-1.33915100	-2.70377800	2.05982000
C	-0.74214500	-3.63249200	-0.22373400
H	-1.24805800	-1.61234000	0.24245900
H	-1.16994700	-1.88419800	2.76437400
H	-2.41548100	-2.78845900	1.88159300
H	-0.99125200	-3.64293000	2.50490600
H	-0.40375700	-3.35436100	-1.22653300
H	-0.12237000	-4.45025400	0.16487100
H	-1.77969700	-3.95815000	-0.31552900
C	3.89778100	-0.68273400	-0.27580400
C	4.58045800	-1.74777200	-1.13351900
C	4.84120600	-0.07084300	0.75357700
H	3.52597700	0.12111300	-0.91064600
H	3.88552500	-2.20529000	-1.84465800

H	5.40037600	-1.29203700	-1.69412600
H	4.99692800	-2.54605300	-0.51159000
H	4.31664600	0.65740600	1.37529900
H	5.28908700	-0.83610800	1.39512000
H	5.65240100	0.44248400	0.23173300
C	0.85920200	-0.01101800	-0.89994900
O	1.20115200	-0.50254400	-2.19604200
C	1.57548900	1.30831800	-0.57342800
C	1.87769100	2.16973500	-1.62731400
C	1.83357200	1.70463200	0.73965500
C	2.46425800	3.40753300	-1.36856700
H	1.63400800	1.86433400	-2.64024900
C	2.40703900	2.94776300	0.99840600
H	1.56314700	1.05483000	1.57059700
C	2.73327800	3.79774200	-0.05722200
H	2.69851700	4.07392600	-2.19282400
H	2.58787600	3.25571600	2.02363400
H	3.17987800	4.76666100	0.14193500
H	2.10655200	-0.83774700	-2.21450700
C	-1.67623900	0.71993000	1.23338100
C	-1.25209700	1.21454200	-0.15643100
C	-2.28170300	1.86551700	2.05807500
C	-2.46113900	1.72463400	-0.96946500
C	-3.14069900	2.81223200	1.20549000
C	-3.63263300	2.11074700	-0.05819700
H	-2.40523800	-0.08935400	1.11187100
H	-2.13235500	2.58167300	-1.56713300
H	-1.49518000	2.47337600	2.52065900
H	-0.80429300	0.30457700	1.76095300
H	-0.59240500	2.07234400	-0.00019600
H	-2.88981700	1.44736600	2.86701900
H	-2.79845800	0.94212000	-1.65247100
H	-3.99346500	3.16831100	1.80052200
H	-4.33961700	2.75161000	-0.60034700
H	-4.18223400	1.20365300	0.22332900
N	-0.52427200	0.23009100	-0.95791800
H	-1.10859000	-0.50690300	-1.35790900
O	-2.30903400	3.93171300	0.87613200
H	-2.77848400	4.48477900	0.24096300
Br	-3.42419200	-1.66259600	-0.98231500

INT5

C	1.67634400	-2.40808800	1.66017900
C	2.49294100	-1.37548000	1.96656700
C	0.89687400	-0.59357400	0.64829100
N	0.67750900	-1.90893900	0.85826700
H	1.73501400	-3.45088500	1.92430500

H	3.39795000	-1.35158600	2.54872200
N	1.99614900	-0.25211900	1.34521200
C	-0.32949000	-2.80218300	0.22477200
C	-1.17238700	-3.47069700	1.30652500
C	0.38231500	-3.79809300	-0.68580100
H	-0.95186100	-2.16157500	-0.39579000
H	-1.63806400	-2.73660600	1.97257400
H	-1.96460800	-4.05586800	0.83201300
H	-0.57360500	-4.15298300	1.91837700
H	1.03973000	-3.27132400	-1.38303100
H	0.98366200	-4.50603700	-0.10535500
H	-0.36633600	-4.36752100	-1.24348500
C	2.77255800	1.01988800	1.35437300
C	4.25377400	0.73318700	1.11937000
C	2.51482800	1.75906800	2.66178500
H	2.41657000	1.59557300	0.50602000
H	4.37657700	0.08654800	0.24686100
H	4.75454700	1.68533200	0.92455800
H	4.73442900	0.28442300	1.99480200
H	1.44911100	1.94616700	2.81058800
H	2.89197500	1.18033400	3.51247400
H	3.03607600	2.72002700	2.64324200
C	-0.09241600	0.25043900	-0.19020000
O	-0.24533700	-0.38755300	-1.43564900
H	0.65669100	-0.62684200	-1.78076000
C	0.34523100	1.70762000	-0.39056800
C	0.03885900	2.67500000	0.57022700
C	1.05537600	2.07703900	-1.53532200
C	0.47293600	3.98936300	0.41184200
H	-0.53874600	2.38507700	1.44247300
C	1.48504900	3.39354800	-1.69304000
H	1.30183600	1.33647000	-2.28755700
C	1.20709900	4.34996800	-0.71767500
H	0.23544600	4.73117200	1.16874800
H	2.04716500	3.66732600	-2.58020400
H	1.54950700	5.37270400	-0.84268400
C	-3.47479000	1.34006000	0.95004100
C	-2.52597500	0.76392200	-0.12011900
C	-4.92470800	1.33474100	0.46875500
C	-3.25933200	-0.29095900	-0.98272200
C	-5.43084400	-0.10022600	0.27918800
C	-4.28510100	-1.04156900	-0.13625300
H	-3.38962100	0.72938400	1.86036100
H	-3.78636300	0.21018500	-1.80333700
H	-4.99982700	1.84055400	-0.50147200
H	-3.14840300	2.34710600	1.22758400
H	-2.18737100	1.57302100	-0.77550500

H	-5.57985200	1.87492500	1.15777300
H	-2.52688300	-0.95512800	-1.44497200
H	-5.87228700	-0.46127600	1.22080200
H	-4.70123600	-1.89966000	-0.67759500
H	-3.80630200	-1.45232100	0.76544900
N	-1.32942000	0.25200700	0.56893200
H	-1.52669700	-0.65554700	0.97975800
O	-6.43933800	-0.03311000	-0.72172900
H	-6.85710300	-0.89704200	-0.81052100
Br	2.77948000	-1.11180900	-1.71983900

TS6

C	1.44844500	-2.55373200	-2.29024800
C	2.14723400	-2.98521600	-1.22109000
C	0.67129700	-1.48936100	-0.49682600
N	0.52435700	-1.64864700	-1.82797400
H	1.54375000	-2.79131900	-3.33617800
H	2.97191700	-3.67383300	-1.15362100
N	1.63779700	-2.34719400	-0.11086000
C	-0.37590800	-0.92512000	-2.75582700
C	-1.43627600	-1.88240500	-3.29475000
C	0.45071900	-0.29788200	-3.87756800
H	-0.82653900	-0.13718400	-2.15294300
H	-2.01566900	-2.35695400	-2.49682400
H	-2.12931000	-1.33251600	-3.93725300
H	-0.97843500	-2.67630200	-3.89424800
H	1.32611300	0.20472400	-3.45388800
H	0.78027500	-1.05489200	-4.59737900
H	-0.16704900	0.42377300	-4.41902500
C	2.26519600	-2.59533900	1.21299100
C	3.69464300	-2.06034000	1.19656300
C	2.17280000	-4.07947400	1.55229200
H	1.68468000	-2.05074600	1.94660800
H	3.72377800	-1.06361500	0.74492800
H	4.07732600	-2.02307200	2.21988800
H	4.34992900	-2.71456200	0.61108800
H	1.13376400	-4.41827400	1.54436100
H	2.74994800	-4.69730900	0.85791100
H	2.58214900	-4.23733100	2.55324200
C	-0.25544400	-0.52147700	0.32229000
O	-0.33151200	0.68396400	-0.29973000
H	0.30027100	1.79406700	-0.03920200
C	0.27010700	-0.34939400	1.75677800
C	-0.34061400	-0.92549600	2.87056600
C	1.43538800	0.40280100	1.92652100
C	0.20291000	-0.73952800	4.14192900
H	-1.21752100	-1.54873800	2.73175200

C	1.98815100	0.56883000	3.19216800
H	1.94112100	0.77213500	1.03433800
C	1.36849000	0.00367900	4.30666600
H	-0.28058900	-1.18943100	5.00383500
H	2.91271300	1.12939800	3.30249600
H	1.79647300	0.13359300	5.29593200
C	-3.77318800	-1.46988300	1.30223700
C	-2.71467500	-0.48640400	0.76537300
C	-5.17087800	-0.85549900	1.25797300
C	-3.32403000	0.39742900	-0.35279900
C	-5.62132400	-0.60616800	-0.18827000
C	-4.41115700	-0.36401700	-1.10628500
H	-3.75219500	-2.38137100	0.68932500
H	-3.78579100	1.28889600	0.09134600
H	-5.16393500	0.11678600	1.76511200
H	-3.50924400	-1.78278600	2.31704800
H	-2.40241500	0.16881700	1.58506600
H	-5.90308000	-1.47784400	1.77902700
H	-2.51968400	0.74120200	-1.00438900
H	-6.18293100	-1.47997100	-0.55455000
H	-4.73932100	0.17923200	-2.00069600
H	-4.02150700	-1.32868600	-1.45974000
N	-1.53426200	-1.26457500	0.36828700
H	-1.72020300	-1.68373100	-0.53928500
O	-6.47088800	0.53101800	-0.14430300
H	-6.83351200	0.66671000	-1.02678600
Br	2.97290100	0.58785400	-1.33556700
N	0.44222700	2.99442900	0.00428400
C	0.99181400	3.45617400	-1.30252000
C	0.22538800	2.89146000	-2.48521300
H	2.01192600	3.07605000	-1.36162700
H	0.99719500	4.55587600	-1.29815900
H	0.79366300	3.08616600	-3.39792800
H	0.15328500	1.81098800	-2.35213800
H	-0.77202400	3.32262200	-2.60466400
C	-0.97787900	3.41878900	0.15998700
C	-1.55461000	3.05749100	1.52136800
H	-1.54350800	2.89759500	-0.61312500
H	-1.03719300	4.49984200	-0.02753300
H	-1.30727500	2.01937600	1.76054500
H	-1.18362300	3.70308100	2.32016400
H	-2.64288000	3.15373900	1.48981300
C	1.25075600	3.52648700	1.14129100
C	2.76194600	3.46555900	0.95413700
H	0.96187300	2.95600100	2.02567200
H	0.93854500	4.56897600	1.30059600
H	3.23308700	3.63078200	1.92718000

H	3.09678900	2.50664400	0.54679100
H	3.11590500	4.24879700	0.27966700

INT6

C	1.93565900	3.09440000	-0.46453400
C	2.88568900	2.23819500	-0.89564700
C	1.26641000	1.02960700	0.04846400
N	0.94304300	2.33704900	0.11601200
H	1.88790400	4.16821100	-0.51612100
H	3.81910700	2.43071100	-1.39182400
N	2.46514500	0.96141100	-0.57279100
C	-0.29743500	2.94830000	0.66093500
C	-1.05900500	3.64087900	-0.46441500
C	0.05644600	3.89513600	1.80027300
H	-0.86442600	2.11645700	1.06825800
H	-1.25961800	2.95591900	-1.29161000
H	-2.01350000	4.00276500	-0.07797700
H	-0.50663500	4.49868900	-0.85612600
H	0.60584800	3.36551200	2.57945500
H	0.65662800	4.73948300	1.45224500
H	-0.86401200	4.29297900	2.23116100
C	3.18744900	-0.24408200	-1.06629800
C	4.68475300	0.02023700	-1.15943900
C	2.58802500	-0.66159700	-2.40350000
H	3.03129800	-1.02214400	-0.32779200
H	5.07632400	0.43485500	-0.22886200
H	5.18204200	-0.93267200	-1.34505600
H	4.93669300	0.68732700	-1.98607100
H	1.51299900	-0.82304000	-2.30880400
H	2.76592100	0.11189900	-3.15561500
H	3.05465600	-1.58958700	-2.74013700
C	0.31228200	-0.06658100	0.68604800
O	-0.06648300	0.34514300	1.88708100
C	1.04880300	-1.42858600	0.77210200
C	0.89944200	-2.45087100	-0.16461100
C	1.89814400	-1.63719700	1.86067300
C	1.61156100	-3.64244800	-0.03723300
H	0.23478600	-2.30231300	-1.00630100
C	2.62695000	-2.81575900	1.98123500
H	1.98464500	-0.85355100	2.60396700
C	2.48970200	-3.82342300	1.02657600
H	1.48391100	-4.42660100	-0.77530900
H	3.30046100	-2.95257900	2.81986300
H	3.05380000	-4.74439400	1.11886900
C	-2.60483000	-1.52120600	-1.23826800
C	-1.93728700	-0.94911700	0.02894200
C	-4.09021500	-1.79464200	-1.00812200

C	-2.96331600	-0.12633200	0.84595300
C	-4.84638800	-0.48143900	-0.79024000
C	-3.95985600	0.55919400	-0.08650900
H	-2.49243400	-0.79485300	-2.05197400
H	-3.51570200	-0.79202800	1.51827600
H	-4.21599800	-2.40952600	-0.11042900
H	-2.08166800	-2.42566200	-1.55718400
H	-1.59374700	-1.77958500	0.65194300
H	-4.53128800	-2.34751200	-1.83997000
H	-2.42230700	0.58072400	1.47300100
H	-5.17369500	-0.08240300	-1.75794500
H	-4.59591000	1.26699900	0.45315700
H	-3.42417200	1.14455900	-0.84346900
N	-0.74019900	-0.19780900	-0.37658500
H	-1.03484800	0.72711300	-0.67847700
O	-6.00118000	-0.80058000	-0.00883800
H	-6.52959000	-0.00283900	0.09014100

TS7

C	3.87659800	-1.29138400	-0.51652000
C	3.24680700	-2.33589700	0.06863300
C	1.68985800	-0.74893100	-0.33879100
N	2.90621300	-0.33505100	-0.76173300
H	4.91403600	-1.15509100	-0.77016500
H	3.63083200	-3.28341600	0.40691100
N	1.91210800	-1.98016900	0.17612400
C	3.18750000	1.01721700	-1.27745100
C	4.07697800	0.94656200	-2.51311500
C	3.79478600	1.87413200	-0.17060900
H	2.21500300	1.41496400	-1.56296700
H	3.64072400	0.29282800	-3.27061800
H	4.18289400	1.94656200	-2.93711000
H	5.07818700	0.58266600	-2.26935700
H	3.13540900	1.89972800	0.70066700
H	4.76983500	1.48130700	0.13208900
H	3.93338500	2.89628900	-0.52979300
C	0.87716300	-2.84326900	0.77380400
C	1.33013000	-3.34879400	2.13888300
C	0.52781900	-3.97934600	-0.18090600
H	0.01104700	-2.19223900	0.88580900
H	1.62153200	-2.51835100	2.78517400
H	0.50825100	-3.88634200	2.61501400
H	2.17393000	-4.03821400	2.05435700
H	0.17880500	-3.58331400	-1.13678900
H	1.39758800	-4.61662700	-0.36393100
H	-0.26287900	-4.59669600	0.25022300
C	-0.02968700	0.41404600	-0.69184300

O	0.06843400	0.75309300	-1.89027300
C	0.27979800	1.43435300	0.39625800
C	0.46074600	1.06457900	1.73096700
C	0.39711100	2.77249000	0.03884500
C	0.76577100	2.02001800	2.69026700
H	0.38147000	0.01637700	2.00493500
C	0.70613600	3.73610600	0.99948700
H	0.25981600	3.04669800	-1.00096300
C	0.89335600	3.36221400	2.32468800
H	0.91231800	1.72336500	3.72248400
H	0.80402800	4.77591900	0.70912900
H	1.13825400	4.10742400	3.07264900
C	-3.18183700	-1.24491000	0.56942000
C	-2.27711100	-0.03157100	0.28464100
C	-4.65041000	-0.82864900	0.62302500
C	-3.02012100	1.01560500	-0.57817300
C	-5.12456400	-0.35543400	-0.75404200
C	-3.98615900	0.32159400	-1.53497400
H	-3.05155000	-1.98868100	-0.22652500
H	-3.58606900	1.68856000	0.07465700
H	-4.77168400	0.00163900	1.32676000
H	-2.87081400	-1.72734500	1.49825700
H	-2.01811700	0.43424800	1.23789300
H	-5.28288500	-1.64465500	0.97744500
H	-2.29589200	1.62884700	-1.11761200
H	-5.49259300	-1.21406100	-1.32845000
H	-4.41209200	1.02188600	-2.25897600
H	-3.44741900	-0.43434400	-2.11763500
N	-1.02962500	-0.54212300	-0.30851100
H	-1.24288700	-1.08389100	-1.14285400
O	-6.21003300	0.54511000	-0.52051700
H	-6.58454400	0.79534800	-1.37051200

PR1

C	1.22598100	1.74084900	-0.20951500
O	1.86803000	2.78785800	-0.17667500
C	1.93372600	0.42093400	-0.10063800
C	2.92373900	0.27535500	0.87052700
C	1.68162300	-0.61857600	-0.99644000
C	3.63634100	-0.91509300	0.96482000
H	3.12708200	1.09601900	1.54865900
C	2.41008300	-1.80043500	-0.91470600
H	0.92923700	-0.49636700	-1.76778000
C	3.38171800	-1.95265600	0.07133100
H	4.39455000	-1.03153900	1.73005600
H	2.22048300	-2.60019900	-1.62045100
H	3.94352800	-2.87676500	0.13922100

C	-1.93202400	0.35170000	-1.32755600
C	-1.07192200	0.66681100	-0.09083200
C	-3.29303700	-0.26684100	-0.95543100
C	-1.96687000	1.04621200	1.09107900
C	-3.19978300	-1.06902800	0.33293700
C	-2.84223500	-0.14810900	1.51102500
H	-2.09811100	1.28073800	-1.88086200
H	-1.35256300	1.38340100	1.92854000
H	-3.65509700	-0.90116200	-1.76668600
H	-1.37793400	-0.31821000	-1.98844700
H	-0.50093900	-0.21664200	0.18916200
H	-4.03828600	0.51928500	-0.80398100
H	-2.59779000	1.89170400	0.79273800
H	-4.15567300	-1.56312500	0.53530600
H	-2.32922500	-0.74215800	2.27355400
H	-3.76541600	0.21836100	1.96661500
N	-0.11541300	1.73431700	-0.38460900
H	-0.50883900	2.66334000	-0.49186400
O	-2.19783300	-2.06786200	0.11569900
H	-2.11273800	-2.59361400	0.91668700

COM2

C	2.85748600	-0.62986100	1.25843300
C	2.72545000	-1.35791800	-0.08464700
C	3.85623700	0.52000400	1.12557600
C	2.71535300	-0.36536900	-1.26809600
C	3.33767200	1.60671800	0.17071400
C	2.31211300	1.03848900	-0.81868000
H	1.87323900	-0.24664400	1.55879400
H	3.71653000	-0.31449700	-1.71055900
H	4.79598900	0.14054500	0.70396400
H	3.17677400	-1.33313600	2.03551100
H	3.59874500	-2.01925600	-0.19587500
H	4.09862600	0.95311900	2.09945600
H	2.03723200	-0.73462800	-2.04617600
H	2.86336400	2.41176700	0.75083300
H	2.22706600	1.71190700	-1.68007100
H	1.32465000	1.00804200	-0.34728100
N	1.48572200	-2.15414900	-0.08602200
H	1.43441500	-2.73710500	-0.91860300
H	1.45500000	-2.77380500	0.72143300
O	4.48612100	2.12115100	-0.49794400
H	4.22270100	2.87186900	-1.04199000
C	-4.22001400	1.17679500	0.86379100
C	-4.33918900	1.06869300	-0.65990700
N	-2.36543400	-0.00381700	0.03225900
H	-5.02992900	0.67926100	1.40216200

H	-4.35236800	2.03507000	-1.16890700
C	-3.09711000	0.30967700	-1.10899800
O	-2.78971100	0.02087100	-2.23849900
C	-2.91491400	0.47553700	1.21684000
O	-2.43219600	0.34601300	2.31436000
Br	-0.72609700	-0.92064600	-0.02332900
H	-4.16547900	2.20508300	1.22802600
H	-5.21741900	0.50989600	-0.99136200

INT3

C	2.40664000	-0.63318200	1.10559600
C	2.55264300	-0.62382300	-0.41093100
C	3.73238500	-0.21343200	1.76542000
C	2.80098400	0.80479700	-0.92704900
C	4.51200800	0.81923200	0.93852700
C	3.56204600	1.66895700	0.09648000
H	1.60579400	0.06049900	1.39054600
H	3.35945200	0.75126800	-1.86814700
H	4.38784500	-1.08043100	1.89643300
H	2.10261400	-1.63017800	1.43820300
H	3.42661900	-1.24130600	-0.66185800
H	3.53347400	0.19578400	2.76085800
H	1.83803300	1.27802400	-1.14815800
H	5.09324400	1.46162300	1.61423600
H	4.10933300	2.47207600	-0.41119900
H	2.85549700	2.15981500	0.77724600
N	1.45319700	-1.34539100	-1.06922200
H	1.59187000	-1.29237000	-2.07911300
H	-2.00373300	-1.83582500	0.24615700
O	5.41128200	0.08880900	0.10124300
H	5.92933100	0.71218600	-0.42090100
C	-4.92218500	-0.58309000	0.95085900
C	-5.20754600	0.87663100	0.59897700
N	-2.94166900	0.30987100	-0.05816400
H	-5.56208000	-1.30562100	0.43711200
H	-5.45376000	1.49899200	1.46152300
C	-3.88563800	1.36612200	-0.01373600
O	-3.67559400	2.48342600	-0.40663700
C	-3.50343900	-0.72337000	0.46418900
O	-2.91367000	-1.89541700	0.59883800
Br	-0.23677200	-0.48913800	-0.83372500
H	-4.96788900	-0.80441400	2.02078700
H	-6.00284600	1.00074000	-0.13918100

TS4

C	2.47473200	-0.54959000	1.21803500
C	2.58862100	-0.73739300	-0.28965700

C	3.74725500	0.12188400	1.76408600
C	2.64758200	0.62058400	-1.01215400
C	4.36622600	1.12354100	0.77762800
C	3.29799000	1.71194000	-0.14194600
H	1.59693100	0.07168600	1.43420900
H	3.20246900	0.50134100	-1.94941300
H	4.51449400	-0.62807300	1.98236000
H	2.30769300	-1.51978500	1.69491100
H	3.52677200	-1.27691500	-0.48434900
H	3.51765300	0.63337500	2.70418600
H	1.62975700	0.92991000	-1.27363700
H	4.86449400	1.92636600	1.33842200
H	3.72456900	2.50184500	-0.77198900
H	2.54007700	2.19547700	0.48680700
N	1.57545700	-1.67369500	-0.79720800
H	1.68467400	-1.75106900	-1.80913900
H	-2.87241900	-1.29027900	0.54685000
O	5.34491900	0.40787800	0.01982600
H	5.75329500	1.01015000	-0.61286100
C	-5.29667300	0.55713400	0.68921800
C	-4.60514500	1.74473700	-0.01551300
N	-3.07035300	-0.05306900	0.11398400
H	-6.16149800	0.16321500	0.14950600
H	-4.53411900	2.63489100	0.61352600
C	-3.17452100	1.26493300	-0.34796100
O	-2.32376000	1.91062300	-0.89966200
C	-4.19284400	-0.45250600	0.68938000
O	-4.05099700	-1.63485900	1.11459000
Br	-0.20008200	-0.99208500	-0.62569100
H	-5.61225800	0.76921200	1.71361700
H	-5.09610500	2.03823400	-0.94599200

INT4

C	1.60591400	-0.22862800	-1.24006900
C	2.20477700	0.68686400	-0.18099200
C	2.30124200	-1.60145700	-1.22840800
C	1.98456300	0.13097500	1.23665800
C	2.80291800	-2.00735900	0.16296800
C	1.91908100	-1.40773100	1.25399300
H	0.53768000	-0.37553900	-1.03679400
H	2.79317700	0.48691700	1.88492000
H	3.16757200	-1.60286900	-1.89780300
H	1.68302300	0.24862700	-2.22113000
H	3.28694600	0.73945500	-0.36862900
H	1.59859000	-2.35868700	-1.58740000
H	1.05076100	0.53859700	1.64160200
H	2.80145900	-3.10281400	0.24006500

H	2.21247100	-1.78961300	2.23952000
H	0.89466100	-1.75324600	1.07053700
N	1.79494200	2.08600000	-0.37582400
H	2.21299900	2.64679700	0.36854100
O	4.14749800	-1.53055100	0.27963000
H	4.49944700	-1.79551600	1.13720600
C	-4.29650500	-1.04670400	0.08854300
C	-3.44395700	-2.30000600	-0.14738200
N	-2.02589800	-0.44515200	0.07736700
H	-4.88378200	-1.08446500	1.00888800
H	-3.63219800	-2.78199100	-1.10958800
C	-2.00129500	-1.81056600	-0.13406100
O	-1.00003900	-2.47413900	-0.28244400
C	-3.29781800	0.09812200	0.20452000
O	-3.53118700	1.26902400	0.37661700
Br	-0.07068400	2.37282200	-0.06786100
H	-4.98417700	-0.82346900	-0.73013100
H	-3.55809700	-3.06097600	0.62785700
H	-1.19361300	0.13837500	0.11164700

COM2'

C	-3.45675700	0.84304300	1.30230600
C	-4.71499100	0.02629200	0.95556500
C	-2.18985200	0.16152800	0.78662100
C	-4.52330300	-0.74413200	-0.36506500
C	-2.19096600	0.09755000	-0.74664100
C	-3.61886800	0.04755200	-1.30474900
H	-3.55482100	1.83465200	0.84096500
H	-4.06921100	-1.72210200	-0.16675600
H	-2.14024800	-0.86960400	1.15931300
H	-3.39475300	1.00083600	2.38419200
H	-4.88052100	-0.70864100	1.76043900
H	-1.29193000	0.67081500	1.14542400
H	-5.50200500	-0.92961300	-0.82084600
H	-1.66327200	0.97093300	-1.15749900
H	-3.60215300	-0.38563200	-2.31242100
H	-4.01290800	1.06550700	-1.40585500
N	-5.84241000	0.95131700	0.80897000
H	-6.71891000	0.44427000	0.72544300
H	-5.92168900	1.55554300	1.62260000
O	-1.46156900	-1.08724100	-1.09714800
H	-1.46043900	-1.18010500	-2.05803600
C	4.70516400	1.31714900	0.17222300
C	4.90014000	0.02342500	0.97022900
N	2.76740000	0.00505900	-0.00837800
H	5.38038900	1.40126400	-0.68293300
H	5.02342200	0.19334100	2.04265700

C	3.62224300	-0.77870500	0.77055200
O	3.36830200	-1.87471500	1.19553800
C	3.28344600	1.25207400	-0.36342400
O	2.69698300	2.09449100	-0.99232300
Br	1.05862400	-0.52044500	-0.45704100
H	4.81061000	2.22641700	0.76734200
H	5.74439800	-0.58187500	0.63400100

INT3'

C	3.58464200	0.90409700	1.35372600
C	4.74287400	0.83798200	0.34092400
C	2.23049400	0.75469500	0.65873900
C	4.36938300	-0.04835400	-0.86082600
C	2.10236200	-0.65061100	0.05233000
C	3.46213900	-1.19040400	-0.41383300
H	3.71558500	0.08749000	2.07680400
H	3.85616300	0.54700000	-1.62446100
H	2.14832900	1.48435800	-0.15758300
H	3.62779900	1.84055000	1.91964800
H	4.93375200	1.85862800	-0.02957000
H	1.40796100	0.95573200	1.35037000
H	5.28425400	-0.43685100	-1.32166500
H	1.66124000	-1.34091400	0.78709000
H	3.29155300	-1.91669600	-1.21366100
H	3.94311400	-1.72068600	0.41626200
N	5.91365800	0.26473700	1.01157800
H	6.73973900	0.33923900	0.42468000
H	6.11421000	0.76046700	1.87611800
O	1.28501000	-0.65321800	-1.12324300
C	-4.88915300	-0.72369800	1.09689800
C	-5.31118900	0.64379300	0.55771600
N	-3.01805000	0.19032500	-0.07979700
H	-5.46647400	-1.56347300	0.70075000
H	-5.60059900	1.35435400	1.33447800
C	-4.05117900	1.16230200	-0.15169500
O	-3.94192100	2.22745000	-0.69588000
C	-3.47217100	-0.80573400	0.59795900
O	-2.77431400	-1.89038000	0.86714800
Br	-0.46206600	-0.17728300	-0.78079300
H	-4.90174800	-0.79960000	2.18763800
H	-6.12566300	0.59324700	-0.16811100
H	-1.88558500	-1.79861600	0.47065600

TS4'

C	2.82503600	1.38302900	-0.44723900
C	4.13753900	0.58377900	-0.33823000

C	1.63669000	0.46465400	-0.73650200
C	3.87078700	-0.84534200	0.17032600
C	1.39739900	-0.45407600	0.46566100
C	2.70860200	-0.84810000	1.15843700
H	2.65966300	1.89917200	0.50893500
H	3.63816400	-1.50712300	-0.67170300
H	1.84936200	-0.16512100	-1.60981100
H	2.91150400	2.15661800	-1.21647200
H	4.58183500	0.51286000	-1.34436500
H	0.73832500	1.04078900	-0.98075500
H	4.77840800	-1.23862700	0.64064700
H	0.73116900	0.03235600	1.19475200
H	2.57334800	-1.82475200	1.63231800
H	2.91990100	-0.12353300	1.95339700
N	5.01952700	1.26804900	0.61148800
H	5.94726000	0.85355300	0.60644800
H	5.12838400	2.24757900	0.36235900
O	0.79869000	-1.69922600	0.08118700
C	-2.51347600	0.91097900	1.71446000
C	-1.76352700	1.84294600	0.73949200
N	-3.40360100	0.64691900	-0.47739800
H	-3.01558200	1.42528800	2.53695500
H	-0.68534300	1.66852000	0.71038900
C	-2.34658800	1.54991800	-0.65899800
O	-1.95881500	2.01728600	-1.69692100
C	-3.50992200	0.28637700	0.79226000
O	-4.45729500	-0.54510100	0.91073000
Br	-0.90235100	-1.44617200	-0.55675300
H	-1.87985500	0.12609800	2.13933900
H	-1.92294600	2.90185700	0.95906000
H	-4.39867200	-0.22294300	-0.39175600

INT4'

C	-1.99611500	-1.72896300	-0.72804500
C	-3.51559700	-1.50476800	-0.84642500
C	-1.23513000	-0.40166500	-0.72738800
C	-3.92448400	-0.16142200	-0.21371900
C	-1.58339000	0.39416500	0.53415600
C	-3.03051700	0.15268500	0.98136900
H	-1.79687500	-2.25376100	0.21574000
H	-3.84176800	0.64285000	-0.95393100
H	-1.51478800	0.19510900	-1.60536900
H	-1.64461400	-2.37740800	-1.53753700
H	-3.77695200	-1.47496500	-1.91707300
H	-0.15612300	-0.57491300	-0.78022200
H	-4.97629000	-0.20809400	0.08874800
H	-0.88408200	0.15389800	1.34166800

H	-3.37677600	1.02986300	1.53578100
H	-3.04628400	-0.69792800	1.67247100
N	-4.19971100	-2.59126600	-0.13908800
H	-5.19964700	-2.56620900	-0.31747700
H	-3.86117800	-3.49704500	-0.45257000
O	-1.53379800	1.81389600	0.28704600
C	3.34169400	-2.07934500	1.06016400
C	4.34695000	-1.73031600	-0.04317500
N	2.53462100	-0.23896700	-0.15509400
H	3.74940700	-1.98185600	2.06900600
H	4.48809100	-2.52896800	-0.77499900
C	3.75236200	-0.52481600	-0.76127200
O	4.22666200	0.08528400	-1.68675300
C	2.21088600	-1.07204200	0.90300000
O	1.19889800	-0.99963500	1.56023200
Br	0.17037900	2.41984700	0.01050200
H	2.92215000	-3.08393300	0.97192200
H	5.33398300	-1.45307000	0.33339900
H	1.94005100	0.53596400	-0.43403700

COM2_a

C	-0.43185800	2.27247900	1.16953700
C	-0.66816300	2.90781300	-0.19881500
C	-0.05227400	3.36013100	2.18579200
C	-1.92008400	3.79767900	-0.15949700
C	-0.76685800	4.69394500	1.91991900
C	-2.10584800	4.46392400	1.21916400
H	-1.34889300	1.75847000	1.48177200
H	-1.84535700	4.55894600	-0.94415600
H	1.02450000	3.56090700	2.15796400
H	0.34317800	1.50067400	1.11001200
H	0.19896500	3.53732400	-0.43787500
H	-0.28906700	3.01569200	3.19724400
H	-2.79929300	3.18410900	-0.38564800
H	-0.93005700	5.21547800	2.87317500
H	-2.65074000	5.40985700	1.11707300
H	-2.71807700	3.82448400	1.86662400
N	-0.80881400	1.86850600	-1.23401200
H	-1.01823000	2.28405000	-2.13965500
H	0.06235000	1.32641600	-1.30795500
O	0.10555600	5.47879700	1.10327000
H	-0.31149200	6.32966400	0.92503500
C	-5.88389700	-2.14111000	-0.39153400
C	-4.82388100	-3.02012100	0.27764100
N	-3.79478500	-1.04630400	-0.49284600
H	-6.69452800	-1.84242900	0.27681200
H	-4.67306500	-3.98371500	-0.21476600

C	-3.53486700	-2.21745700	0.16688000
O	-2.44553000	-2.55927000	0.59552800
C	-5.13353700	-0.88698700	-0.83234900
O	-5.60596800	0.07862100	-1.38096200
Br	-2.42059900	0.30700600	-0.83795000
H	-6.33648300	-2.59699100	-1.27521100
H	-5.01751100	-3.21756600	1.33458000
C	4.33259400	2.50484300	-0.37909700
C	5.19828500	1.75758800	-1.40947000
C	2.86077000	2.11747700	-0.51446700
C	4.59897200	0.37435300	-1.72507500
C	2.64667300	0.63801900	-0.16042300
C	3.89934300	-0.19270200	-0.49301700
H	4.68785700	2.23679300	0.62488000
H	3.87145400	0.45683600	-2.54153400
H	2.53358000	2.26454500	-1.55345200
H	4.46254100	3.58708700	-0.48603300
H	5.21142300	2.34927100	-2.34008400
H	2.22865300	2.75539500	0.11181600
H	5.39463400	-0.29439900	-2.07214800
H	2.43292300	0.54867500	0.91657100
H	3.59946000	-1.23354100	-0.65104400
H	4.59858600	-0.17802700	0.35270500
N	6.54125700	1.58201100	-0.84825100
H	7.18240100	1.22428700	-1.55070100
H	6.91578400	2.47023100	-0.52507000
O	1.51587000	0.17840300	-0.89295700
H	1.07079600	-0.53198100	-0.38125700
C	2.79469200	-3.82244800	1.81885800
C	3.06594600	-4.19643000	0.35073500
C	1.97050000	-2.53870100	1.90509500
C	1.88552900	-3.78505500	-0.55183200
C	0.56939300	-2.74786600	1.31572800
C	0.57538100	-3.83196500	0.22799200
H	2.24628000	-4.64897700	2.28948600
H	2.03698600	-2.76762500	-0.93532100
H	2.47067800	-1.75441500	1.32162000
H	3.74090600	-3.71548700	2.36067700
H	3.96319200	-3.64461400	0.02134600
H	1.90085200	-2.16851000	2.93209300
H	1.85194900	-4.44619800	-1.42504900
H	-0.13395400	-3.03725400	2.10747300
H	-0.29522900	-3.68250600	-0.41777300
H	0.46774100	-4.82089700	0.68946400
N	3.25110700	-5.64844800	0.26699200
H	3.56733500	-5.91796300	-0.66028700
H	3.95911300	-5.95952600	0.92703500

O	0.15176800	-1.48650200	0.78842700
H	-0.79694900	-1.55696900	0.57756500

TS3_a

C	1.49303500	-2.54552600	-0.79713700
C	1.67780400	-1.97953700	0.60898400
C	2.63473800	-3.52721700	-1.10486300
C	1.47026500	-3.08826100	1.65367200
C	3.08421200	-4.32017400	0.13248400
C	1.93771800	-4.46239300	1.13309100
H	0.52551700	-3.05802900	-0.84494400
H	2.00980000	-2.82333300	2.56986900
H	3.51389900	-2.99208400	-1.48123800
H	1.45357600	-1.74119000	-1.53910500
H	2.71321700	-1.61457200	0.68919700
H	2.31845100	-4.22251700	-1.88849600
H	0.40461000	-3.13915500	1.90414500
H	3.43505600	-5.31318500	-0.17999600
H	2.23704800	-5.10623400	1.96852300
H	1.11050500	-4.97667400	0.62966900
N	0.81803300	-0.80496000	0.83972700
H	0.88482500	-0.50614600	1.81289400
H	0.95139500	0.17926400	-0.09903300
O	4.17675500	-3.60271900	0.71413100
H	4.49388700	-4.08782200	1.48464200
C	-5.47052500	-2.31124400	-0.52635800
C	-5.14332700	-1.37084600	-1.68343500
N	-3.33088600	-1.30566200	-0.14277300
H	-5.61525400	-3.35231400	-0.82408500
H	-5.84451400	-0.54081600	-1.80137500
C	-3.77751700	-0.81337100	-1.30098700
O	-3.19014400	0.01768800	-2.02882100
C	-4.23352900	-2.22238700	0.37822800
O	-4.07214200	-2.85937600	1.39665100
Br	-1.11267700	-1.10646000	0.49544500
H	-6.34720300	-2.00922300	0.05191700
H	-5.05944600	-1.86856200	-2.65328500
C	4.47964800	1.40528100	-1.63198300
C	4.84953600	1.50478700	-0.13947000
C	3.10593000	0.75903700	-1.80513800
C	3.58629500	1.65508800	0.72967100
C	2.01310200	1.68426600	-1.25077900
C	2.52022700	2.45578700	-0.01518500
H	4.46192500	2.42038200	-2.05142300
H	3.19432200	0.66309900	0.98952000
H	3.08013000	-0.18584400	-1.24486200
H	5.24858600	0.84664900	-2.17519300

H	5.35677200	0.56991200	0.15047500
H	2.89352600	0.51246900	-2.84945000
H	3.85218600	2.14438100	1.67330900
H	1.71341300	2.39873200	-2.02882600
H	1.66766900	2.68911900	0.63221900
H	2.96202200	3.40990900	-0.32715200
N	5.69943800	2.68280100	0.05344500
H	6.09974200	2.69252700	0.98731300
H	6.47455000	2.68063800	-0.60412800
O	0.85476000	0.91370500	-0.94838500
H	-0.26072600	1.27753800	-1.28150100
C	-1.29091400	4.71453300	0.36899500
C	-1.08742800	3.92745600	1.67932000
C	-0.97544300	3.84535700	-0.84976400
C	-1.38933900	2.43047900	1.47479200
C	-1.97589400	2.68702600	-0.95145100
C	-2.48519400	2.25511300	0.42830300
H	-2.33747800	5.04324800	0.32620300
H	-0.48242100	1.90648200	1.14251600
H	0.03287600	3.42996100	-0.73376300
H	-0.67127500	5.61743300	0.36916600
H	-0.03012400	4.03193000	1.97926000
H	-0.97297300	4.42906400	-1.77448900
H	-1.68256300	1.97633900	2.42793100
H	-2.82464000	2.97497500	-1.58149800
H	-2.84691300	1.22423000	0.37917100
H	-3.33901500	2.88426400	0.70688300
N	-2.00344600	4.46567300	2.68766700
H	-1.82242300	4.05476600	3.59910100
H	-1.88917700	5.47141400	2.78211600
O	-1.33302600	1.59898100	-1.64722700
H	-2.03166300	0.82435100	-1.77597100

COM2c

C	-0.58189600	2.32861100	0.79915300
C	-0.89891800	2.56506200	-0.67483600
C	-0.63958600	3.66148500	1.56311900
C	-2.36146100	3.00640600	-0.83827600
C	-1.72078600	4.60978500	1.02196000
C	-2.85744800	3.82152500	0.37229700
H	-1.31011500	1.61724400	1.20738400
H	-2.46251600	3.59176900	-1.75897000
H	0.31701500	4.18953700	1.49104600
H	0.40151700	1.85650100	0.90240200
H	-0.24489200	3.37247800	-1.03271900
H	-0.82376400	3.46833600	2.62455500
H	-2.98572100	2.11229400	-0.95195200

H	-2.11337600	5.22181400	1.84576400
H	-3.66916400	4.49531300	0.07343300
H	-3.27807800	3.15038500	1.13104900
N	-0.65477700	1.34220300	-1.45528600
H	-0.82458200	1.49659100	-2.44656300
H	0.30680200	1.01544700	-1.32768700
O	-1.08735700	5.46465900	0.06773900
H	-1.73943000	6.08515500	-0.27786900
C	-3.26019700	-4.30363600	0.71312200
C	-1.77095400	-4.46018900	1.03832800
N	-2.10808800	-2.38597400	-0.02029300
H	-3.90382100	-4.31319000	1.59564400
H	-1.29360600	-5.29523500	0.52004100
C	-1.13139300	-3.16786600	0.55206300
O	0.04427100	-2.86601000	0.64306400
C	-3.38266300	-2.93625400	0.04524000
O	-4.39279200	-2.41631000	-0.35960100
Br	-1.62695800	-0.65813300	-0.71961100
H	-3.63962500	-5.05769200	0.01992700
H	-1.56106000	-4.57136800	2.10459400
C	4.88892100	0.82560000	0.34683300
C	5.48256300	-0.28940200	-0.53413300
C	3.38874600	0.97665900	0.09849200
C	4.44326500	-1.39703200	-0.79500700
C	2.63278100	-0.28377700	0.54009000
C	3.50947400	-1.53873300	0.40311500
H	5.06224700	0.56010400	1.39814000
H	3.84992600	-1.15215200	-1.68409900
H	3.20550800	1.11127300	-0.97598500
H	5.41278700	1.77044100	0.16553800
H	5.76399200	0.15488500	-1.50387100
H	2.98707600	1.86138400	0.60345400
H	4.96352300	-2.33778500	-1.00709000
H	2.32072700	-0.17727900	1.59068300
H	2.85715700	-2.41417500	0.31538000
H	4.11189900	-1.67377300	1.30960200
N	6.63576500	-0.86712000	0.16263600
H	7.13578700	-1.51334600	-0.44120700
H	7.29333700	-0.14211400	0.43716400
O	1.47540000	-0.36410900	-0.28223800
H	0.93481800	-1.12727500	-0.01189300

TS3c

C	0.57396200	-2.35146500	0.73767200
C	0.79543100	-2.41749000	-0.77868700
C	1.30950000	-3.51055100	1.41026300
C	2.24157000	-2.83835300	-1.12830600

C	2.83179100	-3.37402600	1.26495200
C	3.20677100	-2.55328400	0.02303000
H	0.93922500	-1.39281500	1.12738800
H	2.26296300	-3.91303000	-1.34249000
H	1.02209900	-4.45553900	0.93128100
H	-0.49804100	-2.39593600	0.95749500
H	0.10531800	-3.17203100	-1.18457400
H	1.03489900	-3.59586500	2.46478100
H	2.56060100	-2.32199600	-2.04087600
H	3.24346600	-2.87682800	2.15515600
H	4.23580600	-2.79165100	-0.27015700
H	3.19229600	-1.48580300	0.26591800
N	0.37876700	-1.15258900	-1.41311700
H	0.38756100	-1.25003200	-2.42777300
H	-0.71014600	-0.48303700	-0.91027600
O	3.33384400	-4.70489800	1.19067700
H	4.29712500	-4.68000900	1.20955200
C	0.73825300	4.35339500	1.14785300
C	2.19471000	4.74348300	0.91275500
N	1.78090100	2.59525500	-0.07219300
H	0.01156000	5.02933100	0.68949600
H	2.76988400	4.89219800	1.82949000
C	2.77330900	3.54204100	0.15151200
O	3.92641400	3.44070800	-0.20441900
C	0.63256100	2.99006900	0.47507300
O	-0.46517400	2.36896600	0.47990400
Br	1.45208200	0.44515100	-0.99268900
H	0.46803100	4.24862100	2.20217400
H	2.31775200	5.63750100	0.29666900
O	-1.41552200	0.31129200	-0.47549800
H	-0.90561800	1.18733100	-0.08180700
C	-4.54930600	-1.55170300	0.11072400
C	-5.39624200	-0.34701700	-0.34321600
C	-3.09407800	-1.39437000	-0.32947900
C	-4.54274900	0.93404000	-0.40799200
C	-2.44972900	-0.19938200	0.38609700
C	-3.46625800	0.91014100	0.67296500
H	-4.59613500	-1.61067300	1.20601400
H	-4.06927700	1.02321600	-1.39292300
H	-3.05605800	-1.20327300	-1.41004900
H	-4.97233700	-2.48356100	-0.27823400
H	-5.77844100	-0.55865700	-1.35573900
H	-2.52228600	-2.31115600	-0.14731200
H	-5.19318300	1.80743300	-0.29067000
H	-1.98125500	-0.52362900	1.32542400
H	-2.93571100	1.86368700	0.75217400
H	-3.94120400	0.72009400	1.64209100

N	-6.47570800	-0.15206200	0.62769600
H	-7.13266200	0.55158300	0.30270800
H	-7.00029500	-1.01168000	0.76586300

COM2a

C	2.31548100	-2.05553600	0.84361000
C	2.03392500	-2.14874900	-0.66200000
C	3.80952100	-2.24283700	1.10170400
C	3.13191600	-1.44651500	-1.49174700
C	4.63185000	-1.09075200	0.50634600
C	3.89301600	-0.41662300	-0.65720400
H	1.97842400	-1.07984100	1.21759300
H	3.84384700	-2.19170100	-1.86416700
H	4.15101900	-3.16625300	0.61634900
H	1.73038700	-2.81467900	1.37367300
H	2.02505700	-3.21532900	-0.93379500
H	4.02211500	-2.35004900	2.16865200
H	2.67447000	-0.97040900	-2.36684300
H	4.82974600	-0.33865500	1.28437000
H	4.61474500	0.12863500	-1.27732700
H	3.19362200	0.32940100	-0.26541100
N	0.71466300	-1.55846500	-0.93710600
H	0.39608800	-1.77560600	-1.87818800
H	0.01800800	-1.87471900	-0.25016300
O	5.86445600	-1.66906200	0.08568600
H	6.45629800	-0.96795900	-0.20927000
C	-0.71629700	4.33919400	1.42344400
C	-0.34830000	4.89803400	0.04480000
N	-0.04866700	2.56578400	0.02848100
H	-1.75606500	4.51677300	1.70749700
H	0.48276100	5.60669200	0.06646200
C	0.07741100	3.68774000	-0.78231500
O	0.45352100	3.68763500	-1.92823900
C	-0.49906300	2.83653000	1.30654400
O	-0.68447600	2.00760300	2.17179400
Br	0.36129000	0.76858700	-0.49150400
H	-0.08471200	4.71523600	2.23173500
H	-1.18180300	5.38552600	-0.46613900
C	-3.02602100	-2.90229500	0.91955700
C	-2.53955300	-1.55087300	1.48032400
C	-4.31978000	-2.73618000	0.12091200
C	-2.97141100	-0.39260100	0.56449100
C	-4.08435800	-1.87709600	-1.12853800
C	-2.96719000	-0.84667100	-0.89126600
H	-2.24083700	-3.30516300	0.26424400
H	-3.98554000	-0.07322500	0.83149800
H	-5.07454700	-2.22704800	0.73253400

H	-3.15999600	-3.62724100	1.72941400
H	-3.00124700	-1.39438600	2.46733000
H	-4.74396700	-3.70346400	-0.16252300
H	-2.31299200	0.46536200	0.73016900
H	-3.80348500	-2.52708900	-1.97166900
H	-3.08987700	-0.00216600	-1.57984300
H	-1.99536800	-1.29879900	-1.12767100
N	-1.07006600	-1.57786100	1.57682700
H	-0.72952000	-0.67711900	1.91745300
H	-0.78361900	-2.27833700	2.25801200
O	-5.32958400	-1.24806200	-1.41383900
H	-5.24786900	-0.74867500	-2.23395200

TS3a

C	2.11933900	-1.97424900	1.09409700
C	1.64113500	-2.19262300	-0.34904300
C	3.58289300	-2.39272500	1.22790400
C	2.74368500	-1.81212600	-1.36850800
C	4.50667200	-1.48109300	0.40801200
C	3.76246900	-0.84045600	-0.77095400
H	2.00260200	-0.91590800	1.36504800
H	3.27337500	-2.71882100	-1.68415300
H	3.70740000	-3.41158800	0.83895100
H	1.49275400	-2.55693600	1.78008300
H	1.43167200	-3.26712300	-0.46413500
H	3.90000700	-2.41285100	2.27399000
H	2.27847100	-1.38283700	-2.26284900
H	4.90355200	-0.68356500	1.05323100
H	4.49018900	-0.53003900	-1.53022300
H	3.25514400	0.07093300	-0.43853600
N	0.35971500	-1.49911400	-0.55935900
H	-0.03797300	-1.78661200	-1.45265700
H	-0.49585800	-1.37045600	0.58675700
O	5.57890400	-2.31112100	-0.03020500
H	6.23640100	-1.76466900	-0.47508100
C	-0.40116400	4.36652100	1.40975300
C	0.25790100	5.02510500	0.19812500
N	0.21930000	2.66884500	-0.12980500
H	-1.44286600	4.65923600	1.56498600
H	1.16593400	5.58374900	0.43689200
C	0.63233600	3.84910100	-0.71514100
O	1.20008500	3.95060600	-1.78200500
C	-0.35573800	2.87527400	1.07999000
O	-0.79803700	1.99746100	1.82987900
Br	0.43797000	0.55158400	-0.60551200
H	0.12921600	4.53369500	2.35084400
H	-0.40463200	5.69545100	-0.35486200

C	-2.97783700	-2.49287500	1.04713100
C	-2.58203500	-1.04478100	1.37790200
C	-4.31814100	-2.51412200	0.31099400
C	-3.04188600	-0.06442300	0.28453000
C	-4.20623100	-1.84025700	-1.06424000
C	-3.11009200	-0.76218800	-1.07025000
H	-2.20285200	-2.94081600	0.40894100
H	-4.04472800	0.29374600	0.54212400
H	-5.06575700	-1.95666100	0.88860700
H	-3.02227100	-3.09574600	1.96022400
H	-3.03425600	-0.74536200	2.32990600
H	-4.69739000	-3.53353100	0.20468200
H	-2.38397100	0.80875100	0.26933000
H	-3.97118500	-2.59895900	-1.82596100
H	-3.30443900	-0.04094500	-1.87158900
H	-2.14347100	-1.22388200	-1.30277600
N	-1.10112400	-0.97244400	1.54991100
H	-0.82259900	0.01551100	1.70011400
H	-0.81628700	-1.51446000	2.36573100
O	-5.48939300	-1.28660400	-1.32673200
H	-5.50267800	-0.92298700	-2.21922700

COM2e

C	0.48604800	1.64327000	0.98374400
C	0.48086500	1.95451300	-0.51053200
C	1.17649300	2.78500700	1.74576200
C	-0.42563500	3.16129400	-0.79679700
C	0.90751900	4.16148400	1.11726500
C	-0.42663700	4.16698500	0.37173000
H	-0.54995800	1.52606700	1.32335800
H	-0.09450900	3.65008000	-1.71981700
H	2.26276800	2.64289800	1.75784000
H	0.98052200	0.68505300	1.17564900
H	1.50738700	2.20899700	-0.80812300
H	0.84011100	2.78708700	2.78715700
H	-1.44797100	2.80449200	-0.96622800
H	0.89817700	4.92639600	1.90613300
H	-0.65813700	5.17529600	0.00875800
H	-1.21481400	3.90949000	1.08971700
N	0.03261700	0.78310000	-1.28365000
H	-0.03296700	1.00556700	-2.27503900
H	0.69135100	0.00307800	-1.15463200
O	1.98856300	4.43006000	0.22095200
H	1.85713800	5.29839200	-0.17718900
C	-6.02269100	-1.24378500	0.01675000
C	-5.29175400	-2.23293100	0.92774600
N	-3.69414200	-0.88132200	-0.15287700

H	-6.69598400	-0.56921400	0.55058700
H	-5.44289300	-3.27993100	0.65415400
C	-3.81672600	-1.89893400	0.75133800
O	-2.89619000	-2.45616400	1.32771800
C	-4.91521400	-0.41208700	-0.62487800
O	-5.05911300	0.49544400	-1.40744400
H	-6.59770600	-1.72226200	-0.77931500
H	-5.54411000	-2.12972500	1.98574500
C	5.10641600	-0.24494100	-0.05722700
C	5.62155800	-1.50568200	-0.77589500
C	3.60235300	-0.07074900	-0.26463600
C	4.53595800	-2.59833200	-0.81544800
C	2.81933800	-1.22055700	0.38664600
C	3.65412300	-2.51086700	0.42628300
H	5.31733000	-0.35280700	1.01494800
H	3.90889800	-2.47340600	-1.70644500
H	3.37559900	-0.08154500	-1.33986600
H	5.65275600	0.63920100	-0.40286800
H	5.87150600	-1.22999600	-1.81410200
H	3.25803500	0.89428200	0.12349100
H	5.01495000	-3.58049000	-0.89700800
H	2.53915500	-0.94479900	1.41488800
H	2.97156900	-3.36431600	0.49834400
H	4.29074700	-2.52295800	1.31916200
N	6.78626200	-2.01303100	-0.04430600
H	7.23909000	-2.76181800	-0.56072700
H	7.47729100	-1.27924500	0.08840600
O	1.63420400	-1.40616700	-0.37991900
H	0.97298700	-1.85708500	0.18512100
O	-0.11481700	-2.31074800	1.50617700
H	-1.06954600	-2.19319800	1.33473000
H	-0.04636100	-3.14359600	1.98302900
Br	-1.96511000	-0.10036400	-0.67614400

TS3_e

C	0.49996100	1.89862500	1.03149000
C	0.58513400	2.05651800	-0.48403000
C	1.21689200	3.07350900	1.71552600
C	-0.24419300	3.27329400	-0.92980300
C	1.05946900	4.39029300	0.93902300
C	-0.23763900	4.39241100	0.13091200
H	-0.55520900	1.87139800	1.32554400
H	0.15292900	3.64723100	-1.88002700
H	2.29140300	2.87752100	1.80289500
H	0.93119500	0.94126100	1.34579900
H	1.63664800	2.23899400	-0.74661200
H	0.82723300	3.19961400	2.73028600

H	-1.27617600	2.95157600	-1.10922200
H	1.06285100	5.23144100	1.64559100
H	-0.39102900	5.36924500	-0.34247700
H	-1.07167200	4.25569600	0.82989000
N	0.21937200	0.81185100	-1.18166000
H	0.20930800	0.97899600	-2.18788700
H	0.92287100	-0.39267600	-0.80975300
O	2.19483800	4.50172900	0.07668300
H	2.13382600	5.32873200	-0.41520500
C	-5.91226900	-1.17702000	0.51295700
C	-5.10438900	-2.38898800	0.96971200
N	-3.60504100	-0.85897300	-0.06413300
H	-6.41329500	-0.64480000	1.32471500
H	-5.39360000	-3.32868100	0.49182100
C	-3.68694500	-2.03425700	0.54163800
O	-2.73649900	-2.82762300	0.77252100
C	-4.85581300	-0.25401500	-0.11045500
O	-5.08132700	0.84126400	-0.57692100
H	-6.66493900	-1.40737200	-0.24486200
H	-5.11671800	-2.55428300	2.05026500
C	4.78092400	-0.51146900	0.34301300
C	5.29962900	-1.74258600	-0.42366000
C	3.33817500	-0.18700700	-0.04471000
C	4.14910800	-2.71793800	-0.73586000
C	2.39486300	-1.32126500	0.38987600
C	3.11077800	-2.67700200	0.38147500
H	4.82912900	-0.73070100	1.41774900
H	3.67183800	-2.44730500	-1.68543000
H	3.26650800	-0.08080500	-1.13581300
H	5.43092800	0.35090600	0.16297300
H	5.72794000	-1.39666700	-1.37895200
H	3.02204500	0.76705600	0.38921000
H	4.55532300	-3.72765400	-0.85927400
H	2.00527600	-1.12168900	1.39860800
H	2.36471400	-3.47157800	0.28132800
H	3.61556000	-2.83260500	1.34158000
N	6.28916400	-2.42496000	0.41360500
H	6.76280300	-3.15734800	-0.10748400
H	7.00225100	-1.77558300	0.73473700
O	1.28507100	-1.37717200	-0.51930200
H	0.38544000	-2.11399300	-0.14006400
O	-0.38753600	-2.91040800	0.25244800
H	-1.46205700	-2.72675800	0.45271500
H	-0.31250900	-3.74376900	-0.22489700
Br	-1.57239300	0.13395000	-0.74395600

C	2.42392900	0.93106600	0.06176700
C	3.09874300	-0.28652100	0.68503700
C	3.46078200	1.76832500	-0.70244100
C	3.60053600	-1.24328100	-0.40903400
C	4.53358400	0.90439600	-1.38514700
C	3.99309300	-0.49047800	-1.69516700
H	1.63661600	0.58554800	-0.62048200
H	4.45346100	-1.81497700	-0.02673700
H	3.98125800	2.45255500	-0.02436800
H	1.93521000	1.52399600	0.84241600
H	3.95957300	0.06931400	1.26755900
H	2.95281900	2.38070300	-1.45436000
H	2.80572400	-1.95999200	-0.64401800
H	4.85998800	1.39418000	-2.31298600
H	4.72962300	-1.06852600	-2.26569600
H	3.11784300	-0.37892000	-2.34670800
N	2.16203100	-0.98752000	1.58188200
H	2.60126700	-1.80547100	1.99881300
H	1.83618400	-0.36495900	2.32916000
O	5.64133500	0.82734600	-0.48453900
H	6.33752500	0.29714500	-0.88935800
C	-2.95339100	-3.49157000	-1.60016200
C	-3.75579900	-2.77141500	-0.51341000
N	-1.46599200	-2.34995800	-0.16274700
H	-3.19114300	-3.16347300	-2.61438200
H	-4.34244500	-3.43856500	0.12240000
C	-2.70752100	-2.08082800	0.34787400
O	-2.94285500	-1.38769100	1.32350000
C	-1.49718700	-3.14341300	-1.30502500
O	-0.52995400	-3.49171300	-1.93769200
Br	0.20844400	-1.71907200	0.63619900
H	-3.05614800	-4.57890300	-1.57169800
H	-4.43339000	-2.00670400	-0.90185400
C	-0.97697900	3.80002900	-0.47553300
C	-2.46027100	4.03613700	-0.81828200
C	-0.83598900	3.01683100	0.82932800
C	-3.33834300	2.90006400	-0.26197400
C	-1.36839900	1.59491700	0.63652700
C	-2.58376100	1.57379100	-0.30834900
H	-0.52444400	3.22188000	-1.29373900
H	-3.62444400	3.12001400	0.77319300
H	-1.42110000	3.49833800	1.62369200
H	-0.44270000	4.75467600	-0.42368200
H	-2.77625600	4.97960200	-0.34275500
H	0.20195200	2.98555000	1.17421300
H	-4.26646900	2.84458100	-0.84221100
H	-0.57386400	0.97119400	0.20246800

H	-3.23416200	0.73704800	-0.03365100
H	-2.24204400	1.40085900	-1.33642400
N	-2.60192700	4.07977800	-2.27728200
H	-3.53496900	4.38460500	-2.53990800
H	-1.94556700	4.74144100	-2.68341300
O	-1.68815300	1.08896700	1.93449300
H	-2.05922100	0.19083400	1.84332400
O	0.76034700	1.01639600	3.10114700
H	-0.16873200	1.01145000	2.77205500
H	0.74980900	1.47167900	3.94784900

TS3_f

C	-2.62209500	-1.33626700	-0.27403700
C	-3.16514200	-0.30209900	0.70577000
C	-3.78330400	-2.10952100	-0.92295400
C	-3.97478800	0.77774500	-0.03292800
C	-5.03761900	-1.24677000	-1.12318500
C	-4.66083000	0.22299400	-1.29625600
H	-2.02775100	-0.82192300	-1.04016100
H	-4.72033200	1.19613800	0.65212800
H	-4.07402900	-2.96240800	-0.30122300
H	-1.94846500	-2.02240400	0.25015300
H	-3.83172900	-0.82551700	1.40502700
H	-3.45978700	-2.50844600	-1.88936800
H	-3.30111300	1.59179300	-0.32055600
H	-5.58592600	-1.60198300	-2.00639500
H	-5.54592100	0.82080300	-1.54306400
H	-3.98586300	0.30195600	-2.15707600
N	-2.08329400	0.26329100	1.53469400
H	-2.47467200	0.93469700	2.19481000
H	-1.24175200	-0.60347200	2.09149800
O	-5.85354600	-1.42646700	0.03699600
H	-6.66534100	-0.91726700	-0.06878300
C	2.41681300	4.15576300	-1.28771600
C	3.19099300	3.59834900	-0.09538700
N	1.16650500	2.36618100	-0.30316000
H	2.92998800	4.02497800	-2.24356700
H	3.33459600	4.31719700	0.71599200
C	2.29572700	2.47114500	0.40388600
O	2.62858400	1.74399300	1.36685000
C	1.12721500	3.32488500	-1.30616900
O	0.21019100	3.48348600	-2.08268200
Br	-0.66837100	1.27333200	0.56772100
H	2.15365300	5.21193800	-1.19631900
H	4.17235400	3.18734400	-0.34577900
C	1.95294200	-3.11334700	-1.13075100
C	3.28648100	-3.67330100	-0.59964200

C	1.25483200	-2.26487700	-0.06822700
C	3.92059400	-2.70747900	0.42040400
C	2.08477100	-1.01123300	0.21820800
C	3.58705200	-1.26407200	0.05586600
H	2.16660700	-2.49612300	-2.01335000
H	3.54392300	-2.92319200	1.42765300
H	1.15108800	-2.84623300	0.85657500
H	1.30360700	-3.93087900	-1.46130400
H	3.07774900	-4.62770200	-0.08782400
H	0.24454700	-1.97888000	-0.37416300
H	5.00398100	-2.86733600	0.44543000
H	1.76481500	-0.19256000	-0.43864600
H	4.13291200	-0.54362000	0.67268300
H	3.87458400	-1.08584300	-0.98693300
N	4.20271900	-3.84069900	-1.73081400
H	5.04044400	-4.34099700	-1.44757700
H	3.76696500	-4.37972500	-2.47434700
O	1.82985600	-0.58382600	1.58140800
H	2.06503300	0.44200700	1.60439200
O	-0.33463800	-1.26337000	2.39695300
H	0.78870700	-0.87241500	1.98556300
H	-0.34681400	-1.52998100	3.32176500

COM2g

C	-2.63499800	1.12996700	0.69121100
C	-2.62682000	0.95583000	-0.83316800
C	-3.74281400	0.27183100	1.30011500
C	-2.90819500	-0.50526800	-1.24247100
C	-3.45623800	-1.22457000	1.11217300
C	-2.56619100	-1.47665500	-0.11327700
H	-1.65740400	0.83619300	1.09451400
H	-3.96932700	-0.61802100	-1.49205800
H	-4.69446800	0.48509900	0.79606000
H	-2.76656200	2.18689700	0.94328800
H	-3.42102000	1.59264500	-1.25159400
H	-3.88982500	0.49934500	2.35915800
H	-2.33684900	-0.74599200	-2.14664900
H	-2.94854200	-1.61672600	2.00593000
H	-2.68996000	-2.51474700	-0.44384200
H	-1.51307600	-1.36396000	0.16485300
N	-1.32246700	1.39393000	-1.35754400
H	-1.33762300	1.47006000	-2.37169600
H	-1.05009400	2.29903500	-0.96465400
O	-4.72816300	-1.85353100	0.97929800
H	-4.60486800	-2.80899700	0.95370300
C	4.38222900	-0.25147300	1.11276800
C	4.24256700	-1.63370800	0.46479900

N	2.35142000	-0.33963700	-0.06877800
H	5.24420700	0.31757300	0.75676400
H	4.23550800	-2.45690400	1.18252100
C	2.89455100	-1.60608400	-0.25074800
O	2.38107500	-2.50602000	-0.86764000
C	3.11611700	0.49294700	0.71565200
O	2.81623700	1.62989200	1.02806600
Br	0.65746400	0.28426900	-0.71762400
H	4.43611200	-0.28193100	2.20359200
H	5.01684100	-1.84797300	-0.27556000
O	0.28120500	3.18668800	0.41502800
H	0.46039300	4.03056600	0.83989200
H	1.06855000	2.63522000	0.56651800

TS3_g

C	-2.38411000	0.93238500	0.98094400
C	-2.44449400	1.03515200	-0.54725500
C	-3.61686700	0.18580100	1.48974100
C	-2.98417500	-0.26118400	-1.19110200
C	-3.62320300	-1.27877900	1.02647600
C	-2.81285000	-1.46483700	-0.26431400
H	-1.47048100	0.40411600	1.28114200
H	-4.05167200	-0.13690100	-1.40550600
H	-4.52403600	0.65508300	1.08760800
H	-2.32886900	1.93577500	1.41603000
H	-3.12385600	1.86047200	-0.80381400
H	-3.69150900	0.24019200	2.57871200
H	-2.48264600	-0.43204100	-2.15044900
H	-3.18982900	-1.91577200	1.81091600
H	-3.13840500	-2.38371900	-0.76531600
H	-1.75393100	-1.60223500	-0.02196000
N	-1.13243600	1.45841400	-1.07699900
H	-1.20870600	1.69777100	-2.06493600
H	-0.42137000	2.32718300	-0.36305300
O	-4.99390900	-1.61828400	0.84249600
H	-5.06573400	-2.56309700	0.66613100
C	4.34517200	0.16587600	1.21724700
C	4.61677600	-1.24793800	0.71173200
N	2.49480600	-0.49538700	-0.12638800
H	5.07084600	0.91162900	0.88232200
H	4.73539000	-1.99067400	1.50360600
C	3.36176500	-1.58569800	-0.10533300
O	3.15745800	-2.64424800	-0.65475800
C	2.98957500	0.49265900	0.60724500
O	2.46858900	1.62465500	0.83633500
Br	0.34827000	0.17874200	-0.92548100
H	4.27170900	0.24631700	2.30521500

H	5.48788500	-1.32086700	0.05629200
O	0.47253100	2.83698900	0.20992200
H	0.25204700	3.45158900	0.91644200
H	1.38426800	2.18448300	0.46191800

COM2_h

C	-2.82427300	0.87439000	0.12772800
C	-2.56208400	0.17148800	-1.20944200
C	-3.84156500	0.06686000	0.93333000
C	-2.49960300	-1.36266400	-1.05090200
C	-3.27906700	-1.30129600	1.34489100
C	-2.17176000	-1.76291900	0.38767100
H	-1.88459800	0.97650800	0.68679800
H	-3.47104000	-1.79447900	-1.31738300
H	-4.73286100	-0.12188900	0.32060500
H	-3.18303600	1.89193600	-0.05563400
H	-3.39099700	0.41710300	-1.88971600
H	-4.17745300	0.61905800	1.81491400
H	-1.76351000	-1.77409900	-1.75135900
H	-2.86525800	-1.23877400	2.36206700
H	-2.05025400	-2.84993400	0.46964000
H	-1.21825200	-1.31670800	0.68817200
N	-1.31040500	0.68870300	-1.79563200
H	-1.20906700	0.38299300	-2.76095100
H	-1.29545000	1.71457300	-1.76206700
O	-4.38622600	-2.19973800	1.34086900
H	-4.10270000	-3.05010000	1.69474000
C	4.25084900	-0.26402100	1.46575200
C	4.51786600	-1.30062900	0.37129400
N	2.42755600	-0.27370600	-0.02408100
H	4.97283800	0.55605300	1.48124600
H	4.60312700	-2.32242700	0.74818600
C	3.29826800	-1.22828000	-0.54411400
O	3.10495500	-1.87742700	-1.54184800
C	2.88380300	0.31018000	1.12365800
O	2.29778300	1.16328000	1.77231100
Br	0.68782100	0.15484600	-0.82219300
H	4.20772800	-0.68394700	2.47338800
H	5.40995600	-1.09298400	-0.22372500
O	-0.13322500	2.49671100	1.55228000
H	-0.13137900	2.97650700	2.38579800
H	0.69432000	1.97510900	1.53473400
O	-1.09179400	3.40738300	-0.86390600
H	-0.74280400	3.14850400	0.01476800
H	-0.52964800	4.12208000	-1.17633900

TS3_h

C	-2.64008600	0.91938900	0.54489600
C	-2.54178000	0.50060100	-0.92719800
C	-3.73169900	0.09983200	1.23266900
C	-2.69001900	-1.02889200	-1.10288100
C	-3.37098900	-1.39171900	1.29826700
C	-2.38067400	-1.78007400	0.19269700
H	-1.67350300	0.76185200	1.04130700
H	-3.72103000	-1.25716700	-1.39687100
H	-4.66517000	0.17988300	0.66060500
H	-2.85397100	1.99070000	0.60815700
H	-3.36310800	0.99252200	-1.46793900
H	-3.94355700	0.48389400	2.23395800
H	-2.04087100	-1.37133900	-1.91656200
H	-2.91893100	-1.61919400	2.27484500
H	-2.42527600	-2.86338900	0.02923900
H	-1.35911200	-1.55620000	0.51596300
N	-1.31299100	1.05968600	-1.52735100
H	-1.33105200	0.92170600	-2.53684600
H	-1.04302300	2.32346600	-1.09044100
O	-4.60350200	-2.09656600	1.17361600
H	-4.44105800	-3.03771900	1.30304500
C	4.43560700	-0.35834300	1.19332800
C	4.45330200	-1.66063500	0.39596800
N	2.41932600	-0.47460900	-0.05956400
H	5.22940800	0.34256300	0.92126100
H	4.47577900	-2.55788000	1.01887800
C	3.12718300	-1.63178000	-0.37611700
O	2.74952500	-2.48664600	-1.14438300
C	3.09479200	0.25217400	0.81751700
O	2.73102500	1.34893400	1.32244600
Br	0.37981800	0.23556600	-0.91694800
H	4.47493300	-0.49299900	2.27728100
H	5.27564600	-1.73417000	-0.31913800
O	0.65164200	2.55753900	1.31238700
H	0.75287700	3.22009200	2.00362400
H	1.58209600	1.94044400	1.21777100
O	-0.70046500	3.26320500	-0.54459800
H	0.03537900	2.92364600	0.40687800
H	-0.24405200	3.85387300	-1.15407700

COM2i

C	-2.39625600	1.93137200	-0.09426600
C	-1.65106900	0.96713400	-1.02891900
C	-3.90493800	1.70653600	-0.19132300
C	-2.35243000	-0.40545500	-1.09239200
C	-4.28973300	0.32069400	0.34332700
C	-3.13143800	-0.67501800	0.19166800

H	-2.05609900	1.75751800	0.93670900
H	-3.04867700	-0.43032600	-1.93888400
H	-4.21418500	1.74815100	-1.24347200
H	-2.13388800	2.96639600	-0.33694800
H	-1.66653700	1.40822300	-2.03884900
H	-4.46455800	2.48572300	0.33338600
H	-1.60480200	-1.18943800	-1.25865900
H	-4.55772000	0.39963000	1.40835100
H	-3.51758100	-1.70100900	0.21359300
H	-2.45630200	-0.59410900	1.05074700
N	-0.27187600	0.80014400	-0.54574000
H	0.27745200	0.33982500	-1.27107300
H	0.15246000	1.71952100	-0.41614300
O	-5.43648000	-0.08449700	-0.39932700
H	-5.73728300	-0.93794500	-0.06759200
C	1.50791100	0.48236200	2.14972100
C	0.28129400	-0.39944300	2.40608600
N	1.48827500	-1.26669100	0.59124300
H	2.22954800	0.48018600	2.97070400
H	-0.65830700	0.14976300	2.31741000
C	0.29382900	-1.44651100	1.31101700
O	-0.51850800	-2.30153700	1.08334700
C	2.17510200	-0.10032100	0.92146000
O	3.12745600	0.32927100	0.31572000
Br	1.76447100	-2.11097100	-0.99574100
H	1.25485300	1.52040000	1.91864500
H	0.29873200	-0.90723900	3.37365500
C	2.69851700	3.21505400	-0.30572500
N	1.62584800	3.33562600	0.10896400
C	4.05385100	3.06435200	-0.82938000
H	4.08493600	3.39077100	-1.87025700
H	4.74342800	3.67158400	-0.24052800
H	4.33472200	2.01236700	-0.75668400

TS3_i

C	-2.66809500	0.95567000	0.74889000
C	-2.61391500	0.73288300	-0.76607400
C	-3.84534700	0.17112600	1.32825400
C	-2.91426000	-0.73290200	-1.15116500
C	-3.64834800	-1.34562000	1.18124300
C	-2.69558700	-1.68313400	0.02614600
H	-1.72903700	0.62125000	1.20734300
H	-3.96024100	-0.80863900	-1.46898200
H	-4.76315400	0.43131100	0.78538000
H	-2.75980000	2.02464200	0.96218200
H	-3.37075700	1.38166600	-1.22864500
H	-4.01597900	0.43304000	2.37538900

H	-2.29716400	-1.02631600	-2.00788600
H	-3.23396000	-1.75605300	2.11326900
H	-2.85751000	-2.72129000	-0.28601100
H	-1.65716600	-1.62232900	0.36818500
N	-1.33623800	1.24602500	-1.31010200
H	-1.36050400	1.23937100	-2.32975900
H	-0.95738500	2.40794700	-0.79920400
O	-4.94866500	-1.88530600	0.96304600
H	-4.89656800	-2.84766900	0.97299100
C	4.61356500	-1.03485700	0.78690300
C	4.10982200	-2.38492400	0.28210900
N	2.40002400	-0.71180200	-0.03387100
H	5.48157800	-0.64743800	0.24689500
H	4.05854100	-3.15483600	1.05507200
C	2.68971900	-2.07686400	-0.20679800
O	1.91783400	-2.87893400	-0.67288300
C	3.42551100	-0.13316400	0.52460200
O	3.52947200	1.10679800	0.86065600
Br	0.24905500	0.25349000	-0.81627600
H	4.85420100	-1.01335100	1.85298400
H	4.68899100	-2.78922000	-0.55111400
C	0.66687400	3.31284400	0.31107000
N	-0.39701200	3.33729200	-0.20855700
C	1.90381800	3.25176800	0.90287700
H	2.66232000	3.87000100	0.42839700
H	1.88692400	3.29642700	1.98926300
H	2.71064300	1.77132700	0.73673100

COM2'a

C	-3.46266500	-4.06334900	0.72660800
C	-4.29371700	-3.10444200	-0.12010600
C	-2.02085900	-3.55013000	0.86518000
C	-4.44118600	-1.75847200	0.61194700
C	-1.94493200	-2.01792900	0.96980900
C	-3.24492200	-1.44862900	1.53018400
H	-3.94540700	-4.15975600	1.70759000
H	-4.56760000	-0.96002500	-0.12798800
H	-1.42440600	-3.85198900	-0.00225000
H	-3.46270400	-5.06407100	0.27866500
H	-3.74249700	-2.92360000	-1.05627000
H	-1.55054400	-3.99755700	1.74711400
H	-5.35863100	-1.79972200	1.21098100
H	-1.10635800	-1.73230700	1.62338400
H	-3.13949900	-0.36912300	1.68740300
H	-3.40283500	-1.89454100	2.52008000
N	-5.62463400	-3.67238900	-0.35474700
H	-6.20967100	-3.00751300	-0.85456300

H	-5.55691900	-4.50162700	-0.93890900
O	-1.69623300	-1.49110100	-0.33875200
H	-1.61169200	-0.51973900	-0.23340700
C	4.78566100	-2.92765800	-1.21532400
C	4.77898700	-2.54401000	0.26882300
N	2.62379500	-2.23397900	-0.60752900
H	5.05566800	-3.97034500	-1.39659900
H	5.42514200	-1.69465100	0.50398300
C	3.34761100	-2.13756100	0.56588900
O	2.90244100	-1.76742900	1.63139400
C	3.35747400	-2.71775200	-1.69956800
O	2.91364600	-2.91809400	-2.79754900
Br	0.79342200	-1.90316700	-0.65049000
H	5.44624800	-2.30512800	-1.82284500
H	5.05174600	-3.36353100	0.93751400
C	-3.89893400	3.21572100	-0.67913000
C	-2.92582900	3.99838800	-1.57954300
C	-3.28169700	1.90201000	-0.19918800
C	-1.46566000	3.75906900	-1.14656000
C	-2.03725400	2.14267600	0.67535600
C	-1.40378600	3.50296400	0.35555000
H	-4.14898600	3.84523300	0.18456400
H	-1.05311200	2.89059100	-1.67510300
H	-2.96636100	1.30856600	-1.06797000
H	-4.83567400	3.02412800	-1.21363300
H	-3.04496800	3.63276100	-2.61278700
H	-4.01996000	1.30171700	0.34104100
H	-0.85739300	4.62637100	-1.42839300
H	-2.31088700	2.10691700	1.74003700
H	-0.37499600	3.51894600	0.72659400
H	-1.94397600	4.30015400	0.88013600
N	-3.23243000	5.42695900	-1.45905600
H	-2.70704100	5.96694700	-2.14095100
H	-4.21834000	5.59970200	-1.63731200
O	-1.13622100	1.07428400	0.38921700
H	-0.37593200	1.03564100	1.00512400
C	2.88712100	3.76327400	1.47817000
C	2.51319000	3.78020400	-0.01584100
C	2.08063000	2.71803700	2.24871600
C	2.12015400	2.37474300	-0.50722900
C	2.38180000	1.29780400	1.75062600
C	2.86040200	1.30660900	0.29046300
H	3.95788500	3.53307200	1.55779400
H	1.04066300	2.21334200	-0.40108400
H	1.00819800	2.90092100	2.10889700
H	2.74349900	4.75807300	1.91388400
H	1.64460600	4.44871300	-0.14556300

H	2.26449900	2.78835200	3.32451000
H	2.34197100	2.29053400	-1.57712100
H	3.15324700	0.83460400	2.37963600
H	2.70202200	0.31652900	-0.14656200
H	3.93815200	1.51316600	0.25640900
N	3.67957000	4.24272700	-0.77595100
H	3.43536400	4.39455100	-1.75072600
H	4.01749500	5.12981900	-0.41140800
O	1.17430700	0.54586400	1.90204800
H	1.40305600	-0.39413300	1.81437900

TS3'_a

C	-1.87236900	4.40527200	1.54658200
C	-3.16673400	3.65037600	1.89958700
C	-0.76007900	3.44018800	1.13573700
C	-3.29388700	2.35886200	1.06693100
C	-1.13091000	2.69565000	-0.16048400
C	-2.65333500	2.55786500	-0.30364100
H	-2.09116800	5.08822600	0.71474100
H	-2.79119700	1.53291800	1.58518700
H	-0.61219300	2.68321200	1.91709600
H	-1.55661300	5.02566900	2.39228700
H	-3.12148700	3.36991500	2.96487200
H	0.19414700	3.96152500	1.01901400
H	-4.35240600	2.08727700	0.97694100
H	-0.72687600	3.23229200	-1.03282700
H	-2.86724100	1.72564800	-0.98427800
H	-3.06980700	3.46320300	-0.76100300
N	-4.30956600	4.52156600	1.60648000
H	-5.16983100	4.12695900	1.97630400
H	-4.18699100	5.43283100	2.04022400
O	-0.59745600	1.37935000	-0.13988000
H	-0.81127900	0.04982000	-1.17730400
C	5.81858200	1.61392100	-0.94730300
C	5.51377700	0.30231800	-1.66762600
N	3.51955300	1.02352800	-0.60372500
H	6.16817100	2.41414400	-1.60265200
H	6.11248700	-0.54941300	-1.33616600
C	4.05814000	0.05325000	-1.32215300
O	3.48714700	-1.00504500	-1.71831700
C	4.47139000	2.02018200	-0.34303300
O	4.24914000	3.03608900	0.26733800
Br	1.32979100	1.30934500	-0.27977200
H	6.54469400	1.50665200	-0.13790800
H	5.60556100	0.36382600	-2.75566600
C	-4.11229800	-1.80763600	-2.92657100
C	-4.74545400	-2.16724700	-1.56631500

C	-2.78058900	-1.05103500	-2.78616200
C	-4.29575400	-1.16566600	-0.50097500
C	-1.99369600	-1.51448300	-1.56562100
C	-2.77762600	-1.24534700	-0.26636500
H	-3.95668300	-2.73325000	-3.49418000
H	-4.57985800	-0.15811100	-0.83136500
H	-2.96765000	0.02662600	-2.68045400
H	-4.81315400	-1.19846500	-3.50667800
H	-5.84104400	-2.11458900	-1.66287100
H	-2.16443800	-1.17503400	-3.68132600
H	-4.83043000	-1.34134300	0.44032800
H	-1.78584500	-2.58565900	-1.65703200
H	-2.42641700	-0.29976900	0.16366200
H	-2.54953800	-2.03160500	0.45847500
N	-4.29396000	-3.50671700	-1.16525900
H	-4.69198100	-3.76433300	-0.26563900
H	-4.60396500	-4.20307800	-1.83708800
O	-0.71848400	-0.86433400	-1.54376500
H	0.56504600	-1.48697900	-1.07589500
C	2.11933200	-3.74841300	2.33458600
C	0.62021500	-3.97727100	2.60415300
C	2.35371300	-3.35814300	0.87567900
C	-0.24794800	-3.07677200	1.70217600
C	1.72964500	-1.98681100	0.59398000
C	0.46543500	-1.75535100	1.42864000
H	2.46792700	-2.94194400	2.99337600
H	-0.46526100	-3.58639500	0.75407400
H	1.87819800	-4.09247700	0.21414100
H	2.69222800	-4.64448700	2.59494500
H	0.38609600	-5.02885900	2.36973700
H	3.41849800	-3.34765600	0.62378000
H	-1.21099800	-2.90228500	2.19478400
H	2.45235300	-1.19023500	0.81451500
H	-0.18167300	-1.02147800	0.93868900
H	0.76268200	-1.31182200	2.38569600
N	0.34606900	-3.64711500	4.00531600
H	-0.59582600	-3.92518000	4.26568700
H	0.98622800	-4.13691700	4.62467300
O	1.46572000	-1.91687500	-0.82992400
H	2.40433300	-1.38106000	-1.32497400

COM2'c

C	-2.81714700	-3.71832900	-0.30487800
C	-3.62873500	-2.44287700	-0.55604100
C	-1.38630300	-3.39793900	0.17777600
C	-3.80568500	-1.65679600	0.76252700
C	-1.30220500	-2.11609300	1.02737900

C	-2.62472800	-1.83656300	1.74522600
H	-3.35300400	-4.32196100	0.43834300
H	-3.94849600	-0.59446100	0.53347500
H	-0.70560700	-3.26682500	-0.67028200
H	-2.77353100	-4.32565700	-1.21738100
H	-3.04689300	-1.81321700	-1.24875200
H	-0.99943800	-4.24111400	0.76045200
H	-4.72866600	-2.00697300	1.23863900
H	-0.49389700	-2.21765000	1.76509500
H	-2.52028300	-0.95680900	2.39032900
H	-2.81934700	-2.68523900	2.41313300
N	-4.95495100	-2.79529200	-1.08867100
H	-5.49713900	-1.94454400	-1.23255400
H	-4.84727200	-3.21092300	-2.01276200
O	-0.97234900	-1.02476100	0.14085500
H	-0.84619000	-0.20809600	0.68118000
C	5.67777400	-0.26635000	-0.42271900
C	5.21892000	0.84739300	0.53564900
N	3.34649400	-0.38700300	-0.15757100
H	6.37300200	-0.97562500	0.03445000
H	5.43932200	1.85528200	0.17299000
C	3.70580500	0.68838500	0.64123600
O	2.93885800	1.36974000	1.29743200
C	4.40691100	-1.02032200	-0.81995100
O	4.30899200	-1.97247700	-1.55481600
Br	1.51624700	-0.88751000	-0.26290200
H	6.15406300	0.11125200	-1.33163400
H	5.64866200	0.76572800	1.53800300
C	-2.61763400	3.84886100	0.47456400
C	-2.71224200	3.31187000	-0.97357700
C	-1.97687800	2.82720800	1.42092400
C	-1.57818300	2.30182700	-1.26827500
C	-0.51473300	2.55801800	1.03262100
C	-0.30332400	2.65671600	-0.49677800
H	-2.00897200	4.76226500	0.45728600
H	-1.90054700	1.28977800	-0.99757700
H	-2.52457600	1.87759100	1.36455100
H	-3.61019300	4.14018800	0.83712500
H	-3.67358700	2.77658800	-1.07561700
H	-2.03557500	3.15595500	2.46324200
H	-1.38123100	2.28160700	-2.34664300
H	0.13487000	3.29286500	1.52755900
H	0.52384600	1.99996100	-0.78319800
H	-0.00919600	3.68006700	-0.75686900
N	-2.60418600	4.44952600	-1.90140600
H	-2.81086600	4.13956200	-2.84925100
H	-3.31107400	5.14678100	-1.67367900

O	-0.18110600	1.25510400	1.54977200
H	0.78682300	1.15495200	1.49540300

TS3'e

C	-2.82403500	-3.52032100	-0.30089200
C	-3.50852900	-2.18224800	-0.59700400
C	-1.40092500	-3.31854700	0.26219100
C	-3.69840600	-1.38465300	0.71186700
C	-1.24999800	-2.03284100	1.10937700
C	-2.58831200	-1.65387600	1.75430800
H	-3.45120900	-4.07365000	0.40959200
H	-3.74926800	-0.31447400	0.47855500
H	-0.66673700	-3.26344700	-0.54847200
H	-2.78162500	-4.13222200	-1.21064500
H	-2.83257400	-1.60473200	-1.24869900
H	-1.12357500	-4.18688100	0.87133000
H	-4.67005600	-1.66436800	1.13532000
H	-0.50240900	-2.20817400	1.89824900
H	-2.45492700	-0.78756800	2.41192800
H	-2.88300200	-2.48923700	2.40217700
N	-4.82440200	-2.42058300	-1.21289200
H	-5.27553400	-1.52651800	-1.40185600
H	-4.69454400	-2.85929300	-2.12340300
O	-0.82497400	-0.92470700	0.30742600
H	-0.23251300	0.44626200	1.11035800
C	5.61560000	-0.12771700	-0.40568500
C	4.99381500	0.95617500	0.48414400
N	3.25786700	-0.47440700	-0.25374400
H	6.34862300	-0.75235400	0.11192000
H	5.12044500	1.97374300	0.10209500
C	3.51384500	0.60516100	0.48783700
O	2.68522100	1.30597700	1.14024000
C	4.42515600	-1.00439500	-0.82985000
O	4.46888200	-1.98317000	-1.53697700
Br	1.15386600	-1.03254500	-0.20174200
H	6.10217900	0.26658600	-1.30189400
H	5.36398200	0.95415400	1.51391100
C	-2.45988300	3.64851600	0.54133500
C	-2.61789500	3.11590200	-0.90489500
C	-1.69620600	2.66393400	1.43642100
C	-1.47085900	2.14640700	-1.27279200
C	-0.25526500	2.50038100	0.93507300
C	-0.15824000	2.56396900	-0.60331200
H	-1.91193200	4.59843100	0.49392700
H	-1.72403400	1.12373600	-0.97307500
H	-2.19199000	1.68578900	1.40656400
H	-3.44006100	3.87262000	0.97611500

H	-3.56509200	2.55018500	-0.95840900
H	-1.69782900	2.98594800	2.48208800
H	-1.34701200	2.12679600	-2.36156600
H	0.39230900	3.26085300	1.37994800
H	0.67252700	1.93871500	-0.94081900
H	0.07223800	3.59506100	-0.89309900
N	-2.59602100	4.26430400	-1.82450400
H	-2.83153900	3.95507500	-2.76572000
H	-3.31745400	4.93285300	-1.55967000
O	0.27991400	1.24495800	1.47602200
H	1.43366500	1.15041900	1.25980000

COM2'd

C	-2.22379100	-3.31066800	1.32699600
C	-3.67352900	-2.85606000	1.01554800
C	-1.22105900	-3.00659800	0.19049300
C	-3.92036000	-2.87554400	-0.49964100
C	-1.61468200	-1.73442600	-0.55286700
C	-2.96541600	-1.93185200	-1.27053900
H	-1.89732100	-2.82004700	2.25226400
H	-3.78490500	-3.90805400	-0.84296000
H	-1.19092200	-3.83544000	-0.52833600
H	-2.22097100	-4.38658800	1.53320900
H	-4.36649900	-3.57617700	1.48408000
H	-0.20814200	-2.90157700	0.59003300
H	-4.96587900	-2.62158100	-0.71579200
H	-1.71113400	-0.92493300	0.17998100
H	-2.75146400	-2.35227500	-2.25951200
H	-3.43698800	-0.95775100	-1.43529600
N	-3.88609600	-1.48600200	1.52444000
H	-4.84886000	-1.20407200	1.34745000
H	-3.77163400	-1.47898900	2.53599900
O	-0.59447800	-1.39614900	-1.50478500
H	-0.67057600	-0.41929000	-1.70698400
C	5.45443300	-0.10233100	1.04890200
C	5.08074700	1.24429800	0.40681500
N	3.34130800	-0.29266600	0.03474300
H	5.59815200	-0.04436300	2.13140900
H	5.76945100	1.55793400	-0.38280200
C	3.69955200	1.02799900	-0.21013500
O	3.02811400	1.84704700	-0.80559800
C	4.27304300	-1.03388700	0.76625200
O	4.15131700	-2.18831000	1.10326100
Br	1.65366000	-0.96185000	-0.56792200
H	6.35850000	-0.55117600	0.62818600
H	5.01689800	2.06836100	1.12291900
C	-0.59249900	2.08708000	0.49297400

C	-1.07977500	2.33465600	-0.95525100
C	-1.67889300	2.38692000	1.54933000
C	-2.60203100	2.18709800	-1.05149400
C	-2.56396200	3.55971700	1.13094600
C	-3.33089200	3.22457800	-0.17228300
H	-0.26615600	1.04615100	0.58707200
H	-2.92960300	2.28029100	-2.09466500
H	-1.21416600	2.60385400	2.51641200
H	0.28967500	2.70633600	0.67688100
H	-0.82702600	3.37165400	-1.21992200
H	-2.32187800	1.50953600	1.69181800
H	-2.87306100	1.17465700	-0.73006900
H	-3.29008900	3.77701300	1.93022900
H	-3.48603700	4.15774500	-0.73010300
H	-4.32964100	2.84808000	0.07827700
N	-0.41612000	1.38277600	-1.87657000
H	-0.58399900	1.67108900	-2.83969100
H	0.59460700	1.43422600	-1.73521200
O	-1.69092500	4.68367000	0.96377700
H	-2.22962200	5.43543000	0.68459300

TS3'a

C	-3.26971000	-2.54028300	1.41465800
C	-4.49118600	-1.65490900	1.05408200
C	-2.22518300	-2.63887600	0.27988700
C	-4.70930900	-1.64520800	-0.46568100
C	-2.16156800	-1.33589800	-0.51685400
C	-3.49794600	-1.06987400	-1.23688900
H	-2.80137200	-2.13520300	2.32040300
H	-4.90122300	-2.67734300	-0.78206900
H	-2.48172100	-3.45202200	-0.41084800
H	-3.61791500	-3.54610500	1.67408000
H	-5.38683100	-2.09585500	1.52499300
H	-1.23740700	-2.87411100	0.68823400
H	-5.61675900	-1.08038600	-0.71488600
H	-1.95744100	-0.51165100	0.17767400
H	-3.44196600	-1.53204500	-2.22896200
H	-3.61230200	0.00672300	-1.39263700
N	-4.25810400	-0.27173700	1.51641000
H	-5.08227900	0.29427800	1.32064300
H	-4.14796200	-0.26810400	2.52851700
O	-1.17379100	-1.35552400	-1.55111100
H	1.21755100	0.91990900	-1.64387500
C	4.88042500	-1.85043000	1.16121600
C	5.15502500	-0.38824200	0.80576400
N	2.96145200	-0.92333900	0.02346800
H	4.90925600	-2.05851900	2.23424000

H	6.00055200	-0.24028700	0.12668000
C	3.86920200	0.03343400	0.10830700
O	3.76354400	1.23530000	-0.32332500
C	3.45205500	-2.09010100	0.63726800
O	2.83574000	-3.12865400	0.73912400
Br	0.60823500	-1.25130800	-0.84123900
H	5.56095800	-2.55654100	0.67720100
H	5.32535700	0.25988500	1.67128200
C	0.68553500	2.22137700	0.80807500
C	0.64576300	2.65217500	-0.66315900
C	-0.20897200	3.13308800	1.68091200
C	-0.78317700	2.52418000	-1.23809700
C	-1.37150800	3.78025700	0.90979200
C	-1.88282900	2.85267900	-0.19547700
H	0.36569500	1.17489500	0.86909200
H	-0.87694400	3.17750500	-2.11303400
H	0.37894700	3.94691200	2.11704400
H	1.71698100	2.25109700	1.17179100
H	0.97012900	3.69436200	-0.72571200
H	-0.61450800	2.55012200	2.51424000
H	-0.93111400	1.49687300	-1.59171500
H	-2.18926000	3.99969400	1.61330200
H	-2.75078100	3.30352800	-0.69371200
H	-2.25249000	1.93333300	0.27497300
N	1.61927600	1.84830900	-1.46549300
H	1.78669700	2.28734300	-2.37000200
H	2.74620300	1.53576700	-0.85699200
O	-0.87069300	5.01190700	0.36418800
H	-1.58274300	5.41466400	-0.15112000

COM2'e

C	-4.35322300	-0.13750200	-1.63783100
C	-5.08497100	-0.21065300	-0.30083900
C	-2.84198300	0.04545500	-1.42442800
C	-4.64921000	-1.47370900	0.46323600
C	-2.32828000	-0.69061900	-0.17823800
C	-3.20321800	-1.89781700	0.14237700
H	-4.56542000	-1.06240100	-2.18982600
H	-4.75973600	-1.30266000	1.53989400
H	-2.59371000	1.10625300	-1.31103400
H	-4.74918000	0.68585900	-2.24363900
H	-4.78662200	0.66788200	0.29197800
H	-2.29816200	-0.31288800	-2.30503700
H	-5.33504900	-2.28404600	0.18923700
H	-1.29045300	-1.01789100	-0.34701700
H	-2.76527600	-2.45918200	0.97439500
H	-3.18803100	-2.55819000	-0.73416500

N	-6.53239700	-0.26371800	-0.52991400
H	-7.02430600	-0.38456200	0.35190300
H	-6.85851500	0.61192500	-0.93055700
O	-2.33232300	0.23177300	0.91834800
H	-1.99291700	-0.25772500	1.69548800
C	2.71269200	4.09466900	-1.07191500
C	3.50103400	3.31536700	-0.01350200
N	1.26869200	2.59681200	0.02931400
H	3.08409700	3.95016400	-2.08865600
H	3.92369100	3.94552400	0.77250200
C	2.49333400	2.37360700	0.62180500
O	2.71878600	1.55749900	1.49174300
C	1.29356000	3.55225600	-0.99775100
O	0.34805300	3.86521000	-1.66930000
Br	-0.28028800	1.66703700	0.48405900
H	2.67469600	5.16983400	-0.88310400
H	4.31379300	2.71303400	-0.42654700
C	1.67934500	-3.58050900	-0.95027300
C	3.18010300	-3.86674200	-0.75027800
C	1.09936800	-2.84123200	0.25463200
C	3.83223700	-2.78369100	0.12993400
C	1.71457500	-1.44234300	0.35942100
C	3.17348000	-1.43192100	-0.12796200
H	1.56544600	-2.95888300	-1.84899400
H	3.72335300	-3.04290100	1.18963900
H	1.33859200	-3.38548000	1.17745600
H	1.13667000	-4.51325800	-1.13599000
H	3.27868900	-4.83608700	-0.23420300
H	0.00769000	-2.77589300	0.20564900
H	4.90692600	-2.74590500	-0.08053700
H	1.12658500	-0.73641100	-0.24625300
H	3.70789800	-0.61741400	0.37275100
H	3.19896700	-1.22924900	-1.20584400
N	3.83254900	-3.87161100	-2.06326500
H	4.78792600	-4.20996000	-1.99114500
H	3.34398400	-4.48855400	-2.70678300
O	1.62238100	-1.05343700	1.73268400
H	1.93374600	-0.13511300	1.81981600
O	-0.91057600	-1.39221000	2.57528500
H	0.03770200	-1.25887000	2.33860400
H	-0.93851700	-1.67199900	3.49457600

TS3'e

C	-2.95347700	-3.34022900	-0.63369400
C	-3.63438200	-1.98186300	-0.82503600
C	-1.58582400	-3.19523500	0.06692700
C	-3.95886300	-1.36172500	0.54957400

C	-1.52669800	-2.01347100	1.06454600
C	-2.91666500	-1.71267400	1.63881500
H	-3.62803700	-3.97864500	-0.04894400
H	-4.04972700	-0.27425600	0.44598800
H	-0.78868500	-3.04395300	-0.66766000
H	-2.82380600	-3.83865500	-1.60234800
H	-2.91342900	-1.31939600	-1.33163600
H	-1.34662100	-4.12573900	0.59523400
H	-4.94372800	-1.73223700	0.85728500
H	-0.84748600	-2.27923000	1.89100000
H	-2.84465600	-0.90868800	2.37926100
H	-3.23911400	-2.60938000	2.18315200
N	-4.88340800	-2.15163100	-1.58501900
H	-5.33658800	-1.24575900	-1.69693800
H	-4.66260200	-2.46625700	-2.52868600
O	-1.04501800	-0.81938300	0.43659200
H	-0.89420400	0.48718700	1.35595700
C	5.24646100	-0.85059000	-1.30837000
C	5.27663700	0.21971500	-0.21117500
N	3.10560900	-0.72664200	-0.25119900
H	5.92876300	-1.68472700	-1.12162600
H	5.46709000	1.23097400	-0.58400700
C	3.87275900	0.16906700	0.37457700
O	3.54397000	0.91396800	1.33746900
C	3.80265100	-1.37546900	-1.28572100
O	3.32941900	-2.20711300	-2.02452000
H	5.47054000	-0.46804600	-2.30752500
H	6.00486800	0.03081800	0.58297400
C	-2.53459800	3.62886200	-0.26425000
C	-1.78213200	3.21929200	-1.55364400
C	-2.34620000	2.59781100	0.85550000
C	-0.53284900	2.36927800	-1.22462500
C	-0.87282000	2.53355000	1.29660700
C	0.08428700	2.79601500	0.11117800
H	-2.14476400	4.60152000	0.06279700
H	-0.79567500	1.30712100	-1.18693900
H	-2.63698100	1.60676000	0.48593700
H	-3.60029900	3.77332800	-0.47541300
H	-2.46191700	2.59484400	-2.16019300
H	-2.98798800	2.81476900	1.71511900
H	0.20072900	2.47449900	-2.03236700
H	-0.68695800	3.27921600	2.07733500
H	1.03666100	2.28791900	0.28816800
H	0.30158500	3.86941300	0.06596300
N	-1.36645300	4.44317400	-2.25796600
H	-0.99668000	4.20060500	-3.17537200
H	-2.17877700	5.03329100	-2.43021100

O	-0.62932200	1.26376300	1.95281900
H	0.65345400	1.01052100	2.40546400
O	1.61880500	0.69527100	2.79211100
H	2.46496500	0.79036700	2.04181500
H	1.52266200	-0.25627700	2.94627100
Br	0.95413200	-0.88863600	0.05046900

COM2'f

C	4.40155000	-0.63245800	-1.54363100
C	5.57425100	-0.41226600	-0.55892100
C	3.11964800	-1.05850900	-0.81966800
C	5.05898400	0.05558800	0.82361100
C	2.62201600	0.04784300	0.12819300
C	3.78793500	0.89520200	0.67840800
H	4.22822800	0.31007000	-2.07887200
H	4.84512000	-0.81685400	1.45205600
H	3.31546600	-1.95057000	-0.21270800
H	4.67809400	-1.37559100	-2.30041400
H	6.08631500	-1.38067100	-0.41691100
H	2.33364300	-1.33376600	-1.52884700
H	5.84643700	0.62421300	1.33213300
H	1.92184300	0.70744800	-0.40494600
H	3.48340400	1.34740700	1.62802000
H	3.98760000	1.72161900	-0.01369400
N	6.46708400	0.61668700	-1.11751700
H	7.32168300	0.66461300	-0.56550500
H	6.75521500	0.34628000	-2.05648500
O	1.91819100	-0.60537800	1.20275900
H	1.54116400	0.09079100	1.80964600
C	-3.45025300	-3.70312900	-1.05618000
C	-4.16592500	-2.70483000	-0.13345600
N	-1.85059200	-2.30756100	-0.02466700
H	-3.72840400	-3.59852300	-2.10862000
H	-4.70855200	-3.18065200	0.68861300
C	-3.05431300	-1.84224000	0.45792600
O	-3.21418800	-0.90488500	1.22504000
C	-1.96025300	-3.38630200	-0.91472000
O	-1.03698000	-3.94374700	-1.45813700
Br	-0.14664100	-1.55627200	0.49522500
H	-3.61229100	-4.74911900	-0.78248200
H	-4.87545100	-2.05395000	-0.65170200
C	-0.85283800	4.11489900	-0.69917000
C	-2.07569800	3.89666300	-1.62762500
C	-0.98029700	3.40795600	0.66797200
C	-3.33508500	3.63447200	-0.78915900
C	-1.75469100	2.09968800	0.54305400
C	-3.20581300	2.37172200	0.09577600

H	0.04581300	3.76076900	-1.21916600
H	-3.50890300	4.51752800	-0.16236600
H	-1.51101000	4.05148600	1.38183000
H	-0.70939400	5.18874700	-0.53567200
H	-2.23617800	4.82202300	-2.20821000
H	0.00895600	3.22035900	1.09617200
H	-4.21320500	3.55235400	-1.44229800
H	-1.26001600	1.45932600	-0.19709500
H	-3.81155400	2.49658900	1.00024900
H	-3.59370300	1.49330500	-0.42768800
N	-1.82950400	2.73305100	-2.49760300
H	-2.61769900	2.60445600	-3.12976500
H	-1.01877600	2.91064400	-3.08685600
O	-1.73355200	1.43741200	1.82369100
H	-2.15123900	0.56073500	1.70259700
O	0.79080900	1.27147500	2.70589000
H	-0.16216700	1.30752900	2.41922900
H	0.77351800	1.11087300	3.65699800

TS3'_f

C	-4.71547300	-0.06623600	-1.49439300
C	-5.70873300	-0.55364300	-0.41285500
C	-3.47726200	0.59355800	-0.87647400
C	-4.96838400	-0.92362200	0.89460500
C	-2.66122400	-0.41841600	-0.04348900
C	-3.57721500	-1.48709300	0.59642600
H	-4.40935100	-0.93642300	-2.08985700
H	-4.86992200	-0.03359900	1.52669500
H	-3.78270300	1.40369900	-0.20343400
H	-5.21635500	0.62338300	-2.18385500
H	-6.39923100	0.27761000	-0.18405700
H	-2.84600500	1.05011500	-1.64458000
H	-5.56819100	-1.64673200	1.46022800
H	-1.93244500	-0.92471400	-0.69760700
H	-3.09320800	-1.87238000	1.50017500
H	-3.68241000	-2.33190100	-0.09423400
N	-6.41392400	-1.74157700	-0.92319600
H	-7.18286800	-1.97820300	-0.29854500
H	-6.84019000	-1.52553400	-1.82282400
O	-1.96779100	0.24852200	1.01414300
H	-1.01775700	-0.63355900	1.96333600
C	2.61936400	4.50977500	-0.86714900
C	3.47399800	3.59821500	0.02012600
N	1.32324800	2.61745900	-0.17129200
H	2.99964800	4.60493600	-1.88809300
H	3.80776400	4.06951700	0.94997200
C	2.52954800	2.45452400	0.35683400

O	2.93142100	1.48436200	1.06896900
C	1.24841800	3.81503300	-0.90804200
O	0.26031700	4.21639800	-1.47682200
Br	-0.45965900	1.39692800	0.35757800
H	2.49450000	5.52176900	-0.47312400
H	4.36531700	3.19793300	-0.47204800
C	1.91553400	-3.81798500	-0.69362300
C	3.44173600	-4.02132200	-0.53942000
C	1.36350900	-2.82290600	0.33473500
C	4.11278600	-2.75228300	0.03722900
C	1.95580100	-1.42285700	0.09929700
C	3.39442400	-1.48775100	-0.44024600
H	1.72346900	-3.44223300	-1.70672700
H	4.09748600	-2.78948500	1.13275100
H	1.63311400	-3.14839300	1.34632000
H	1.39304300	-4.77731400	-0.61051000
H	3.60636600	-4.84492400	0.17778500
H	0.27108800	-2.78613000	0.30383400
H	5.16757800	-2.73078100	-0.25944800
H	1.31907700	-0.84750900	-0.58245800
H	3.93265400	-0.58200800	-0.14599300
H	3.35778600	-1.49622300	-1.53502400
N	4.01073000	-4.30711600	-1.86565100
H	4.98106300	-4.60037100	-1.76834100
H	3.52067700	-5.09293600	-2.28952900
O	1.97198100	-0.69830000	1.37321600
H	2.32353800	0.42921700	1.22171700
O	-0.30518400	-1.09007000	2.51452700
H	1.06641400	-0.79577300	1.84306900
H	-0.37918800	-0.70412000	3.39650300

COM2'g

C	-3.61849600	0.14596600	1.46347000
C	-3.52326200	-1.30795300	0.94288300
C	-2.50904300	1.03036800	0.88221900
C	-2.90321600	-1.35437300	-0.47459400
C	-2.65702000	1.16948400	-0.64961100
C	-3.25980100	-0.10003700	-1.27804700
H	-4.59725600	0.54643500	1.16957100
H	-1.81391700	-1.44397200	-0.39939900
H	-1.52982300	0.58333000	1.09015400
H	-3.59004100	0.15956900	2.55939400
H	-2.85460500	-1.86872200	1.62028300
H	-2.51127100	2.01960800	1.35514100
H	-3.25227400	-2.25485100	-0.99312700
H	-3.31757500	2.02047700	-0.87375700
H	-2.90696700	-0.16821800	-2.31177700

H	-4.35045400	-0.00490600	-1.31337900
N	-4.88053700	-1.87556500	0.89823000
H	-4.82838500	-2.87184400	0.69372500
H	-0.95002900	2.17673400	-0.83060400
O	-1.39144500	1.42132900	-1.28191800
C	4.48820300	-0.06699700	1.04925200
C	4.41687600	-1.49855800	0.48861100
N	2.43274600	-0.35804900	-0.04687100
H	5.30883300	0.52535800	0.63512100
H	4.48538800	-2.27259900	1.25768500
C	3.05086300	-1.60845900	-0.19164700
O	2.57528000	-2.56720500	-0.74877500
C	3.16843800	0.58607500	0.65271600
O	2.81069500	1.72432200	0.89814400
Br	0.70639000	0.10055300	-0.69177300
H	4.58239200	-0.02870800	2.13822300
H	5.19039500	-1.71281300	-0.25396200
O	0.22399400	3.22588500	0.16376000
H	-0.05263400	3.39476500	1.07294600
H	1.04523300	2.70876300	0.25879300
H	-5.31556400	-1.80020800	1.81630300

TS3'_g

C	-3.64189700	0.28109800	1.42029000
C	-3.66950100	-1.20008300	0.97038300
C	-2.38689700	1.00703400	0.92055700
C	-2.87216900	-1.40190700	-0.33874400
C	-2.38629300	1.09674500	-0.61998500
C	-2.97818300	-0.18217200	-1.26085600
H	-4.53162900	0.77424000	1.00712000
H	-1.81994400	-1.59167400	-0.10324000
H	-1.48882300	0.46545800	1.24112500
H	-3.72229900	0.34945500	2.51151900
H	-3.17993700	-1.80372500	1.75546400
H	-2.32461500	2.01354100	1.35426900
H	-3.23997300	-2.29873900	-0.85141400
H	-3.01674500	1.94930900	-0.91801500
H	-2.46299400	-0.35383200	-2.21108200
H	-4.03587800	-0.01505100	-1.49294600
N	-5.07158500	-1.59416500	0.75502400
H	-5.12328600	-2.59806600	0.59167900
H	-0.22607300	2.36289700	-0.40845800
O	-1.09883100	1.41595200	-1.15057300
C	4.38853300	0.13619200	1.07347200
C	4.51510200	-1.33499500	0.65588400
N	2.41080600	-0.47599800	-0.07051900
H	5.14315600	0.79164900	0.62830300

H	4.62602300	-2.02193100	1.49918000
C	3.19466400	-1.64460300	-0.06783600
O	2.86792700	-2.70078100	-0.55340600
C	3.01671900	0.53607700	0.55488300
O	2.57474000	1.70876600	0.73792000
Br	0.45831400	0.09773700	-0.78325600
H	4.42432600	0.29702400	2.15522400
H	5.34604400	-1.52568100	-0.02853200
O	0.54134900	2.88583700	0.11048900
H	0.16882500	3.25497600	0.92209700
H	1.49802400	2.20208400	0.36527900
H	-5.61168900	-1.42011300	1.60111300

COM2'h

C	-3.37417500	-1.39285600	1.27317900
C	-4.60818900	-1.32877900	0.35553200
C	-2.08896000	-1.11584400	0.49383800
C	-4.39805400	-0.30488000	-0.77607900
C	-2.07961800	0.31687000	-0.05883500
C	-3.50384300	0.83531000	-0.29834200
H	-3.49664800	-0.63927600	2.06218700
H	-3.92469700	-0.79142000	-1.63719500
H	-2.01877000	-1.80013400	-0.36201900
H	-3.32237600	-2.36853200	1.76901100
H	-4.74821700	-2.32311600	-0.10028300
H	-1.20667100	-1.29482500	1.11456200
H	-5.37207900	0.06753900	-1.11256600
H	-1.55088700	0.98843000	0.63385000
H	-3.46298900	1.65970500	-1.01770900
H	-3.91019400	1.24520900	0.63409300
N	-5.76497400	-0.92466500	1.16151800
H	-6.62364000	-1.00153600	0.62372500
H	-5.86501700	-1.52650600	1.97473400
O	-1.34878900	0.28207200	-1.29313100
H	-1.27203000	1.21115100	-1.58944400
C	4.71614000	-0.03515800	1.22144800
C	4.89197700	-1.27397900	0.33734700
N	2.76143700	-0.34733200	-0.03931000
H	5.39997500	0.77895300	0.96869400
H	5.01175500	-2.19852100	0.90728400
C	3.60343100	-1.38451700	-0.46594000
O	3.32682100	-2.19787400	-1.30504800
C	3.30118900	0.44242300	0.94955200
O	2.74262100	1.37619700	1.49156800
Br	1.01578300	-0.11163400	-0.66089600
H	4.81877900	-0.23274500	2.29048700
H	5.73007200	-1.20513600	-0.35907000

O	0.28829400	2.74249600	1.11378700
H	1.09010700	2.19277300	1.18396800
H	0.31120400	3.35814500	1.85221900
O	-0.99134300	2.99318500	-1.30446700
H	-0.50977600	3.55492600	-1.91801500
H	-0.50578300	3.01593300	-0.45447400

TS3'h

C	-3.74475900	-1.67943800	0.58170200
C	-4.80157600	-0.97386000	-0.28737300
C	-2.33096800	-1.25565700	0.18499900
C	-4.31434900	0.42282900	-0.71871000
C	-2.10994200	0.23993600	0.47145100
C	-3.42611400	1.02605900	0.36507100
H	-3.92952900	-1.41048300	1.63050300
H	-3.74326200	0.34993700	-1.65158200
H	-2.18230300	-1.41143700	-0.89140900
H	-3.85960600	-2.76625900	0.50738100
H	-4.95918700	-1.57920500	-1.19546800
H	-1.57633900	-1.86017700	0.69562600
H	-5.18163800	1.06147700	-0.92100900
H	-1.68811700	0.36990800	1.48118200
H	-3.19706600	2.07913500	0.17079300
H	-3.95771800	0.98499500	1.32324800
N	-6.03069400	-0.82980600	0.49957600
H	-6.79854800	-0.50915900	-0.08353200
H	-6.30923500	-1.72224100	0.89882800
O	-1.19697100	0.78132800	-0.47828600
H	-0.85270300	2.15661100	-0.29005000
C	4.98866700	-0.56397100	0.29262800
C	4.56672400	-2.01850600	0.08957700
N	2.65166500	-0.59479900	-0.06658900
H	5.68416200	-0.18871500	-0.46226500
H	4.77285800	-2.66174900	0.94770300
C	3.05306200	-1.94109300	-0.11518800
O	2.30741700	-2.86908200	-0.29138400
C	3.68353900	0.19572000	0.17254200
O	3.66376300	1.45118900	0.29689100
Br	0.63679800	0.05598800	-0.28192800
H	5.42649000	-0.35890400	1.27296200
H	5.01307700	-2.48654200	-0.79063100
O	1.96255800	3.11415800	0.30005600
H	2.70190700	2.18209000	0.25880900
H	2.08867100	3.61900800	1.11097500
O	-0.44773300	3.11376200	-0.14909700
H	-0.70306000	3.66087800	-0.89928900
H	0.91844900	3.06054900	0.07817200

COM2'i

C	-3.38651200	-1.46141000	1.29229800
C	-4.65827900	-1.36992400	0.42901700
C	-2.12834000	-1.25898800	0.44929200
C	-4.45226200	-0.40033700	-0.75041000
C	-2.08875800	0.15759300	-0.14068000
C	-3.50042500	0.72211800	-0.34773100
H	-3.44311500	-0.68283300	2.06478900
H	-4.02985700	-0.93720700	-1.60797200
H	-2.12298700	-1.96493900	-0.39088600
H	-3.35095700	-2.42432600	1.81314100
H	-4.86792100	-2.37168700	0.01886200
H	-1.22393100	-1.45602100	1.03139600
H	-5.42278100	-0.00270500	-1.06689900
H	-1.52186300	0.82130000	0.53264200
H	-3.46149100	1.51884100	-1.09867100
H	-3.85904300	1.17747800	0.58340500
N	-5.75377400	-0.87623300	1.26919300
H	-6.63996300	-0.92900800	0.77489900
H	-5.84556000	-1.44063300	2.10978300
O	-1.38788500	0.06180100	-1.38318200
H	-1.36125800	0.94705800	-1.78143300
C	4.75765300	-0.00599600	1.22718100
C	4.93275900	-1.29564300	0.41865100
N	2.79751400	-0.40696800	-0.00047200
H	5.44019500	0.79167600	0.92400600
H	5.06983100	-2.18249000	1.04207100
C	3.63760900	-1.46840100	-0.36111900
O	3.35689000	-2.34201200	-1.13647200
C	3.33987600	0.45770600	0.93639600
O	2.77807800	1.41624100	1.41382400
Br	1.07340700	-0.22466400	-0.65610000
H	4.86466800	-0.14062600	2.30550200
H	5.76099700	-1.26163800	-0.29218500
C	-0.46014000	3.14188800	-0.38578700
N	-0.95583500	2.97380900	-1.41724900
C	0.15891800	3.33557700	0.92260900
H	0.92596700	2.57156200	1.08103300
H	0.61977500	4.32408300	0.96853300
H	-0.60453400	3.25775500	1.69950400

TS3'i

C	-3.78209400	-1.59746700	0.75674800
C	-4.83656200	-1.01346000	-0.20086700
C	-2.36661800	-1.23618500	0.30661700
C	-4.34390800	0.30951900	-0.81825600

C	-2.14720600	0.28145800	0.40156900
C	-3.45469800	1.05378800	0.17335400
H	-3.96408300	-1.18528800	1.75838100
H	-3.77621500	0.11006600	-1.73462000
H	-2.22023200	-1.53125000	-0.74045600
H	-3.89884900	-2.68371900	0.83274400
H	-4.99619500	-1.73721500	-1.01714500
H	-1.61506600	-1.77194300	0.89251600
H	-5.20789000	0.91966900	-1.10347600
H	-1.72886500	0.54431700	1.38624000
H	-3.22043100	2.06735700	-0.16723400
H	-3.98873200	1.15051000	1.12605300
N	-6.06361700	-0.75844500	0.55984200
H	-6.82899600	-0.51106200	-0.06090000
H	-6.34951800	-1.58871000	1.07215300
O	-1.21968500	0.70451200	-0.60513700
H	-0.86918400	2.04858200	-0.39214500
C	4.97834200	-0.73345500	0.33322000
C	4.51355200	-2.17050700	0.10467100
N	2.64179900	-0.67189600	-0.05416700
H	5.69584200	-0.36888800	-0.40623200
H	4.68911500	-2.83199000	0.95548200
C	3.00641400	-2.03929900	-0.11585300
O	2.22853200	-2.93268700	-0.31178500
C	3.69631100	0.05585200	0.20165000
O	3.75232200	1.32950400	0.34568100
Br	0.57661600	-0.01292800	-0.33940700
H	5.40556100	-0.55264500	1.32300300
H	4.95535500	-2.63887000	-0.77754600
C	0.75247800	3.22762800	0.09588500
N	-0.39516000	3.04092000	-0.13939200
C	2.07300600	3.42220400	0.36809800
H	2.88870900	1.94849200	0.28607700
H	2.63541200	3.95922300	-0.39047200
H	2.30810600	3.66069200	1.40176200

TS6a

C	2.58497800	-1.67694500	1.74370300
C	3.42965600	-0.68478300	1.37497700
C	1.32409900	0.00503500	0.89178900
N	1.31195200	-1.23122400	1.44875900
H	2.78821700	-2.64983300	2.16175300
H	4.50636400	-0.63355100	1.40976100
N	2.64045500	0.33180600	0.87182000
C	0.09523400	-1.99896200	1.71728200
C	-0.22309900	-1.98437200	3.21080700
C	0.20032000	-3.41386300	1.15613900

H	-0.69075200	-1.45724300	1.18989900
H	-0.28365400	-0.95675800	3.58111700
H	-1.18044400	-2.48087600	3.39388500
H	0.55305000	-2.51053100	3.77707000
H	0.47433900	-3.38909600	0.09781300
H	0.95244900	-3.99703000	1.69828800
H	-0.75928100	-3.92583400	1.27819800
C	3.18099300	1.59712700	0.36154800
C	4.18226000	1.32628800	-0.75848400
C	3.78266500	2.41063300	1.50443200
H	2.32061500	2.13108000	-0.04515300
H	3.76153400	0.63712000	-1.49473600
H	4.44801000	2.26475500	-1.25314100
H	5.10323200	0.88393900	-0.36257900
H	3.03419300	2.59746200	2.27959100
H	4.62889900	1.88427500	1.95905500
H	4.14586400	3.37117800	1.12783900
C	0.03271700	0.82896800	-0.89607900
O	1.08591300	0.95256400	-1.66543200
C	-0.45804200	2.11550200	-0.31161200
C	-0.49746200	3.20776600	-1.18177700
C	-0.91949600	2.24735200	0.99818300
C	-1.01309300	4.42661200	-0.74469500
H	-0.11959900	3.09407400	-2.19300800
C	-1.44666000	3.46277700	1.42492500
H	-0.82520600	1.40814200	1.67909200
C	-1.49829600	4.55298900	0.55488500
H	-1.03714800	5.27504000	-1.42109700
H	-1.80037300	3.56567200	2.44608700
H	-1.90106900	5.50150700	0.89629800
H	1.42764600	0.01663800	-1.93949100
C	-2.56695300	-1.81714800	-0.79682600
C	-2.14346500	-0.35832300	-0.55277100
C	-4.09516500	-2.00058600	-0.71515900
C	-3.20356200	0.57809900	-1.14079400
C	-4.72119300	-0.97763100	0.22170900
C	-4.50438500	0.44576000	-0.32797200
H	-2.21975800	-2.12165500	-1.79202300
H	-2.86338900	1.61634900	-1.13781900
H	-4.33651900	-3.01210400	-0.37833400
H	-2.06982400	-2.46995300	-0.07520000
H	-2.09214900	-0.18007200	0.52678300
H	-4.54935200	-1.87066400	-1.70408900
H	-3.36798300	0.29659000	-2.18895200
H	-5.79709000	-1.17440600	0.32232100
H	-4.48812100	1.14708800	0.51638300
H	-5.35883000	0.72592200	-0.95322100

N	-0.81603300	-0.17032000	-1.13840400
H	-0.37607900	-0.97884000	-1.59282100
O	-4.09083700	-1.16348500	1.49067200
H	-4.51820800	-0.59634800	2.14186400
Br	1.86979700	-1.90257900	-1.92096700

INT6a

C	0.13459000	-1.35215300	0.26927500
O	-0.51725800	-2.46871900	0.26393800
C	1.60161700	-1.46933200	0.12204500
C	2.09955400	-2.50769200	-0.66994000
C	2.47923500	-0.61137400	0.79012800
C	3.47173800	-2.66170800	-0.82112300
H	1.40320600	-3.18137400	-1.15726500
C	3.85116300	-0.77946000	0.64522900
H	2.09147300	0.16470100	1.44173400
C	4.34659000	-1.79770500	-0.16587900
H	3.85900600	-3.45992200	-1.44506300
H	4.53222500	-0.11948800	1.17140300
H	5.41841500	-1.92445200	-0.27981700
H	-1.55215600	-2.30218700	0.18681200
C	-0.08353500	2.02546300	1.35515400
C	-0.05069000	1.14371400	0.09299600
C	-0.30890500	3.51233000	1.01850500
C	-0.98336600	1.71509300	-0.98057800
C	0.27884800	3.84896700	-0.34435600
C	-0.47805800	3.09052000	-1.44896100
H	-0.88757900	1.67093500	2.00845300
H	-1.06266700	1.01588800	-1.81739700
H	0.14344700	4.14372300	1.78703700
H	0.85465100	1.90778500	1.90464100
H	0.96482900	1.09972200	-0.30443800
H	-1.37958700	3.74166100	0.99606700
H	-1.99158900	1.79351100	-0.55460700
H	0.20614900	4.93032200	-0.52648500
H	0.19127300	2.97587100	-2.31037000
H	-1.32579200	3.69318400	-1.78928900
N	-0.49895100	-0.21439500	0.40720000
H	-1.53888000	-0.33426700	0.47247000
O	1.64752800	3.46012500	-0.28388200
H	2.06148900	3.68676500	-1.12401000
Br	-3.30543100	-1.45351000	-0.01501900

TS7a

C	-0.72279600	-0.77471400	0.26557100
O	0.29355500	-1.44324200	0.46428700
C	-0.65067000	0.47437900	-0.56075400

C	0.10216300	0.45302500	-1.73398800
C	-1.23440300	1.66706000	-0.13165900
C	0.25236200	1.61358100	-2.48548800
H	0.56855400	-0.47383800	-2.05089200
C	-1.06153300	2.83161700	-0.86983200
H	-1.79774400	1.69090200	0.79448000
C	-0.32366000	2.80409300	-2.05151600
H	0.83293600	1.59258800	-3.40022600
H	-1.49906600	3.75995000	-0.52230000
H	-0.19385900	3.71173800	-2.62912800
H	2.23026700	-1.35300500	-0.22229400
C	-4.01681300	-0.14445300	1.64467700
C	-3.25440800	-0.70228400	0.43028100
C	-5.54355300	-0.27576600	1.48657100
C	-4.02859500	-1.86730500	-0.18787900
C	-5.95775800	-0.19913500	0.02089400
C	-5.36314300	-1.37037400	-0.76957800
H	-3.69887100	-0.69144800	2.53694600
H	-3.42777400	-2.34190300	-0.96640900
H	-6.05227900	0.49906300	2.06613500
H	-3.73731400	0.90052000	1.79783400
H	-3.15556800	0.07284900	-0.32758800
H	-5.88621100	-1.23811200	1.87919400
H	-4.20641200	-2.62108000	0.58815500
H	-7.04918300	-0.22151300	-0.06072300
H	-5.22620400	-1.03767700	-1.80143300
H	-6.08159600	-2.19241700	-0.78778200
N	-1.90535200	-1.11725100	0.81821200
H	-1.84952600	-1.94842500	1.39770100
O	-5.47366900	1.00979700	-0.57764800
H	-5.81867600	1.75560600	-0.07640700
Br	3.13865100	-2.20750400	-0.95354700
N	3.18489200	0.86793200	0.95468300
C	2.21782500	1.96307400	1.09231200
C	1.17542300	1.73644700	2.18166200
H	1.69686100	2.07301700	0.13808500
H	2.74844900	2.91501900	1.28719700
H	0.38073300	2.47750600	2.07646300
H	0.73178100	0.74145700	2.08326700
H	1.59132700	1.83705600	3.18515700
C	3.81879500	0.57833400	2.24510900
C	4.85952400	-0.53470200	2.19810700
H	3.03537200	0.27561400	2.94050600
H	4.27866800	1.49725600	2.65688600
H	4.45818600	-1.41121400	1.68477700
H	5.77847400	-0.23095200	1.69496800
H	5.12286800	-0.82350000	3.21764500

C	4.20145800	1.19875600	-0.04688800
C	3.63901700	1.54965200	-1.41812500
H	4.84876000	0.32791700	-0.16215900
H	4.83501200	2.03086700	0.31626600
H	4.45822300	1.61058700	-2.13791900
H	2.94498500	0.77666000	-1.75403800
H	3.11475000	2.50663100	-1.42846800

TS5'

C	2.23299400	-2.27690800	1.61160700
C	2.97716000	-1.16916400	1.81412000
C	1.66962100	-0.80128300	0.02307900
N	1.43146700	-2.05788900	0.50780200
H	2.18723600	-3.19785300	2.16962700
H	3.71968400	-0.95480000	2.56503700
N	2.65069000	-0.25655400	0.82039900
C	0.46741800	-3.06913900	0.02315200
C	-0.49424300	-3.45536800	1.13985200
C	1.23342200	-4.25492000	-0.55499000
H	-0.10399300	-2.59418000	-0.76509700
H	-1.01014500	-2.56487400	1.50604900
H	-1.25025000	-4.13498600	0.73882600
H	0.01706600	-3.95742800	1.96898300
H	1.88173500	-3.92789500	-1.37216600
H	1.84622400	-4.74833100	0.20812600
H	0.52405900	-4.98903300	-0.94595500
C	3.63911400	0.75406200	0.37996100
C	4.86244800	0.04873000	-0.20368900
C	3.99282100	1.68924200	1.53020700
H	3.16342000	1.33042400	-0.40990000
H	4.56475000	-0.62505400	-1.01210500
H	5.55735800	0.78936900	-0.60889400
H	5.38664000	-0.53237200	0.56196000
H	3.09725000	2.15096400	1.95350700
H	4.52560000	1.16290000	2.32901300
H	4.64988400	2.48137500	1.16245000
C	1.00240400	-0.18314400	-1.07216700
O	0.74060800	-1.02510200	-2.13610600
C	0.92812500	1.24477300	-1.31445500
C	0.66987700	1.70769800	-2.62276600
C	0.97914700	2.20910600	-0.28135400
C	0.47268400	3.05868500	-2.87972700
H	0.62930200	0.98837100	-3.43309200
C	0.78818700	3.55913700	-0.55057300
H	1.14961600	1.89865600	0.74591400
C	0.52928600	3.99892600	-1.84891600
H	0.27548700	3.38219400	-3.89764200

H	0.83043200	4.27261000	0.26857500
H	0.37446600	5.05319200	-2.05368000
H	-0.22261400	-1.01588400	-2.26809100
C	-3.17949600	0.97113200	2.34239300
C	-2.70982400	2.40219200	2.07404300
C	-2.23561800	-0.07616400	1.72255600
C	-2.71437900	2.68978900	0.55793700
C	-1.58197000	0.44242500	0.43411600
C	-2.47859900	1.43246600	-0.29955200
H	-3.28423200	0.79917000	3.42061600
H	-3.67348400	3.14142800	0.28292700
H	-2.79841000	-0.98615900	1.49367800
H	-4.18404900	0.86565400	1.91453900
H	-3.41283600	3.09561100	2.56182700
H	-1.44561800	-0.34250300	2.43434800
H	-1.94049800	3.43625700	0.34095500
H	-0.68501800	0.99469400	0.73871000
H	-3.42983700	0.93896800	-0.53199900
H	-2.00820100	1.70024500	-1.25232300
N	-1.34483000	2.56462500	2.60422900
H	-1.02971900	3.52092200	2.46330400
H	-1.33572600	2.39546600	3.60734700
O	-1.07652200	-0.58398300	-0.39985500
Br	-2.72408600	-1.83541000	-1.03639100

INT5'

C	2.95932300	-0.91849100	1.63285700
C	3.55020200	-0.23909100	0.62184800
C	1.36473000	0.02716800	0.43532100
N	1.60022100	-0.71461600	1.53335300
H	3.39205700	-1.53000300	2.40533500
H	4.58799800	-0.15409000	0.34675400
N	2.54951300	0.36905100	-0.09386700
C	0.63935300	-1.33253100	2.49068400
C	1.22273000	-1.29939800	3.90072000
C	0.27377000	-2.73980700	2.03686900
H	-0.24487700	-0.70124500	2.46325400
H	1.59089000	-0.30305000	4.16340500
H	0.43051900	-1.56901400	4.60362300
H	2.03094300	-2.02467900	4.03423400
H	-0.16363400	-2.72334200	1.03744100
H	1.16305800	-3.37784400	1.99917400
H	-0.43690700	-3.16677300	2.75198700
C	2.80179300	1.21372500	-1.28713600
C	3.73008500	0.48008700	-2.24934000
C	3.33304500	2.56980500	-0.83386200
H	1.83448700	1.33532200	-1.76929200

H	3.34750500	-0.52509400	-2.44769200
H	3.77679200	1.03878500	-3.18770800
H	4.74927300	0.40964800	-1.85443600
H	2.62497800	3.06167000	-0.15923100
H	4.29613900	2.46304800	-0.32291600
H	3.48098300	3.21092800	-1.70731200
C	0.02040700	0.46056500	-0.18113700
O	0.01260100	0.22325100	-1.53666200
C	-0.18156600	1.95951500	0.06449300
C	-0.33838600	2.85423900	-0.99138300
C	-0.20451100	2.42868500	1.37997300
C	-0.51114000	4.21458900	-0.73073300
H	-0.33000200	2.47651600	-2.00851700
C	-0.37399000	3.78490000	1.63965600
H	-0.09440400	1.72371700	2.20187500
C	-0.52460500	4.68237400	0.58092900
H	-0.63770700	4.90842500	-1.55607900
H	-0.38894700	4.14306200	2.66430100
H	-0.65623100	5.74126500	0.78064600
H	0.35319700	-0.71506300	-1.67825700
C	-4.60873700	-0.72745800	0.85275100
C	-4.96591600	-0.72651800	-0.63523300
C	-3.24556100	-0.05602200	1.10978800
C	-3.93024400	-1.55257300	-1.42701200
C	-2.26588600	-0.26813900	-0.05087400

TS6'

C	1.48337600	-2.92786000	-1.80402000
C	2.20391800	-3.12069400	-0.67723600
C	0.76586200	-1.48083300	-0.28451100
N	0.58886200	-1.91781100	-1.54375200
H	1.53925000	-3.41801900	-2.75982500
H	3.00206200	-3.81085300	-0.47501500
N	1.74850600	-2.22138500	0.26233300
C	-0.39996200	-1.44532400	-2.54688100
C	-1.08250600	-2.63854800	-3.20530300
C	0.29439400	-0.52984600	-3.54596600
H	-1.13493300	-0.88462400	-1.98130300
H	-1.48455600	-3.32378400	-2.45671900
H	-1.90980900	-2.26870800	-3.81357900
H	-0.40820900	-3.18925100	-3.86447200
H	0.73989800	0.31834600	-3.02437700
H	1.07436700	-1.07011700	-4.08989100
H	-0.43474100	-0.16066300	-4.27052600
C	2.25165400	-2.24295900	1.66410800
C	3.73426500	-2.59188600	1.69322800
C	1.40086900	-3.20927300	2.47907900

H	2.14314900	-1.23543100	2.04719700
H	4.28940100	-1.96666900	0.99123900
H	4.10544800	-2.40139300	2.70124700
H	3.91601900	-3.64532600	1.47131900
H	0.34604700	-2.93120000	2.43841200
H	1.51158400	-4.22724300	2.09643300
H	1.72678800	-3.19148400	3.52082900
C	-0.11576000	-0.33917400	0.29632900
O	-0.19896000	0.63666100	-0.62946600
H	-0.21428600	1.89603000	-0.44995800
C	0.40707200	0.20028300	1.63431800
C	-0.14981200	-0.16804500	2.85602000
C	1.47789000	1.09445400	1.61374600
C	0.35081200	0.36018600	4.04453500
H	-0.96695800	-0.87693800	2.88188400
C	1.98723900	1.61283500	2.79919300
H	1.94096200	1.34439300	0.66619900
C	1.41956100	1.25131700	4.01949900
H	-0.09360300	0.07120900	4.98988700
H	2.82886500	2.29602900	2.76988900
H	1.81138500	1.65742400	4.94480400
C	-3.38159100	-1.14012000	1.73905100
C	-2.52553700	-0.29023700	0.77994100
C	-4.87577300	-0.95455500	1.47711500
C	-3.30374000	0.01657100	-0.50570200
C	-5.25788500	-1.45573700	0.07543500
C	-4.11374700	-1.20534700	-0.92600700
H	-3.11455900	-2.18996400	1.57703700
H	-3.98633200	0.85452900	-0.32445100
H	-5.13560100	0.10695400	1.55314500
H	-3.14281700	-0.90573800	2.77834200
H	-2.23069800	0.64725500	1.26274100
H	-5.46365900	-1.47866300	2.23464900
H	-2.60394200	0.33779800	-1.27363800
H	-5.43419500	-2.53840900	0.13605700
H	-4.52998800	-1.08369600	-1.92964600
H	-3.45082700	-2.07631300	-0.95883600
Br	4.00141800	0.29833800	-1.19980500
N	-0.39153100	3.10517300	-0.57199200
C	-0.47480300	3.35219000	-2.04061300
C	-1.59309600	2.59925500	-2.74346200
H	0.47844700	3.03707500	-2.46436800
H	-0.57418600	4.43337600	-2.19292000
H	-1.50130000	2.77699500	-3.81635700
H	-1.49584900	1.52812800	-2.56540700
H	-2.58568000	2.92907800	-2.43494800
C	-1.69717900	3.37941200	0.08833600

C	-1.63224600	3.34981400	1.61021800
H	-2.38666300	2.61079300	-0.26269600
H	-2.06489100	4.35008700	-0.26342700
H	-1.08947700	2.47184600	1.97096000
H	-1.15611600	4.24123500	2.01937800
H	-2.64982800	3.30401900	2.00197800
C	0.69516800	3.92890400	0.02561800
C	2.03397500	3.78878700	-0.68607100
H	0.79840600	3.61569900	1.06279500
H	0.36421900	4.97441800	0.02192100
H	2.81679000	4.18516300	-0.03684800
H	2.27466300	2.74417700	-0.90053700
H	2.06313300	4.34801400	-1.62163500
O	-1.34575000	-1.06122700	0.49900200
N	-6.46217100	-0.73920000	-0.36988500
H	-6.82484400	-1.16852100	-1.21621100
H	-7.19444700	-0.83124200	0.32924100

INT6'

C	3.10891000	-2.14165100	0.36574000
C	3.73552600	-1.11168300	-0.24414300
C	1.55474800	-0.67107500	-0.23894400
N	1.75653600	-1.85351400	0.37710500
H	3.50988000	-3.04563500	0.78666200
H	4.78056300	-0.94670800	-0.43985500
N	2.76154900	-0.21191900	-0.61444900
C	0.74838500	-2.78624300	0.95665200
C	1.34318500	-3.54842000	2.13378500
C	0.23096600	-3.71375400	-0.13494000
H	-0.06008400	-2.15506300	1.30884600
H	1.81296600	-2.87299800	2.85130600
H	0.53116800	-4.07308700	2.63926400
H	2.07106000	-4.29892200	1.81829300
H	-0.22187800	-3.13292600	-0.93871300
H	1.04462400	-4.32380500	-0.53688800
H	-0.52461400	-4.38182400	0.28388700
C	3.05906900	1.10282000	-1.23485200
C	3.96618300	0.91013000	-2.44335000
C	3.65697300	2.03397800	-0.18593200
H	2.09731000	1.47407200	-1.57713000
H	3.52525900	0.20656100	-3.15154100
H	4.09393000	1.87168300	-2.94297100
H	4.95719200	0.55096600	-2.15667000
H	2.98017200	2.14539400	0.66433800
H	4.61902700	1.65596400	0.17078200
H	3.81977300	3.01786400	-0.63040900
C	0.24426900	0.13016200	-0.58314700

O	0.17982400	0.39645200	-1.85607100
C	0.25915200	1.37444300	0.35569600
C	0.16934100	2.65243900	-0.18310200
C	0.38270700	1.22632400	1.73811600
C	0.20857800	3.77406800	0.64405600
H	0.07817100	2.74931300	-1.25927800
C	0.43067500	2.34151600	2.56862200
H	0.44483200	0.22902400	2.16606900
C	0.34562200	3.62129000	2.02052200
H	0.13646600	4.76686300	0.21394000
H	0.53378500	2.21568700	3.64060900
H	0.38331000	4.49217200	2.66485800
C	-4.42979300	-0.77079200	0.68081700
C	-4.91983500	0.02793800	-0.52641800
C	-2.93670400	-0.52829000	0.96813200
C	-4.14879300	-0.39482600	-1.79572200
C	-2.12149600	-0.27629800	-0.30822100
C	-2.76203200	-0.98712300	-1.49257400
H	-5.03073500	-0.52446400	1.56138000
H	-4.74102600	-1.12562000	-2.35225900
H	-2.51755500	-1.41258000	1.45850400
H	-4.60387700	-1.83103100	0.47232400
H	-5.98463200	-0.19244900	-0.67755400
H	-2.80188300	0.31221000	1.65353500
H	-4.04323700	0.48161100	-2.44327100
H	-2.09330700	0.79613400	-0.52114700
H	-2.84870700	-2.05259200	-1.24612000
H	-2.10141300	-0.90396100	-2.35662500
N	-4.70955500	1.46274500	-0.26703600
H	-5.08456000	2.00656300	-1.03860000
H	-5.23710400	1.74039500	0.55640800
O	-0.79712600	-0.74766600	-0.07843700

TS7'

C	-3.30318800	2.18449500	0.42732200
C	-3.94928000	1.11187300	-0.08600800
C	-1.72626100	0.74428200	-0.33027000
N	-1.94936600	1.93788600	0.27034600
H	-3.69004100	3.08507600	0.87439200
H	-5.00275400	0.90015100	-0.15913100
N	-2.96834600	0.25034500	-0.54716200
C	-0.88942200	2.86012500	0.70812200
C	-0.99513300	3.11624100	2.20786000
C	-0.94331300	4.15013200	-0.10325300
H	0.03574700	2.32921500	0.49107400
H	-0.98348900	2.17724900	2.76485200
H	-0.14997100	3.72502100	2.53469700

H	-1.91317600	3.65540500	2.45561200
H	-0.86361900	3.93766000	-1.17093700
H	-1.87812100	4.68791200	0.07714700
H	-0.11670800	4.80235300	0.18498000
C	-3.23469900	-1.08669400	-1.10121500
C	-4.23683900	-1.00451200	-2.24690800
C	-3.69698500	-2.02295800	0.01160800
H	-2.27563900	-1.42515900	-1.49226700
H	-3.88984200	-0.31240900	-3.01624300
H	-4.35731300	-1.99210200	-2.69563000
H	-5.21806200	-0.67528900	-1.89617300
H	-2.96517700	-2.04632900	0.82292000
H	-4.66097100	-1.69655200	0.41226100
H	-3.81358600	-3.03585600	-0.37980900
C	0.09250500	-0.43275600	-0.87939100
O	-0.01569000	-0.73178500	-2.05888300
C	-0.11898200	-1.46545900	0.20926900
C	-0.32029800	-2.79424500	-0.15107600
C	-0.09121900	-1.11232300	1.55884800
C	-0.50836200	-3.76661300	0.82987200
H	-0.33226600	-3.05654700	-1.20292500
C	-0.28223600	-2.07885100	2.53790600
H	0.06679500	-0.07282500	1.82604500
C	-0.49372700	-3.40995300	2.17390300
H	-0.66806600	-4.79967600	0.54346000
H	-0.26823800	-1.79916100	3.58510700
H	-0.64417400	-4.16346400	2.93837800
C	4.48864900	1.19357400	0.47794000
C	5.13043400	0.05460000	-0.31392900
C	2.98517500	0.95579900	0.71331400
C	4.48541500	-0.05195900	-1.71130900
C	2.33065300	0.19095600	-0.43995200
C	3.04142400	0.47991800	-1.75326500
H	5.00292200	1.32394600	1.43428400
H	5.09125600	0.50155300	-2.43264300
H	2.47596000	1.92021900	0.80429800
H	4.63780800	2.11990200	-0.08501300
H	6.19721900	0.27893800	-0.44078200
H	2.81666500	0.41226600	1.64570800
H	4.50408600	-1.10084700	-2.02351600
H	2.37762800	-0.88350600	-0.23641400
H	3.03811700	1.56481900	-1.90838900
H	2.48764900	0.03152700	-2.57979300
N	4.93645300	-1.20611700	0.42224600
H	5.41202800	-1.96131500	-0.06291800
H	5.37558800	-1.13758400	1.33646700
O	0.94752500	0.59885900	-0.49154600

PR2

C	1.16495200	1.71493100	-0.22987700
O	1.70998000	2.78336200	-0.09153500
C	1.91294900	0.42588900	-0.09299500
C	2.88480000	0.31702700	0.90069200
C	1.71282000	-0.61976000	-0.99524000
C	3.63530800	-0.84815300	1.00908600
H	3.04178000	1.14246500	1.58494700
C	2.48057000	-1.77380600	-0.89849300
H	0.97423900	-0.52182500	-1.78258000
C	3.43528100	-1.89183100	0.10885500
H	4.38004300	-0.94024300	1.79037500
H	2.33442500	-2.57872900	-1.60831100
H	4.02704800	-2.79604200	0.18842600
C	-3.22551800	-0.34883800	-0.98055100
C	-3.24094000	-0.97853000	0.41233500
C	-1.81443400	0.13083400	-1.37175900
C	-2.85446200	0.07633600	1.46933900
C	-1.02298900	0.61648500	-0.15655800
C	-1.94881900	1.18555000	0.90525600
H	-3.59476400	-1.06181300	-1.72228800
H	-3.76017500	0.53127100	1.87607400
H	-1.89309100	0.96178300	-2.07765200
H	-3.92319100	0.49347500	-0.97989200
H	-4.25832800	-1.32879200	0.62583000
H	-1.26845300	-0.67169500	-1.87122800
H	-2.35255100	-0.42796200	2.30035100
H	-0.43911400	-0.19631700	0.27235100
H	-2.55111000	1.97609900	0.44574800
H	-1.36304100	1.64580100	1.70392800
N	-2.27275400	-2.08678300	0.44452800
H	-2.31138800	-2.54890300	1.34809200
H	-2.53108400	-2.78836500	-0.24396500
O	-0.12486400	1.67669700	-0.58877000

TS6a'

C	-0.96546200	1.90495300	2.61098500
C	-1.43282000	2.70160200	1.61708300
C	-1.22079500	0.61229600	0.75712300
N	-0.84354800	0.63970500	2.06183800
H	-0.69868000	2.14096700	3.62851200
H	-1.63287500	3.76050600	1.61134500
N	-1.59217700	1.89243600	0.51001100
C	-0.51790300	-0.58086000	2.80657400
C	-1.80012600	-1.21877500	3.33930200
C	0.48461500	-0.30195000	3.92111100

H	-0.06717700	-1.25083400	2.06902000
H	-2.48492300	-1.43651300	2.51475700
H	-1.57234000	-2.15062500	3.86665800
H	-2.30061600	-0.53935500	4.03783400
H	1.34520700	0.26167000	3.55102800
H	0.02311800	0.26053500	4.73968300
H	0.84104500	-1.24899800	4.33556000
C	-2.15032100	2.31824500	-0.78216600
C	-1.87069700	3.79006800	-1.05860800
C	-3.64455200	2.00096900	-0.81897500
H	-1.62727900	1.71831200	-1.53124800
H	-0.80309700	4.00222600	-0.96372900
H	-2.18033700	4.02337300	-2.08088500
H	-2.44354500	4.43993500	-0.38751000
H	-3.81866200	0.94383800	-0.59868100
H	-4.18000000	2.60255600	-0.07594700
H	-4.05571900	2.23006200	-1.80739900
C	-0.40748000	-1.03587100	-0.96906100
O	-0.17288200	-0.15718000	-1.85950400
C	-1.69451500	-1.76811400	-1.02157000
C	-2.68048700	-1.33123900	-1.90722600
C	-1.91815300	-2.87905800	-0.20621600
C	-3.89799200	-2.00056300	-1.96839100
H	-2.48396000	-0.46774400	-2.53459800
C	-3.14054100	-3.54060900	-0.26633500
H	-1.14079600	-3.21075800	0.47422700
C	-4.13173800	-3.10149200	-1.14454400
H	-4.66611600	-1.66056700	-2.65567200
H	-3.32090500	-4.40075500	0.37058100
H	-5.08440600	-3.62011700	-1.18937600
H	0.49608000	0.66396200	-1.59114900
C	4.19774400	-2.30281800	-0.17519500
C	4.62289200	-0.82984600	-0.22894900
C	2.72355100	-2.47880600	-0.60559200
C	3.80422100	-0.02841400	0.80107900
C	1.92408400	-1.20506000	-0.34256800
C	2.35578800	-0.53641800	0.94764100
H	4.84465600	-2.91107500	-0.81648300
H	4.30522500	-0.08910600	1.77283300
H	2.26638200	-3.30262700	-0.04475800
H	4.34269800	-2.66534100	0.85027000
H	5.68520200	-0.75788300	0.05093000
H	2.65854800	-2.72395900	-1.66898300
H	3.78542800	1.02644500	0.50870000
H	2.03723900	-0.51947300	-1.17782300
H	2.28688900	-1.27620300	1.75834100
H	1.68396400	0.29649400	1.17259200

N	4.37512300	-0.32138500	-1.58268200
H	4.29716700	0.69186600	-1.60355300
H	5.10607400	-0.60314000	-2.22735900
O	0.51611900	-1.59240600	-0.23754100
Br	1.43997000	2.14755100	-1.03824400

INT6a'

C	1.33050100	0.08693600	-0.07936800
O	0.86720400	1.26700100	-0.07503900
C	2.78863800	-0.07502300	-0.04214700
C	3.60115300	1.06248700	-0.01497200
C	3.34978900	-1.35573000	-0.03262300
C	4.97957600	0.91378300	0.01947500
H	3.15182200	2.04709100	-0.02250900
C	4.72927400	-1.49334900	0.00305300
H	2.70872500	-2.22770600	-0.05262100
C	5.54162900	-0.36105200	0.02891600
H	5.61553000	1.78970500	0.03884700
H	5.17183400	-2.48128100	0.01125300
H	6.61894400	-0.47359100	0.05640400
H	-0.15072700	1.51151800	-0.08566800
C	-2.89889600	-0.83946400	1.27107700
C	-3.49633400	-1.76377100	0.19303000
C	-1.35916200	-0.82989400	1.27641700
C	-2.52845700	-2.90708000	-0.10674000
C	-0.84353100	-1.01313900	-0.13847800
C	-1.20944700	-2.38410400	-0.70573400
H	-3.26338100	0.17766200	1.10989800
H	-2.33337300	-3.44602100	0.82463700
H	-0.97085000	-1.65285100	1.88460300
H	-3.24490400	-1.16051500	2.25552700
H	-4.43129000	-2.18697500	0.57974600
H	-0.99599800	0.10548800	1.70844700
H	-2.98307400	-3.62229800	-0.79657200
H	-1.17857600	-0.20782800	-0.79203700
H	-0.40069800	-3.07815300	-0.46498600
H	-1.27567600	-2.31682300	-1.79174200
N	-3.71643600	-1.00065300	-1.04466500
H	-4.16924400	-1.59026000	-1.73746100
H	-4.34923000	-0.22669500	-0.86666200
O	0.63678800	-0.98502600	-0.11899600
Br	-1.81271800	2.55842000	-0.08644600

TS7a'

C	-0.88113800	-1.32930500	-0.43617900
O	-0.54456000	-0.27919300	-0.93108900
C	-2.30207700	-1.77475200	-0.31271200

C	-3.28007400	-1.01773000	-0.95932600
C	-2.66587400	-2.88690700	0.44842000
C	-4.62326700	-1.36607200	-0.84368400
H	-2.97043100	-0.15774900	-1.54797700
C	-4.00798500	-3.22620900	0.56716800
H	-1.90552400	-3.46703800	0.94713800
C	-4.98424600	-2.47154300	-0.07724500
H	-5.37796400	-0.77806100	-1.34793600
H	-4.29577800	-4.08908100	1.16273000
H	-6.02885800	-2.73851900	0.01522500
H	0.31975600	1.72164000	-0.44314700
C	3.49703300	-1.59111300	-1.19523300
C	4.18183000	-1.92680400	0.14304800
C	2.01855500	-2.02124600	-1.25149100
C	3.47664900	-3.11341100	0.79870500
C	1.37544900	-1.85239400	0.11185700
C	2.01946600	-2.76889700	1.15599500
H	3.57046900	-0.51282600	-1.37171100
H	3.51071500	-3.95461700	0.10619800
H	1.92995500	-3.06877600	-1.54636200
H	4.03488700	-2.08766500	-2.01063000
H	5.22208800	-2.20200800	-0.05953600
H	1.48520800	-1.41691000	-1.99395600
H	4.01987300	-3.42369300	1.70029400
H	1.44752900	-0.79945400	0.42064900
H	1.42935400	-3.68779500	1.20917500
H	1.97004400	-2.28577100	2.13768900
N	4.09586300	-0.76470900	1.04497000
H	4.57979000	-0.97239000	1.91454200
H	4.57381400	0.02668400	0.63340000
O	-0.02911600	-2.21062100	0.08450500
Br	1.60476900	1.96128800	-1.11672000
N	-0.88019500	2.52591800	0.70273500
C	-0.06327100	3.17340800	1.73935200
C	0.61607600	4.47164900	1.31541300
H	0.70313300	2.45413400	2.05282300
H	-0.68623800	3.38110400	2.62680500
H	1.26477800	4.80922300	2.12216800
H	1.22790800	4.32351100	0.42457700
H	-0.10633000	5.26648400	1.11659100
C	-1.61895100	3.51180000	-0.10429000
C	-2.51971600	2.88380300	-1.16121700
H	-0.87470700	4.12390600	-0.62337700
H	-2.20480700	4.18355600	0.54108500
H	-1.97301900	2.13229500	-1.73547800
H	-3.40173600	2.41717400	-0.72130700
H	-2.86487000	3.66664000	-1.83860600

C	-1.77127800	1.52765400	1.29654300
C	-1.02460900	0.50431400	2.14554100
H	-2.27653300	1.00143600	0.48337500
H	-2.54518000	2.02288100	1.90553800
H	-1.65556300	-0.37949600	2.29986100
H	-0.11277200	0.18388100	1.63537100
H	-0.75162100	0.89478000	3.12474700