

Supporting Information

**Mechanism, Regio- and Stereoselectivity in an NHC-catalyzed
Mannich/Lactamization Domino Reaction**

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1: Test results of computational methods at different levels

To examine the effects of the functional and basis set on the stereoselectivity of the reaction, single point energy calculations with different functionals (ω B97X-D, M06-2X-D3, B3LYP-D3 and B3PW91-D3 with 6-311++G(2df,2pd) basis set) and basis set (6-311++G(d,p) together with M06-2X-D3) have been conducted (for details see Table S1). The results are collected in Table S2. As can be seen from Table S2, the relative free energies calculated by these levels (**L2-L6**) are similar to those calculated at SMD(toluene)M06-2X-D3/6-311++G(2df,2pd) (**L1**). Thus the computational level is reliable for the reaction system studied in this work.

Table S1. Different computational levels.

Level	Functional	Basis set	Solvent model
L1	M06-2X-D3	6-311++G(2df,2pd)	SMD
L2	M06-2X-D3	6-311++G(2df,2pd)	IEFPCM
L3	ω B97X-D	6-311++G(2df,2pd)	SMD
L4	B3LYP-D3	6-311++G(2df,2pd)	SMD
L5	B3PW91-D3	6-311++G(2df,2pd)	SMD
L6	M06-2X-D3	6-311++G(d,p)	SMD

Table S2. Comparison of the relative free energies (in kcal/mol) of the stereoselective transition states at different levels.

	L1	L2	L3	L4	L5	L6
TS5(RR)	14.2	16.9	12.3	13.4	14.4	15.5
TS5(RS)	9.9	12.2	8.2	8.9	9.5	10.4
TS5(SR)	5.5	4.4	4.7	3.9	3.9	4.7
TS5(SS)	0.0	0.0	0.0	0.0	0.0	0.0

Fig. S1 Free energy surface and optimized structures for Step 1. Free energies (in kcal/mol) are at SMD(toluene)M06-2X-D3/6-311++G(2df,2pd) level. Bond lengths are given in Å.

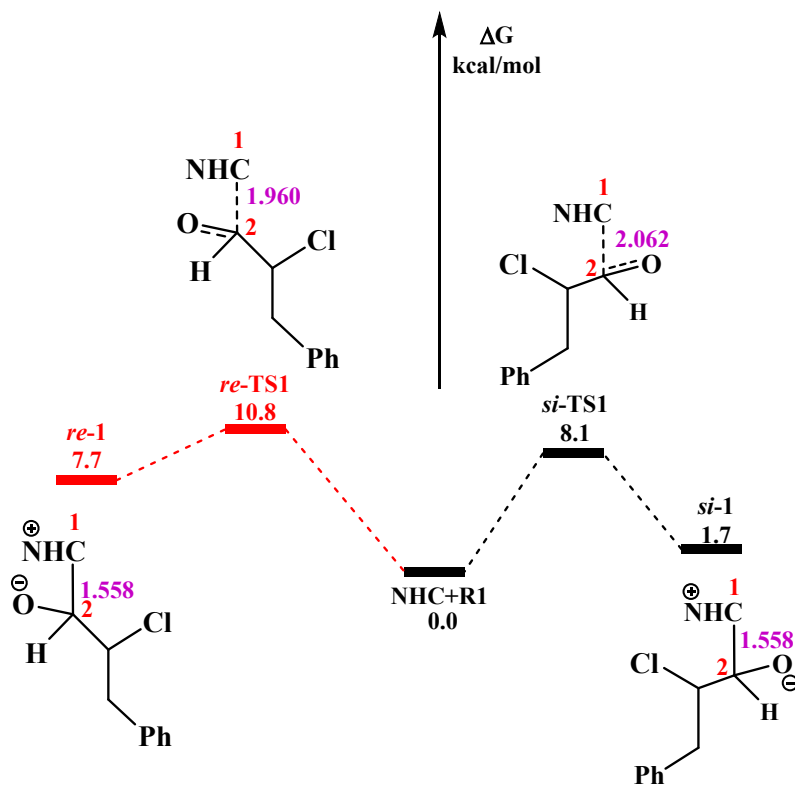


Fig. S2 Free energy surface and optimized transition states for Step 2. Free energies (in kcal/mol) are at SMD(toluene)M06-2X-D3/6-311++G(2df,2pd) level. Bond lengths are given in Å.

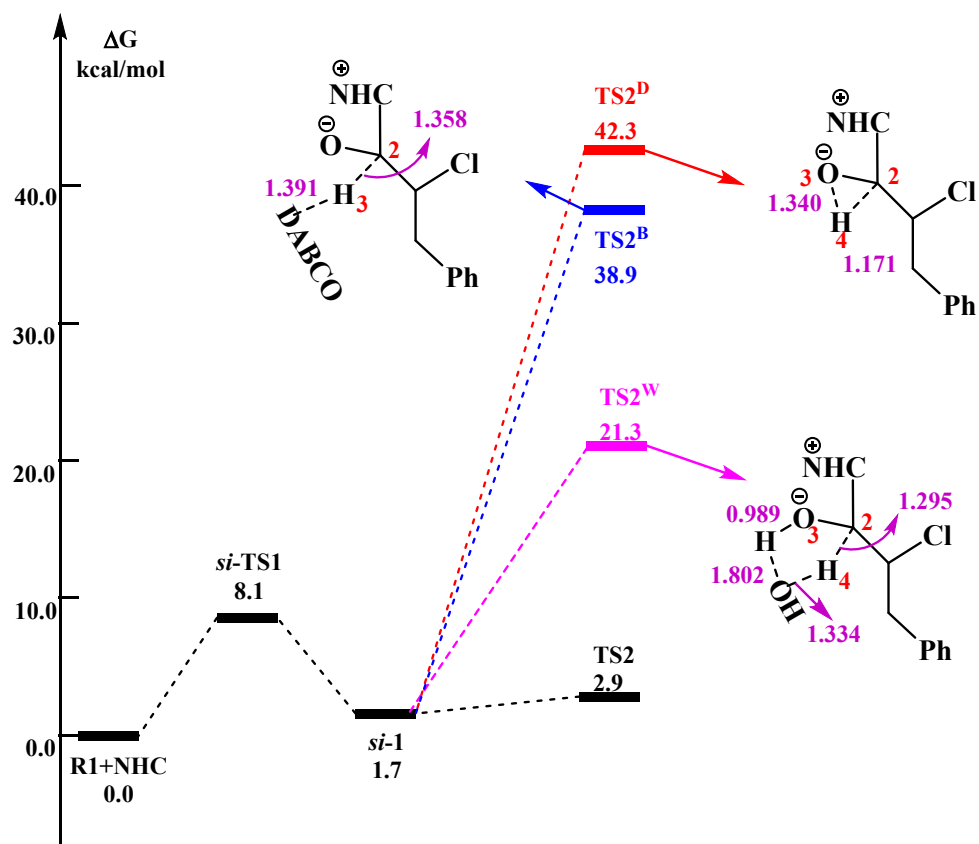


Fig. S3 3-D structures involved in the C5–C6 bond formation step. Bond lengths are given in Å.

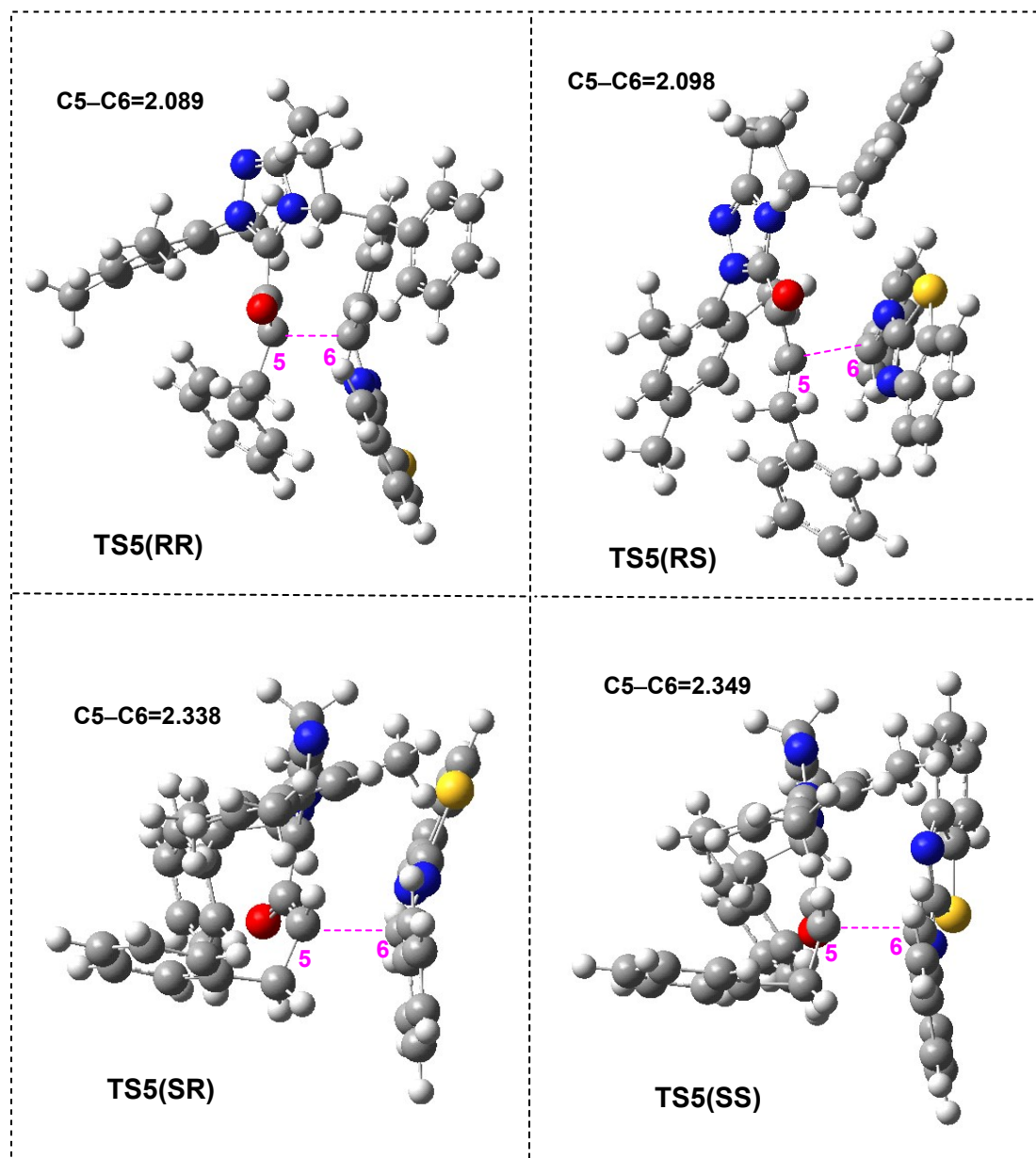
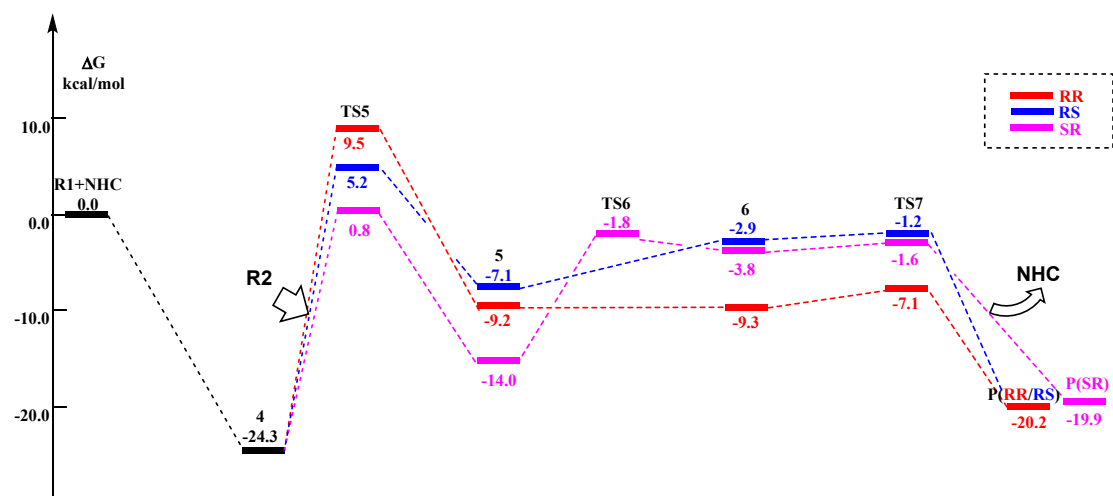


Fig. S4 Free energy surface for the unfavored pathways. Free energies (in kcal/mol) are at SMD(toluene)M06-2X-D3/6-311++G(2df,2pd) level.



Coordinates

NHC

C	0.31031000	-0.26475700	0.05366200
C	-0.07422900	1.96162900	0.01073700
C	-1.12193300	3.02413900	-0.07803000
C	-2.38426400	2.20478200	0.28308600
C	-2.09801600	0.75209700	-0.16883600
H	-0.93893700	3.86006400	0.59774800
H	-1.17643000	3.41610800	-1.09893200
H	-3.29757300	2.59554700	-0.16877100
H	-2.35090300	0.62658000	-1.22867100
N	1.21200400	1.88955100	0.12268800
N	1.41630700	0.51476200	0.14465900
N	-0.63753800	0.71258800	-0.03371500
H	-2.51471300	2.20502100	1.37094100
C	2.75437800	0.02908800	0.28501700
C	3.44254700	0.28706200	1.47602300
C	3.33142700	-0.68372800	-0.76780600
C	4.74553200	-0.18852000	1.59257600
C	4.63752600	-1.14702700	-0.60150500
C	5.35949300	-0.90655800	0.56478900
H	5.29309300	-0.00072300	2.51369700
H	5.10181900	-1.70555700	-1.41072900
C	-2.83450400	-0.30751600	0.66271500
H	-3.77365600	0.13768300	1.01033800
H	-2.22875300	-0.51422800	1.55250500
C	-3.15454300	-1.58619500	-0.08076300
C	-4.48094500	-1.90709400	-0.37482000
C	-2.13991800	-2.45408600	-0.49848600
C	-4.79724800	-3.07141600	-1.07074300
H	-5.27663400	-1.24011800	-0.05159500
C	-2.45678100	-3.61664200	-1.19457700
H	-1.10535900	-2.19945800	-0.27956200
C	-3.78354100	-3.93023100	-1.48272400
H	-5.83452300	-3.30601600	-1.28843600
H	-1.66118000	-4.28351000	-1.51232200
H	-4.02535600	-4.83914600	-2.02447700
C	6.77464000	-1.40139300	0.72219100
H	7.47729200	-0.56473700	0.78526200
H	6.88544400	-1.99019500	1.63734500
H	7.07181400	-2.02725100	-0.12188900
C	2.78329500	1.04262900	2.59868500
H	2.65588700	2.09643700	2.33782700
H	1.78674600	0.63863200	2.80233100

H	3.38056500	0.97407200	3.50993700
C	2.57039100	-0.94632000	-2.03984100
H	1.71651200	-1.60222000	-1.85199300
H	2.17258700	-0.01480200	-2.45388700
H	3.21920100	-1.40915500	-2.78589300

R1

C	-2.84993400	-1.07612800	0.74673600
C	-1.51294500	-1.29589100	0.43096500
C	-0.81828100	-0.40608500	-0.39149900
C	-1.48878100	0.70961500	-0.89456800
C	-2.82655600	0.93236400	-0.58144100
C	-3.50986200	0.04052100	0.24017400
H	-3.37836400	-1.77959200	1.38232600
H	-1.00210100	-2.17436500	0.81950800
H	-0.95539900	1.40707400	-1.53455500
H	-3.33561900	1.80342100	-0.98160000
H	-4.55370000	0.21288900	0.48183200
C	3.01322300	-0.54620700	0.18889800
O	3.31870200	-1.46028900	-0.52977400
H	3.76516800	0.02679800	0.76573000
C	1.56840500	-0.10300500	0.38552700
H	1.23858700	-0.43698000	1.37633900
C1	1.56534300	1.69545600	0.45876700
C	0.63954000	-0.63913900	-0.69765800
H	0.92125200	-0.18548200	-1.65290700
H	0.85087200	-1.71048100	-0.78032200

R2

C	-2.55174400	0.69528100	-0.00010800
C	-3.01311600	-0.63935700	0.00004100
C	-4.37637200	-0.93653100	0.00014100
C	-5.27544800	0.11883500	0.00008800
C	-4.82874700	1.45001800	-0.00006600
C	-3.47709100	1.74685400	-0.00016700
H	-4.72291200	-1.96429000	0.00025200
H	-6.34034800	-0.08861600	0.00016300
H	-5.55521400	2.25585700	-0.00011100
H	-3.11410100	2.76871200	-0.00029000
N	-1.17920100	0.84842500	-0.00019200
S	-1.64693600	-1.71603600	0.00005400
C	-0.59423700	-0.30444400	-0.00010400
N	0.77070400	-0.56961600	-0.00018700
C	1.56159900	0.43895700	0.00027500

H	1.17206900	1.46365100	0.00075400
C	3.01638400	0.27342400	0.00014500
C	3.60254200	-0.99914500	-0.00002700
C	3.82970500	1.41063000	0.00018900
C	4.98358000	-1.12394300	-0.00014900
H	2.95465200	-1.86923400	-0.00006100
C	5.21436900	1.28255500	0.00005400
H	3.37048500	2.39579000	0.00032600
C	5.79099300	0.01560600	-0.00011400
H	5.43798500	-2.10941100	-0.00029000
H	5.84183300	2.16754400	0.00007100
H	6.87148900	-0.08752100	-0.00022100

H₂O

O	0.00000000	0.00000000	0.11780500
H	0.00000000	0.76028500	-0.47122100
H	0.00000000	-0.76028500	-0.47122100

DABCO

C	0.77935000	-0.08884800	-1.37397900
C	-0.77935000	-0.08884800	-1.37397900
H	1.18085600	0.75971400	-1.93836800
H	1.18113200	-1.00314900	-1.82404200
H	-1.18085600	0.75971300	-1.93836800
H	-1.18113200	-1.00314900	-1.82404300
C	0.77917800	1.23448000	0.61003800
H	1.18104300	1.29933200	1.62691800
H	1.18067300	2.08141400	0.04282200
C	-0.77917900	1.23448000	0.61003800
H	-1.18104400	1.29933200	1.62691800
H	-1.18067300	2.08141300	0.04282200
C	-0.77942400	-1.14569600	0.76395200
H	-1.18101200	-1.07799600	1.78078400
H	-1.18110300	-2.05852500	0.31087000
C	0.77942400	-1.14569600	0.76395200
H	1.18101200	-1.07799600	1.78078400
H	1.18110400	-2.05852500	0.31087000
N	1.28403600	-0.00005800	0.00013500
N	-1.28403600	-0.00005900	0.00013500

DABCO·H⁺

C	0.81476000	1.21767300	-0.64820500
C	-0.73171700	1.32576300	-0.53647200
H	1.28548800	2.08181400	-0.17485000

H	1.12463800	1.20025700	-1.69532000
H	-1.05866400	2.09311400	0.16818200
H	-1.22469700	1.49085400	-1.49632800
C	0.81599600	-0.05105000	1.37778300
H	1.28344800	-0.89453500	1.88986700
H	1.12992900	0.86329800	1.88580200
C	-0.73121600	-0.19499600	1.41673000
H	-1.06229600	-1.18763600	1.72883800
H	-1.22021200	0.55518800	2.04088600
C	-0.73763500	-1.12642500	-0.87639300
H	-1.23073900	-2.03939300	-0.53747500
H	-1.06859600	-0.89943700	-1.89204500
C	0.80943500	-1.17144400	-0.73391000
H	1.11966100	-2.06984600	-0.19581900
H	1.27545800	-1.19589800	-1.72104900
N	1.28705500	-0.00263600	-0.00260200
N	-1.22229500	0.00261500	0.00231800
H	-2.24447500	0.00524200	0.00409500

re-TS1

C	0.07518100	-1.16391100	-0.22638000
C	-0.70652700	-3.03293600	-1.14196500
C	-1.93891200	-3.82193400	-1.45933400
C	-3.04783200	-2.74256100	-1.32125600
C	-2.47239100	-1.63147200	-0.40854900
H	-1.90736200	-4.28124800	-2.44808900
H	-2.05578000	-4.61952900	-0.71956200
H	-3.98006100	-3.14538600	-0.92443000
H	-2.65861200	-1.82290400	0.65338800
N	0.58022100	-3.21449900	-1.13896300
N	1.03785100	-2.03657100	-0.57423900
N	-1.03636400	-1.81749400	-0.61795000
H	-3.26049500	-2.31279900	-2.30570700
C	2.42705100	-1.88925300	-0.25614700
C	3.27524800	-1.26135500	-1.16904000
C	2.86717100	-2.39057800	0.97223600
C	4.61101100	-1.10674600	-0.80321700
C	4.21133300	-2.21107700	1.29342700
C	5.09141400	-1.56476000	0.42462500
H	5.29402600	-0.62228300	-1.49695000
H	4.58002400	-2.58838800	2.24405100
C	-2.92626700	-0.21286800	-0.73657300
H	-2.90249600	-0.05773000	-1.82159600
H	-2.20896800	0.47239500	-0.27710800

C	-4.29919300	0.04967000	-0.17046800
C	-5.44037700	0.03401300	-0.97101400
C	-4.42629500	0.26719700	1.20570900
C	-6.69896500	0.23732300	-0.40829100
H	-5.34243100	-0.13125300	-2.04155800
C	-5.68271200	0.47000400	1.76576300
H	-3.52505200	0.27068100	1.81818000
C	-6.82109900	0.45553000	0.96031600
H	-7.58201200	0.22844100	-1.03951800
H	-5.77520000	0.64334600	2.83330100
H	-7.80044900	0.61622000	1.39987800
C	6.53186200	-1.34922300	0.81058000
H	6.65780500	-0.37945600	1.30285600
H	6.87609200	-2.11937400	1.50446900
H	7.18243800	-1.36079300	-0.06706200
C	2.75828300	-0.78752100	-2.50087800
H	2.20319000	-1.58272600	-3.00636300
H	2.07977600	0.06286800	-2.38128300
H	3.58264800	-0.47488300	-3.14404300
C	1.92070700	-3.12557600	1.88571900
H	1.03054400	-2.53237400	2.12227400
H	1.57622500	-4.04833700	1.40806300
H	2.41639300	-3.38539600	2.82241900
C	0.33266500	5.17262500	-1.54337500
C	0.18086000	3.82342800	-1.24210000
C	1.18740900	3.12166700	-0.57442600
C	2.35232600	3.79909000	-0.21445800
C	2.51041300	5.14857700	-0.51705900
C	1.50133600	5.83886200	-1.18238700
H	-0.45914900	5.70319800	-2.06282200
H	-0.73063200	3.30259000	-1.52906700
H	3.13578500	3.26282700	0.31396200
H	3.42262400	5.66265800	-0.23077900
H	1.62440000	6.89101900	-1.41837200
C	-0.06271700	-0.06299600	1.38944600
O	-1.11145900	-0.46285800	1.93254800
H	0.93376700	-0.40639200	1.74732300
C	0.05175000	1.40555100	0.92767900
H	-0.94878400	1.80191300	0.73728900
Cl	0.63020000	2.29484900	2.39594200
C	0.99376900	1.66344600	-0.24283700
H	1.95586700	1.17650200	-0.03409100
H	0.55318800	1.15367400	-1.10686600

si-TS1

C	-0.63902000	-0.92656900	0.29268700
C	-1.93303100	-2.65005600	-0.28454200
C	-3.34247300	-3.12334800	-0.44812700
C	-4.12289300	-2.06328800	0.37757400
C	-3.23256400	-0.79344000	0.42111300
H	-3.61969800	-3.10522700	-1.50674400
H	-3.49187800	-4.13887900	-0.08002000
H	-4.26639000	-2.43496300	1.39476400
H	-3.26890800	-0.31229000	1.40254100
N	-0.73189600	-3.08371300	-0.51349900
N	0.04520300	-2.00026200	-0.14057100
N	-1.90914500	-1.37465700	0.20973500
H	-5.10713900	-1.84218900	-0.03949000
C	1.47489500	-2.06583300	-0.24242500
C	2.07418100	-1.59619100	-1.41254000
C	2.20536400	-2.53114500	0.85412100
C	3.46800400	-1.57061500	-1.45945300
C	3.59482300	-2.49606900	0.75536400
C	4.23950800	-2.01096800	-0.38495100
H	3.95804400	-1.18613500	-2.35027800
H	4.18928400	-2.84543600	1.59663900
C	-3.53235700	0.24094500	-0.67276900
H	-3.52616400	-0.26425100	-1.64656500
H	-2.71045100	0.96718100	-0.67901800
C	-4.85285000	0.93001100	-0.44066200
C	-5.98952500	0.58199600	-1.17256700
C	-4.96505400	1.91096200	0.54907000
C	-7.21373800	1.19718900	-0.92230700
H	-5.91007000	-0.17038800	-1.95399900
C	-6.18582000	2.52683100	0.80282000
H	-4.08214000	2.19929600	1.11566400
C	-7.31446300	2.16983900	0.06743200
H	-8.08689100	0.91929400	-1.50398600
H	-6.25696800	3.29025800	1.57095600
H	-8.26667300	2.65247000	0.26200900
C	5.74498200	-1.95573900	-0.43554000
H	6.17885100	-2.95579600	-0.34111700
H	6.09526600	-1.52163800	-1.37462100
H	6.13952400	-1.35167500	0.38838800
C	1.23101000	-1.10359300	-2.55780800
H	0.51443400	-1.87029700	-2.86788100
H	0.66101000	-0.21494400	-2.26641600
H	1.85634500	-0.84336800	-3.41327600

C	1. 50504400	-3. 02239100	2. 09095700
H	1. 01267200	-2. 18281600	2. 59293600
H	0. 74637000	-3. 76822200	1. 83580300
H	2. 21983300	-3. 47589600	2. 78023600
C	5. 31709200	1. 84849400	-0. 32593300
C	4. 20437500	1. 53864600	0. 44804300
C	3. 21123100	2. 49425400	0. 68624200
C	3. 35644200	3. 76606600	0. 13372000
C	4. 47280200	4. 08169200	-0. 63793000
C	5. 45515500	3. 12427300	-0. 87026600
H	6. 08066300	1. 09593200	-0. 50041400
H	4. 09389300	0. 54075700	0. 87043800
H	2. 58374900	4. 51099400	0. 30374200
H	4. 57272600	5. 07643500	-1. 06104100
H	6. 32471000	3. 37032800	-1. 47148500
C	0. 01952300	0. 52869500	1. 60745900
O	0. 40853400	-0. 04380400	2. 62749300
H	-0. 96752700	1. 04148600	1. 56619100
C	1. 06757500	1. 18581600	0. 68990400
H	1. 67090300	0. 41803300	0. 20450200
Cl	0. 23613600	2. 08696400	-0. 63910400
C	1. 98894100	2. 10963800	1. 48140400
H	1. 43570800	2. 99335200	1. 81625500
H	2. 27224200	1. 53445600	2. 36991200

re-1

C	0. 13364300	-0. 89168300	0. 03334800
C	-0. 73432700	-2. 30475300	-1. 40113700
C	-1. 98667700	-2. 93515300	-1. 92239800
C	-3. 07152100	-1. 96297400	-1. 39319900
C	-2. 45493800	-1. 21148200	-0. 18926200
H	-1. 98947200	-3. 03667400	-3. 00832400
H	-2. 08537300	-3. 93505500	-1. 48999000
H	-3. 99359300	-2. 47086300	-1. 11046100
H	-2. 55330600	-1. 75972800	0. 75299400
N	0. 53972300	-2. 55886900	-1. 45118000
N	1. 06639600	-1. 65183400	-0. 55549600
N	-1. 01963000	-1. 29274700	-0. 53075700
H	-3. 31847600	-1. 23251400	-2. 17065200
C	2. 44817900	-1. 72964900	-0. 17358300
C	3. 42689900	-1. 23116100	-1. 03276300
C	2. 73652500	-2. 33783400	1. 05528000
C	4. 75273700	-1. 32030800	-0. 60781800
C	4. 07507200	-2. 39147700	1. 43407100

C	5.09131100	-1.88117100	0.62247500
H	5.53784000	-0.94195500	-1.25747500
H	4.33263700	-2.85469500	2.38323000
C	-2.99551200	0.19710500	0.02549600
H	-2.92339600	0.77408300	-0.90452300
H	-2.38585100	0.65756400	0.80622100
C	-4.42208700	0.10914700	0.51048200
C	-5.51194900	0.26691600	-0.34550000
C	-4.64942700	-0.18509400	1.85876500
C	-6.81294300	0.13414800	0.13548600
H	-5.34132000	0.50707100	-1.39244200
C	-5.94754300	-0.31975500	2.33897900
H	-3.79072600	-0.29285100	2.51899700
C	-7.03224500	-0.16125300	1.47771400
H	-7.65438000	0.26651000	-0.53739400
H	-6.11460300	-0.54098800	3.38834500
H	-8.04534700	-0.26147600	1.85376800
C	6.52622700	-1.93164300	1.07901900
H	7.21458200	-1.82558900	0.23803200
H	6.73379900	-1.12150100	1.78525500
H	6.74545300	-2.87409300	1.58677300
C	3.07058800	-0.62875200	-2.36689900
H	2.33616100	-1.24351800	-2.89265000
H	2.64721400	0.37578700	-2.25302000
H	3.96080700	-0.54013500	-2.99191000
C	1.64670600	-2.94668900	1.90236600
H	0.89034900	-2.22162800	2.22972000
H	1.12462400	-3.72425100	1.33351300
H	2.07933500	-3.41288500	2.78901900
C	0.90952500	4.16732200	-2.77567500
C	1.01061800	3.03467500	-1.97421900
C	1.42956100	3.13121600	-0.64434400
C	1.73933000	4.39070300	-0.12910700
C	1.63903400	5.52694400	-0.92726100
C	1.22602700	5.41860100	-2.25241900
H	0.58656000	4.07419900	-3.80786700
H	0.75771700	2.05677900	-2.38145600
H	2.05337500	4.47571900	0.90725900
H	1.88318500	6.49973700	-0.51235000
H	1.15061700	6.30454300	-2.87455100
C	0.17753700	-0.00279400	1.31265300
O	-0.80099400	-0.44048600	2.07005700
H	1.21971600	-0.13461400	1.70504500
C	0.14965000	1.48045800	0.80401200

H	-0.64043000	1.62261000	0.06110300
Cl	-0.29129100	2.55457100	2.17205100
C	1.49727100	1.89593400	0.21474800
H	2.21218900	2.02329800	1.03354900
H	1.85927500	1.05248600	-0.38854100

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C	-0.52734700	-0.91111400	0.33688700
C	-1.74697600	-2.55906800	-0.45890000
C	-3.13406400	-3.06266000	-0.70001000
C	-3.95609300	-2.14897700	0.24862100
C	-3.13978400	-0.84025000	0.41279100
H	-3.40526600	-2.91503200	-1.75008000
H	-3.24114000	-4.12273600	-0.46935100
H	-4.05387900	-2.63554400	1.22182800
H	-3.19581200	-0.44785700	1.43126300
N	-0.52597300	-2.93465500	-0.68642600
N	0.22318100	-1.89686300	-0.18071000
N	-1.78408300	-1.34339100	0.16420300
H	-4.95900300	-1.93978600	-0.12710000
C	1.66125000	-1.97172000	-0.20239200
C	2.32708300	-1.50361300	-1.33617700
C	2.31744500	-2.50960700	0.90875400
C	3.72125200	-1.51446700	-1.31119900
C	3.71024600	-2.50353100	0.87912200
C	4.42479400	-1.99525000	-0.20781100
H	4.26520100	-1.12985500	-2.17005000
H	4.25111900	-2.90340900	1.73371000
C	-3.49562900	0.25931000	-0.59684200
H	-3.45385500	-0.16232100	-1.60872000
H	-2.72675400	1.03801300	-0.53903100
C	-4.86071300	0.83549800	-0.31700400
C	-5.96970900	0.47684700	-1.08526800
C	-5.03849400	1.71854800	0.75165500
C	-7.23230400	0.98658700	-0.79298400
H	-5.83966900	-0.19965900	-1.92710500
C	-6.29795700	2.22870800	1.04714600
H	-4.17729400	2.01485700	1.34676100
C	-7.39882700	1.86239800	0.27513300
H	-8.08415200	0.70302100	-1.40274900
H	-6.41998700	2.91870600	1.87580200
H	-8.38110600	2.26350800	0.50256800
C	5.93137200	-1.96991500	-0.17710600
H	6.33931600	-2.97490500	-0.03441500

H	6.34109900	-1.56459200	-1.10474300
H	6.28977900	-1.35231700	0.65257500
C	1.56441500	-0.98775300	-2.52726500
H	0.84152600	-1.73127000	-2.87654000
H	1.01044000	-0.07429400	-2.28476700
H	2.24759400	-0.75843200	-3.34651400
C	1.54334700	-3.06703300	2.06800600
H	0.97732100	-2.24795100	2.52798000
H	0.84719200	-3.84026000	1.72581500
H	2.21915000	-3.51161100	2.80083500
C	5.11964500	2.07673400	-0.11491800
C	3.93891700	1.71858900	0.52422500
C	2.89116500	2.63700100	0.65963800
C	3.05454400	3.92144800	0.14406000
C	4.24066700	4.28645000	-0.49073000
C	5.27504500	3.36592900	-0.62353800
H	5.92115600	1.35024000	-0.21529800
H	3.81338400	0.71210300	0.92249000
H	2.24241500	4.63786700	0.23493800
H	4.35332300	5.29079400	-0.88744300
H	6.19704300	3.64940700	-1.12141000
C	-0.06957700	0.26542900	1.25058300
O	0.50274100	-0.24496300	2.31112900
H	-1.02211000	0.85155300	1.40156600
C	0.87294100	1.18332100	0.42235500
H	1.61253700	0.57015900	-0.09442400
Cl	-0.05665000	2.01505600	-0.91059100
C	1.60445100	2.18527900	1.30097200
H	0.95102700	3.03040700	1.54023600
H	1.80202400	1.63061300	2.22609900

TS2^D

C	-0.90187800	0.19049900	0.45441500
C	-0.83705300	-0.27093100	2.63259800
C	-0.02969500	-0.83657800	3.76252500
C	1.10105600	-1.57501800	3.00183800
C	1.23371500	-0.84471400	1.64325400
H	0.35706400	-0.02064800	4.38141900
H	-0.61300200	-1.49483100	4.40739300
H	0.80283200	-2.61271000	2.82550400
H	1.52468600	-1.53477600	0.84162000
N	-1.96503400	0.33701300	2.50418300
N	-2.02661000	0.63725700	1.12826700
N	-0.14038300	-0.39405800	1.45610200

H	2. 04924800	-1. 58693900	3. 54256700
C	-2. 67035700	1. 87371900	0. 75854100
C	-1. 99235500	3. 07190600	1. 00244300
C	-3. 94366300	1. 85504500	0. 18445800
C	-2. 62786800	4. 27103500	0. 67914200
C	-4. 54135300	3. 07366200	-0. 12300300
C	-3. 90147800	4. 29029500	0. 11766100
H	-2. 11275400	5. 20956700	0. 87086000
H	-5. 53189600	3. 07285200	-0. 57288300
C	2. 20726300	0. 35044500	1. 68751400
H	2. 02123600	0. 91239200	2. 61202800
H	1. 97412900	1. 02295100	0. 85413900
C	3. 64996600	-0. 07556000	1. 59338000
C	4. 42280100	-0. 28997300	2. 73648200
C	4. 22913300	-0. 28643200	0. 33781400
C	5. 74413900	-0. 71667300	2. 63197100
H	3. 99045000	-0. 10377800	3. 71736400
C	5. 55028200	-0. 70844000	0. 23119900
H	3. 65246700	-0. 09452100	-0. 56636600
C	6. 30985000	-0. 92871800	1. 37780200
H	6. 33309300	-0. 87547200	3. 52990700
H	5. 98606600	-0. 85226900	-0. 75254800
H	7. 34141900	-1. 25563000	1. 29472800
C	-4. 57711500	5. 58915300	-0. 24015000
H	-3. 98256200	6. 44784200	0. 07936600
H	-4. 72544200	5. 66571500	-1. 32177700
H	-5. 56203800	5. 66347400	0. 23020600
C	-0. 60369500	3. 07378800	1. 58827700
H	-0. 56717400	2. 50776400	2. 52480500
H	0. 11075900	2. 61339800	0. 89544400
H	-0. 27028700	4. 09394800	1. 78911800
C	-4. 61207700	0. 55195400	-0. 13785300
H	-3. 98900700	0. 05262400	-0. 89002700
H	-4. 68022100	-0. 08237500	0. 75190100
H	-5. 61764600	0. 71287000	-0. 53204200
C	4. 12956000	2. 81106000	-1. 27507100
C	2. 76279900	2. 55993300	-1. 36227100
C	2. 25027900	1. 66604200	-2. 30881100
C	3. 14424500	1. 04416600	-3. 18705400
C	4. 51207100	1. 29301900	-3. 10259400
C	5. 01014300	2. 17196300	-2. 14288600
H	4. 50647000	3. 50329800	-0. 52876100
H	2. 07597800	3. 06698600	-0. 68716700
H	2. 76051200	0. 35333100	-3. 93165500

H	5.19137100	0.80045000	-3.79194000
H	6.07680900	2.36057300	-2.07497800
C	-0.88133200	-0.03374800	-0.97040400
O	-1.86210200	0.34087900	-1.73166200
H	-1.11852100	-1.32773900	-0.63453800
C	0.53253300	0.01091300	-1.53511200
H	1.29273500	-0.12403100	-0.76649500
Cl	0.84714000	-1.41537700	-2.66319900
C	0.78399300	1.31816900	-2.29573000
H	0.35347200	1.23172200	-3.29560400
H	0.20841400	2.09471200	-1.77808100
C	-0.73309900	-3.70859500	-0.33299700
C	-1.50688700	-5.05038100	-0.48218700
H	0.09960900	-3.61927600	-1.03584000
H	-0.34318500	-3.57168700	0.68250900
H	-1.20234600	-5.57723400	-1.39171400
H	-1.30971400	-5.71245300	0.36660900
C	-2.33444000	-2.80832000	-1.90860100
H	-2.86279600	-1.88213700	-2.14817200
H	-1.53919700	-2.92755700	-2.64828000
C	-3.23516500	-4.06802700	-1.80364200
H	-4.29574800	-3.79792400	-1.79414900
H	-3.07273300	-4.73891700	-2.65262900
C	-3.34794000	-3.97331400	0.57600600
H	-4.43912400	-3.89829900	0.59335800
H	-3.03635000	-4.48537200	1.49230800
C	-2.70031900	-2.56655300	0.46835400
H	-3.41822600	-1.79389000	0.18898300
H	-2.22214200	-2.25133800	1.40269900
N	-1.67348600	-2.60295700	-0.59532900
N	-2.94843200	-4.80283300	-0.56398800

TS2^B

C	-0.53751600	-0.71455100	-0.32859800
C	-1.66792000	-2.53365600	0.21849000
C	-2.99031900	-3.08589800	0.64898000
C	-3.70070000	-1.80245900	1.15694000
C	-3.07868700	-0.62342000	0.36777100
H	-3.50510500	-3.52449200	-0.21163000
H	-2.89268300	-3.85737100	1.41293700
H	-3.49617700	-1.67630100	2.22302000
H	-2.95644900	0.27790500	0.96382000
N	-0.48495100	-2.98761000	-0.04364000
N	0.22201400	-1.84886800	-0.39508800

N	-1.74986400	-1.17795600	0.07167900
H	-4.78373700	-1.83449900	1.02240600
C	1.62187400	-1.92641100	-0.66699300
C	2.07052300	-1.71280600	-1.97209500
C	2.49376400	-2.13538900	0.40834100
C	3.44969600	-1.68343400	-2.18206300
C	3.85988700	-2.10712500	0.14649800
C	4.35463000	-1.86729300	-1.13841500
H	3.82223800	-1.49862000	-3.18617900
H	4.55720200	-2.25172300	0.96880300
C	-3.83246800	-0.27954300	-0.92297300
H	-4.11840000	-1.20187700	-1.44413400
H	-3.14711100	0.28822100	-1.55631800
C	-5.03930200	0.56910400	-0.61271700
C	-6.33616500	0.05886500	-0.64965200
C	-4.83851100	1.90306600	-0.23985200
C	-7.42363500	0.86691600	-0.32131400
H	-6.49758100	-0.97453600	-0.94846300
C	-5.92304600	2.70868600	0.08714100
H	-3.82056000	2.29016700	-0.21904800
C	-7.21813700	2.19214100	0.04793200
H	-8.42966500	0.46098600	-0.35785700
H	-5.76006300	3.74394500	0.36957400
H	-8.06384800	2.82335900	0.30124300
C	5.83948800	-1.77244900	-1.37260300
H	6.37516200	-2.56302100	-0.84082200
H	6.08017600	-1.84762900	-2.43481100
H	6.21972600	-0.81226200	-1.00926100
C	1.09649100	-1.47124400	-3.09247600
H	0.30481200	-2.22608200	-3.09078600
H	0.62206200	-0.48920600	-2.98224600
H	1.60541700	-1.49868900	-4.05706900
C	1.95814300	-2.33058600	1.80141200
H	1.28965300	-1.50693200	2.07888700
H	1.37732500	-3.25399500	1.87341900
H	2.77324400	-2.36845600	2.52642400
C	4.81855700	1.76714300	1.89895600
C	3.49882700	1.43562500	1.61283600
C	2.59241400	2.40701200	1.17673400
C	3.03843000	3.72069900	1.03381100
C	4.35817900	4.05895100	1.32344200
C	5.25171800	3.08390800	1.75670600
H	5.50864700	0.99956900	2.23667200
H	3.16350000	0.40527400	1.72166100

H	2.34459900	4.47907300	0.68241100
H	4.68932400	5.08607300	1.20673500
H	6.28020000	3.34728400	1.98214600
C	-0.27338500	0.64361000	-0.68022500
O	-1.36292100	1.55405100	-0.42109200
H	-0.92269600	1.03207500	-1.57406500
C	1.10749400	1.20490300	-0.47150800
H	1.87530700	0.43156900	-0.46578100
Cl	1.57644300	2.27701600	-1.87332600
C	1.18131900	2.01392000	0.82545300
H	0.51627400	2.87437700	0.73224800
H	0.76361700	1.37008600	1.61243200

TS2^W

TS2

2 C	-0.50249400	-0.82372800	0.30198400
C	-1.85666400	-2.54902000	0.13753000
C	-3.27111900	-3.02649800	0.24147000
C	-3.92748400	-1.83378700	0.98828900
C	-3.11039100	-0.58515000	0.57661800
H	-3.69433800	-3.16563500	-0.75830800
H	-3.35107900	-3.97199800	0.77837300
H	-3.83877600	-1.99062600	2.06640900
H	-3.03544000	0.17906800	1.35211800
N	-0.68566200	-3.05063800	-0.11382700
N	0.15300400	-1.96338500	0.00136000
N	-1.78918900	-1.21172500	0.38666500
H	-4.98335300	-1.70882100	0.74372700
C	1.57211000	-2.17787400	-0.02040200
C	2.18112200	-2.49687600	-1.23509100
C	2.27006400	-2.09535200	1.18845200
C	3.56116400	-2.68689100	-1.22625600
C	3.64961100	-2.28540700	1.14026100
C	4.31047000	-2.56829900	-0.05601600
H	4.06361500	-2.92276100	-2.16084000
H	4.22061400	-2.21878500	2.06321600
C	-3.59644400	0.04891900	-0.73515700
H	-3.64612400	-0.72543000	-1.51178800
H	-2.86695300	0.81121400	-1.02092000
C	-4.94933200	0.68979000	-0.54044200
C	-6.11036800	0.10548100	-1.04913500
C	-5.04494200	1.87802500	0.19277900
C	-7.35471600	0.69442600	-0.83363500

H	-6.03875100	-0.81392000	-1.62723100
C	-6.28914200	2.46259100	0.40824400
H	-4.12232900	2.32300700	0.56658200
C	-7.44546200	1.87444900	-0.10219700
H	-8.24994600	0.23361300	-1.23961300
H	-6.35751300	3.38675300	0.97426600
H	-8.41331600	2.33638300	0.06620700
C	5.80885200	-2.72083900	-0.08411500
H	6.18248400	-3.13876200	0.85364900
H	6.12623200	-3.37086600	-0.90249900
H	6.28855500	-1.74723700	-0.22801700
C	1.37084100	-2.63345300	-2.49421800
H	0.71942400	-3.51067800	-2.44036000
H	0.73697400	-1.75427600	-2.64090400
H	2.02580600	-2.73541800	-3.36105700
C	1.56035100	-1.81353500	2.48744600
H	1.17646600	-0.78827100	2.54162200
H	0.70347400	-2.48385700	2.61202900
H	2.23888100	-1.97079600	3.32774500
C	5.37350400	2.82100700	0.78683500
C	4.06758200	2.44213200	1.07953300
C	3.00308900	2.86434900	0.27876600
C	3.27496800	3.67387000	-0.82457200
C	4.58006300	4.05778000	-1.12019900
C	5.63273900	3.63269900	-0.31503000
H	6.18903700	2.48914300	1.42206500
H	3.86424400	1.81304900	1.94389800
H	2.45396700	3.99827800	-1.45815900
H	4.77537200	4.68918300	-1.98140400
H	6.65039700	3.93326300	-0.54345000
C	-0.08201700	0.56017900	0.57102700
O	-0.35266700	0.83069600	1.94191600
H	-0.96849800	1.39125000	0.12339800
C	1.32125200	0.97748500	0.16329700
H	2.12869700	0.33404200	0.52781400
Cl	1.43143600	0.84386100	-1.64911400
C	1.59921300	2.41732700	0.59414800
H	0.85568900	3.07350600	0.12984800
H	1.42644200	2.44346600	1.67501100
O	-1.92460200	2.25624900	0.46758700
H	-0.99023800	1.58216600	1.85327100
H	-1.71157300	3.11699800	0.09154500

TS3

C	0.57476400	-0.86029900	-0.42330300
C	1.83809700	-2.65203300	-0.13724700
C	3.23533300	-3.18753000	-0.10284800
C	4.01603100	-2.06703900	-0.84008000
C	3.19055900	-0.76923200	-0.65354000
H	3.55887700	-3.29649500	0.93701800
H	3.32498500	-4.16106500	-0.58565000
H	4.07554400	-2.30694000	-1.90441800
H	3.21639500	-0.12599900	-1.53346700
N	0.64947100	-3.07844300	0.13979000
N	-0.14451800	-1.95992900	-0.05166900
N	1.84842600	-1.33243800	-0.50092800
H	5.03361300	-1.94198300	-0.46490900
C	-1.55737200	-2.00615300	0.15583100
C	-2.04855700	-1.80859100	1.45031400
C	-2.38663900	-2.12298000	-0.96138700
C	-3.42974600	-1.71643900	1.60306100
C	-3.76139900	-2.01612200	-0.75901800
C	-4.29652800	-1.79745800	0.51103200
H	-3.83824400	-1.54499300	2.59597500
H	-4.42857800	-2.08588700	-1.61519000
C	3.57637900	0.03855500	0.59422200
H	3.63721100	-0.63886000	1.45500800
H	2.77202600	0.75274800	0.80149400
C	4.88536900	0.75762900	0.38859100
C	6.05920400	0.32774000	1.00776300
C	4.94051600	1.85840300	-0.47201000
C	7.26602800	0.98437900	0.77689200
H	6.02502700	-0.52241800	1.68511200
C	6.14320800	2.51556900	-0.70519500
H	4.02686800	2.20038900	-0.95414000
C	7.31018300	2.07877600	-0.08079400
H	8.17024500	0.64232600	1.27035700
H	6.16994000	3.37291500	-1.37007400
H	8.24891600	2.59289000	-0.25965800
C	-5.77691700	-1.60166300	0.70350500
H	-6.34170400	-1.95739300	-0.16131900
H	-6.13476800	-2.12964300	1.59117600
H	-5.99722500	-0.53662400	0.83490100
C	-1.10389300	-1.60910400	2.60346200
H	-1.64021300	-1.65925700	3.55254100
H	-0.31540400	-2.36645600	2.60321200
H	-0.63484400	-0.61929400	2.53144700
C	-1.79485700	-2.28022400	-2.33560800

H	-1.05605600	-3.08640700	-2.35752700
H	-2.57171200	-2.49736800	-3.07090000
H	-1.28520000	-1.35591900	-2.63387100
C	-5.40291900	1.64648500	-0.98426600
C	-4.06187900	1.55227500	-1.34284300
C	-3.09923700	2.36196800	-0.73437800
C	-3.50110300	3.26482500	0.25022100
C	-4.84280500	3.36294100	0.61005600
C	-5.79676300	2.55615700	-0.00505600
H	-6.14007300	1.01382900	-1.47083100
H	-3.75161400	0.83888800	-2.10411000
H	-2.75085800	3.87273400	0.74689400
H	-5.14365700	4.06913500	1.37765700
H	-6.84259300	2.63694500	0.27515300
C	0.15217300	0.43488500	-0.76163800
O	1.15707500	1.30093700	-1.18255700
H	1.17852700	1.99089100	-0.49264100
C	-1.05437200	0.99585700	-0.36199500
H	-1.79173200	0.34016000	0.08520500
Cl	-0.44934700	2.06355400	1.56966400
C	-1.64579300	2.18472700	-1.09815800
H	-1.07000900	3.09087700	-0.90131800
H	-1.55743300	1.96820000	-2.17082200

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C	0.42058100	-0.79935400	-0.81767800
C	1.64051700	-2.60610200	-0.64347100
C	3.02303700	-3.17898600	-0.67253000
C	3.82180100	-1.99478800	-1.28268500
C	3.05855100	-0.71830300	-0.85965600
H	3.34802100	-3.41619200	0.34488600
H	3.07993200	-4.09065200	-1.26776000
H	3.82299900	-2.08275000	-2.37236100
H	3.11589700	0.09454300	-1.58272500
N	0.42168800	-3.03224100	-0.48095700
N	-0.33052500	-1.89147500	-0.58200200
N	1.68065200	-1.25687500	-0.83941400
H	4.85726200	-1.95882800	-0.94143700
C	-1.75042900	-1.90588100	-0.35799800
C	-2.22639300	-1.35443100	0.83419400
C	-2.57754900	-2.34771500	-1.39356100
C	-3.60904100	-1.20943800	0.94843600
C	-3.94955400	-2.19193700	-1.22114900
C	-4.47778400	-1.60486500	-0.06725500

H	-4.01142100	-0.74338800	1.84390900
H	-4.62034200	-2.51296400	-2.01454500
C	3.43800400	-0.22188800	0.54520800
H	3.57667200	-1.09010800	1.20271500
H	2.61601300	0.37560800	0.95517200
C	4.69099900	0.61448400	0.49461200
C	5.95853100	0.05751700	0.67245300
C	4.58008300	1.98288300	0.23123000
C	7.10094000	0.84831200	0.57510500
H	6.05170700	-0.99985700	0.91235300
C	5.71996800	2.77374700	0.13567000
H	3.58989100	2.42142200	0.13110200
C	6.98260500	2.20768300	0.30210200
H	8.08062600	0.40438300	0.72185800
H	5.62178400	3.83712700	-0.05769400
H	7.87105300	2.82729300	0.23305700
C	-5.96436600	-1.41738300	0.08309300
H	-6.41353400	-1.08251500	-0.85588800
H	-6.44900900	-2.35740100	0.36645900
H	-6.18360000	-0.67297200	0.85140000
C	-1.29487900	-0.88710800	1.91730900
H	-1.84583700	-0.72825100	2.84583800
H	-0.50759500	-1.62395300	2.10570200
H	-0.80445400	0.06247200	1.66437300
C	-1.98881200	-2.90998900	-2.65992000
H	-1.37462800	-3.79034500	-2.45142400
H	-2.77766800	-3.19241300	-3.35876800
H	-1.34623000	-2.17137800	-3.15288100
C	-5.23908400	2.09041800	0.28247100
C	-4.21085700	2.19404800	-0.65201900
C	-2.88785400	2.34937200	-0.23643100
C	-2.59916500	2.38515700	1.13129800
C	-3.62737200	2.27922200	2.06400500
C	-4.94880100	2.13089500	1.64431100
H	-6.26620400	1.98191100	-0.05398200
H	-4.43841500	2.15704200	-1.71501600
H	-1.56481000	2.48578500	1.45986500
H	-3.39169000	2.31508000	3.12344500
H	-5.74930000	2.05437300	2.37441200
C	0.03560000	0.60450500	-1.01995100
O	1.07022900	1.46206800	-0.90433100
H	1.08799200	1.79325700	0.07749900
C	-1.23360800	0.94905800	-1.29141800
H	-1.97977400	0.17784900	-1.44597000

C1	0.96829600	2.07063800	1.86984900
C	-1.75041400	2.35416200	-1.24291600
H	-0.94884800	3.03132800	-0.93742300
H	-2.11976800	2.66809000	-2.22601200

TS4

C	1.07576200	-0.51201700	-0.18120600
C	0.79684200	-2.67357800	-0.33992500
C	-0.17867300	-3.80655100	-0.37988000
C	-1.49785400	-3.05507800	-0.68626100
C	-1.31997000	-1.64138800	-0.09527900
H	0.08194500	-4.55851100	-1.12526600
H	-0.21118000	-4.29173100	0.60077300
H	-2.37624300	-3.54631500	-0.26757400
H	-1.48043800	-1.65486500	0.98784600
N	2.08828100	-2.52260600	-0.29968100
N	2.24053200	-1.16612500	-0.19652600
N	0.14458500	-1.47303100	-0.27311200
H	-1.63673700	-2.97149900	-1.76999100
C	3.54735000	-0.56707900	-0.14722000
C	4.16931200	-0.25148500	-1.35508800
C	4.12200800	-0.33644600	1.10284100
C	5.44005500	0.31241000	-1.28872000
C	5.39503900	0.23022700	1.11424000
C	6.06395400	0.56009100	-0.06460600
H	5.95275200	0.56786100	-2.21267400
H	5.87296100	0.42160500	2.07167200
C	-2.18171500	-0.54425000	-0.70596500
H	-2.00781800	-0.48670500	-1.78692700
H	-1.89821700	0.41897700	-0.26932300
C	-3.63480700	-0.82459300	-0.40364100
C	-4.52149300	-1.25089300	-1.39132900
C	-4.09926100	-0.66997700	0.90665300
C	-5.85519100	-1.51211700	-1.08090900
H	-4.16849000	-1.36609700	-2.41336400
C	-5.42770200	-0.93537400	1.21896800
H	-3.41139200	-0.31732900	1.67344400
C	-6.30975600	-1.35619500	0.22442100
H	-6.53768400	-1.83578600	-1.86057700
H	-5.77864300	-0.80657200	2.23802400
H	-7.34816600	-1.55876300	0.46672200
C	7.42434900	1.20563400	-0.01694900
H	8.01429800	0.95306700	-0.90101400
H	7.33000500	2.29578400	0.01947600

H	7.98040100	0.89249000	0.86961200
C	3.46894500	-0.49508000	-2.66443800
H	3.15572100	-1.53938100	-2.75851100
H	2.57419600	0.13384400	-2.73341900
H	4.12247300	-0.25295500	-3.50387000
C	3.37593800	-0.66006500	2.36670600
H	2.51482700	0.01061300	2.45554100
H	3.00681100	-1.69014700	2.35830500
H	4.01885000	-0.53041300	3.23859900
C	-3.80321800	2.81846700	-1.18838200
C	-2.48014300	3.01312200	-1.58088800
C	-1.45408900	3.04833400	-0.63584800
C	-1.77697900	2.89899200	0.71783600
C	-3.09762000	2.70473500	1.11102800
C	-4.11506400	2.65847900	0.15847500
H	-4.59001500	2.77996400	-1.93592800
H	-2.23696200	3.12046300	-2.63579400
H	-0.97380400	2.89062300	1.45057200
H	-3.32818200	2.57039900	2.16386100
H	-5.14190600	2.48168200	0.46306400
C	0.89759500	0.97265800	-0.04335800
O	1.19133800	1.45875700	1.12666000
H	0.26259900	0.75357300	2.10955800
C	0.43684800	1.61273300	-1.14015100
H	0.21250200	1.04173800	-2.03784500
Cl	-0.60706200	-0.03348700	2.87786600
C	0.00082800	3.05248600	-1.05975800
H	0.61108200	3.56847300	-0.31345900
H	0.12225100	3.56027200	-2.02149800

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C	-0.37542300	-0.81201400	-0.05537300
C	-0.38086100	-2.83050200	0.81352000
C	0.44442400	-4.03069200	1.15960900
C	1.72785300	-3.76327600	0.32468600
C	1.82094400	-2.22608800	0.16113200
H	0.64782300	-4.04090700	2.23479200
H	-0.05062300	-4.96689000	0.90101400
H	1.62305700	-4.23290500	-0.65654200
H	2.20600000	-1.90553700	-0.80528700
N	-1.61672900	-2.44291600	0.92066800
N	-1.59886700	-1.17666800	0.37838000
N	0.39539200	-1.87254200	0.23763900
H	2.62971500	-4.15919400	0.79548200

C	-2.80936900	-0.40581700	0.37742900
C	-2.92664000	0.66850100	1.26276900
C	-3.82029500	-0.77779000	-0.51174400
C	-4.12278300	1.38355600	1.23712400
C	-4.99700400	-0.03373600	-0.49348400
C	-5.16332000	1.04961600	0.37066900
H	-4.23989500	2.22742100	1.91226800
H	-5.79952400	-0.30259500	-1.17577500
C	2.60436700	-1.52867100	1.28202500
H	2.37875200	-2.00749000	2.24352200
H	2.26611200	-0.49018000	1.30035100
C	4.08149400	-1.57428300	0.98539700
C	4.94781800	-2.44103200	1.65002700
C	4.58350800	-0.73960100	-0.02027200
C	6.30186100	-2.47793000	1.32024400
H	4.56330200	-3.08301500	2.43966900
C	5.93376500	-0.77751700	-0.34855700
H	3.89396400	-0.06509800	-0.52636800
C	6.79570300	-1.64706100	0.32000400
H	6.96902100	-3.15291700	1.84710300
H	6.31813600	-0.12382900	-1.12519200
H	7.84993500	-1.67277300	0.06332200
C	-6.42990800	1.86521700	0.34481300
H	-6.65719100	2.27325400	1.33226300
H	-6.32990300	2.70849500	-0.34605600
H	-7.28121500	1.26533500	0.01545000
C	-1.79630600	1.07655500	2.16641200
H	-1.29315000	0.20766700	2.60042400
H	-1.05522800	1.65165600	1.59802300
H	-2.16484900	1.70429500	2.97935500
C	-3.62110900	-1.92407800	-1.46645900
H	-2.71500700	-1.77304400	-2.06290600
H	-3.50839000	-2.86935400	-0.92853400
H	-4.46932200	-2.00789900	-2.14755900
C	-0.99574500	5.82181700	-0.12582300
C	-0.98583300	4.80338900	-1.07914400
C	-0.17720300	3.68047500	-0.91502900
C	0.62930000	3.59006100	0.22792500
C	0.62036300	4.60463000	1.17809600
C	-0.19353100	5.72536700	1.00549600
H	-1.63153500	6.69044400	-0.26995200
H	-1.61515500	4.88191800	-1.96230900
H	1.25896700	2.70942800	0.34432100
H	1.25417400	4.52640800	2.05671600

H	-0.19763500	6.51764100	1.74765400
C	0.19698800	0.41602000	-0.70091000
O	1.47053800	0.48016900	-0.61360900
C	-0.68445700	1.26953200	-1.30032600
H	-1.75153900	1.08540300	-1.27869200
C	-0.17037600	2.54023500	-1.91601500
H	0.86041800	2.36242700	-2.24285600
H	-0.76268400	2.82123900	-2.79334100

TS5(RR)

C	0.64331600	-1.83835900	0.52868900
C	0.48825700	-3.96659800	0.06323600
C	-0.44771500	-5.11744000	-0.13525500
C	-1.74007000	-4.55997100	0.52720800
C	-1.68299000	-3.01999200	0.35741000
H	-0.58358000	-5.31016700	-1.20390400
H	-0.08464700	-6.03233900	0.33238300
H	-1.73423200	-4.80986600	1.59077100
H	-2.05738700	-2.46700500	1.22093200
N	1.77075600	-3.74847100	0.12853700
N	1.85054000	-2.40673200	0.41831200
N	-0.22286000	-2.83002800	0.30917700
H	-2.65196500	-4.96725200	0.08809100
C	3.09607300	-1.83274900	0.87181400
C	4.04457900	-1.40744600	-0.05515900
C	3.27981600	-1.74232200	2.25845200
C	5.22587300	-0.85964000	0.44984800
C	4.46978900	-1.17875100	2.70686400
C	5.44988900	-0.72678800	1.81753600
H	5.97807600	-0.51084000	-0.25311600
H	4.63811700	-1.09119000	3.77724900
C	-2.35542400	-2.51482700	-0.92564900
H	-2.10434300	-3.18348100	-1.75940000
H	-1.95372800	-1.52502000	-1.15952400
C	-3.84741800	-2.39859000	-0.73777700
C	-4.72513500	-3.41297800	-1.11936400
C	-4.35086900	-1.24501800	-0.12898300
C	-6.09283300	-3.28221900	-0.88640100
H	-4.34210300	-4.30090100	-1.61813200
C	-5.71581200	-1.11387600	0.10228500
H	-3.66272300	-0.44397500	0.14085400
C	-6.58801800	-2.13485400	-0.27335600
H	-6.77080500	-4.07294400	-1.19148800
H	-6.09076100	-0.20661100	0.56680800

H	-7.65394100	-2.03160300	-0.09765100
C	6.70164900	-0.07065600	2.33802200
H	7.10569100	-0.61257600	3.19682500
H	7.47364500	-0.01989200	1.56750200
H	6.48506300	0.95158200	2.66588300
C	3.78781900	-1.45933600	-1.53305400
H	3.18040600	-2.32125100	-1.81530100
H	3.25523000	-0.55621700	-1.85337300
H	4.72910100	-1.50077900	-2.08466400
C	2.23324900	-2.24210200	3.22131500
H	1.33242200	-1.61905000	3.20400400
H	1.93597700	-3.26689900	2.97427500
H	2.62509000	-2.24038000	4.23935100
C	4.60062400	2.86042400	0.27114900
C	3.48855300	2.21175900	0.79536700
C	2.20054600	2.72224100	0.60208400
C	2.04882300	3.90410700	-0.12308400
C	3.16309600	4.56161900	-0.64398800
C	4.44022000	4.04180500	-0.45199500
H	5.59237900	2.44246600	0.42495600
H	3.61011500	1.28603000	1.35598700
H	1.04764800	4.28648200	-0.30252400
H	3.03034200	5.47950400	-1.20854900
H	5.30510600	4.55256900	-0.86364700
C	0.26325200	-0.46126000	1.05503200
O	-0.59656300	-0.50777800	1.94010100
C	0.91369300	0.61725800	0.41836800
H	1.80843500	0.32394300	-0.12453900
C	1.01010300	1.95107700	1.12027800
H	0.09553300	2.53313500	0.97954300
H	1.10751900	1.77886700	2.20028300
C	-3.44312400	2.25624900	0.89685200
C	-3.70325900	3.58562400	0.48963400
C	-4.77794700	4.30554600	1.00163700
C	-5.60211500	3.69357500	1.94065000
C	-5.34593300	2.38510300	2.36740100
C	-4.27280700	1.66543800	1.85853800
H	-4.96825800	5.32325000	0.67676400
H	-6.44511700	4.24032700	2.34993700
H	-5.98938800	1.93015300	3.11416600
H	-4.04848100	0.65937200	2.19990500
N	-2.35766800	1.64490700	0.30781400
S	-2.49740600	4.07094400	-0.67627100
C	-1.75886800	2.45160800	-0.53266000

N	-0.65347900	2.21924000	-1.26726100
C	-0.25635500	0.94185700	-1.28176700
H	-1.00629600	0.18314700	-1.04250200
C	0.69570900	0.54325600	-2.35538300
C	1.61997800	1.45868800	-2.87179300
C	0.63909600	-0.74384700	-2.89435600
C	2.45902200	1.08793700	-3.91609300
H	1.65255500	2.45750800	-2.44738100
C	1.47008800	-1.10987600	-3.95184000
H	-0.08387700	-1.45663900	-2.50122900
C	2.38317500	-0.19401800	-4.46507400
H	3.17206400	1.80467900	-4.31136400
H	1.40170300	-2.10732300	-4.37552800
H	3.03181500	-0.47404400	-5.28899600

TS5(RS)

C	-0.57928400	-1.77947300	-0.87481100
C	-0.26193900	-3.93593300	-0.71613400
C	0.74012500	-5.03978600	-0.62540900
C	2.01476500	-4.33511900	-1.16155100
C	1.83326100	-2.81406700	-0.90709000
H	0.84903700	-5.34879900	0.41885500
H	0.45146900	-5.91389200	-1.20922500
H	2.10117200	-4.51547200	-2.23562900
H	2.15601300	-2.20133900	-1.74847500
N	-1.55768700	-3.80601500	-0.71064100
N	-1.74070100	-2.45339300	-0.81911400
N	0.36113200	-2.73152100	-0.83659700
H	2.92702800	-4.69833800	-0.68569000
C	-3.06782100	-1.91662500	-0.95486600
C	-3.90570300	-1.95682200	0.15914600
C	-3.44273000	-1.35914700	-2.18218900
C	-5.15867300	-1.35592100	0.03466500
C	-4.70689900	-0.78176000	-2.25399600
C	-5.56888200	-0.75554800	-1.15381700
H	-5.82349700	-1.35382800	0.89430700
H	-5.02533500	-0.33230300	-3.19189800
C	2.47383900	-2.29331900	0.38168400
H	2.10263300	-2.88283900	1.23059300
H	2.15471700	-1.25021200	0.52443000
C	3.97592000	-2.39874400	0.28784100
C	4.69010800	-3.31429600	1.06180200
C	4.67066600	-1.59617100	-0.62236600
C	6.07310200	-3.42567700	0.93692400

H	4. 15843500	-3. 93754700	1. 77741600
C	6. 05095700	-1. 70678500	-0. 74998700
H	4. 12244000	-0. 86400700	-1. 21085500
C	6. 75562900	-2. 62300600	0. 02857700
H	6. 61606800	-4. 13709800	1. 55117000
H	6. 57887600	-1. 07064300	-1. 45333800
H	7. 83330700	-2. 70623300	-0. 06941100
C	-6. 90993000	-0. 07822200	-1. 26382700
H	-7. 47884400	-0. 16986600	-0. 33676700
H	-6. 78644800	0. 98702800	-1. 48373900
H	-7. 50317300	-0. 51228100	-2. 07384700
C	-3. 46104600	-2. 61510000	1. 43355400
H	-3. 40320800	-3. 69993000	1. 30355600
H	-2. 47015600	-2. 26016800	1. 73465200
H	-4. 15577600	-2. 39301300	2. 24412100
C	-2. 51715100	-1. 35361400	-3. 36997800
H	-1. 75811500	-0. 56875500	-3. 27743800
H	-1. 99635100	-2. 31005300	-3. 47503200
H	-3. 07985500	-1. 17003600	-4. 28671300
C	-4. 53586500	3. 33951000	0. 18409600
C	-3. 63158100	2. 56040700	-0. 53037200
C	-2. 26983200	2. 88248300	-0. 55503900
C	-1. 83303200	4. 00765700	0. 14760400
C	-2. 73829000	4. 79035100	0. 86272900
C	-4. 08980100	4. 45940300	0. 88453600
H	-5. 58942700	3. 07450000	0. 19623000
H	-3. 97746600	1. 68081700	-1. 07252700
H	-0. 77067800	4. 24110100	0. 14825100
H	-2. 38381800	5. 65875900	1. 40958400
H	-4. 79240900	5. 06849700	1. 44459900
C	-0. 27204800	-0. 31833900	-1. 10767400
O	0. 85004100	-0. 11587500	-1. 59232000
C	-1. 19364100	0. 62584100	-0. 61767200
H	-2. 13436500	0. 23122000	-0. 24393400
C	-1. 29661800	1. 98582600	-1. 28581000
H	-0. 30924200	2. 44737400	-1. 34400200
H	-1. 65881500	1. 84037300	-2. 31533800
C	2. 60831100	3. 74633500	-0. 30936300
C	3. 88060500	3. 16171100	-0. 11617200
C	5. 05026900	3. 83594700	-0. 45090700
C	4. 94924700	5. 11422600	-0. 99001300
C	3. 69580200	5. 70417900	-1. 19050300
C	2. 52867000	5. 03194500	-0. 85619300
H	6. 02032600	3. 37552200	-0. 29310100

H	5. 85050600	5. 65667000	-1. 25607800
H	3. 63538400	6. 70207900	-1. 61341800
H	1. 55227300	5. 48071300	-1. 00897000
N	1. 52722800	2. 97685600	0. 06534200
S	3. 67475400	1. 57259700	0. 57524200
C	1. 90526600	1. 81817100	0. 53534100
N	1. 16169300	0. 80800800	1. 03800600
C	-0. 15000900	1. 03108100	1. 15705700
H	-0. 51099200	2. 06025900	1. 08735900
C	-0. 89574800	0. 20955600	2. 15588600
C	-0. 27691000	-0. 85092900	2. 82395200
C	-2. 19461000	0. 58172500	2. 52554100
C	-0. 93920600	-1. 51610300	3. 85419800
H	0. 74730200	-1. 09598400	2. 56097900
C	-2. 84803000	-0. 07486600	3. 56285200
H	-2. 67644000	1. 41113600	2. 00913500
C	-2. 22052000	-1. 12392300	4. 23454300
H	-0. 44235000	-2. 32641500	4. 37959400
H	-3. 84585300	0. 23874700	3. 85497700
H	-2. 72688100	-1. 63017900	5. 05061800

TS5(SR)

C	0. 25081800	0. 08017700	0. 74504200
C	1. 58751100	-0. 69626000	2. 29351900
C	3. 00194700	-0. 87903600	2. 74114800
C	3. 80050300	-0. 43021800	1. 48314200
C	2. 84229100	0. 42970500	0. 62173600
H	3. 20065700	-0. 25543900	3. 61753900
H	3. 20558600	-1. 91756400	3. 00917300
H	4. 11991300	-1. 30843900	0. 92290000
H	2. 91884500	0. 22947100	-0. 44733300
N	0. 39375600	-0. 94713700	2. 75108500
N	-0. 43316100	-0. 45874500	1. 77274600
N	1. 53677900	-0. 05729400	1. 09595800
H	4. 69148300	0. 14490800	1. 74352800
C	-1. 84444800	-0. 34292600	2. 03927700
C	-2. 36644200	0. 94762800	2. 20302500
C	-2. 62049100	-1. 49956900	2. 15589700
C	-3. 74134300	1. 06006000	2. 39411300
C	-3. 98954500	-1. 32449800	2. 36104000
C	-4. 56966400	-0. 06043700	2. 45401900
H	-4. 17024300	2. 05397400	2. 49687700
H	-4. 61759000	-2. 20845000	2. 44479900
C	2. 96833900	1. 93646700	0. 89731200

H	3.09163200	2.09713300	1.97618800
H	2.04285300	2.41418800	0.56733000
C	4.13586400	2.50557200	0.13206700
C	5.33754700	2.84121400	0.75397900
C	4.01664100	2.66562200	-1.25308800
C	6.40828200	3.33135400	0.00846600
H	5.43311000	2.72809400	1.83170200
C	5.08426400	3.15391400	-1.99706200
H	3.07186800	2.40715100	-1.72832800
C	6.28354500	3.48707500	-1.36796200
H	7.33754700	3.59275600	0.50494600
H	4.98097700	3.28012800	-3.07036100
H	7.11599100	3.86970600	-1.94994200
C	-6.06010100	0.09508000	2.60617300
H	-6.30808700	0.97476100	3.20479600
H	-6.53333300	0.21846900	1.62621300
H	-6.50518800	-0.78213500	3.08115000
C	-1.50106600	2.17976700	2.16888400
H	-0.55231600	2.01574400	2.69085600
H	-1.27929800	2.48566200	1.14026600
H	-2.01855700	3.01251800	2.64853800
C	-2.03127600	-2.87908600	2.04717100
H	-2.76367400	-3.62471100	2.36348400
H	-1.74562500	-3.08226200	1.00866100
H	-1.13809800	-2.97917400	2.66830900
C	-3.88422800	4.03439000	0.13110700
C	-3.58259700	2.90837400	-0.62914900
C	-2.36324800	2.80730700	-1.30641900
C	-1.44874400	3.86051200	-1.20624200
C	-1.74987700	4.98805300	-0.44445000
C	-2.96624300	5.07886800	0.22784600
H	-4.83963300	4.10049100	0.64464400
H	-4.29270500	2.08601000	-0.69326900
H	-0.48894300	3.76939800	-1.70585300
H	-1.02981000	5.79784100	-0.37416200
H	-3.20097300	5.95906700	0.81823000
C	-0.17236300	0.77968400	-0.52670400
O	0.71582800	1.50293100	-1.03607900
C	-1.46857800	0.55508300	-0.99060800
H	-2.19108900	0.09579400	-0.32817200
C	-1.99888700	1.52252700	-2.01907600
H	-1.22882700	1.71479800	-2.77314500
H	-2.88075600	1.10783800	-2.51652200
C	2.67198200	-2.43915600	-1.12396600

C	2.66038400	-3.38069000	-0.06819600
C	3.84083200	-3.93354600	0.42798900
C	5.04641800	-3.53752400	-0.13931700
C	5.07238300	-2.60391800	-1.18659700
C	3.89951100	-2.05355100	-1.68125400
H	3.81707800	-4.66381300	1.23070100
H	5.97560700	-3.95849400	0.23010600
H	6.02436600	-2.30916200	-1.61587000
H	3.90431600	-1.33348300	-2.49320700
N	1.44126500	-1.97424700	-1.53224500
S	1.01231900	-3.68794200	0.40336500
C	0.47738200	-2.54700600	-0.86503800
N	-0.86287500	-2.40295100	-1.01034200
C	-1.26415000	-1.56795900	-1.94776900
H	-0.55245700	-1.15524100	-2.66789500
C	-2.68564200	-1.58243900	-2.34298000
C	-3.67988700	-1.97548900	-1.43933400
C	-3.04901000	-1.20197000	-3.63700200
C	-5.01336300	-1.97028900	-1.82267200
H	-3.38774400	-2.26711100	-0.43500700
C	-4.38637800	-1.21313300	-4.02581000
H	-2.27715300	-0.89374000	-4.33773300
C	-5.37073500	-1.59182800	-3.11826100
H	-5.77994700	-2.26393800	-1.11176600
H	-4.65845100	-0.92128900	-5.03500800
H	-6.41425800	-1.59263300	-3.41696000

TS5(SS)

C	0.15343600	-0.04572500	1.06481300
C	1.55895200	-0.58648600	2.65212100
C	2.98790900	-0.61687200	3.09136600
C	3.73611400	-0.25167700	1.77782000
C	2.71449500	0.45723600	0.85261000
H	3.14912900	0.11494700	3.88840100
H	3.27099100	-1.60218900	3.46561800
H	4.09444900	-1.16365900	1.29804700
H	2.77232700	0.12256300	-0.18416600
N	0.39940200	-0.94797000	3.12346900
N	-0.47050400	-0.58789100	2.12233400
N	1.44525300	-0.02024300	1.42183800
H	4.59599000	0.39676900	1.95968600
C	-1.88592300	-0.73645200	2.29676100
C	-2.62935000	0.40831100	2.60027300
C	-2.45463800	-1.99539500	2.09798800

C	-4.01351400	0.26703300	2.66387400
C	-3.84433000	-2.08273900	2.17881500
C	-4.63570300	-0.96357000	2.44384900
H	-4.61866300	1.14359500	2.88296100
H	-4.31839800	-3.04935900	2.02630900
C	2.78712300	1.98896900	0.91166500
H	2.92057200	2.30691600	1.95356700
H	1.83849000	2.38403000	0.54028200
C	3.91995400	2.48269200	0.04756100
C	5.09735000	2.99351800	0.59185500
C	3.79560500	2.38574500	-1.34312100
C	6.13978600	3.40546800	-0.23666800
H	5.19622100	3.07758000	1.67192900
C	4.83575900	2.79485500	-2.16936200
H	2.87162000	1.98841900	-1.76006200
C	6.01065100	3.30533100	-1.61783900
H	7.05074000	3.80519700	0.19778900
H	4.72973400	2.71781200	-3.24692500
H	6.82147200	3.62555000	-2.26439800
C	-6.13811100	-1.07515500	2.46929500
H	-6.55560600	-0.86191600	1.47961700
H	-6.45700500	-2.08039500	2.75364800
H	-6.57532400	-0.36263500	3.17246700
C	-1.96524200	1.74553600	2.78648700
H	-1.07984100	1.66196800	3.42400200
H	-1.65661600	2.16356200	1.81940700
H	-2.65736000	2.45712300	3.23946200
C	-1.59353700	-3.19669600	1.81487600
H	-2.20949200	-4.05381400	1.53664200
H	-0.87800800	-2.99765900	1.00819500
H	-1.01536800	-3.46386900	2.70604200
C	-3.94996200	3.95025600	0.71639800
C	-3.71302600	2.86906800	-0.12776400
C	-2.48211500	2.72004200	-0.77353100
C	-1.48921600	3.68205000	-0.55830100
C	-1.72469200	4.76412400	0.28638500
C	-2.95385400	4.90108000	0.92892000
H	-4.91394400	4.05364800	1.20670600
H	-4.48556600	2.11914400	-0.28524600
H	-0.52557600	3.55585800	-1.04467100
H	-0.94636200	5.50518800	0.44238200
H	-3.13652900	5.74609600	1.58536300
C	-0.33088200	0.53965900	-0.23485400
O	0.58262600	1.05421500	-0.92361700

C	-1.67149400	0.43427500	-0.60444200
H	-2.39348200	0.00505600	0.07963300
C	-2.19068200	1.46855100	-1.57328000
H	-1.43232300	1.65502400	-2.33961000
H	-3.10392500	1.12084400	-2.06510000
C	2.12870500	-2.73341300	-0.13453000
C	3.18311200	-2.52121100	-1.05373200
C	4.48238200	-2.93625700	-0.77103000
C	4.72892900	-3.57799400	0.43928200
C	3.69245300	-3.79503300	1.35750800
C	2.39821600	-3.37211300	1.08320500
H	5.28353900	-2.77132300	-1.48386700
H	5.73382700	-3.91544800	0.67009400
H	3.90319100	-4.30505000	2.29249200
H	1.58523300	-3.53444500	1.78549000
N	0.88532200	-2.29778100	-0.53949900
S	2.55280700	-1.73509400	-2.47708400
C	0.93150300	-1.77721500	-1.74164700
N	-0.09741200	-1.32128600	-2.49287100
C	-1.28733400	-1.45406400	-1.94722300
H	-1.42115200	-2.05025400	-1.04088400
C	-2.49648900	-1.25568900	-2.76375600
C	-2.41339600	-0.75595000	-4.06626400
C	-3.74845000	-1.56096700	-2.22042100
C	-3.57150200	-0.55864200	-4.80980900
H	-1.43147300	-0.53160700	-4.46994900
C	-4.90468900	-1.36158100	-2.96480800
H	-3.80689000	-1.93686300	-1.20027900
C	-4.81780200	-0.85754900	-4.26210100
H	-3.50363300	-0.16837800	-5.82039900
H	-5.87406300	-1.59735400	-2.53669500
H	-5.72024800	-0.69882100	-4.84406600

5(RR)

C	0.07524600	-1.08930200	0.69633300
C	0.92964700	-1.98229900	2.50850500
C	2.16137100	-2.26738300	3.30120700
C	3.25026000	-2.07793200	2.21871000
C	2.68273900	-1.05581400	1.20047000
H	2.25903700	-1.54118600	4.11449400
H	2.15206700	-3.26657500	3.73680800
H	3.42128500	-3.02961800	1.70938300
H	2.97484100	-1.31009700	0.18136500
N	-0.34129500	-2.21836500	2.60960200

N	-0.86152100	-1.66000500	1.46951800
N	1.22824200	-1.30165100	1.35644800
H	4.20168200	-1.73278700	2.62552100
C	-2.26540600	-1.86722700	1.19231400
C	-3.20917700	-0.99326000	1.73092300
C	-2.61617900	-3.01393100	0.47001400
C	-4.55406900	-1.26672500	1.48345600
C	-3.97155600	-3.24942100	0.26741000
C	-4.95173100	-2.38749100	0.76199600
H	-5.30432100	-0.57504500	1.85974300
H	-4.26934800	-4.12981700	-0.29676100
C	3.05207500	0.39801800	1.51748700
H	2.70276700	0.64801200	2.52729300
H	2.53920300	1.06376600	0.81524900
C	4.54532800	0.60054400	1.41548000
C	5.31237700	0.90026700	2.54188900
C	5.18441100	0.45921100	0.18005000
C	6.69168300	1.06503800	2.43899600
H	4.82351700	1.01624300	3.50632800
C	6.56163700	0.62035200	0.07586700
H	4.59830800	0.23143400	-0.70811700
C	7.31913100	0.92446300	1.20516100
H	7.27373300	1.30634400	3.32267000
H	7.04298300	0.51283600	-0.89083700
H	8.39331000	1.05423800	1.12199500
C	-6.41350000	-2.66951100	0.53668400
H	-6.96484400	-1.73993700	0.37415800
H	-6.56327700	-3.31582600	-0.33161800
H	-6.85219200	-3.17098300	1.40568000
C	-2.84472900	0.20421100	2.56656500
H	-1.76644500	0.29152400	2.71997700
H	-3.20163300	1.11964500	2.08281100
H	-3.31777800	0.13586100	3.55023100
C	-1.57180200	-3.94110800	-0.08290100
H	-1.10254800	-3.44851400	-0.94023000
H	-0.80015200	-4.16060500	0.66299800
H	-2.02139300	-4.88496600	-0.39645200
C	-5.17822700	-0.39120800	-1.79258400
C	-3.81446100	-0.17084000	-1.96664500
C	-3.23372700	1.02583200	-1.54199400
C	-4.03062100	1.97446200	-0.89174700
C	-5.39071900	1.74399900	-0.69946000
C	-5.97180600	0.56551200	-1.16370800
H	-5.62158800	-1.32108900	-2.13994900

H	-3.17386000	-0.92519600	-2.41442900
H	-3.57971800	2.90476500	-0.54616300
H	-6.00059500	2.49417000	-0.20432400
H	-7.03773700	0.39641100	-1.03761000
C	-0.23863300	-0.46351400	-0.71125600
O	-0.83908300	-1.32559100	-1.44390100
C	-0.96608900	0.89974500	-0.46525500
H	-1.68388500	0.71770100	0.34008100
C	-1.75723300	1.27865800	-1.73165900
H	-1.59625900	2.33424300	-1.96754300
H	-1.38876400	0.68169100	-2.56962100
C	1.90852100	-0.98936700	-2.04120500
C	2.87734200	-0.38612600	-2.85970600
C	3.74469400	-1.14745900	-3.63136300
C	3.63575500	-2.53617600	-3.58979400
C	2.67288300	-3.13963800	-2.78297600
C	1.80432600	-2.38061000	-2.00131900
H	4.48852100	-0.66601100	-4.25785700
H	4.30117900	-3.14534200	-4.19181000
H	2.58866700	-4.22134200	-2.76439600
H	1.03157500	-2.84146900	-1.39876400
N	1.18707600	-0.07895800	-1.26910000
S	2.81803000	1.36806500	-2.72705000
C	1.51634700	1.24323000	-1.51114700
N	1.03481000	2.28282700	-0.95639600
C	-0.00223800	2.00234600	0.02293000
H	0.47019700	1.62598100	0.95208100
C	-0.75807100	3.26487400	0.38432200
C	-0.84790400	4.33381400	-0.50811600
C	-1.44360700	3.34319900	1.59752100
C	-1.64418200	5.43714700	-0.20930700
H	-0.27854200	4.28855600	-1.43087300
C	-2.23996800	4.44343500	1.89966400
H	-1.34883100	2.53314200	2.31579600
C	-2.35093300	5.49188900	0.98912200
H	-1.71117000	6.25816100	-0.91643600
H	-2.76794300	4.48556300	2.84751100
H	-2.97227700	6.35143200	1.21954400

5(RS)

C	-0.41324900	-1.66140200	-0.67166000
C	0.27706600	-3.74532200	-0.67604700
C	1.46455200	-4.65216900	-0.74820800
C	2.55461600	-3.65654300	-1.22802300

C	2.14082200	-2.27988100	-0.65553500
H	1.68769300	-5.06597300	0.24029200
H	1.30668800	-5.48233100	-1.43682300
H	2.54030900	-3.60833500	-2.31976000
H	2.40839200	-1.44678500	-1.30864500
N	-1.01778500	-3.84823600	-0.67396700
N	-1.42905600	-2.53524600	-0.66890000
N	0.67809900	-2.44093300	-0.65945400
H	3.56015300	-3.93474100	-0.91160100
C	-2.82485500	-2.20756200	-0.62019100
C	-3.44040000	-2.20418700	0.63437400
C	-3.45936700	-1.81978100	-1.79942500
C	-4.75062600	-1.73822300	0.69452800
C	-4.77509300	-1.36765400	-1.68406000
C	-5.42299800	-1.30103500	-0.45005500
H	-5.25107200	-1.69783100	1.65932500
H	-5.29868700	-1.04354400	-2.58031300
C	2.63409200	-2.03625200	0.78152100
H	2.42210900	-2.92977200	1.38344700
H	2.04407500	-1.21209000	1.19390900
C	4.10321000	-1.69351500	0.82374100
C	5.09162200	-2.67610700	0.91673100
C	4.49270000	-0.35575100	0.73664300
C	6.44003600	-2.32768200	0.89216400
H	4.80670300	-3.72039000	1.02844000
C	5.83715400	-0.00203200	0.70322200
H	3.73196400	0.41716600	0.72003400
C	6.81505100	-0.99158400	0.77480100
H	7.19801800	-3.10074000	0.97121300
H	6.10787300	1.04758800	0.62519100
H	7.86650200	-0.72325600	0.75268200
C	-6.81444300	-0.73407300	-0.33757900
H	-7.45789400	-1.37923400	0.26643800
H	-6.78466000	0.24699000	0.14935000
H	-7.27546300	-0.60897300	-1.31937400
C	-2.69211700	-2.65439600	1.85956800
H	-2.36720700	-3.69363000	1.75192900
H	-1.80206200	-2.03613800	2.02759300
H	-3.32153300	-2.57025000	2.74660300
C	-2.73513500	-1.85708800	-3.11841900
H	-1.85849400	-1.19564800	-3.11346700
H	-2.37925000	-2.87115300	-3.32813600
H	-3.40272600	-1.55432900	-3.92712200
C	-5.23679200	3.20249100	-0.12968600

C	-4.33470100	2.34410300	-0.74954700
C	-3.00186600	2.72423300	-0.94616200
C	-2.59893700	3.98643400	-0.50585500
C	-3.49891400	4.84790100	0.11843500
C	-4.82035100	4.45864200	0.30905500
H	-6.27072800	2.89737100	0.00445200
H	-4.65959400	1.36263100	-1.09091700
H	-1.56862000	4.29778400	-0.66026800
H	-3.16516200	5.82492400	0.45352900
H	-5.52393300	5.12970200	0.79127100
C	-0.39152800	-0.14546500	-1.08143500
O	-0.00961800	-0.12155800	-2.30691000
C	-1.61798100	0.68930400	-0.54813600
H	-2.50171500	0.13852100	-0.22080300
C	-2.01666200	1.76054600	-1.55828000
H	-1.11854600	2.28188000	-1.90759200
H	-2.44725600	1.26340300	-2.43525200
C	3.17864400	2.78009600	0.05997600
C	3.58912300	2.33170700	-1.21054100
C	4.76360700	2.79487400	-1.79856700
C	5.53343300	3.71847800	-1.09992900
C	5.13372500	4.17101200	0.16462900
C	3.96403600	3.70831300	0.75055100
H	5.07271800	2.44138300	-2.77690500
H	6.45246300	4.09147300	-1.53995800
H	5.74862200	4.89210200	0.69367900
H	3.64371600	4.04398200	1.73090900
N	2.02626300	2.19438000	0.55814800
S	2.42075700	1.18899200	-1.84075700
C	1.54577400	1.33448400	-0.29259600
N	0.45741100	0.56858200	-0.01226000
C	-0.73203700	1.19819500	0.60729600
H	-0.62382400	2.28982100	0.64274000
C	-1.08332500	0.67883600	1.97819900
C	-0.10165900	0.16911000	2.82760700
C	-2.40911800	0.73585200	2.41940700
C	-0.44433000	-0.30961800	4.09069200
H	0.93257000	0.17919200	2.49471600
C	-2.74857200	0.26655200	3.68453400
H	-3.17430300	1.14919900	1.76426500
C	-1.76866900	-0.26812100	4.51923300
H	0.32575200	-0.70710200	4.74463800
H	-3.78119900	0.31319800	4.01794000
H	-2.03530600	-0.64164500	5.50295800

5(SR)

C	-0.33232900	1.06766100	0.76027900
C	0.87066800	1.52461600	2.51526000
C	2.23680500	1.77478900	3.06100000
C	3.01608200	2.16776500	1.78342400
C	2.26357500	1.53577800	0.58967000
H	2.24550400	2.54594300	3.83187000
H	2.61248300	0.84113700	3.48889400
H	4.05223500	1.82985000	1.80075600
H	2.59266800	0.50449400	0.43707200
N	-0.30893200	1.27682000	2.99816000
N	-1.06215400	1.01706200	1.87989100
N	0.88971300	1.46616800	1.14752500
H	3.01487600	3.25660900	1.66368700
C	-2.44677900	0.65316300	1.99498200
C	-3.42276600	1.53520700	1.52955400
C	-2.74609300	-0.59628100	2.56296800
C	-4.75494700	1.12648100	1.63534300
C	-4.08883700	-0.95301800	2.63020800
C	-5.10465000	-0.10746400	2.17223200
H	-5.53054100	1.79668300	1.27464000
H	-4.34965800	-1.92020100	3.05313000
C	2.40597100	2.30136200	-0.72260500
H	2.01740200	3.31863100	-0.60749100
H	1.81637000	1.80616500	-1.49756200
C	3.86680200	2.30378100	-1.10827400
C	4.64924900	3.45413800	-1.01190700
C	4.46366700	1.10377500	-1.50618900
C	6.00948000	3.40881300	-1.31104200
H	4.19036900	4.39118700	-0.70584000
C	5.82348800	1.05406000	-1.79086600
H	3.85534000	0.20470500	-1.58590200
C	6.59920500	2.20825000	-1.69591000
H	6.60823200	4.31133600	-1.23926900
H	6.27321700	0.10884200	-2.07802500
H	7.66025100	2.17152800	-1.92080500
C	-6.54827000	-0.52398000	2.28232900
H	-6.89734900	-0.44259800	3.31649900
H	-7.19063800	0.10463100	1.66172700
H	-6.68161900	-1.56368100	1.97251700
C	-3.09202600	2.86393200	0.90181400
H	-2.16152400	3.28328000	1.29259900
H	-2.99663800	2.76994100	-0.18662900

H	-3.89694700	3.57658400	1.09218900
C	-1.66223700	-1.52042700	3.04613300
H	-2.09588000	-2.45439300	3.40790700
H	-0.97070700	-1.73967800	2.22376800
H	-1.09038700	-1.06304900	3.85809700
C	-5.58980900	1.72038000	-1.63673900
C	-4.56736700	0.78469900	-1.76704300
C	-3.37038400	1.11846500	-2.40679100
C	-3.21838700	2.41287300	-2.91129900
C	-4.23806000	3.35224400	-2.77907100
C	-5.42696100	3.00929100	-2.13943700
H	-6.51698800	1.43975600	-1.14515600
H	-4.69556900	-0.21880300	-1.36539900
H	-2.28454800	2.68418500	-3.39442200
H	-4.10284200	4.35366000	-3.17535800
H	-6.22363700	3.73950100	-2.03927800
C	-0.84961500	1.06169400	-0.66590800
O	-0.55141600	2.01452200	-1.34950800
C	-1.59283000	-0.15270100	-1.15026900
H	-2.34312900	-0.42360600	-0.39553500
C	-2.25754800	0.10153700	-2.50213800
H	-1.49977200	0.43638100	-3.21744700
H	-2.64988100	-0.85533500	-2.86239800
C	3.44806400	-2.07965700	-0.20104500
C	3.59018500	-2.01179800	1.20782800
C	4.82241000	-2.17178300	1.82884500
C	5.94628600	-2.40932400	1.04006500
C	5.82329700	-2.49231200	-0.34984600
C	4.59127300	-2.33225600	-0.97228000
H	4.90746500	-2.11939100	2.90994200
H	6.91569800	-2.53696800	1.50961200
H	6.70410200	-2.68900800	-0.95399900
H	4.48802100	-2.39861300	-2.05107300
N	2.19140000	-1.85242200	-0.71139500
S	2.01588000	-1.72550700	1.92608300
C	1.30997200	-1.62611000	0.24772200
N	0.04144900	-1.28742900	0.18053700
C	-0.52801600	-1.28305300	-1.15638900
H	0.22433000	-1.03755500	-1.92265400
C	-1.15471700	-2.61579500	-1.51457600
C	-2.13567600	-3.17024300	-0.68652600
C	-0.76505500	-3.30503200	-2.66074600
C	-2.72450100	-4.38662500	-1.00987400
H	-2.42208800	-2.64563700	0.22329300

C	-1.35163200	-4.52758300	-2.98489100
H	0.01497500	-2.88584000	-3.29038500
C	-2.33469000	-5.06806400	-2.16307000
H	-3.48475300	-4.81013800	-0.36072400
H	-1.03555700	-5.05857500	-3.87730800
H	-2.79258300	-6.01962900	-2.41383400

5(SS)

C	-0.25988300	0.21459400	-1.04946100
C	-1.63859400	-0.20757200	-2.67891400
C	-3.06859400	-0.33636400	-3.09649200
C	-3.81731500	-0.21168500	-1.73793100
C	-2.84722700	0.47205000	-0.73999100
H	-3.32980900	0.45713000	-3.80282100
H	-3.25006500	-1.30107300	-3.57315800
H	-4.08019300	-1.20566600	-1.37279200
H	-2.82804200	-0.02113200	0.23641200
N	-0.45801100	-0.42858800	-3.19197800
N	0.39478900	-0.14211200	-2.15819100
N	-1.55191600	0.22626300	-1.39559500
H	-4.73521600	0.37307400	-1.82867200
C	1.82025400	-0.18846900	-2.32617100
C	2.50467600	1.02829900	-2.39178800
C	2.44862200	-1.43572800	-2.35676200
C	3.89663000	0.97162800	-2.43592700
C	3.84149700	-1.43349200	-2.41467100
C	4.57777600	-0.24640300	-2.43250500
H	4.45742700	1.90269700	-2.46372600
H	4.36494300	-2.38638200	-2.42845400
C	-3.10063000	1.97780000	-0.58429300
H	-3.26318400	2.41731900	-1.57634000
H	-2.21173400	2.43927500	-0.14751800
C	-4.29582300	2.21551600	0.30575100
C	-5.49835400	2.70973700	-0.19845500
C	-4.20486200	1.90508400	1.66663700
C	-6.59520200	2.89611900	0.64058100
H	-5.57408400	2.95833000	-1.25458000
C	-5.29868900	2.08874100	2.50428000
H	-3.26782200	1.51936800	2.06331100
C	-6.49681200	2.58532900	1.99263500
H	-7.52474200	3.28468200	0.23676100
H	-5.21637300	1.84465500	3.55849100
H	-7.34975000	2.72931200	2.64805700
C	6.08359300	-0.28427100	-2.41663200

H	6.45110800	-0.37469800	-1.38865900
H	6.46441800	-1.13979900	-2.97914100
H	6.50885900	0.62714900	-2.84219600
C	1.77049100	2.34245400	-2.36428600
H	0.90344500	2.32521800	-3.03144600
H	1.42130600	2.58510800	-1.35199400
H	2.43095100	3.15431600	-2.67181300
C	1.65034000	-2.70997500	-2.32445400
H	2.31165400	-3.57129100	-2.21662900
H	0.93393800	-2.70377900	-1.49334900
H	1.08291300	-2.82322000	-3.25432100
C	3.74747500	4.02566300	-0.00425500
C	3.46527100	2.84032400	0.66630200
C	2.22865100	2.64481700	1.29307100
C	1.27897000	3.66767500	1.23202600
C	1.55784900	4.85589300	0.55724500
C	2.79046500	5.03784300	-0.06380700
H	4.71662100	4.16444600	-0.47507900
H	4.20846000	2.04572800	0.71132100
H	0.31592500	3.52235400	1.71416500
H	0.81067000	5.64287700	0.52058100
H	3.00774700	5.96507000	-0.58451200
C	0.20479400	0.59941800	0.33379300
O	-0.64947800	1.13227600	1.01368500
C	1.57073200	0.27507800	0.86607200
H	2.31470000	0.31247200	0.06509800
C	1.93455700	1.31388000	1.94011400
H	1.11726500	1.38230500	2.66117100
H	2.82308100	0.96200900	2.46946700
C	-1.85716300	-2.69310700	-0.19328200
C	-2.84754400	-2.80647200	0.81903600
C	-4.10374500	-3.32766300	0.54703700
C	-4.39193400	-3.77188800	-0.74753300
C	-3.42155300	-3.69145500	-1.74787100
C	-2.16566600	-3.14917500	-1.48330400
H	-4.84949400	-3.40502500	1.33211500
H	-5.36774400	-4.19280600	-0.96534200
H	-3.64509900	-4.05982400	-2.74530100
H	-1.40542700	-3.08816600	-2.25821700
N	-0.65609700	-2.15463900	0.18349900
S	-2.19131400	-2.22106200	2.33699900
C	-0.60648400	-1.91062200	1.50954600
N	0.39169900	-1.47425100	2.21071500
C	1.55820100	-1.22519700	1.41240700

H	1. 58158700	-1. 85516900	0. 51101200
C	2. 84982700	-1. 46616300	2. 16879000
C	2. 85543200	-1. 67575900	3. 54628000
C	4. 06402400	-1. 45673400	1. 47554900
C	4. 05985500	-1. 86648200	4. 22114100
H	1. 90235100	-1. 69268200	4. 06359100
C	5. 26598900	-1. 64508800	2. 14968000
H	4. 06146300	-1. 30806200	0. 39584100
C	5. 26699500	-1. 84851600	3. 52874400
H	4. 05395200	-2. 03184800	5. 29428700
H	6. 20263100	-1. 64188500	1. 59961500
H	6. 20359100	-1. 99828700	4. 05655200

TS6(SR)

C	0. 44419400	-0. 44884900	0. 65336400
C	1. 60347100	-1. 10804800	2. 39539300
C	2. 96389900	-1. 29829100	2. 98954600
C	3. 86911100	-1. 09005200	1. 74552600
C	3. 06057100	-0. 19679700	0. 78175600
H	3. 13820600	-0. 54590400	3. 76516000
H	3. 08023200	-2. 28341300	3. 44388800
H	4. 05559700	-2. 05275900	1. 26009700
H	3. 26299400	-0. 40768100	-0. 26154300
N	0. 36915000	-1. 21102800	2. 78315100
N	-0. 35151500	-0. 79484700	1. 68648900
N	1. 68902400	-0. 62908700	1. 12254800
H	4. 82994300	-0. 63191600	1. 99075300
C	-1. 72401600	-0. 42741100	1. 94879700
C	-1. 97587200	0. 94608800	2. 10187500
C	-2. 68004000	-1. 40936200	2. 20353600
C	-3. 27539700	1. 32809900	2. 41677800
C	-3. 95772500	-0. 96832400	2. 56447600
C	-4. 27846200	0. 38322600	2. 65549800
H	-3. 50082200	2. 38838600	2. 50742600
H	-4. 72489800	-1. 71386900	2. 75963600
C	3. 19916000	1. 30947100	1. 04895000
H	3. 20074500	1. 50063800	2. 13042700
H	2. 32856900	1. 80329600	0. 60605200
C	4. 46046700	1. 82826000	0. 40599400
C	5. 59204800	2. 15796500	1. 15051000
C	4. 50434500	1. 94204100	-0. 98843600
C	6. 75293100	2. 59913100	0. 51681900
H	5. 56213200	2. 07824400	2. 23517000
C	5. 66146300	2. 38136400	-1. 62125900

H	3.61414400	1.68467000	-1.56087500
C	6.78936900	2.71063400	-0.86933500
H	7.62652700	2.85730500	1.10766200
H	5.68450600	2.47230600	-2.70302300
H	7.69197200	3.05564400	-1.36410600
C	-5.66775000	0.83086200	3.03171000
H	-6.01912500	1.62126600	2.36146000
H	-6.37796000	0.00157600	2.98618400
H	-5.68554800	1.23362700	4.05014900
C	-0.87227000	1.96513900	1.97132100
H	-0.03304800	1.70444100	2.62857200
H	-0.48653700	2.04527800	0.94787900
H	-1.23337000	2.95648300	2.25090400
C	-2.39452000	-2.87697500	2.06121600
H	-2.53178000	-3.16160600	1.01155600
H	-1.37033500	-3.12182100	2.35103000
H	-3.08276300	-3.45785400	2.68001700
C	-2.41401300	4.41686900	-0.08773900
C	-2.39743800	3.25436900	-0.85248200
C	-1.21706000	2.81331000	-1.46253400
C	-0.05109300	3.56198800	-1.28779800
C	-0.06471800	4.72512000	-0.51881400
C	-1.24414000	5.15647900	0.08316100
H	-3.34074800	4.74875300	0.37260600
H	-3.30709900	2.66732400	-0.97561000
H	0.87156800	3.20705800	-1.73668700
H	0.85051000	5.29602300	-0.39083200
H	-1.25352200	6.06447600	0.67885600
C	0.24747100	0.00364700	-0.83370700
O	1.19847000	0.73577900	-1.19811500
C	-1.21581300	0.30792200	-1.24820000
H	-1.76747700	0.60017500	-0.35063400
C	-1.22360900	1.50519900	-2.21679000
H	-0.35729000	1.43383400	-2.87873700
H	-2.13068900	1.45252300	-2.82825900
C	1.68098400	-2.27524700	-1.48355500
C	1.71409700	-3.48453200	-0.75882100
C	2.89765000	-4.19416800	-0.60377900
C	4.06470300	-3.68387900	-1.17747700
C	4.03459700	-2.49861500	-1.91516500
C	2.84333200	-1.79556100	-2.08811000
H	2.91409900	-5.13206500	-0.05727900
H	4.99641800	-4.22964900	-1.06687100
H	4.94599900	-2.12570300	-2.37216900

H	2.79228800	-0.87846800	-2.66551200
N	0.43907700	-1.66845600	-1.55641900
S	0.10005000	-3.91037800	-0.19382300
C	-0.55274600	-2.44451100	-1.01833700
N	-1.78827500	-2.11684500	-1.02457100
C	-1.97907100	-0.91347600	-1.83817100
H	-1.54395300	-1.08865300	-2.83425600
C	-3.44975600	-0.59693000	-1.99674400
C	-4.23232600	-0.33168800	-0.87179600
C	-4.04232300	-0.53301100	-3.25675400
C	-5.57794000	-0.00765100	-1.00111500
H	-3.77770700	-0.38948600	0.11104700
C	-5.39120600	-0.20659300	-3.39326200
H	-3.44196900	-0.74123500	-4.13934500
C	-6.16246900	0.05788000	-2.26578900
H	-6.17198200	0.18928200	-0.11226000
H	-5.83806000	-0.16077300	-4.38188300
H	-7.21309800	0.31135800	-2.37049800

TS6(SS)

C	0.24076000	-0.51922000	1.09925600
C	1.33764300	-0.94360700	2.94695400
C	2.68308700	-1.07703500	3.58780900
C	3.59785200	-1.18155300	2.33670400
C	2.86022600	-0.44215500	1.19572600
H	2.89705000	-0.18519300	4.18474600
H	2.74613900	-1.94596000	4.24313700
H	3.71367000	-2.23349400	2.06193600
H	2.97231400	-0.92116800	0.22469700
N	0.08651300	-1.05221500	3.29135100
N	-0.58781100	-0.78668100	2.12383900
N	1.46225500	-0.61710700	1.63314000
H	4.58952900	-0.75494200	2.49942000
C	-2.01989600	-0.64540500	2.18809700
C	-2.50817600	0.58577700	2.64138300
C	-2.84285500	-1.73314300	1.89292200
C	-3.88984300	0.73626500	2.72286700
C	-4.22029200	-1.52202600	1.97302900
C	-4.75885200	-0.29723300	2.36492200
H	-4.29705000	1.68743500	3.05673500
H	-4.88781300	-2.34283700	1.72440100
C	3.16861100	1.05717100	1.10425400
H	3.28887000	1.47270900	2.11321900
H	2.30939100	1.54186400	0.63171200

C	4. 39607800	1. 31692100	0. 27013100
C	5. 56178700	1. 84969900	0. 81734000
C	4. 35458400	1. 02187800	-1. 09857300
C	6. 67480600	2. 09330200	0. 01343400
H	5. 59546800	2. 08741200	1. 87805600
C	5. 46454000	1. 26496200	-1. 89932400
H	3. 43670300	0. 61075800	-1. 51621200
C	6. 62714600	1. 80216600	-1. 34561900
H	7. 57590900	2. 51245700	0. 45000700
H	5. 42331900	1. 03839500	-2. 96006900
H	7. 49132800	1. 99344300	-1. 97371000
C	-6. 24756300	-0. 07601000	2. 35403800
H	-6. 56150800	0. 27041300	1. 36305700
H	-6. 78975200	-0. 99925800	2. 56960500
H	-6. 54441900	0. 68043100	3. 08392900
C	-1. 56691100	1. 68976800	3. 04413200
H	-1. 02202500	1. 41371700	3. 95248800
H	-0. 82503600	1. 89992200	2. 26536000
H	-2. 11742700	2. 61191000	3. 23908800
C	-2. 27414500	-3. 07513500	1. 52511200
H	-3. 06535500	-3. 82551100	1. 48826300
H	-1. 78065600	-3. 03025100	0. 54934600
H	-1. 53322800	-3. 39360300	2. 26537100
C	0. 43004800	4. 43848100	0. 82723800
C	-0. 36210900	3. 52882000	0. 12929200
C	0. 15453900	2. 79914800	-0. 94587800
C	1. 47935400	3. 02833600	-1. 32479400
C	2. 27305200	3. 94537300	-0. 64092200
C	1. 75338700	4. 64700300	0. 44543600
H	0. 00978900	4. 99192200	1. 66216100
H	-1. 40427900	3. 38745300	0. 41321000
H	1. 89379200	2. 45340600	-2. 14716500
H	3. 30588100	4. 09202000	-0. 94409700
H	2. 37281700	5. 35595600	0. 98567600
C	0. 07602100	-0. 24427700	-0. 42483300
O	1. 18807400	0. 04222000	-0. 94503600
C	-1. 17056900	0. 63028000	-0. 78326100
H	-1. 58847600	1. 03805700	0. 14557700
C	-0. 71068200	1. 79762100	-1. 67239500
H	-0. 17289300	1. 38907500	-2. 53016000
H	-1. 60545200	2. 30661700	-2. 04693200
C	0. 62914000	-2. 82103900	-0. 84614600
C	1. 08850500	-3. 31412500	-2. 08215700
C	2. 10647600	-4. 25487900	-2. 15289300

C	2. 67767600	-4. 72313100	-0. 97030100
C	2. 19794600	-4. 28327600	0. 26126400
C	1. 16564400	-3. 34771800	0. 33067100
H	2. 44854700	-4. 62216000	-3. 11476900
H	3. 47839400	-5. 45353400	-1. 01323600
H	2. 60913600	-4. 69253800	1. 17909300
H	0. 75308600	-3. 06537600	1. 29489100
N	-0. 39838600	-1. 87422400	-0. 92461300
S	0. 15695700	-2. 64270900	-3. 41002000
C	-0. 80925200	-1. 69928400	-2. 24081700
N	-1. 72982600	-0. 90122900	-2. 60971300
C	-2. 29223500	-0. 20163600	-1. 46978900
H	-2. 63357100	-0. 93154200	-0. 71669400
C	-3. 48196000	0. 65084200	-1. 85836800
C	-3. 84508600	0. 84224800	-3. 19038600
C	-4. 23220200	1. 27157700	-0. 85570700
C	-4. 94007500	1. 64302500	-3. 51175000
H	-3. 26046700	0. 35117200	-3. 96006700
C	-5. 32306400	2. 07274900	-1. 17578900
H	-3. 95690800	1. 11947400	0. 18524400
C	-5. 68147900	2. 26124800	-2. 50958500
H	-5. 21388300	1. 78429300	-4. 55288900
H	-5. 89336500	2. 55126400	-0. 38440400
H	-6. 53268400	2. 88491800	-2. 76378800

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C	-0. 03230000	-1. 09462800	0. 76601200
C	0. 78823600	-1. 98588000	2. 59476800
C	2. 00584100	-2. 27745500	3. 40659300
C	3. 11152400	-2. 10433800	2. 33869800
C	2. 56810900	-1. 08172200	1. 30761100
H	2. 09868800	-1. 54724600	4. 21685300
H	1. 98089500	-3. 27384400	3. 84795400
H	3. 28037200	-3. 06023500	1. 83658700
H	2. 87163500	-1. 34344200	0. 29371400
N	-0. 48587200	-2. 21147500	2. 67812000
N	-0. 98486800	-1. 65450400	1. 52780300
N	1. 10914300	-1. 31304100	1. 44419600
H	4. 06053800	-1. 76607100	2. 75686100
C	-2. 38667200	-1. 85190200	1. 23305000
C	-3. 33075700	-0. 97159000	1. 76232200
C	-2. 73737800	-2. 99675800	0. 50865900
C	-4. 67436500	-1. 23754400	1. 50295300
C	-4. 09281700	-3. 22382400	0. 29247100

C	-5.07220700	-2.35651700	0.77765800
H	-5.42445300	-0.54222400	1.87312100
H	-4.39019500	-4.10341900	-0.27305400
C	2.94799000	0.36952800	1.62363200
H	2.58885800	0.62731000	2.62800400
H	2.45095600	1.03788200	0.91258100
C	4.44455200	0.55625800	1.53928600
C	5.20025400	0.86048300	2.67218300
C	5.09786900	0.39630200	0.31366600
C	6.58226800	1.01178700	2.58484800
H	4.70062800	0.99056800	3.62925400
C	6.47768600	0.54388700	0.22505500
H	4.52130200	0.16477100	-0.57965500
C	7.22380200	0.85289200	1.36056900
H	7.15547000	1.25661200	3.47332100
H	6.96985200	0.42217100	-0.73447500
H	8.30007600	0.97214900	1.28969100
C	-6.53437300	-2.62316000	0.53647500
H	-7.04602200	-1.70511200	0.23450600
H	-6.67818000	-3.37145200	-0.24628100
H	-7.01946000	-2.99066500	1.44654000
C	-2.96627700	0.22573900	2.59826700
H	-3.30371600	1.14299800	2.10421900
H	-3.45669400	0.16819900	3.57405400
H	-1.88981300	0.30099500	2.76953800
C	-1.69424000	-3.93286400	-0.03157500
H	-1.21375200	-3.44669900	-0.88636700
H	-0.93057000	-4.15423600	0.72198500
H	-2.14725300	-4.87512100	-0.34501500
C	-5.24026500	-0.34431600	-1.77155600
C	-3.87143400	-0.14537800	-1.92997800
C	-3.28393800	1.05833000	-1.53519100
C	-4.07959800	2.03698800	-0.92982800
C	-5.44529900	1.82840500	-0.75309400
C	-6.03258700	0.64182200	-1.18790900
H	-5.68881700	-1.28018900	-2.09565100
H	-3.23117900	-0.92181600	-2.33905300
H	-3.62263200	2.97191500	-0.60557500
H	-6.05428400	2.60101000	-0.29259000
H	-7.10248700	0.48938200	-1.07395100
C	-0.31925100	-0.47239000	-0.64904300
O	-0.91651000	-1.33285600	-1.38661900
C	-1.03795800	0.89822000	-0.42081500
H	-1.77344300	0.72475600	0.37051100

C	-1.80052700	1.28287600	-1.70324300
H	-1.61541200	2.33321500	-1.94468500
H	-1.42980300	0.67200700	-2.53021800
C	1.84270400	-1.02219600	-1.94407300
C	2.83104700	-0.43066600	-2.74773800
C	3.70476700	-1.20275500	-3.50132400
C	3.58242800	-2.59027100	-3.45685400
C	2.60014100	-3.18197600	-2.66483800
C	1.72516300	-2.41226800	-1.90110900
H	4.46388300	-0.73024800	-4.11619900
H	4.25263300	-3.20747700	-4.04521500
H	2.50573000	-4.26279400	-2.64385700
H	0.93830800	-2.86427700	-1.31030000
N	1.11715300	-0.10268400	-1.18687900
S	2.78591900	1.32438100	-2.62125000
C	1.46290900	1.21589700	-1.42671600
N	0.98271900	2.26147900	-0.88208300
C	-0.07234100	1.99272600	0.08137600
H	0.38196300	1.61423500	1.01863100
C	-0.82300100	3.26210400	0.42886400
C	-0.89015600	4.33175400	-0.46462400
C	-1.52715500	3.34565400	1.63097900
C	-1.68292900	5.44100300	-0.17806400
H	-0.30643300	4.28254200	-1.37817900
C	-2.32008100	4.45141700	1.92076300
H	-1.44925700	2.53485100	2.35036100
C	-2.40863500	5.50075400	1.00883700
H	-1.73235000	6.26292300	-0.88561300
H	-2.86292100	4.49701100	2.85999300
H	-3.02726300	6.36483000	1.22944300

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C	-0.33704800	0.86132700	0.84908100
C	0.44840700	2.90506100	0.76108200
C	1.63635200	3.77452500	0.52866000
C	2.77670500	2.77905400	0.83785000
C	2.24142100	1.37579600	0.45189000
H	1.64975900	4.09190800	-0.52000500
H	1.64141500	4.66081200	1.16264000
H	2.99468000	2.80137900	1.90878800
H	2.58172300	0.61617900	1.15706000
N	-0.80551000	3.06608000	1.04801400
N	-1.28636600	1.78107000	1.11670000
N	0.78198200	1.57926500	0.65983700

H	3.69679000	3.00350400	0.29641800
C	-2.61608000	1.59241500	1.66062700
C	-3.74044900	1.84925700	0.87126900
C	-2.71425400	1.28984600	3.02612400
C	-4.99471200	1.69035100	1.46457900
C	-3.98891300	1.14698900	3.56509300
C	-5.14025000	1.31790000	2.79759500
H	-5.87994500	1.87977900	0.86161300
H	-4.08217000	0.90180100	4.62020600
C	2.58019900	0.97099600	-0.98238600
H	2.16889100	1.71097100	-1.67820700
H	2.09571400	0.01890300	-1.20692100
C	4.07185700	0.84177400	-1.17039300
C	4.75004500	1.65812400	-2.07625800
C	4.79922000	-0.09637800	-0.43076500
C	6.12824200	1.54286700	-2.24419700
H	4.18605700	2.38054400	-2.66221900
C	6.17556700	-0.20964200	-0.59377600
H	4.28379000	-0.75099500	0.27044600
C	6.84430300	0.60986100	-1.50067600
H	6.64095600	2.18086800	-2.95724400
H	6.72632600	-0.94493800	-0.01565700
H	7.91787600	0.51752600	-1.63010700
C	-6.50403300	1.11067800	3.40158400
H	-7.27188400	1.65547400	2.84785300
H	-6.77170600	0.04925900	3.38646800
H	-6.52900400	1.44147300	4.44274400
C	-3.66461100	2.30929400	-0.56090600
H	-4.58671100	2.82962600	-0.82767400
H	-2.83270700	3.00030900	-0.71739000
H	-3.55823600	1.46588400	-1.25291000
C	-1.50280100	1.11965100	3.89822700
H	-1.12867800	0.10093600	3.76364600
H	-0.70861000	1.82196100	3.62234100
H	-1.75992800	1.29371800	4.94479800
C	-5.78009800	-1.31479700	-1.67453400
C	-4.66648200	-1.35135600	-0.84277900
C	-3.59811700	-2.21632900	-1.10875800
C	-3.68070200	-3.05026000	-2.22526300
C	-4.79766700	-3.02049100	-3.05891400
C	-5.84923700	-2.15121000	-2.78796200
H	-6.60038700	-0.63891400	-1.44978700
H	-4.61877200	-0.70815400	0.03493300
H	-2.85776400	-3.72782500	-2.44068100

H	-4.84347500	-3.67755900	-3.92198100
H	-6.71936400	-2.12713100	-3.43627100
C	-0.63870600	-0.68302400	0.81118700
O	-1.14193100	-1.04682400	1.93359400
C	-1.52883400	-0.93557700	-0.47073100
H	-2.23089000	-0.09547400	-0.52493700
C	-2.38120900	-2.19479000	-0.22027700
H	-1.77004100	-3.08902300	-0.38584200
H	-2.66550100	-2.17709000	0.83452400
C	1.59985600	-1.68427500	1.55030800
C	2.57024600	-2.63355500	1.19125900
C	3.57004100	-3.01507500	2.07597200
C	3.59700900	-2.44321100	3.34649100
C	2.63150300	-1.50705400	3.71136000
C	1.62759000	-1.11900000	2.82614300
H	4.31294000	-3.74830200	1.77854800
H	4.36882600	-2.73425600	4.05070800
H	2.65172700	-1.07435500	4.70634800
H	0.85671800	-0.41717300	3.11702500
N	0.73267800	-1.35296000	0.50860300
S	2.33975500	-3.18354000	-0.46096200
C	0.93044100	-2.09844400	-0.64482400
N	0.29215300	-2.06359700	-1.74325000
C	-0.78256600	-1.07156200	-1.81284700
H	-1.52141200	-1.47702400	-2.51805300
C	-0.24678700	0.19292400	-2.49334700
C	0.68193300	0.04640300	-3.53398500
C	-0.67108500	1.48199500	-2.17717000
C	1.17881300	1.15284200	-4.21230000
H	1.02594200	-0.95156000	-3.78472600
C	-0.17409100	2.59855000	-2.85229500
H	-1.40501600	1.63048900	-1.39860400
C	0.75724000	2.43979600	-3.87249000
H	1.90241800	1.01177200	-5.00934500
H	-0.52896300	3.58910000	-2.57865800
H	1.14430600	3.30350100	-4.40440200

6(SR)

C	0.44475100	-0.49314400	0.70429600
C	1.57719200	-1.02464900	2.51171700
C	2.92783300	-1.14709900	3.14510200
C	3.85479100	-1.00850800	1.90757500
C	3.05172200	-0.19845400	0.86957500
H	3.07085600	-0.33814700	3.86764900

H	3.05232800	-2.09430400	3.67106000
H	4.06661800	-1.99957000	1.49506800
H	3.27680000	-0.47205100	-0.15398200
N	0.33704300	-1.12608600	2.88069300
N	-0.36585700	-0.79407800	1.74130500
N	1.68072300	-0.62950300	1.21154900
H	4.80292500	-0.51789900	2.13706600
C	-1.74551600	-0.42090300	1.95848600
C	-1.98603300	0.95372400	2.11666600
C	-2.72165600	-1.39179000	2.16944600
C	-3.28984800	1.34978600	2.39269300
C	-4.00615300	-0.93947600	2.49027900
C	-4.31196500	0.41485100	2.58765300
H	-3.50471700	2.41162200	2.48707500
H	-4.78795300	-1.67768100	2.65101500
C	3.15580200	1.32535600	1.03467900
H	3.17459400	1.58872400	2.10041200
H	2.26326300	1.76181700	0.57571400
C	4.38572300	1.83572400	0.32893800
C	5.52470700	2.24415100	1.02075100
C	4.38928100	1.86086200	-1.07091800
C	6.65512000	2.67741500	0.32933200
H	5.52394100	2.23304000	2.10842800
C	5.51649700	2.29303300	-1.75999800
H	3.49078500	1.53920300	-1.59688800
C	6.65253400	2.70175400	-1.06123100
H	7.53546100	2.99629900	0.87864500
H	5.51014900	2.31621200	-2.84530400
H	7.53132300	3.03981100	-1.60116600
C	-5.70457900	0.87498500	2.93357400
H	-6.43666400	0.08023700	2.77461300
H	-5.76220800	1.17876200	3.98383600
H	-5.99406600	1.73743500	2.32717900
C	-0.86092000	1.95226200	2.03433400
H	-0.06143700	1.67827700	2.73332500
H	-0.42507200	2.01407500	1.03010600
H	-1.21483100	2.95168800	2.28964700
C	-2.44658200	-2.86090200	2.02896200
H	-2.64402000	-3.15953300	0.99360000
H	-1.40864700	-3.10280500	2.26397900
H	-3.09915700	-3.43384100	2.69126500
C	-2.11673300	4.46882200	-0.06809200
C	-2.15449000	3.31568200	-0.84656100
C	-0.98483700	2.79169400	-1.40827600

C	0.22681700	3.44410700	-1.16838200
C	0.26715200	4.59640800	-0.38457800
C	-0.90290900	5.11332400	0.16676500
H	-3.03530400	4.86710300	0.35371400
H	-3.09919600	2.80156500	-1.01926200
H	1.13773300	3.01798900	-1.57782200
H	1.21731100	5.09143700	-0.20623800
H	-0.87097800	6.01319100	0.77333600
C	0.30400600	-0.17901900	-0.86031900
O	1.30322600	0.53254300	-1.21784000
C	-1.14144900	0.28201900	-1.25271500
H	-1.67580700	0.58520900	-0.34898100
C	-1.05291200	1.50155700	-2.18829400
H	-0.17198100	1.39067000	-2.82414800
H	-1.94451100	1.52177300	-2.82336100
C	1.62216700	-2.37880000	-1.37028500
C	1.54085300	-3.64564800	-0.76758800
C	2.66690200	-4.44653700	-0.63029500
C	3.88809500	-3.97143800	-1.10938400
C	3.96566500	-2.73068500	-1.74351600
C	2.83300300	-1.93343000	-1.89710900
H	2.59400700	-5.42668300	-0.17059200
H	4.77627000	-4.58699000	-1.01181200
H	4.91573000	-2.38472000	-2.13776100
H	2.86135900	-0.97162200	-2.39544200
N	0.40628800	-1.69578800	-1.43259400
S	-0.12053100	-4.03135500	-0.31710100
C	-0.66232500	-2.47297600	-1.02502000
N	-1.87711100	-2.10283800	-1.10949500
C	-1.97714400	-0.85937700	-1.88564100
H	-1.54006500	-1.04567800	-2.87980700
C	-3.42118100	-0.44707900	-2.05665900
C	-4.20417000	-0.18829000	-0.93120000
C	-3.98385200	-0.28240700	-3.32090400
C	-5.52250400	0.23092700	-1.06422600
H	-3.77083600	-0.32682500	0.05292700
C	-5.30556000	0.13923600	-3.46042000
H	-3.38224100	-0.48655300	-4.20330900
C	-6.07765800	0.39818600	-2.33265000
H	-6.11708500	0.42538400	-0.17553200
H	-5.73093500	0.26407600	-4.45132900
H	-7.10650100	0.72714400	-2.44017100

6(SS)

C	0.15708700	-0.81956600	1.14748100
C	1.12357500	-1.32451200	3.05725900
C	2.41166400	-1.53363500	3.78519400
C	3.39603400	-1.72620400	2.60241400
C	2.77737500	-0.99431200	1.38486500
H	2.64643000	-0.64337200	4.37671100
H	2.37407900	-2.38833600	4.46075600
H	3.48583600	-2.79268900	2.38047000
H	2.89234500	-1.54210000	0.45343600
N	-0.14584400	-1.33938600	3.33690200
N	-0.73232600	-1.02936400	2.13636400
N	1.34341400	-1.02001600	1.74755100
H	4.39501900	-1.34100600	2.81546600
C	-2.15066100	-0.80954500	2.09274200
C	-2.60783600	0.40893100	2.61944000
C	-2.99205800	-1.74504500	1.49560900
C	-3.95002100	0.71732800	2.44916200
C	-4.33263700	-1.37668700	1.33772900
C	-4.81969700	-0.15078700	1.77800600
H	-4.32298700	1.67163900	2.81270700
H	-5.00435800	-2.07103100	0.83912500
C	3.27453000	0.43985200	1.18917500
H	3.34159800	0.95072600	2.15808600
H	2.55011800	0.96349200	0.55666400
C	4.61364200	0.42895900	0.49497900
C	5.75211500	0.98180600	1.07700200
C	4.70683100	-0.13613300	-0.78332400
C	6.96826900	0.98301300	0.39444400
H	5.68383900	1.43039900	2.06511800
C	5.91948300	-0.14022600	-1.46193600
H	3.80557200	-0.53683400	-1.24523100
C	7.05426300	0.42175100	-0.87508500
H	7.84641000	1.42368800	0.85593700
H	5.97996700	-0.57337000	-2.45547100
H	7.99974900	0.42227700	-1.40790900
C	-6.24324300	0.26226100	1.51591000
H	-6.27384200	0.99821000	0.70610600
H	-6.85773100	-0.59021700	1.22059200
H	-6.69083000	0.72347500	2.39999600
C	-1.66299400	1.36149000	3.30367500
H	-1.28217100	0.93201700	4.23451100
H	-0.79501500	1.58868500	2.67267100
H	-2.16943100	2.30041600	3.53448000
C	-2.53153800	-3.10183700	1.03621100

H	-3.05099200	-3.87531300	1.60980800
H	-2.76926900	-3.25324900	-0.02105300
H	-1.45800600	-3.24820300	1.16097200
C	2.18150600	4.39648500	-0.22901100
C	1.09229200	3.62830400	-0.62796900
C	1.26579600	2.50069200	-1.43904000
C	2.55687200	2.17208900	-1.85286900
C	3.65089900	2.94088400	-1.45970000
C	3.46757400	4.05176600	-0.64137900
H	2.02689700	5.26789200	0.40049300
H	0.08636900	3.90349400	-0.31350400
H	2.69868900	1.28351300	-2.46040100
H	4.65094200	2.65305700	-1.77220400
H	4.32067700	4.64521100	-0.32764800
C	0.11553200	-0.43607900	-0.42237600
O	1.31839300	-0.53164500	-0.85955500
C	-0.58202500	0.96361700	-0.61703400
H	-0.35666900	1.55528000	0.28050700
C	0.06836300	1.66625200	-1.82863700
H	0.36292400	0.91520900	-2.56435400
H	-0.67963700	2.31828200	-2.29240600
C	-0.33317300	-2.76477400	-1.36077200
C	-1.04824400	-3.41814800	-2.37654600
C	-0.72673000	-4.70750600	-2.77572100
C	0.33304600	-5.36095000	-2.15019700
C	1.04973100	-4.71907700	-1.14308900
C	0.72780800	-3.42459500	-0.74179900
H	-1.29258900	-5.19344600	-3.56368200
H	0.59874200	-6.36790200	-2.45262400
H	1.87909800	-5.22917400	-0.66407400
H	1.30419200	-2.92686500	0.02602800
N	-0.83550200	-1.50066300	-1.04350300
S	-2.33876800	-2.40016400	-2.99930000
C	-1.88420700	-1.09997400	-1.86243000
N	-2.51566600	0.00074800	-1.84540100
C	-2.11876100	0.87891400	-0.75786100
H	-2.51787800	0.44627800	0.16384400
C	-2.76227900	2.24643100	-0.88688800
C	-3.46451000	2.62040300	-2.03190100
C	-2.66128300	3.15925000	0.16827900
C	-4.04425800	3.88482400	-2.12293400
H	-3.55106200	1.90226500	-2.83960900
C	-3.23859900	4.42169000	0.07888700
H	-2.12263700	2.87646900	1.07057600

C	-3.93325600	4.78963700	-1.07192500
H	-4.58481100	4.16336400	-3.02243700
H	-3.14835000	5.11810300	0.90713900
H	-4.38426300	5.77400700	-1.14597600

TS7(RR)

C	-0.39858000	-1.44875000	-0.08639500
C	-1.59501000	-3.17698400	-0.81817800
C	-2.95772400	-3.68588200	-1.15678100
C	-3.85254300	-2.65812900	-0.42115400
C	-3.01914900	-1.35623600	-0.30554600
H	-3.10534300	-3.65702000	-2.24109500
H	-3.11854700	-4.71132600	-0.82256900
H	-4.07318100	-3.02604300	0.58408500
H	-3.20565900	-0.85572100	0.64618600
N	-0.37168800	-3.59515000	-0.90625200
N	0.34742400	-2.51307800	-0.44072600
N	-1.65176000	-1.90092700	-0.31907400
H	-4.79943700	-2.47536700	-0.93131900
C	1.78206200	-2.58090900	-0.43055600
C	2.46156900	-2.20189100	-1.59318900
C	2.43684700	-3.02827300	0.71726700
C	3.85268600	-2.18763700	-1.55170000
C	3.83290100	-2.99673600	0.70746700
C	4.55353600	-2.55589600	-0.40061900
H	4.40358700	-1.88043800	-2.43827700
H	4.36835300	-3.32365700	1.59595100
C	-3.21192500	-0.38144000	-1.47519100
H	-2.88507700	-0.87410200	-2.39965100
H	-2.55072800	0.48233900	-1.32473700
C	-4.64926200	0.06115100	-1.61600500
C	-5.34320400	-0.15289300	-2.80771700
C	-5.32070700	0.66466900	-0.54779200
C	-6.67340300	0.23823400	-2.94020200
H	-4.83313300	-0.62540000	-3.64349000
C	-6.65039700	1.05152600	-0.67587100
H	-4.80109300	0.83661600	0.39140100
C	-7.33092000	0.84189600	-1.87315500
H	-7.19415000	0.06900100	-3.87731000
H	-7.15556100	1.52102200	0.16248900
H	-8.36748300	1.14726200	-1.97251400
C	6.05585600	-2.46667600	-0.36929600
H	6.49487600	-2.85978800	-1.29029800
H	6.36566200	-1.42112100	-0.26743300

H	6.46974600	-3.02313200	0.47487100
C	1.70793600	-1.85098600	-2.84927000
H	1.00603700	-1.02700700	-2.68686600
H	2.39672000	-1.55307000	-3.64189600
H	1.12500700	-2.71030700	-3.19519800
C	1.66698400	-3.53969600	1.90341200
H	1.13514700	-2.71627300	2.38731600
H	0.93364200	-4.28817400	1.58755500
H	2.34399600	-4.00245000	2.62410900
C	5.35952300	0.14327100	1.90859400
C	3.98692000	0.36387200	1.91277100
C	3.45258800	1.53499500	1.36617600
C	4.31657100	2.47577400	0.80690900
C	5.69236500	2.25517900	0.79832000
C	6.21841800	1.09151800	1.35194100
H	5.76166100	-0.77091000	2.33752700
H	3.30394400	-0.37525400	2.32924900
H	3.90455600	3.37214500	0.34805400
H	6.35261400	2.99304400	0.35249500
H	7.29099700	0.92103000	1.34901100
C	0.18253000	-0.03824600	1.19818300
O	0.47684500	-0.66804900	2.22321200
C	1.26433900	0.69919200	0.40488300
H	1.99486600	-0.06400700	0.12364300
C	1.95358300	1.71642800	1.35520300
H	1.69479200	2.73764100	1.05676600
H	1.57361800	1.56098800	2.36995100
C	-2.03835500	0.67143800	2.22057300
C	-2.98357900	1.70774300	2.13935000
C	-4.08584000	1.74682100	2.98215500
C	-4.24679400	0.73240900	3.92406700
C	-3.31335500	-0.29859800	4.00479300
C	-2.20517200	-0.34799600	3.15977700
H	-4.80593400	2.55517200	2.90326800
H	-5.10091600	0.74991300	4.59204600
H	-3.44351100	-1.08370900	4.74235000
H	-1.46644400	-1.13426100	3.22598300
N	-1.04277200	0.78153500	1.24483300
S	-2.59948200	2.84347300	0.85195800
C	-1.16668300	1.88583800	0.40221000
N	-0.42994200	2.23222400	-0.56909600
C	0.71192400	1.37268500	-0.86188700
H	0.35725000	0.58054400	-1.53872300
C	1.80204000	2.14779500	-1.58359800

C	1. 73054100	3. 53092700	-1. 74229500
C	2. 93031000	1. 47034200	-2. 05401900
C	2. 77484700	4. 22527100	-2. 35251800
H	0. 84868700	4. 05062500	-1. 38429200
C	3. 97070200	2. 16151900	-2. 66311700
H	3. 01471200	0. 39610300	-1. 90685700
C	3. 89795700	3. 54518600	-2. 81266400
H	2. 70754100	5. 30306700	-2. 46679200
H	4. 84720100	1. 62058300	-3. 00710100
H	4. 71150000	4. 08710300	-3. 28473900

TS7(RS)

C	-0. 19413100	-0. 31885300	-1. 20599400
C	-1. 36976500	0. 08459100	-3. 04903400
C	-2. 72015900	0. 34575800	-3. 62921800
C	-3. 63735300	-0. 13737900	-2. 47976400
C	-2. 81170400	0. 00751600	-1. 17650100
H	-2. 83962200	1. 41562100	-3. 82719700
H	-2. 88534700	-0. 19052800	-4. 56421400
H	-3. 87712800	-1. 19386100	-2. 62670200
H	-3. 03004500	-0. 80750400	-0. 48725000
N	-0. 14507600	0. 04842400	-3. 46920000
N	0. 56143800	-0. 20978200	-2. 31663700
N	-1. 44196500	-0. 14232700	-1. 69811800
H	-4. 57249800	0. 42092600	-2. 41884700
C	1. 99710500	-0. 22262600	-2. 36225800
C	2. 63468700	1. 01827600	-2. 23228000
C	2. 69302500	-1. 41847800	-2. 53754600
C	4. 02294100	1. 02606300	-2. 14415100
C	4. 08731800	-1. 35385100	-2. 45565700
C	4. 76243300	-0. 15597400	-2. 23169000
H	4. 53600100	1. 97549500	-2. 01028900
H	4. 65635000	-2. 27456100	-2. 56960500
C	-2. 95599600	1. 36458900	-0. 48302100
H	-2. 58713200	2. 14616000	-1. 16033400
H	-2. 28930000	1. 37013400	0. 38906100
C	-4. 37137700	1. 69196200	-0. 06269300
C	-4. 81098800	3. 01690700	-0. 10435200
C	-5. 26165300	0. 70866400	0. 38165000
C	-6. 09771500	3. 35944100	0. 29966300
H	-4. 13128400	3. 78988400	-0. 45436800
C	-6. 55179400	1. 04750900	0. 77922500
H	-4. 95224700	-0. 33294300	0. 42212100
C	-6. 97417900	2. 37328100	0. 74246300

H	-6.41659000	4.39629500	0.26276000
H	-7.22903100	0.27054600	1.12006400
H	-7.98020100	2.63533500	1.05343000
C	6.26625100	-0.12966300	-2.13147700
H	6.60469700	0.71767400	-1.52993100
H	6.64726800	-1.04933500	-1.67899900
H	6.72292400	-0.03602000	-3.12232100
C	1.83032000	2.28916700	-2.24447000
H	1.25455800	2.35360900	-3.17321100
H	1.12601500	2.33147000	-1.40768100
H	2.48411300	3.15866800	-2.17528500
C	2.01999700	-2.72404500	-2.86341300
H	2.19143500	-3.45029900	-2.06798400
H	0.94133100	-2.60768800	-2.96408500
H	2.42647600	-3.11370100	-3.80179700
C	5.80603900	-0.32287800	1.66581200
C	4.59989000	-0.92543500	1.32633700
C	3.57321400	-1.05784600	2.26949800
C	3.79318600	-0.58291300	3.56321800
C	5.00052100	0.02339600	3.90735400
C	6.00893000	0.15809100	2.95934900
H	6.59167600	-0.23002100	0.92156300
H	4.43658400	-1.28903300	0.31333400
H	3.00958300	-0.68944000	4.30956100
H	5.15008200	0.39146700	4.91754300
H	6.94875500	0.63138700	3.22525600
C	0.37468700	-1.44609100	0.22611800
O	0.71900400	-2.48360300	-0.37371600
C	1.45195800	-0.63898400	0.97713900
H	2.13049500	-0.27045800	0.20116500
C	2.24914600	-1.64086400	1.84511400
H	1.65365000	-1.92089500	2.72291100
H	2.40665900	-2.54224000	1.24725200
C	-1.88500600	-2.46016900	0.82671000
C	-3.02172000	-2.17195900	1.60534900
C	-4.17669500	-2.93508800	1.50847100
C	-4.19905300	-4.00995400	0.62085000
C	-3.07603500	-4.29733400	-0.15120500
C	-1.91132100	-3.53498000	-0.06319000
H	-5.04347000	-2.69248400	2.11548000
H	-5.09234200	-4.61935900	0.53704900
H	-3.09852300	-5.13682300	-0.83847500
H	-1.03236500	-3.75126800	-0.65320300
N	-0.85627300	-1.53352100	1.02838300

S	-2.78911500	-0.73793300	2.59659600
C	-1.15335400	-0.51081500	1.91815400
N	-0.44715700	0.48213400	2.25904100
C	0.94281400	0.55389700	1.83230200
H	1.51861800	0.51729600	2.76851200
C	1.26875500	1.92922700	1.26792900
C	0.29190800	2.90854400	1.09097000
C	2.60754800	2.25850300	1.02190000
C	0.64133500	4.18856300	0.65922500
H	-0.73824700	2.67086900	1.33288500
C	2.95608800	3.53777800	0.60540800
H	3.38325600	1.51041300	1.17554000
C	1.97262800	4.50919000	0.41847600
H	-0.13081600	4.94083200	0.52807400
H	4.00065900	3.77869100	0.42945200
H	2.24569800	5.50853900	0.09407700

TS7(SR)

C	-0.19413100	-0.31885300	-1.20599400
C	-1.36976500	0.08459100	-3.04903400
C	-2.72015900	0.34575800	-3.62921800
C	-3.63735300	-0.13737900	-2.47976400
C	-2.81170400	0.00751600	-1.17650100
H	-2.83962200	1.41562100	-3.82719700
H	-2.88534700	-0.19052800	-4.56421400
H	-3.87712800	-1.19386100	-2.62670200
H	-3.03004500	-0.80750400	-0.48725000
N	-0.14507600	0.04842400	-3.46920000
N	0.56143800	-0.20978200	-2.31663700
N	-1.44196500	-0.14232700	-1.69811800
H	-4.57249800	0.42092600	-2.41884700
C	1.99710500	-0.22262600	-2.36225800
C	2.63468700	1.01827600	-2.23228000
C	2.69302500	-1.41847800	-2.53754600
C	4.02294100	1.02606300	-2.14415100
C	4.08731800	-1.35385100	-2.45565700
C	4.76243300	-0.15597400	-2.23169000
H	4.53600100	1.97549500	-2.01028900
H	4.65635000	-2.27456100	-2.56960500
C	-2.95599600	1.36458900	-0.48302100
H	-2.58713200	2.14616000	-1.16033400
H	-2.28930000	1.37013400	0.38906100
C	-4.37137700	1.69196200	-0.06269300
C	-4.81098800	3.01690700	-0.10435200

C	-5.26165300	0.70866400	0.38165000
C	-6.09771500	3.35944100	0.29966300
H	-4.13128400	3.78988400	-0.45436800
C	-6.55179400	1.04750900	0.77922500
H	-4.95224700	-0.33294300	0.42212100
C	-6.97417900	2.37328100	0.74246300
H	-6.41659000	4.39629500	0.26276000
H	-7.22903100	0.27054600	1.12006400
H	-7.98020100	2.63533500	1.05343000
C	6.26625100	-0.12966300	-2.13147700
H	6.60469700	0.71767400	-1.52993100
H	6.64726800	-1.04933500	-1.67899900
H	6.72292400	-0.03602000	-3.12232100
C	1.83032000	2.28916700	-2.24447000
H	1.25455800	2.35360900	-3.17321100
H	1.12601500	2.33147000	-1.40768100
H	2.48411300	3.15866800	-2.17528500
C	2.01999700	-2.72404500	-2.86341300
H	2.19143500	-3.45029900	-2.06798400
H	0.94133100	-2.60768800	-2.96408500
H	2.42647600	-3.11370100	-3.80179700
C	5.80603900	-0.32287800	1.66581200
C	4.59989000	-0.92543500	1.32633700
C	3.57321400	-1.05784600	2.26949800
C	3.79318600	-0.58291300	3.56321800
C	5.00052100	0.02339600	3.90735400
C	6.00893000	0.15809100	2.95934900
H	6.59167600	-0.23002100	0.92156300
H	4.43658400	-1.28903300	0.31333400
H	3.00958300	-0.68944000	4.30956100
H	5.15008200	0.39146700	4.91754300
H	6.94875500	0.63138700	3.22525600
C	0.37468700	-1.44609100	0.22611800
O	0.71900400	-2.48360300	-0.37371600
C	1.45195800	-0.63898400	0.97713900
H	2.13049500	-0.27045800	0.20116500
C	2.24914600	-1.64086400	1.84511400
H	1.65365000	-1.92089500	2.72291100
H	2.40665900	-2.54224000	1.24725200
C	-1.88500600	-2.46016900	0.82671000
C	-3.02172000	-2.17195900	1.60534900
C	-4.17669500	-2.93508800	1.50847100
C	-4.19905300	-4.00995400	0.62085000
C	-3.07603500	-4.29733400	-0.15120500

C	-1.91132100	-3.53498000	-0.06319000
H	-5.04347000	-2.69248400	2.11548000
H	-5.09234200	-4.61935900	0.53704900
H	-3.09852300	-5.13682300	-0.83847500
H	-1.03236500	-3.75126800	-0.65320300
N	-0.85627300	-1.53352100	1.02838300
S	-2.78911500	-0.73793300	2.59659600
C	-1.15335400	-0.51081500	1.91815400
N	-0.44715700	0.48213400	2.25904100
C	0.94281400	0.55389700	1.83230200
H	1.51861800	0.51729600	2.76851200
C	1.26875500	1.92922700	1.26792900
C	0.29190800	2.90854400	1.09097000
C	2.60754800	2.25850300	1.02190000
C	0.64133500	4.18856300	0.65922500
H	-0.73824700	2.67086900	1.33288500
C	2.95608800	3.53777800	0.60540800
H	3.38325600	1.51041300	1.17554000
C	1.97262800	4.50919000	0.41847600
H	-0.13081600	4.94083200	0.52807400
H	4.00065900	3.77869100	0.42945200
H	2.24569800	5.50853900	0.09407700

TS7(SS)

C	-0.19413100	-0.31885300	-1.20599400
C	-1.36976500	0.08459100	-3.04903400
C	-2.72015900	0.34575800	-3.62921800
C	-3.63735300	-0.13737900	-2.47976400
C	-2.81170400	0.00751600	-1.17650100
H	-2.83962200	1.41562100	-3.82719700
H	-2.88534700	-0.19052800	-4.56421400
H	-3.87712800	-1.19386100	-2.62670200
H	-3.03004500	-0.80750400	-0.48725000
N	-0.14507600	0.04842400	-3.46920000
N	0.56143800	-0.20978200	-2.31663700
N	-1.44196500	-0.14232700	-1.69811800
H	-4.57249800	0.42092600	-2.41884700
C	1.99710500	-0.22262600	-2.36225800
C	2.63468700	1.01827600	-2.23228000
C	2.69302500	-1.41847800	-2.53754600
C	4.02294100	1.02606300	-2.14415100
C	4.08731800	-1.35385100	-2.45565700
C	4.76243300	-0.15597400	-2.23169000
H	4.53600100	1.97549500	-2.01028900

H	4.65635000	-2.27456100	-2.56960500
C	-2.95599600	1.36458900	-0.48302100
H	-2.58713200	2.14616000	-1.16033400
H	-2.28930000	1.37013400	0.38906100
C	-4.37137700	1.69196200	-0.06269300
C	-4.81098800	3.01690700	-0.10435200
C	-5.26165300	0.70866400	0.38165000
C	-6.09771500	3.35944100	0.29966300
H	-4.13128400	3.78988400	-0.45436800
C	-6.55179400	1.04750900	0.77922500
H	-4.95224700	-0.33294300	0.42212100
C	-6.97417900	2.37328100	0.74246300
H	-6.41659000	4.39629500	0.26276000
H	-7.22903100	0.27054600	1.12006400
H	-7.98020100	2.63533500	1.05343000
C	6.26625100	-0.12966300	-2.13147700
H	6.60469700	0.71767400	-1.52993100
H	6.64726800	-1.04933500	-1.67899900
H	6.72292400	-0.03602000	-3.12232100
C	1.83032000	2.28916700	-2.24447000
H	1.25455800	2.35360900	-3.17321100
H	1.12601500	2.33147000	-1.40768100
H	2.48411300	3.15866800	-2.17528500
C	2.01999700	-2.72404500	-2.86341300
H	2.19143500	-3.45029900	-2.06798400
H	0.94133100	-2.60768800	-2.96408500
H	2.42647600	-3.11370100	-3.80179700
C	5.80603900	-0.32287800	1.66581200
C	4.59989000	-0.92543500	1.32633700
C	3.57321400	-1.05784600	2.26949800
C	3.79318600	-0.58291300	3.56321800
C	5.00052100	0.02339600	3.90735400
C	6.00893000	0.15809100	2.95934900
H	6.59167600	-0.23002100	0.92156300
H	4.43658400	-1.28903300	0.31333400
H	3.00958300	-0.68944000	4.30956100
H	5.15008200	0.39146700	4.91754300
H	6.94875500	0.63138700	3.22525600
C	0.37468700	-1.44609100	0.22611800
O	0.71900400	-2.48360300	-0.37371600
C	1.45195800	-0.63898400	0.97713900
H	2.13049500	-0.27045800	0.20116500
C	2.24914600	-1.64086400	1.84511400
H	1.65365000	-1.92089500	2.72291100

H	2.40665900	-2.54224000	1.24725200
C	-1.88500600	-2.46016900	0.82671000
C	-3.02172000	-2.17195900	1.60534900
C	-4.17669500	-2.93508800	1.50847100
C	-4.19905300	-4.00995400	0.62085000
C	-3.07603500	-4.29733400	-0.15120500
C	-1.91132100	-3.53498000	-0.06319000
H	-5.04347000	-2.69248400	2.11548000
H	-5.09234200	-4.61935900	0.53704900
H	-3.09852300	-5.13682300	-0.83847500
H	-1.03236500	-3.75126800	-0.65320300
N	-0.85627300	-1.53352100	1.02838300
S	-2.78911500	-0.73793300	2.59659600
C	-1.15335400	-0.51081500	1.91815400
N	-0.44715700	0.48213400	2.25904100
C	0.94281400	0.55389700	1.83230200
H	1.51861800	0.51729600	2.76851200
C	1.26875500	1.92922700	1.26792900
C	0.29190800	2.90854400	1.09097000
C	2.60754800	2.25850300	1.02190000
C	0.64133500	4.18856300	0.65922500
H	-0.73824700	2.67086900	1.33288500
C	2.95608800	3.53777800	0.60540800
H	3.38325600	1.51041300	1.17554000
C	1.97262800	4.50919000	0.41847600
H	-0.13081600	4.94083200	0.52807400
H	4.00065900	3.77869100	0.42945200
H	2.24569800	5.50853900	0.09407700

P(RR)

C	4.10931600	2.69447700	-0.14157500
C	2.74574900	2.42225900	-0.12921500
C	2.22737700	1.33601800	-0.83972200
C	3.09985200	0.54460600	-1.58465900
C	4.46615300	0.81094900	-1.59588000
C	4.97617600	1.88329400	-0.87076200
H	4.49580500	3.54157000	0.41682800
H	2.07178000	3.05903200	0.44079000
H	2.71036000	-0.30743400	-2.13441000
H	5.13211600	0.17055000	-2.16593400
H	6.04169500	2.08960700	-0.87581100
C	-1.17146000	1.13059600	0.80912700
O	-1.49260300	2.25042600	1.13411000
C	0.26907800	0.68150400	0.66403300

H	0.83128600	1.28800600	1.37865000
C	0.74644600	1.03271700	-0.77121400
H	0.49526500	0.20682300	-1.44648300
H	0.19053800	1.91422500	-1.11113400
C	-3.48598800	0.40424600	0.19940200
C	-4.10340000	-0.68000000	-0.43636700
C	-5.44825400	-0.63897600	-0.77279000
C	-6.17858200	0.50652300	-0.46410700
C	-5.56472500	1.58246600	0.17140100
C	-4.21380700	1.54779300	0.51420400
H	-5.91748800	-1.48377700	-1.26530100
H	-7.23141200	0.55420000	-0.72016500
H	-6.14293400	2.46799000	0.41178900
H	-3.73171300	2.37844400	1.00814700
N	-2.11432600	0.16142100	0.44259100
S	-2.99112800	-2.01688600	-0.72430100
C	-1.67513700	-1.12939500	0.06681400
N	-0.53368000	-1.63064800	0.26270400
C	0.40773700	-0.81112900	1.01926800
H	0.14007400	-0.91721700	2.08406900
C	1.83096300	-1.30618000	0.84218500
C	2.14388800	-2.30978700	-0.07020900
C	2.85834500	-0.71163300	1.58091000
C	3.47055900	-2.69625400	-0.26029800
H	1.34134100	-2.78064400	-0.62669500
C	4.17990900	-1.08695000	1.38275200
H	2.62607600	0.07041700	2.30066900
C	4.49071500	-2.08149900	0.45591200
H	3.70339100	-3.47921800	-0.97574900
H	4.96947500	-0.59996800	1.94606900
H	5.52379700	-2.37512500	0.29827900

P(RS)

C	5.27038400	-1.63131900	-0.95131700
C	3.92458200	-1.62659600	-1.30527800
C	2.93074800	-1.65770500	-0.32512300
C	3.30863900	-1.68923400	1.01957100
C	4.65408700	-1.69295200	1.37652400
C	5.63764900	-1.66546300	0.39152100
H	6.03256700	-1.61170300	-1.72400100
H	3.63824200	-1.60525500	-2.35430500
H	2.53627800	-1.70047600	1.78618100
H	4.93397600	-1.71866200	2.42491000
H	6.68683300	-1.67136100	0.66894600

C	-0.49041000	-0.27280400	-1.35785500
O	-0.85273900	-0.33408100	-2.51079200
C	0.95667200	-0.16979700	-0.92386100
H	1.51047000	0.27541000	-1.75495100
C	1.47319400	-1.61631600	-0.70873200
H	0.87415100	-2.10260300	0.06894800
H	1.31096400	-2.16729100	-1.64088900
C	-2.73584200	-0.77965700	-0.37764400
C	-3.28554500	-1.06550900	0.87802700
C	-4.60142200	-1.48502000	1.00364100
C	-5.37247800	-1.61651700	-0.14901300
C	-4.82641100	-1.32807500	-1.39663900
C	-3.50495000	-0.90474500	-1.53052100
H	-5.01753400	-1.70246100	1.98154500
H	-6.40370000	-1.94268300	-0.06860700
H	-5.43627000	-1.42811600	-2.28806800
H	-3.07660000	-0.67855100	-2.49588400
N	-1.38212600	-0.38373300	-0.28292500
S	-2.13261400	-0.82736800	2.18983500
C	-0.89939200	-0.27030600	1.04335400
N	0.22717700	0.16908100	1.41117100
C	1.07778400	0.69410000	0.33023500
H	2.11123700	0.63302400	0.68684300
C	0.74517200	2.16837000	0.11944500
C	0.37516200	2.70728700	-1.11226500
C	0.82090400	3.01529900	1.23141300
C	0.09087000	4.06856800	-1.23052600
H	0.29889800	2.08196800	-1.99670200
C	0.53982200	4.36915100	1.11311200
H	1.09370900	2.59301300	2.19442300
C	0.17351200	4.90181400	-0.12285100
H	-0.19835600	4.47121500	-2.19604900
H	0.60446700	5.01206500	1.98527400
H	-0.04735000	5.96012300	-0.21767600

P(SR)

C	4.43945100	1.97214600	-0.91853800
C	3.63448000	1.24689700	-0.04364900
C	2.44024600	1.79296500	0.43194500
C	2.05884400	3.06840100	0.00972800
C	2.86319200	3.79295200	-0.86443500
C	4.05686200	3.24641800	-1.32973100
H	5.36768800	1.54026400	-1.27993100
H	3.93005600	0.24757000	0.27114300

H	1. 12119700	3. 48330500	0. 37179100
H	2. 55899000	4. 78553500	-1. 18183400
H	4. 68613000	3. 81186300	-2. 00975300
C	-0. 92615700	0. 81632400	0. 74720100
O	-1. 12979900	1. 93692800	1. 15669700
C	0. 45789700	0. 22434600	0. 53045200
H	0. 64714000	0. 36455300	-0. 54532200
C	1. 52779100	0. 99543500	1. 33228000
H	1. 02432700	1. 66654300	2. 03243300
H	2. 12104400	0. 28708300	1. 91677900
C	-3. 31898300	0. 36946900	0. 17825000
C	-4. 06364400	-0. 60569500	-0. 49608300
C	-5. 40685500	-0. 40988700	-0. 78094300
C	-6. 00740300	0. 78148400	-0. 38055600
C	-5. 26743600	1. 74889900	0. 29337700
C	-3. 91739200	1. 55854900	0. 58448700
H	-5. 97292300	-1. 17268400	-1. 30465100
H	-7. 05683800	0. 95101100	-0. 59539500
H	-5. 74422800	2. 67219900	0. 60441200
H	-3. 34130500	2. 30700700	1. 10806200
N	-1. 97261800	-0. 02675600	0. 35778500
S	-3. 10671900	-2. 02890200	-0. 90166700
C	-1. 68069800	-1. 32978400	-0. 11119600
N	-0. 59605400	-1. 96313900	0. 01390800
C	0. 46219300	-1. 29859700	0. 77012500
H	0. 27960700	-1. 48424900	1. 84112400
C	1. 81335800	-1. 87746500	0. 40659100
C	2. 17858700	-1. 98951600	-0. 93593100
C	2. 73150600	-2. 23487200	1. 39203400
C	3. 44935600	-2. 43135600	-1. 28536400
H	1. 45386700	-1. 73749200	-1. 70549700
C	4. 00651900	-2. 67878400	1. 04547900
H	2. 44773100	-2. 16576300	2. 43957000
C	4. 36935100	-2. 77153600	-0. 29456200
H	3. 72364000	-2. 51218200	-2. 33232400
H	4. 71243000	-2. 95355200	1. 82277500
H	5. 36165800	-3. 11550500	-0. 56790400

P(SS)

C	-4. 46607200	0. 81054700	-1. 59593100
C	-3. 09973000	0. 54442200	-1. 58475100
C	-2. 22735800	1. 33596500	-0. 83983200
C	-2. 74587800	2. 42214100	-0. 12933600
C	-4. 10948800	2. 69415400	-0. 14166800

C	-4.97624400	1.88281700	-0.87080600
H	-5.13195000	0.17003300	-2.16595500
H	-2.71012300	-0.30756300	-2.13450600
H	-2.07199700	3.05902400	0.44065000
H	-4.49608900	3.54120200	0.41672500
H	-6.04179600	2.08896000	-0.87582700
C	1.17152000	1.13069800	0.80904600
O	1.49270500	2.25053000	1.13398200
C	-0.26903700	0.68165800	0.66396800
H	-0.83122000	1.28821700	1.37855600
C	-0.74639200	1.03283900	-0.77129100
H	-0.19057200	1.91441800	-1.11116900
H	-0.49509400	0.20698100	-1.44656400
C	3.48602700	0.40422600	0.19938600
C	4.10340100	-0.68006900	-0.43633700
C	5.44826200	-0.63911700	-0.77273800
C	6.17863800	0.50635800	-0.46407900
C	5.56482000	1.58235000	0.17138400
C	4.21389400	1.54775000	0.51416300
H	5.91746700	-1.48395500	-1.26521300
H	7.23147500	0.55397800	-0.72011900
H	6.14306400	2.46785500	0.41175500
H	3.73182900	2.37843800	1.00807200
N	2.11435300	0.16146900	0.44256700
S	2.99107400	-2.01691600	-0.72424000
C	1.67511500	-1.12934500	0.06683900
N	0.53363700	-1.63054400	0.26274500
C	-0.40774800	-0.81095400	1.01927800
H	-0.14006800	-0.91699300	2.08408200
C	-1.83099200	-1.30598100	0.84225200
C	-2.14393900	-2.30972400	-0.06998200
C	-2.85836400	-0.71128400	1.58087300
C	-3.47062200	-2.69617300	-0.26003300
H	-1.34140000	-2.78070100	-0.62638000
C	-4.17994000	-1.08656700	1.38273400
H	-2.62608100	0.07087700	2.30050700
C	-4.49076800	-2.08125600	0.45605300
H	-3.70347000	-3.47924700	-0.97535700
H	-4.96950000	-0.59945300	1.94594600
H	-5.52386000	-2.37486100	0.29844200

TS6a(SS)

C	0.37026300	-0.13956200	-1.02296800
C	0.95648000	0.95946300	-2.82056900

C	1. 93915800	1. 91029200	-3. 42597600
C	2. 69019100	2. 42052000	-2. 16352300
C	2. 54898200	1. 31046500	-1. 09198000
H	2. 59910600	1. 37737300	-4. 11732500
H	1. 44369200	2. 70998900	-3. 97713900
H	2. 21190900	3. 33410200	-1. 80430500
H	2. 40447500	1. 69918200	-0. 08262900
N	-0. 13053300	0. 33775600	-3. 17146900
N	-0. 48933600	-0. 33947700	-2. 03070300
N	1. 29848800	0. 67601800	-1. 53375400
H	3. 74244900	2. 63716300	-2. 35762200
C	-1. 56265000	-1. 29467200	-2. 07304100
C	-1. 19841100	-2. 63877900	-2. 23019000
C	-2. 88114800	-0. 86257200	-1. 94793400
C	-2. 21777400	-3. 58231700	-2. 20453300
C	-3. 86658000	-1. 85442600	-1. 93603700
C	-3. 55626300	-3. 20663500	-2. 04998800
H	-1. 96134400	-4. 63449300	-2. 30483900
H	-4. 90535300	-1. 55095900	-1. 83060200
C	3. 69136700	0. 28457300	-1. 11109600
H	3. 93419000	0. 03580000	-2. 15203100
H	3. 33043900	-0. 61684900	-0. 60915400
C	4. 90072000	0. 82579000	-0. 39218700
C	6. 02677300	1. 27878600	-1. 07849700
C	4. 87579200	0. 90388900	1. 00430000
C	7. 11585100	1. 80221100	-0. 38436400
H	6. 05676400	1. 21005200	-2. 16372600
C	5. 96109800	1. 42698700	1. 69745800
H	3. 99538200	0. 54270900	1. 53298800
C	7. 08358900	1. 87823600	1. 00413700
H	7. 98930500	2. 14648800	-0. 92919700
H	5. 93429500	1. 48066600	2. 78115500
H	7. 93131500	2. 28487800	1. 54624800
C	-4. 63893900	-4. 25421700	-2. 04022800
H	-5. 58119800	-3. 84877300	-1. 66660500
H	-4. 81464200	-4. 63839600	-3. 05008100
H	-4. 35709500	-5. 10340900	-1. 41187100
C	0. 24458400	-3. 03322800	-2. 39359200
H	0. 32384500	-4. 08000200	-2. 68915300
H	0. 73498800	-2. 41552300	-3. 15298200
H	0. 79619400	-2. 92263300	-1. 45163200
C	-3. 25273500	0. 58722900	-1. 79813500
H	-4. 15925700	0. 80175800	-2. 36896900
H	-3. 44849200	0. 83216000	-0. 74883300

H	-2.46261400	1.25623300	-2.14714800
C	0.15189700	-5.65581600	-0.15270200
C	-0.37851100	-4.62313900	0.61545400
C	0.44927200	-3.64104500	1.16805500
C	1.82402100	-3.71036500	0.92339800
C	2.35759400	-4.74129700	0.15272300
C	1.52421100	-5.71844700	-0.38606400
H	-0.50589500	-6.41676700	-0.56346700
H	-1.45073800	-4.57610100	0.79509500
H	2.46613800	-2.93660000	1.33418800
H	3.42816300	-4.78369300	-0.02332400
H	1.94116000	-6.52527400	-0.98077100
C	0.42560300	-0.53934100	0.45177800
O	1.57651200	-0.52282700	0.91765500
C	-0.69661000	-1.40274300	1.08665900
H	-1.33578500	-1.84595500	0.31748900
C	-0.13851900	-2.51091100	1.97715100
H	0.61919400	-2.08654000	2.64004400
H	-0.95362500	-2.88275100	2.60879000
C	-2.90947100	3.45246200	0.35892200
C	-1.91138300	4.06969400	-0.42799000
C	-2.13605900	5.26663100	-1.09592600
C	-3.38745400	5.86611700	-0.97980500
C	-4.38797500	5.26834900	-0.20755300
C	-4.16024000	4.07145400	0.45902200
H	-1.35455400	5.72682700	-1.69216800
H	-3.58252100	6.80290200	-1.49084200
H	-5.35841700	5.74781900	-0.12544700
H	-4.92905500	3.60136500	1.06278000
N	-2.57148300	2.25814400	0.95989200
S	-0.45978100	3.08756400	-0.37768800
C	-1.34026000	1.91343900	0.67837900
N	-0.69973600	0.82014500	1.07558700
C	-1.45024100	-0.22701600	1.76534900
H	-2.51323900	-0.21985200	1.49189400
C	-1.33607200	-0.15064300	3.27162600
C	-0.13246500	0.23250600	3.86974000
C	-2.41663900	-0.49771900	4.08090000
C	-0.01612900	0.26091600	5.25499600
H	0.70376100	0.50269500	3.22994400
C	-2.30173400	-0.46842400	5.46904100
H	-3.35925800	-0.78094200	3.61867900
C	-1.10010200	-0.08953700	6.05875900
H	0.92235300	0.56061100	5.71165300

H	-3.15338900	-0.73354300	6.08792700
H	-1.00854800	-0.06117400	7.14006800

6a(SS)

C	-0.70461200	-0.60395200	-1.18081200
C	0.30585100	-0.34808400	-3.08580700
C	1.58841700	-0.45124000	-3.84109200
C	2.43465900	-1.37738100	-2.92984000
C	1.75011000	-1.43332700	-1.53728800
H	1.44590400	-0.85378200	-4.84510000
H	2.02352400	0.54754700	-3.92652900
H	3.46094800	-1.02417200	-2.82950300
H	2.17196400	-0.68707400	-0.85462800
N	-0.83418900	0.25624600	-3.24921800
N	-1.46672600	0.05706700	-2.04963100
N	0.39555200	-0.95044900	-1.86208100
H	2.46885000	-2.38856400	-3.34647400
C	-2.79865000	0.53882200	-1.81539800
C	-3.83897800	-0.38941300	-1.76852600
C	-2.96728300	1.91075500	-1.60034900
C	-5.11006100	0.10021500	-1.47270400
C	-4.25589500	2.34263300	-1.29983000
C	-5.33151600	1.45314500	-1.22515600
H	-5.93928900	-0.59847300	-1.41111000
H	-4.42220300	3.39992900	-1.10738900
C	1.77752800	-2.82997800	-0.91672200
H	1.27878700	-3.52826800	-1.59841300
H	1.21147600	-2.83975800	0.01876300
C	3.20773900	-3.26326200	-0.68226900
C	3.72583500	-4.39049700	-1.32044300
C	4.04341700	-2.52690400	0.16553600
C	5.04600900	-4.78391800	-1.11362000
H	3.08570300	-4.97148600	-1.97981400
C	5.36268000	-2.91657900	0.37117600
H	3.66593400	-1.64191400	0.67359000
C	5.86797700	-4.04709900	-0.26731500
H	5.43056000	-5.66657500	-1.61483200
H	5.99631400	-2.33283200	1.03103300
H	6.89729700	-4.35017900	-0.10548700
C	-6.70958800	1.95633800	-0.88585200
H	-6.68320800	2.58827000	0.00673500
H	-7.11811000	2.55839600	-1.70354600
H	-7.39488900	1.12716300	-0.69635300
C	-3.60458800	-1.85525300	-2.03001200

H	-4.55890000	-2.37917700	-2.10484000
H	-3.05319700	-2.00367500	-2.96382300
H	-3.03413200	-2.32606900	-1.22258200
C	-1.79103100	2.84756300	-1.65412200
H	-2.07752700	3.84193700	-1.30844100
H	-0.96738700	2.47551000	-1.03114100
H	-1.40895600	2.93187100	-2.67589600
C	-6.05443300	-0.11583400	1.80864200
C	-4.73158500	0.17615600	2.12653800
C	-3.73072600	-0.79171500	2.00046400
C	-4.08369600	-2.05814800	1.52446800
C	-5.40429100	-2.34892600	1.18853300
C	-6.39543900	-1.38128800	1.33728400
H	-6.82124600	0.64209200	1.93878000
H	-4.46972200	1.16452400	2.49746300
H	-3.31455600	-2.82052500	1.43295400
H	-5.66224800	-3.34103000	0.82963200
H	-7.42819100	-1.61474100	1.09560500
C	-1.10228100	-1.01039400	0.22742000
O	-1.03306100	-2.18872600	0.49765500
C	-1.50282600	0.08779600	1.18598500
H	-2.11260300	0.81043600	0.63166100
C	-2.30272100	-0.46214300	2.36847800
H	-1.79294400	-1.34323500	2.76921400
H	-2.29466200	0.29667700	3.15845700
C	3.08567200	3.31593300	0.83485900
C	3.44441100	3.20192100	-0.53142200
C	4.50524900	3.91156300	-1.07582100
C	5.23654300	4.76100300	-0.24766600
C	4.89902400	4.88649000	1.10208400
C	3.83600100	4.17546600	1.64557400
H	4.75984400	3.80873100	-2.12611300
H	6.06902500	5.32427500	-0.65628600
H	5.47766900	5.54937800	1.73831600
H	3.57010100	4.26508100	2.69338500
N	2.02133300	2.55645300	1.26653100
S	2.34878500	2.07473500	-1.31043500
C	1.51429100	1.83811100	0.29336900
N	0.50047400	0.99452300	0.29245500
C	-0.18372000	0.84745100	1.55688000
H	-0.47622800	1.82066200	1.98530600
C	0.59916500	0.10581600	2.63017300
C	1.44301100	-0.95134900	2.29173300
C	0.46496900	0.44340700	3.97681800

C	2. 12570300	-1. 66982100	3. 26728600
H	1. 57621200	-1. 18501300	1. 24146000
C	1. 14310500	-0. 27118700	4. 96098900
H	-0. 16052600	1. 28864600	4. 25384800
C	1. 97191700	-1. 33348200	4. 61012200
H	2. 78062100	-2. 48676200	2. 97609000
H	1. 03304100	0. 00995300	6. 00384400
H	2. 50363000	-1. 88708700	5. 37741300

TS7a(SS)

C	-0. 32991200	0. 67235500	1. 15747000
C	-1. 32502900	1. 91604000	2. 70498300
C	-2. 51609000	2. 76247800	3. 02718800
C	-3. 08431200	3. 03855000	1. 60787200
C	-2. 62012800	1. 85840800	0. 71941300
H	-3. 21692300	2. 19378500	3. 64645400
H	-2. 25132000	3. 67187900	3. 56744900
H	-2. 66239400	3. 97188400	1. 22666600
H	-2. 36469500	2. 16023800	-0. 29536000
N	-0. 26517700	1. 47014100	3. 31231400
N	0. 32930200	0. 70721900	2. 33005200
N	-1. 39082100	1. 46000600	1. 41852200
H	-4. 17261500	3. 12887700	1. 59693100
C	1. 53638700	-0. 02369900	2. 57131500
C	1. 43116600	-1. 32333300	3. 07346000
C	2. 75523200	0. 55652700	2. 21053500
C	2. 59666800	-2. 08761200	3. 12572100
C	3. 89009100	-0. 25061800	2. 27041700
C	3. 82525100	-1. 57654100	2. 70175900
H	2. 54151500	-3. 10804500	3. 49793300
H	4. 84408800	0. 16518700	1. 95612100
C	-3. 61162900	0. 68830700	0. 68330400
H	-4. 01368200	0. 51548000	1. 69010700
H	-3. 06621500	-0. 20982800	0. 37452300
C	-4. 72696700	0. 94788100	-0. 29682800
C	-6. 05376200	1. 07172300	0. 11032900
C	-4. 42233100	1. 04001200	-1. 66086300
C	-7. 06830400	1. 27633800	-0. 82468800
H	-6. 29809500	0. 99034800	1. 16711900
C	-5. 43231500	1. 24808800	-2. 59273700
H	-3. 38790500	0. 91304700	-1. 97520000
C	-6. 75933000	1. 36492800	-2. 17786200
H	-8. 09851900	1. 36387800	-0. 49361000
H	-5. 18701600	1. 31106800	-3. 64855000

H	-7.54694700	1.52208600	-2.90794300
C	5.05638300	-2.44540900	2.68471200
H	5.94761500	-1.87367300	2.95394700
H	4.96172700	-3.28311400	3.37929700
H	5.21887100	-2.85558700	1.68236800
C	0.11522500	-1.86353700	3.57168800
H	0.14307400	-2.95371100	3.63252400
H	-0.09858400	-1.47061600	4.57084900
H	-0.72143800	-1.57272200	2.92922500
C	2.83852900	2.00724100	1.82196800
H	2.70704300	2.63514000	2.70972800
H	3.80620400	2.23483000	1.37238400
H	2.05702200	2.28618100	1.10958000
C	-3.95652400	-3.24552500	1.07769000
C	-2.63472900	-3.26403000	0.64368200
C	-2.28290600	-2.75917600	-0.61261400
C	-3.28982700	-2.23868000	-1.42688600
C	-4.61665200	-2.22813900	-1.00154600
C	-4.95316300	-2.72583000	0.25396100
H	-4.20965300	-3.64059600	2.05706300
H	-1.86069300	-3.67654500	1.28863600
H	-3.02346200	-1.81184500	-2.38968800
H	-5.38284300	-1.79837300	-1.64043700
H	-5.98526100	-2.70405900	0.58955100
C	-0.30884900	-0.26255500	-0.60244700
O	-1.24931600	0.25274500	-1.21357100
C	-0.05578600	-1.74049500	-0.17644100
H	-0.22514500	-1.94618200	0.88076300
C	-0.83141400	-2.73333100	-1.03618900
H	-0.74833300	-2.45608000	-2.09181200
H	-0.38215600	-3.72827900	-0.92849200
C	3.61243800	2.19669500	-1.42072000
C	2.62585400	3.18278300	-1.63155200
C	2.96173300	4.51745600	-1.83647600
C	4.30718600	4.86810000	-1.82869200
C	5.29633200	3.89932600	-1.62035300
C	4.96033000	2.56816900	-1.41727700
H	2.19363900	5.26679300	-1.99740300
H	4.59011700	5.90330800	-1.98752500
H	6.34080400	4.19411400	-1.61922700
H	5.71495900	1.80573800	-1.25579700
N	3.14612300	0.91192800	-1.19187800
S	1.03683100	2.44365900	-1.58183400
C	1.85240300	0.90015400	-1.23694000

N	1. 07739200	-0. 18712400	-1. 03597000
C	1. 45668300	-1. 49393800	-0. 50231900
H	2. 06423600	-1. 40542200	0. 40544400
C	2. 13401300	-2. 43460900	-1. 46047900
C	2. 07890500	-2. 25096000	-2. 84122300
C	2. 80268300	-3. 54605300	-0. 94403100
C	2. 68503500	-3. 16996100	-3. 69358700
H	1. 56826100	-1. 37822400	-3. 23830800
C	3. 40117400	-4. 46902800	-1. 79537600
H	2. 85399600	-3. 67788100	0. 13550500
C	3. 34374200	-4. 28126100	-3. 17456800
H	2. 64471100	-3. 01558300	-4. 76729600
H	3. 91777600	-5. 33059900	-1. 38369200
H	3. 81483600	-4. 99599800	-3. 84182000

Pa(SS)

C	-6. 45867500	-0. 59414900	-0. 12662300
C	-5. 28220400	0. 15059500	-0. 12227500
C	-4. 04466900	-0. 46720300	0. 06659900
C	-4. 00392400	-1. 85334700	0. 24782000
C	-5. 17952600	-2. 59832900	0. 23963400
C	-6. 40981600	-1. 97291200	0. 05372000
H	-7. 41203500	-0. 09668800	-0. 27492500
H	-5. 32436400	1. 22716000	-0. 26722100
H	-3. 04907000	-2. 35104600	0. 39624800
H	-5. 13260000	-3. 67370500	0. 38024000
H	-7. 32436600	-2. 55723500	0. 04794600
C	-0. 70569700	-1. 22324400	-0. 20555800
O	-0. 75773600	-2. 31544300	0. 29891200
C	-1. 67271400	-0. 19739200	-0. 81470000
H	-2. 08760900	-0. 56096800	-1. 75977200
C	-2. 77955900	0. 36297000	0. 07819500
H	-2. 39996200	0. 46876500	1. 10190100
H	-3. 00784300	1. 37891500	-0. 26337900
C	3. 87749900	-0. 14055400	-0. 39009300
C	3. 95585400	-1. 41174700	0. 21112500
C	5. 18019900	-1. 98784500	0. 54146400
C	6. 33566400	-1. 26991700	0. 26308500
C	6. 27052300	-0. 00322200	-0. 33369200
C	5. 05146600	0. 56785700	-0. 66293900
H	5. 23107200	-2. 96841800	1. 00258200
H	7. 30113100	-1. 69792400	0. 51137100
H	7. 18853900	0. 53650300	-0. 54094100
H	4. 98124100	1. 54669300	-1. 12429400

N	2.59435600	0.31099700	-0.66653900
S	2.34605700	-2.06158300	0.43637800
C	1.73685800	-0.57485800	-0.29337600
N	0.38214900	-0.40362400	-0.44320600
C	-0.38789500	0.69126000	-1.04184600
H	-0.14213500	0.82422700	-2.10006200
C	-0.32603500	2.00926000	-0.31952400
C	0.03407600	2.09454500	1.02578200
C	-0.69780800	3.16815700	-1.00171200
C	0.01771600	3.32327700	1.67798400
H	0.33787800	1.19886900	1.56071900
C	-0.72036100	4.39609900	-0.34805900
H	-0.96743600	3.10760400	-2.05339100
C	-0.36217800	4.47574300	0.99485700
H	0.30658600	3.38046800	2.72249300
H	-1.00967500	5.29084000	-0.88973400
H	-0.37269000	5.43293200	1.50588500

TS5(SS)_NHC1

C	-0.05193700	-0.51754700	-1.21907200
C	-1.61134400	-1.52117000	-2.38253700
C	-3.07998000	-1.72688500	-2.56970900
C	-3.65272500	-1.08822900	-1.27300800
C	-2.59076400	-0.08848100	-0.75083100
H	-3.41863100	-1.21821800	-3.47733900
H	-3.32638200	-2.78641400	-2.65489100
H	-3.80585500	-1.86972000	-0.52528300
H	-2.46115400	-0.14028200	0.33044500
N	-0.50315700	-1.97678200	-2.88910300
N	0.46543500	-1.32922300	-2.15592800
N	-1.37636100	-0.63185100	-1.38090900
H	-4.60588800	-0.58280100	-1.44240900
C	1.83740300	-1.70971700	-2.31915000
C	2.57199200	-1.18446600	-3.37466300
C	2.38310400	-2.60912800	-1.40967100
C	3.90522500	-1.55880300	-3.50948400
C	3.71898800	-2.97284100	-1.55577300
C	4.47748100	-2.44618400	-2.59931500
H	4.49801100	-1.15435300	-4.32273300
H	4.16488500	-3.66796300	-0.85201600
C	-2.81693500	1.36693100	-1.17999700
H	-3.13609000	1.39451500	-2.22951200
H	-1.86467500	1.89866200	-1.09149800
C	-3.84340100	2.01660700	-0.28625500

C	-5.12864400	2.31948100	-0.73244900
C	-3.49940700	2.29049100	1.04271800
C	-6.06126800	2.89235700	0.13089400
H	-5.39895000	2.11388400	-1.76585000
C	-4.42948000	2.86050400	1.90395000
H	-2.49480800	2.04826300	1.38606200
C	-5.71282300	3.16288400	1.45005500
H	-7.05800000	3.12767500	-0.22901200
H	-4.15331800	3.07205800	2.93216800
H	-6.43737800	3.60875900	2.12398600
C	2.15419300	4.55514500	-2.39087900
C	2.59206900	3.55559400	-1.52730700
C	1.81753700	3.16227100	-0.43247900
C	0.58961300	3.79692700	-0.21987400
C	0.14683600	4.79462600	-1.08506600
C	0.92669700	5.17701000	-2.17357500
H	2.77288800	4.85270800	-3.23232800
H	3.55192300	3.07274000	-1.69809800
H	-0.01894800	3.48990700	0.62492200
H	-0.80951100	5.27673600	-0.90435900
H	0.58352100	5.95790200	-2.84501100
C	0.52476100	0.45529300	-0.22794800
O	-0.32968400	0.97240300	0.51963400
C	1.90351100	0.69243300	-0.13335700
H	2.56982100	0.27597000	-0.88403800
C	2.27382000	2.03378900	0.46780700
H	1.79331400	2.12132500	1.44819800
H	3.35614300	2.08612600	0.61914300
C	-1.22025100	-2.82438600	0.94017200
C	-2.12791500	-2.46975100	1.96618400
C	-3.39432300	-3.04369900	2.04157400
C	-3.75957800	-3.98694400	1.08477500
C	-2.87177000	-4.34508000	0.06233200
C	-1.61018100	-3.76771200	-0.01970000
H	-4.08020200	-2.76633900	2.83538200
H	-4.73985900	-4.44902200	1.13703200
H	-3.16992000	-5.08858300	-0.67076400
H	-0.91325300	-4.04111300	-0.80736300
N	0.00677500	-2.19534200	0.97958600
S	-1.37918300	-1.29310000	3.01419200
C	0.08528800	-1.36785800	2.00128100
N	1.12152200	-0.59207500	2.36496500
C	2.19891700	-0.68100400	1.59318400
H	2.31048800	-1.51930500	0.90413100

C	3.46800700	-0.09898000	2.07949400
C	3.50027200	0.68690800	3.23440100
C	4.65105700	-0.32829200	1.37031200
C	4.69990100	1.24214100	3.66587400
H	2.57251500	0.84290200	3.77503000
C	5.84914700	0.22780600	1.80269000
H	4.61874800	-0.93504800	0.46689000
C	5.87507700	1.01725100	2.95197700
H	4.71937200	1.85322600	4.56278800
H	6.76392300	0.04678200	1.24692800
H	6.80987700	1.45277400	3.29075000
H	5.51894300	-2.73104100	-2.70720900
H	1.75966800	-2.98244000	-0.60069900
H	2.10465500	-0.48873600	-4.06331500

TS5(SS)_NHC2

C	-1.06722300	0.70339300	-1.19437900
C	-0.19489000	2.07589600	-2.66295400
C	1.06885000	2.64861000	-3.22025600
C	2.10559700	1.59729000	-2.73659000
C	1.52730400	1.00178400	-1.43120800
H	1.03464600	2.76727500	-4.30293600
H	1.24761800	3.62800000	-2.76244200
H	3.09085900	2.02822500	-2.54887500
N	-1.47038500	2.11712900	-2.91438600
N	-2.00430900	1.24452600	-1.99205200
N	0.08681600	1.23106400	-1.63324600
H	2.21769800	0.80602400	-3.48374500
C	-3.40149200	0.91912200	-2.06993600
C	-3.75786400	-0.28577200	-2.68660600
C	-4.33857600	1.83696200	-1.58882500
C	-5.11346400	-0.60291400	-2.73399500
C	-5.68331200	1.47357500	-1.66915600
C	-6.08591000	0.25578600	-2.21799300
H	-5.41752900	-1.53978900	-3.19436900
H	-6.43322000	2.16511000	-1.29328700
C	-7.54129900	-0.13220300	-2.24152300
H	-7.79919000	-0.70815700	-1.34644300
H	-8.18619300	0.74889800	-2.26430900
H	-7.77252600	-0.75246000	-3.11055600
C	-2.71664800	-1.21029300	-3.26011800
H	-1.98626700	-0.65528600	-3.85670400
H	-2.17376900	-1.73808000	-2.46677800
H	-3.18555600	-1.95813400	-3.90188500

C	-3.91474800	3.17308200	-1.04427700
H	-4.77044400	3.70227000	-0.62129600
H	-3.14522300	3.06057400	-0.27338800
H	-3.49260600	3.78579300	-1.84820900
C	-1.14062200	-5.08030500	-1.40551500
C	-1.84610100	-4.14936100	-0.64894200
C	-1.19296300	-3.33336100	0.28023900
C	0.18921700	-3.46836300	0.43788200
C	0.89526300	-4.40982400	-0.30964200
C	0.23624700	-5.21503900	-1.23595900
H	-1.66586100	-5.70904200	-2.11849700
H	-2.92316400	-4.05163600	-0.77361100
H	0.70660400	-2.82244200	1.14251500
H	1.96865900	-4.50882500	-0.16408600
H	0.78924400	-5.94988700	-1.81359400
C	-1.06395000	-0.32611900	-0.09477000
O	0.03103300	-0.41210100	0.50689600
C	-2.20488200	-1.06461200	0.21557500
H	-3.08674800	-1.02201000	-0.41158800
C	-1.97028100	-2.29317800	1.06002100
H	-1.40387700	-2.00055400	1.95278900
H	-2.92898800	-2.71035400	1.38364000
C	-0.39487600	3.49269000	0.91660100
C	0.51502100	3.58851900	1.99444200
C	1.54455200	4.52463800	1.99073200
C	1.65991500	5.38216200	0.90094300
C	0.75475100	5.30905200	-0.16563700
C	-0.27175900	4.37262900	-0.16635800
H	2.24790600	4.57988300	2.81504600
H	2.45861900	6.11598500	0.88084900
H	0.85332900	5.99835000	-0.99887900
H	-0.98277500	4.30653200	-0.98618900
N	-1.33242400	2.48812500	1.01246100
S	0.14147700	2.35354800	3.16803900
C	-1.18280500	1.80056000	2.11715800
N	-1.92567800	0.76192100	2.56322800
C	-2.95956200	0.43902100	1.81399500
H	-3.28648100	1.09278600	1.00039800
C	-3.97858500	-0.48484300	2.34607600
C	-3.79020500	-1.11811200	3.57783200
C	-5.14345400	-0.73399200	1.61279700
C	-4.75234500	-1.99597200	4.06386800
H	-2.88379900	-0.90132100	4.13323700
C	-6.10284000	-1.61327100	2.10078900

H	-5.28363400	-0.24071400	0.65145400
C	-5.90766600	-2.24850200	3.32700100
H	-4.60215000	-2.48542600	5.02098500
H	-7.00468200	-1.80635400	1.52794600
H	-6.65609800	-2.93633300	3.70766500
H	1.67304300	-0.07287400	-1.35091000
C	2.06139200	1.67945400	-0.17167400
H	1.98097200	2.76851800	-0.26826900
H	1.45892900	1.34231400	0.67531900
O	3.42878700	1.37184300	-0.00327200
Si	4.17260000	-0.11821200	0.16931500
C	3.33269600	-1.16653500	1.47815100
C	3.60222900	-2.54235900	1.57261900
C	2.47522500	-0.60021600	2.42979600
C	3.04037300	-3.31997200	2.58112800
H	4.25493500	-3.01605500	0.84046100
C	1.88732300	-1.37704200	3.42507600
H	2.24921500	0.46194000	2.39667900
C	2.17415100	-2.73689300	3.50518300
H	3.26210800	-4.38150300	2.63653200
H	1.19862200	-0.91799800	4.12794600
H	1.71736100	-3.34540400	4.27968000
C	4.11005500	-1.10066800	-1.44754100
C	3.08801600	-2.04574800	-1.64362800
C	5.01092500	-0.89705500	-2.50278800
C	2.96853400	-2.75518300	-2.83514900
H	2.35672400	-2.22083400	-0.85598200
C	4.90060300	-1.60400900	-3.69888600
H	5.81670600	-0.17631800	-2.39755300
C	3.87927600	-2.53523200	-3.86686900
H	2.16501700	-3.47829300	-2.94652200
H	5.61471500	-1.42959400	-4.49796200
H	3.79503100	-3.08795700	-4.79772500
C	5.92302400	0.35323300	0.72538000
C	6.50436200	1.48983400	-0.12775900
C	5.81898700	0.85448900	2.17616900
C	6.84604300	-0.87119100	0.67940100
H	6.67813000	1.19215200	-1.16628800
H	5.84146500	2.35970900	-0.13050500
H	7.47430300	1.80011500	0.28337400
H	5.44800000	0.07547100	2.84932600
H	6.80876000	1.16856000	2.53248300
H	5.14646500	1.71647900	2.25020000
H	7.84387400	-0.60502400	1.05182400

H	6.46529000	-1.68203900	1.31125400
H	6.95954100	-1.26119500	-0.33783800

TS5(SS)_NHC3

C	-2.17814200	4.46586000	-2.60059000
C	-2.49286900	3.12887400	-2.37578700
C	-1.58596800	2.11237000	-2.69202100
C	-0.35308800	2.46567300	-3.24999400
C	-0.03564700	3.80403500	-3.47445300
C	-0.94384700	4.80826600	-3.14855300
H	-2.89908800	5.24069400	-2.35692000
H	-3.45876500	2.86116400	-1.95110700
H	0.35661200	1.68021400	-3.49034000
H	0.92269800	4.06199500	-3.91638000
H	-0.69769200	5.84966000	-3.33144600
C	-0.22422500	0.52289400	-0.57063000
O	0.72466300	0.34430900	-1.35380800
C	-1.58506700	0.41559900	-0.89867200
H	-2.32904000	0.70553600	-0.16527000
C	-1.90817300	0.67267100	-2.35540000
H	-1.31541700	-0.01339600	-2.97048000
H	-2.96746600	0.47037600	-2.53789100
C	1.93868000	-3.25802500	0.27214500
C	2.51191400	-3.76530600	-0.91728400
C	3.72093400	-4.45608600	-0.90592500
C	4.37442300	-4.63428700	0.30931000
C	3.82812100	-4.11957400	1.49197500
C	2.62145800	-3.43358900	1.48208100
H	4.14184200	-4.84811200	-1.82608200
H	5.31494300	-5.17438200	0.33840400
H	4.35433600	-4.26117200	2.43051300
H	2.19162000	-3.03728000	2.39676600
N	0.71966500	-2.62415700	0.12978900
S	1.46250400	-3.39884000	-2.25770500
C	0.32560200	-2.63895700	-1.12075900
N	-0.85378900	-2.24588700	-1.65097000
C	-1.75805300	-1.76318900	-0.81645000
H	-1.59502600	-1.80677200	0.26486500
C	-3.18291200	-1.78039000	-1.23074300
C	-3.55649100	-2.20953200	-2.50636200
C	-4.16756500	-1.36829500	-0.32897200
C	-4.89858600	-2.20988300	-2.87448500
H	-2.77874900	-2.54106800	-3.18640000
C	-5.50679300	-1.36644400	-0.69858800

H	-3.86794000	-1.03693100	0.66202700
C	-5.87600600	-1.78642400	-1.97613600
H	-5.18471700	-2.54373900	-3.86699000
H	-6.26283600	-1.03434200	0.00747200
H	-6.92141900	-1.78667600	-2.26856900
C	3.44188600	1.15514800	-0.07795500
C	4.65137600	1.84035000	-0.19542500
C	5.83911000	1.13835700	-0.34196200
C	5.79215400	-0.25589500	-0.35218900
C	4.57961800	-0.93365200	-0.22737200
C	3.38263900	-0.22900500	-0.09976500
C	2.31920800	2.16045500	0.04287900
C	3.05653400	3.42057900	0.55621200
C	4.42116600	3.33348300	-0.12992500
H	6.78671600	1.66166900	-0.43092700
H	6.71323400	-0.82166100	-0.45272200
H	4.56071300	-2.01833900	-0.23233900
H	2.42948800	-0.74356000	-0.03120200
H	1.83932900	2.33870400	-0.92386900
H	2.50149200	4.34765400	0.35397900
H	4.36837100	3.77631300	-1.13148200
C	1.16440000	2.32215000	2.25124600
C	2.15860300	3.33287200	2.73703800
C	0.13940500	1.04094000	0.80023300
H	2.44263800	3.11222900	3.76741200
H	5.17206800	3.87672300	0.44862800
N	1.24402000	1.80300000	0.98989000
N	0.09443200	1.91606600	2.86722200
N	-0.53529100	1.11936700	1.95453600
O	3.31582400	3.30053500	1.94973800
H	1.68238300	4.32558800	2.71092400
C	-1.79751400	0.53760800	2.33146900
C	-2.93560000	1.34270000	2.23049300
C	-1.80567800	-0.74539700	2.88245400
C	-4.14437800	0.79193300	2.65171900
C	-3.04186600	-1.24804200	3.28810300
C	-4.21569100	-0.50194900	3.17181600
H	-5.04997900	1.38787300	2.57247700
H	-3.08545000	-2.24887700	3.71007800
C	-5.53890700	-1.10640600	3.56092500
H	-6.30078000	-0.33857500	3.71001600
H	-5.89003700	-1.78250300	2.77380400
H	-5.45213000	-1.69079500	4.48022600
C	-0.53316800	-1.52929600	3.04429900

H	-0.71851400	-2.43586100	3.62328300
H	-0.11765000	-1.82456000	2.07183300
H	0.21976300	-0.93256300	3.57010000
C	-2.84396400	2.74839500	1.69772200
H	-2.22978900	3.36939300	2.35729200
H	-2.38905400	2.77277400	0.70041600
H	-3.83613500	3.19702700	1.62816200