

SUPPORTING MATERIAL FOR
A DFT study on the PBU₃-catalyzed intramolecular cyclizations of N-allylic substituted α -amino nitriles for the formation of functionalized pyrrolidines: mechanisms, selectivities, and role of catalyst

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Table S1. The single-point energies (SPE) calculated at the M06-2X/6-31+G(d, p) level and

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the Gibbs free energy corrections (GFEC) calculated by the THERMO program of all the optimized structures (OS) (unit: a.u.)

OS	SPE	GFEC	OS	SPE	GFEC
cat	-814.645590	0.329107	P(RS)	-994.458042	0.290337
React-(R)+Cat	-994.408557	0.286110	P(RR)	-994.459111	0.289012
React-(S)+Cat	-994.408557	0.286110	M2(SS)	-1809.079933	0.647644
TS1(R)	-1809.062209	0.640028	M2(SR)	-1809.076817	0.644514
M1(R)	-1809.080139	0.641879	TS3(SS)	-1809.040144	0.642345
TS2(RS)	-1809.059768	0.638456	TS3(SR)	-1809.032910	0.641888
TS2(RR)	-1809.063291	0.638546	P(SS)	-994.459111	0.289012
TS2(R)	-1809.015841	0.638813	P(SR)	-994.458042	0.290337
M2(RS)	-1809.076817	0.644514	TS1(S)	-1809.061740	0.641243
M2(RR)	-1809.079933	0.647644	M1(S)	-1809.080139	0.641879
TS3(RS)	-1809.040136	0.641394	TS2(SS)	-1809.065425	0.638936
TS3(RR)	-1809.035895	0.641974	TS2(SR)	-1809.063837	0.639824
R-TS1	-1809.056011	0.644361	TS2(S)	-1809.016257	0.639289
R-TS2	-1809.052232	0.645725			

Table S2. The relative Gibbs free energies of **TS3(RR&SR&RS&SS)** and **TS3'(RR&SR&RS&SS)**

with the energy of **React-(R&S)+Cat** as 0.0 kcal/mol (unit: kcal/mol)

SP	Energ
	y
TS3(RR)	28.2
TS3(SR)	30.1
TS3(RS)	25.2
TS3(SS)	25.8
TS3'(RR)	28.6
TS3'(SR)	30.8
TS3'(RS)	26.1
TS3'(SS)	26.5

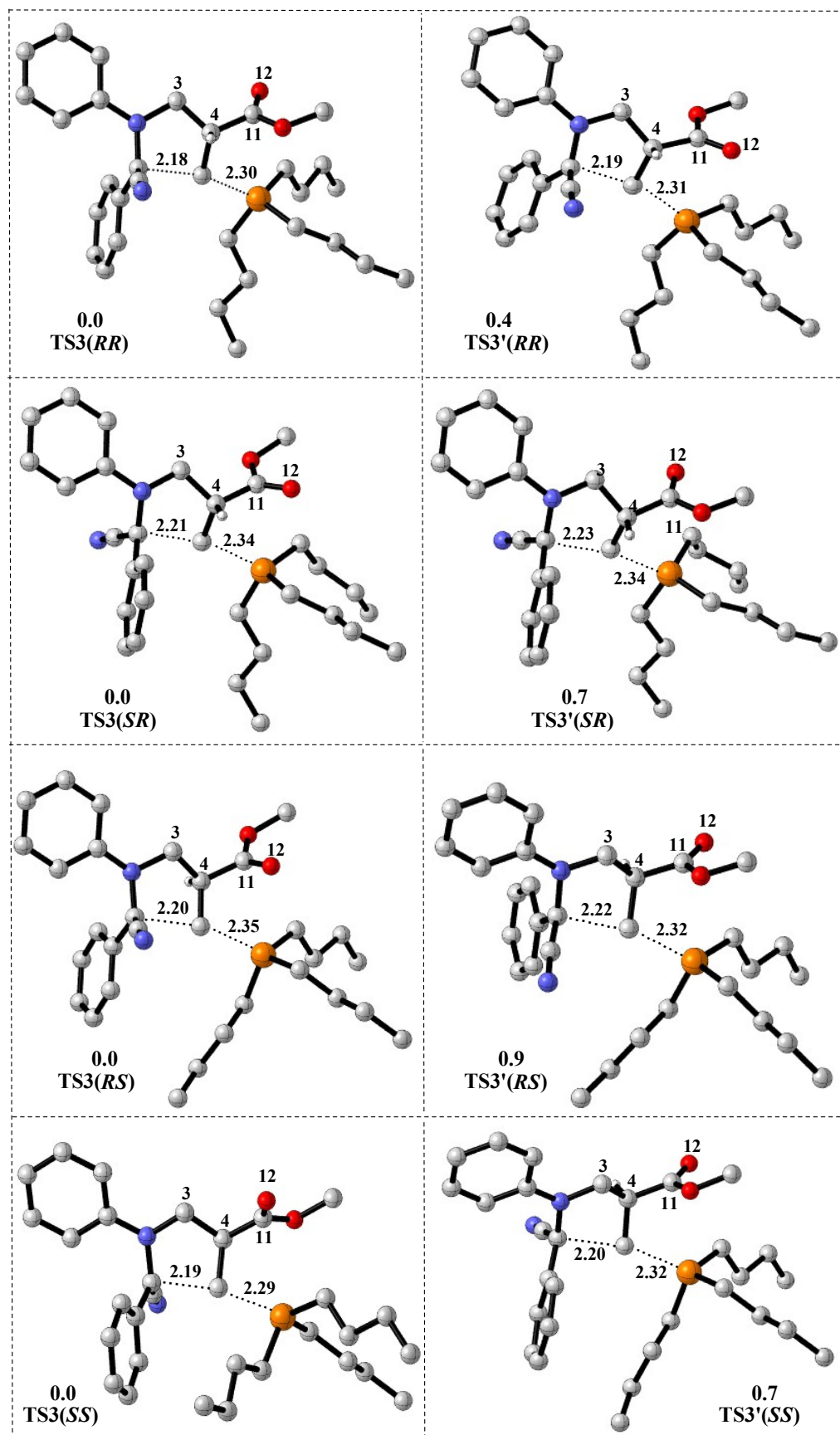


Fig. S1 The optimized structures of transition states $TS3(RR&SR&RS&SS)$ and $TS3'(RR&SR&RS&SS)$

Coordinates of stationary points (SP) of PBU₃-catalyzed intramolecular cyclizations of N-allylic substituted α -amino nitriles in MeCN solvent

Cat				
P	0.00026600	-0.00172200	-2.12975500	
C	-1.12866800	-1.27364400	-1.35677400	
C	-1.66860200	-1.08354700	0.06172300	
H	-1.97998900	-1.36035300	-2.04327800	
H	-0.59399900	-2.23039400	-1.43253400	
C	-2.60876600	-2.21748100	0.47306500	
H	-2.21140400	-0.13113000	0.12484700	
H	-0.84705500	-1.02199800	0.78384500	
C	-3.17236800	-2.02592200	1.87840800	
H	-2.06747700	-3.17040700	0.41625200	
H	-3.43014100	-2.28522700	-0.25137500	
H	-3.83991200	-2.84477600	2.15923500	
H	-3.73863100	-1.09157200	1.94637700	
H	-2.36659500	-1.98017200	2.61794600	
C	-0.53610700	1.61314600	-1.35937700	
C	-0.10516100	1.98471600	0.06070900	
H	-0.18115500	2.39266500	-2.04514500	
H	-1.63173600	1.63164500	-1.43838700	
C	-0.61528600	3.36734300	0.46980800	
H	0.99093900	1.97613100	0.12805100	
H	-0.46746900	1.24342300	0.78144700	
C	-0.17632000	3.75703600	1.87871200	
H	-1.71072900	3.37876100	0.40541700	
H	-0.25561800	4.11180500	-0.25153800	
H	-0.54868600	4.74649200	2.15679800	
H	0.91553700	3.77483300	1.95529200	
H	-0.54903800	3.03817800	2.61526400	
C	1.66640900	-0.34203700	-1.35670800	
C	1.77300300	-0.90415300	0.06228400	
H	2.16846500	-1.03530000	-2.04301400	
H	2.22662500	0.59997900	-1.43205500	
C	3.22612700	-1.14622300	0.47337900	
H	1.22329800	-1.85250600	0.12649500	
H	1.30702800	-0.22429500	0.78414700	
C	3.34515800	-1.72708500	1.87972800	
H	3.77766700	-0.19934800	0.41440500	
H	3.69705600	-1.82349400	-0.25022000	
H	4.38894700	-1.89164400	2.15978200	
H	2.82241700	-2.68626400	1.95019400	
H	2.90112900	-1.05210300	2.61834400	

React-(R)

C	-0.55438700	-0.96121300	0.73689400
C	-0.71569900	-0.85602000	2.21696900
C	1.84024200	-1.29704400	-1.65699900
C	2.37958600	-0.85266400	-0.52398500
C	1.65368000	0.01986700	0.48218400
N	0.22648900	0.13622700	0.20582900
H	2.39925000	-1.94668800	-2.32151100
H	1.81192900	-0.39602500	1.49033800
H	2.08268600	1.02317400	0.51143500
N	-0.79520900	-0.75736700	3.36608700
H	0.83095200	-1.01630100	-1.93860200
C	-0.32945300	1.43638900	0.12941700
C	0.32187300	2.38866400	-0.66818200
C	-1.51677600	1.79593500	0.77676300
C	-0.18392900	3.67683000	-0.78606600
H	1.21613500	2.10360400	-1.21561900
C	-2.02359000	3.08687300	0.63864800
H	-2.05664300	1.08160700	1.38775200
C	-1.36186000	4.03626600	-0.13264100
H	0.33789900	4.39722500	-1.40781700
H	-2.94456700	3.34668900	1.15070000
H	-1.76148700	5.03956900	-0.23175100
C	-1.88933000	-1.19319300	0.03403700
C	-2.91810700	-1.87544300	0.68414400
C	-2.06113800	-0.78785500	-1.28978600
C	-4.10723500	-2.15329300	0.01477300
H	-2.79525600	-2.19106100	1.71648600
C	-3.25177900	-1.06576100	-1.95569700
H	-1.27347800	-0.23693800	-1.79297000
C	-4.27725900	-1.74935000	-1.30674100
H	-4.90133800	-2.68287400	0.53054700
H	-3.37800000	-0.74060100	-2.98314500
H	-5.20547800	-1.96183400	-1.82670100
C	3.76106100	-1.32446000	-0.15840600
O	4.05072100	-2.49531500	-0.09988700
O	4.69489200	-0.40982100	0.14876300
C	4.55971600	0.96070600	-0.23995800
H	3.85627800	1.07372400	-1.06779900
H	4.24376900	1.56061800	0.61572500
H	5.54732900	1.28730400	-0.56350500
H	0.05244300	-1.86352900	0.57981900

TS1 (R)

C	3. 37213800	-0. 72001900	-0. 46767300
C	4. 10477700	-0. 69965600	-1. 75967100
C	-0. 09589500	-0. 83623500	0. 93063800
C	0. 51290100	-0. 54362100	-0. 28006400
C	1. 32050000	0. 70350300	-0. 47506700
N	2. 76235100	0. 55835000	-0. 16849200
H	-0. 44447500	-1. 84618900	1. 12180500
H	1. 19699400	1. 07976600	-1. 50127000
H	0. 93518500	1. 46700400	0. 20933500
N	4. 65620600	-0. 68113100	-2. 77570400
H	0. 20716100	-0. 28299400	1. 81502800
C	3. 55559800	1. 71388300	-0. 19559400
C	2. 97971900	2. 98965200	-0. 34667200
C	4. 95666500	1. 64371200	-0. 05988400
C	3. 77114000	4. 13495900	-0. 33323800
H	1. 91361400	3. 10459100	-0. 48882400
C	5. 73216900	2. 79663200	-0. 05395600
H	5. 45051500	0. 68682100	0. 05405300
C	5. 15151100	4. 05577500	-0. 18458900
H	3. 29093800	5. 10158000	-0. 45196300
H	6. 80821300	2. 70097700	0. 05553400
H	5. 76195600	4. 95201800	-0. 17860200
C	4. 21011700	-1. 30534000	0. 66921200
C	5. 31025200	-2. 12724200	0. 42657400
C	3. 80672100	-1. 06324900	1. 98233500
C	6. 00476900	-2. 69821100	1. 49130700
H	5. 63363900	-2. 31816000	-0. 59304000
C	4. 50134000	-1. 63549300	3. 04385800
H	2. 95516800	-0. 41425300	2. 16169000
C	5. 60297100	-2. 45428100	2. 80177200
H	6. 86310500	-3. 33169700	1. 29210000
H	4. 18364000	-1. 43807800	4. 06276800
H	6. 14624100	-2. 89729700	3. 63004800
C	0. 24842300	-1. 34394200	-1. 45252400
O	0. 85670300	-1. 27619100	-2. 51487300
O	-0. 78649600	-2. 21210600	-1. 28134900
C	-1. 08091200	-3. 04315100	-2. 40110100
H	-0. 22654400	-3. 67644200	-2. 64975500
H	-1. 93158800	-3. 65496100	-2. 10300400
H	-1. 33801100	-2. 43671500	-3. 27229600
P	-2. 37418300	-0. 11468400	0. 87389200
C	-2. 40477200	0. 66776500	-0. 79396100
C	-3. 57784300	1. 57483000	-1. 16635000

H	-2.31160900	-0.15776700	-1.51085400
H	-1.46226600	1.22911400	-0.86790200
C	-3.39396600	2.19902600	-2.55006700
H	-4.51551200	1.00703700	-1.15068100
H	-3.68373300	2.37605400	-0.42368900
C	-4.56111700	3.10303500	-2.93676100
H	-2.45801800	2.77102000	-2.56442900
H	-3.27999000	1.39917700	-3.29206200
H	-4.41392200	3.54630800	-3.92483200
H	-5.49965000	2.54027600	-2.95642400
H	-4.67708200	3.91816300	-2.21553400
C	-3.40214400	-1.64622100	0.75754400
C	-4.60901400	-1.63839900	-0.18352500
H	-3.71046600	-1.89384200	1.78122500
H	-2.70745900	-2.43375600	0.43998900
C	-5.31791600	-2.99294200	-0.21055500
H	-5.32418300	-0.86261900	0.11453700
H	-4.27858800	-1.38924300	-1.20065000
C	-6.51782700	-2.99902900	-1.15343600
H	-4.60110600	-3.76673700	-0.51323900
H	-5.64111600	-3.24989300	0.80582400
H	-7.01174000	-3.97402500	-1.16649600
H	-7.25654200	-2.25147900	-0.84766100
H	-6.21001100	-2.76369400	-2.17710200
C	-3.24695200	1.03417400	2.03903900
C	-4.77789500	1.04403400	2.05808100
H	-2.85587800	2.03626900	1.82104900
H	-2.87681300	0.77749800	3.03875000
C	-5.32491500	2.03811600	3.08364800
H	-5.17310900	1.29584200	1.06739400
H	-5.15005500	0.03992400	2.29970300
C	-6.85040500	2.04158000	3.12883500
H	-4.92312700	1.79112600	4.07410000
H	-4.95689500	3.04255700	2.84054300
H	-7.22729400	2.75857500	3.86258700
H	-7.26807700	2.30775100	2.15272000
H	-7.23423300	1.05217000	3.39675600
H	2.54309400	-1.41756100	-0.62538700

M1 (R)

C	3.31882100	-0.79647600	-0.26645500
C	3.97852000	-1.25854100	-1.52106200
C	-0.43537900	-0.60312700	0.86420400
C	0.32594700	-1.19021900	-0.28261100

C	1. 11200700	-0. 28087900	-1. 15894100
N	2. 35194200	0. 25465400	-0. 50246700
H	-0. 01488400	0. 36069500	1. 18709600
H	0. 54644200	0. 59716800	-1. 47975100
H	1. 40712000	-0. 82228400	-2. 06918400
N	4. 45835800	-1. 61078000	-2. 51289800
H	-0. 45826800	-1. 25906500	1. 74208800
C	2. 81005100	1. 53230300	-0. 88941500
C	1. 90677500	2. 60944200	-0. 84506000
C	4. 13314600	1. 80202500	-1. 26858000
C	2. 30118700	3. 89192200	-1. 19921200
H	0. 89168100	2. 43744800	-0. 50075000
C	4. 52509700	3. 09671300	-1. 60676400
H	4. 87114900	1. 00968000	-1. 30382700
C	3. 61665800	4. 14848500	-1. 58639300
H	1. 57795100	4. 70045600	-1. 15431000
H	5. 55663200	3. 27403900	-1. 89563300
H	3. 92675300	5. 15212800	-1. 85644500
C	4. 31591300	-0. 47650900	0. 83978500
C	3. 82591000	0. 11491500	2. 00618600
C	5. 66857000	-0. 79943400	0. 75045200
C	4. 68177300	0. 38172100	3. 06943400
H	2. 77169200	0. 36916700	2. 06389900
C	6. 52553300	-0. 53125400	1. 81719600
H	6. 06058800	-1. 25513500	-0. 15476000
C	6. 03557500	0. 05989900	2. 97766100
H	4. 29197300	0. 84232400	3. 97161600
H	7. 57810900	-0. 78240100	1. 73532700
H	6. 70368400	0. 27113200	3. 80627700
C	0. 52116900	-2. 56756000	-0. 40601300
O	1. 26927600	-3. 16946000	-1. 20192600
O	-0. 22771200	-3. 31418000	0. 50480800
C	-0. 04007600	-4. 71562200	0. 42943900
H	-0. 29727300	-5. 10018700	-0. 56123700
H	-0. 70240400	-5. 15207000	1. 17844400
H	0. 99571200	-4. 99291400	0. 64563000
P	-2. 20063900	-0. 27288200	0. 47240600
C	-2. 23819900	0. 79045700	-1. 00964900
C	-3. 58314500	1. 42308800	-1. 41074100
H	-1. 50515200	1. 58443200	-0. 81884400
H	-1. 81748000	0. 16576300	-1. 80464300
C	-3. 83444600	2. 77683500	-0. 74377600
H	-4. 42010800	0. 74669400	-1. 20295600
H	-3. 58097900	1. 56393200	-2. 49717500

C	-5.23166000	3.30956600	-1.04450800
H	-3.07576500	3.48665300	-1.09328200
H	-3.70015900	2.69918300	0.34168400
H	-5.38707400	4.29298700	-0.59491600
H	-5.99850800	2.63333000	-0.65098600
H	-5.39094500	3.40091600	-2.12340300
C	-2.97719600	0.56480400	1.89503900
C	-4.50993800	0.58290800	1.92917700
H	-2.59089000	0.05124400	2.78436800
H	-2.56531900	1.58095300	1.92046500
C	-5.03168900	1.47446100	3.05533700
H	-4.88395100	-0.43865800	2.06708000
H	-4.91957900	0.94053800	0.97678600
C	-6.55604800	1.49402500	3.11145600
H	-4.65128700	2.49304700	2.90731000
H	-4.62326700	1.12419100	4.01083200
H	-6.91468800	2.13901500	3.91717800
H	-6.95395600	0.48892600	3.28085900
H	-6.97419200	1.86563900	2.17046600
C	-3.01212800	-1.88331800	0.21057600
C	-4.34595400	-1.92345400	-0.55165100
H	-2.25779400	-2.50160800	-0.28807900
H	-3.11940300	-2.29151500	1.22278300
C	-4.18081300	-1.93677800	-2.07136100
H	-5.00329500	-1.10006800	-0.25020400
H	-4.86693800	-2.83989200	-0.25265700
C	-5.52685600	-1.91852100	-2.78866300
H	-3.61356400	-2.83115900	-2.35420400
H	-3.58196400	-1.08013100	-2.40030100
H	-5.40053400	-1.96285100	-3.87293500
H	-6.08184900	-1.00489700	-2.55067000
H	-6.14208400	-2.77102200	-2.48444500
H	2.72428500	-1.66184100	0.05331300

TS2 (RR)

C	2.85811500	-0.97175200	-0.02262600
C	3.93844000	-1.52196400	-0.80556300
C	-0.27500800	-1.49997600	0.65261400
C	0.46711900	-1.78319200	-0.64156600
C	0.93007600	-0.60048400	-1.44861300
N	2.07138900	0.01216400	-0.72070700
H	-0.65688400	-2.42691800	1.08714100
H	1.23130900	-0.94011100	-2.44865100
H	0.16125800	0.16744900	-1.58759900

N	4. 77152000	-2. 00964300	-1. 45551200
H	0. 38322700	-1. 03386400	1. 39763300
C	2. 62861400	1. 19543500	-1. 20846500
C	1. 95799200	1. 98022500	-2. 16625400
C	3. 86907700	1. 66161800	-0. 72935700
C	2. 49654500	3. 18987800	-2. 59758900
H	1. 01881000	1. 65173200	-2. 59434600
C	4. 39496000	2. 86743900	-1. 17593600
H	4. 41607800	1. 07540100	0. 00025700
C	3. 71560700	3. 64900100	-2. 10923200
H	1. 95164200	3. 77013100	-3. 33651100
H	5. 35336100	3. 19781500	-0. 78646100
H	4. 13183400	4. 58942900	-2. 45345800
C	3. 18182500	-0. 71668100	1. 40849600
C	2. 56007200	0. 32256900	2. 11762300
C	4. 09305600	-1. 53110100	2. 09808400
C	2. 82297200	0. 52333200	3. 46940500
H	1. 87375100	0. 98001200	1. 59143600
C	4. 35713600	-1. 32442100	3. 44801700
H	4. 59584100	-2. 33578100	1. 56775400
C	3. 72093900	-0. 29902100	4. 14679200
H	2. 32780500	1. 33566000	3. 99324500
H	5. 06493400	-1. 97142500	3. 95773200
H	3. 92705200	-0. 14006300	5. 20000600
C	0. 07347800	-2. 93914800	-1. 42392000
O	0. 46099200	-3. 21560300	-2. 55241400
O	-0. 77565700	-3. 77536800	-0. 75685200
C	-1. 11639500	-4. 97251300	-1. 45011900
H	-0. 22196600	-5. 55357700	-1. 68412500
H	-1. 76584100	-5. 53340000	-0. 77960500
H	-1. 64149500	-4. 74448900	-2. 38047300
P	-1. 69787400	-0. 36334100	0. 50080500
C	-2. 58032600	-0. 77521700	-1. 03803100
C	-4. 02923000	-0. 28817900	-1. 13564700
H	-2. 53793400	-1. 87105700	-1. 09134000
H	-1. 98071300	-0. 39757600	-1. 87389300
C	-4. 64969200	-0. 66721000	-2. 48034200
H	-4. 62313700	-0. 73214400	-0. 32741800
H	-4. 07959800	0. 79983400	-1. 01019600
C	-6. 10423600	-0. 21879700	-2. 58390000
H	-4. 06026100	-0. 21527800	-3. 28688100
H	-4. 58152200	-1. 75360600	-2. 61291700
H	-6. 53534600	-0. 49529800	-3. 54899000
H	-6. 71083400	-0. 67985700	-1. 79849900

H	-6.18612000	0.86713900	-2.47629400
C	-2.79958600	-0.60224000	1.93126600
C	-3.73361300	0.57095800	2.25190400
H	-2.14174700	-0.80355200	2.78533700
H	-3.36504600	-1.52261000	1.74207800
C	-4.64050800	0.24858900	3.43986100
H	-3.14041900	1.46371600	2.48420500
H	-4.35491400	0.82075100	1.38444400
C	-5.54993600	1.41985000	3.79888500
H	-5.24431900	-0.63412600	3.19855300
H	-4.02003300	-0.02189900	4.30239800
H	-6.19762800	1.17215100	4.64313600
H	-4.96170000	2.30105800	4.07213900
H	-6.18763400	1.69215800	2.95236700
C	-1.05156800	1.34773900	0.52433600
C	-1.83678900	2.37968600	-0.29024200
H	-0.01461000	1.29204000	0.17144100
H	-1.00029000	1.63689200	1.58126400
C	-1.12264700	3.73104500	-0.29483600
H	-1.94955400	2.03148300	-1.32588100
H	-2.84793600	2.49816200	0.11890000
C	-1.87797200	4.77620000	-1.10997800
H	-1.00008000	4.07723900	0.73834300
H	-0.11352400	3.59385800	-0.70366100
H	-1.34857700	5.73197800	-1.11410400
H	-1.99364500	4.45020000	-2.14828700
H	-2.87760400	4.94561600	-0.69829800
H	1.79799100	-1.88503800	-0.15673600
TS2 (RS)			
C	2.85488200	-0.04864700	-1.03541500
C	-0.45431200	-0.53465800	-1.03114800
C	0.60505200	-0.80412400	0.01599600
C	1.19143000	0.36593100	0.75666700
N	2.41259200	0.80914100	0.02144600
H	-0.61516700	-1.42535900	-1.64518500
H	0.50448600	1.21947400	0.82638000
H	1.45412400	0.06861100	1.77961700
H	-0.13135800	0.26974000	-1.70592600
C	3.17291600	1.85943400	0.49988400
C	2.78743600	2.58385000	1.64676200
C	4.36158800	2.24987800	-0.15377600
C	3.55861400	3.64868700	2.10511400
H	1.88729800	2.31609200	2.18708900
C	5.11706600	3.31320200	0.31959700

H	4.69082800	1.70816100	-1.03300400
C	4.72801400	4.02777100	1.45262100
H	3.23393500	4.18573700	2.99188200
H	6.02623800	3.58551800	-0.20873200
H	5.32337900	4.85799800	1.81662900
C	0.52808800	-2.05139200	0.75842700
O	1.11930900	-2.32319700	1.79437700
O	-0.26730000	-2.97249100	0.14311200
C	-0.37989100	-4.22262500	0.81715800
H	-0.82970900	-4.08721400	1.80445700
H	-1.02166700	-4.84306900	0.19363100
H	0.60008400	-4.68852500	0.93648300
H	1.72512500	-0.86376300	-0.79170300
P	-2.13129400	-0.04145300	-0.45045500
C	-2.58797800	-1.11037300	0.95066400
C	-3.80082400	-0.70740300	1.79150500
H	-1.69430700	-1.13942500	1.58651900
H	-2.70832900	-2.11562500	0.53064200
C	-4.04337500	-1.72228400	2.91009000
H	-3.63853400	0.28363000	2.23178700
H	-4.70018800	-0.64097100	1.16975400
C	-5.23855700	-1.34068200	3.77824300
H	-4.20386700	-2.71180000	2.46585800
H	-3.14019200	-1.79815000	3.52749000
H	-5.41038900	-2.08302700	4.56116500
H	-5.07726300	-0.37174400	4.26018500
H	-6.14965800	-1.26853300	3.17646800
C	-2.08005800	1.73633400	0.01260200
C	-3.28151800	2.61566700	-0.37234100
H	-1.18529100	2.11082300	-0.49485600
H	-1.88134700	1.79176000	1.08928700
C	-4.45057200	2.59051600	0.60863900
H	-3.62856000	2.36341000	-1.38205300
H	-2.91033900	3.64396900	-0.43877100
C	-5.60758400	3.45829800	0.12215500
H	-4.80638300	1.56614500	0.75953900
H	-4.10060500	2.93857700	1.58794600
H	-6.42980500	3.46426900	0.84122300
H	-5.28283400	4.49196200	-0.03126400
H	-5.99614000	3.08595700	-0.83216200
C	-3.22710700	-0.30028800	-1.88536600
C	-4.73819200	-0.31113000	-1.63331300
H	-2.91442600	-1.25654700	-2.31995100
H	-2.95535800	0.47652500	-2.61140900

C	-5.51434400	-0.36017900	-2.94945400
H	-5.00103700	-1.18250800	-1.02239800
H	-5.04901900	0.57786900	-1.07348800
C	-7.02209000	-0.39849600	-2.72063700
H	-5.25002600	0.51871700	-3.54996700
H	-5.19806600	-1.23942400	-3.52321400
H	-7.56521400	-0.42244900	-3.66827700
H	-7.30756300	-1.28418000	-2.14513800
H	-7.35298300	0.48413200	-2.16404200
C	4.05478400	-0.89044500	-0.79268500
C	4.30847400	-1.36035400	0.50529100
C	4.92484500	-1.28046400	-1.82105900
C	5.39534800	-2.18924800	0.76206800
H	3.63442500	-1.07813000	1.30984800
C	6.00993200	-2.11233300	-1.55984200
H	4.75196100	-0.92231800	-2.83273700
C	6.25548200	-2.57119600	-0.26724500
H	5.57188600	-2.54082300	1.77452500
H	6.67175300	-2.39675400	-2.37269500
H	7.10431900	-3.21578900	-0.06360100
C	2.73984200	0.53321200	-2.34482300
N	2.60237700	0.98451500	-3.40990500

M2 (RR)

C	2.66505700	-0.62058400	-1.28097800
C	2.86271800	-0.26500400	-2.61677700
C	-0.24885300	0.79751900	-1.68708700
C	0.85987200	1.65666400	-1.06888800
C	1.63044200	1.07711200	0.14113300
N	2.84436700	0.39272800	-0.28475100
H	-0.66999800	1.34413700	-2.53424200
H	1.90090400	1.90790600	0.79338700
H	0.98021500	0.39975800	0.72482700
N	3.01301900	0.03098800	-3.74446300
H	0.18482700	-0.13558500	-2.06419500
C	3.92785400	0.31327900	0.59843900
C	3.88730000	0.82239800	1.90909800
C	5.12460000	-0.29335000	0.16925400
C	5.01002200	0.75591100	2.73337900
H	2.97777000	1.25142800	2.31159000
C	6.23215000	-0.35501000	1.00172700
H	5.16167200	-0.70935200	-0.83138800
C	6.19304700	0.17435800	2.29319300
H	4.94260500	1.15853000	3.73994700

H	7.14160400	-0.82176700	0.63408900
H	7.06201400	0.12484700	2.94027200
C	2.07505400	-1.88108500	-0.92394000
C	1.53779000	-2.76792000	-1.89351500
C	1.96353700	-2.28496200	0.43160500
C	0.90934800	-3.94856800	-1.52784700
H	1.60590500	-2.49660000	-2.94443400
C	1.33896100	-3.47786300	0.78267200
H	2.37623800	-1.64907400	1.20978500
C	0.78929400	-4.31934600	-0.18437100
H	0.49719400	-4.58966200	-2.30303100
H	1.28123100	-3.75232300	1.83338100
H	0.29594000	-5.24362600	0.09632000
C	0.35241600	3.07620800	-0.86093600
O	-0.73147300	3.47399700	-1.23508600
O	1.25776500	3.86011300	-0.28213900
C	0.87476600	5.23280600	-0.11710800
H	-0.02862700	5.29782300	0.49102100
H	1.71156600	5.71428800	0.38277000
H	0.69214400	5.68933100	-1.09094300
P	-1.69528100	0.27281600	-0.67175600
C	-1.86293900	1.34825300	0.79906600
C	-3.11288400	1.20382900	1.68632500
H	-1.80690000	2.37089400	0.41668500
H	-0.94732500	1.17368800	1.37456300
C	-4.24763700	2.13692900	1.26381400
H	-3.46624500	0.16816700	1.72848900
H	-2.81754900	1.45130400	2.71194400
C	-5.50682500	1.92104900	2.09603000
H	-3.90303000	3.17254700	1.36527200
H	-4.47694100	1.99438100	0.20190700
H	-6.29607500	2.61934100	1.80788300
H	-5.89344600	0.90415400	1.96813700
H	-5.29808400	2.06604300	3.16043100
C	-3.10792200	0.35168000	-1.84438400
C	-4.20070800	-0.72353600	-1.74198500
H	-2.61841600	0.25769900	-2.81957500
H	-3.52192800	1.36516000	-1.80111100
C	-5.27012400	-0.48944200	-0.67985100
H	-4.69085100	-0.76553500	-2.72086500
H	-3.74306800	-1.71052300	-1.60059300
C	-6.27125600	-1.63929800	-0.62213100
H	-4.80785600	-0.36591300	0.30568700
H	-5.79156700	0.45163400	-0.89330700

H	-7.04670500	-1.45067000	0.12411900
H	-6.75962300	-1.78016400	-1.59111800
H	-5.77041200	-2.57705300	-0.36025400
C	-1.37299500	-1.46989300	-0.25065200
C	-2.23541700	-2.14052500	0.82588800
H	-0.31647300	-1.52232000	0.03676000
H	-1.43990700	-1.99289900	-1.21281400
C	-1.71726300	-1.89307400	2.24344200
H	-3.28782100	-1.84089200	0.74690400
H	-2.21498900	-3.21862400	0.63082600
C	-2.67039500	-2.43867800	3.30137900
H	-0.73160600	-2.36312600	2.33510300
H	-1.55688300	-0.82171100	2.41215900
H	-2.27174000	-2.29690100	4.30852300
H	-3.64103300	-1.93328900	3.24735200
H	-2.84452000	-3.50887100	3.15281000
H	1.61090400	1.77315700	-1.86242000

M2 (RS)

C	2.52199900	0.18273200	-1.00132300
C	-0.08337300	-1.75411200	-0.41944200
C	1.05240600	-1.62244300	0.62825800
C	1.31980500	-0.21503900	1.15254000
N	1.78394200	0.69359900	0.11271700
H	-0.44420100	-2.78866400	-0.45100000
H	0.39884400	0.18067700	1.60154400
H	2.03974700	-0.29385000	1.98299500
H	0.29968500	-1.52104200	-1.41884900
C	1.86342100	2.05003300	0.44597000
C	1.48399100	2.53470200	1.71265600
C	2.30537000	2.98700100	-0.50952600
C	1.53236000	3.89976900	1.99448700
H	1.16888700	1.85816300	2.49729400
C	2.35037300	4.34071100	-0.21087300
H	2.61464600	2.62960700	-1.48459500
C	1.96094800	4.81674100	1.04263300
H	1.23492900	4.23930400	2.98232900
H	2.69558700	5.03526100	-0.97136900
H	1.99754900	5.87665600	1.26954300
C	0.77116900	-2.54398000	1.80752000
O	0.31178900	-2.15092300	2.85608100
O	0.99397300	-3.85686500	1.66133900
C	1.75737200	-4.37661900	0.56588300
H	2.77521700	-3.98169700	0.58228000

H	1.78307700	-5.45334200	0.72011400
H	1.28707600	-4.16336400	-0.39627600
H	1.96083400	-1.95842800	0.12162400
P	-1.61214900	-0.75185700	-0.26643200
C	-2.34143300	-1.05880800	1.37448400
C	-3.42112400	-0.08353300	1.85046200
H	-1.50496200	-1.05955200	2.08182100
H	-2.72107500	-2.08815700	1.33994800
C	-3.89113000	-0.43668300	3.26204100
H	-3.02120600	0.93772600	1.84939400
H	-4.28265700	-0.09392800	1.17367400
C	-4.95040000	0.53783200	3.76799500
H	-4.29021800	-1.45780200	3.26249500
H	-3.02769500	-0.43650000	3.93772500
H	-5.27972800	0.27465000	4.77594500
H	-4.55810700	1.55893100	3.79709000
H	-5.82816800	0.53451200	3.11462300
C	-1.24267100	1.00879700	-0.61558800
C	-2.26427300	1.80985700	-1.43937400
H	-0.30041200	0.95576400	-1.16929800
H	-1.01668500	1.50819900	0.33506300
C	-3.41962400	2.42756300	-0.65585800
H	-2.65048800	1.20159600	-2.26676300
H	-1.70147300	2.62119900	-1.91405500
C	-4.37037800	3.18845600	-1.57543700
H	-3.97987900	1.65708900	-0.11620500
H	-3.01168300	3.09979800	0.10865800
H	-5.18094500	3.65564000	-1.01165700
H	-3.83985700	3.97419500	-2.12181700
H	-4.81722500	2.51277600	-2.31294200
C	-2.67443800	-1.42696500	-1.58453700
C	-4.16806000	-1.10740000	-1.46253700
H	-2.52337800	-2.51208000	-1.57683100
H	-2.26216400	-1.05504300	-2.53084900
C	-4.93714900	-1.57196000	-2.69881900
H	-4.57422900	-1.60096600	-0.57154500
H	-4.32723200	-0.03153500	-1.33016000
C	-6.42864900	-1.27246700	-2.58447100
H	-4.52232300	-1.07355300	-3.58332200
H	-4.77805000	-2.64742500	-2.84023700
H	-6.96776800	-1.60100300	-3.47605400
H	-6.86406100	-1.78151400	-1.71927800
H	-6.60048500	-0.19830600	-2.46262900
C	3.89617600	-0.21680400	-0.85655000

C	4.58453500	-0.03639000	0.36669200
C	4.62218200	-0.82499700	-1.91088800
C	5.90481800	-0.44502300	0.52059500
H	4.07397100	0.44855600	1.19442400
C	5.93887100	-1.22587400	-1.74516300
H	4.12846900	-0.97999900	-2.86731500
C	6.60110300	-1.04607600	-0.52708200
H	6.39710800	-0.28650100	1.47678700
H	6.45847600	-1.69052300	-2.57935200
H	7.63027200	-1.36481600	-0.40151900
C	1.84213100	0.09579800	-2.21428400
N	1.21179700	0.02219200	-3.20659100

TS3 (RR)

C	-2.56044900	0.23234800	-0.93492300
C	-2.75395800	-0.00226500	-2.32911100
C	-0.50588200	-0.37821400	-0.55191300
C	-1.01894100	-1.80953800	-0.57373900
C	-2.27682200	-1.87962900	0.29203400
N	-3.12547600	-0.74893000	-0.06594000
H	-0.65766600	0.21601200	0.34181000
H	-1.98954900	-1.85906600	1.35316600
H	-2.79830000	-2.82786400	0.11131400
N	-2.82966300	-0.26288300	-3.46396700
H	-0.22999700	0.13372900	-1.46730000
C	-4.46461300	-0.74177200	0.30341900
C	-5.35258400	0.22119700	-0.21477100
C	-4.96913000	-1.68482000	1.21936600
C	-6.68892400	0.22428400	0.16302400
H	-4.98621900	0.96242100	-0.91591200
C	-6.31209600	-1.66707600	1.58415900
H	-4.31294800	-2.42751400	1.65816200
C	-7.18667200	-0.71815500	1.06250900
H	-7.35123900	0.97601500	-0.25625600
H	-6.67324000	-2.40810800	2.29124900
H	-8.23195900	-0.70985800	1.35154100
C	-2.41277800	1.62057100	-0.48934100
C	-2.54259500	1.95819600	0.86935900
C	-1.98480600	2.62312500	-1.37946100
C	-2.25343500	3.24475800	1.31498900
H	-2.87098300	1.19775500	1.57259400
C	-1.69449300	3.90522700	-0.92600800
H	-1.87494500	2.38698500	-2.43511200
C	-1.82477100	4.22812600	0.42512900

H	-2.36484300	3.47913000	2.36971700
H	-1.36170700	4.65817300	-1.63470700
H	-1.59778700	5.22907600	0.77660600
C	0.00235400	-2.82114100	-0.08883800
O	0.15579500	-3.16741500	1.05981100
O	0.73457200	-3.29075800	-1.10645100
C	1.73290600	-4.25920800	-0.76072200
H	2.47909200	-3.81903800	-0.09546800
H	2.19298400	-4.55780700	-1.70009700
H	1.27051500	-5.11453900	-0.26621900
P	1.73162500	-0.29957900	-0.02215400
C	2.49965100	-1.02805200	1.49115000
C	3.63402300	-0.23881900	2.15081900
H	1.67721500	-1.17010200	2.20194300
H	2.83536800	-2.03587700	1.21957600
C	4.19649700	-0.97151600	3.36931100
H	3.26414900	0.74598400	2.46252800
H	4.44186300	-0.05950500	1.43244200
C	5.30746800	-0.17979400	4.05329000
H	4.57591700	-1.95126500	3.05441700
H	3.38380300	-1.16531800	4.07992600
H	5.70501800	-0.71657700	4.91830500
H	4.93801900	0.79045800	4.39936200
H	6.13530900	0.00550300	3.36180600
C	1.68515600	1.52410300	0.23592100
C	2.92632400	2.35271100	-0.09832500
H	0.83740100	1.89019200	-0.36324600
H	1.39284800	1.67401500	1.28408100
C	2.67150700	3.84457400	0.12088400
H	3.21119300	2.18657800	-1.14517800
H	3.77800200	2.03551600	0.51440500
C	3.88442900	4.69839700	-0.23707100
H	2.39486200	4.01002400	1.16952200
H	1.80542400	4.15141700	-0.47914400
H	3.68793400	5.76032300	-0.06984600
H	4.15632600	4.56710500	-1.28902600
H	4.75107000	4.41673000	0.36905200
C	2.81872200	-0.64593700	-1.47056600
C	4.33158000	-0.68657700	-1.24048800
H	2.47678100	-1.60901900	-1.86813600
H	2.56056200	0.10484100	-2.22859600
C	5.08698200	-1.03401600	-2.52369000
H	4.56746100	-1.43498200	-0.47241900
H	4.68814000	0.27857900	-0.86152900

C	6.59518700	-1.10482200	-2.30270400
H	4.85649200	-0.28413600	-3.29022400
H	4.71951500	-1.99410400	-2.90635900
H	7.12251500	-1.35335200	-3.22701600
H	6.84357400	-1.86692300	-1.55738100
H	6.98156800	-0.14673800	-1.94150500
H	-1.25990200	-2.06070900	-1.61021900

TS3 (RS)

C	-2.38036100	0.44941600	-0.40960100
C	-2.46884700	0.80485800	-1.78871900
C	-0.26401500	-0.14885300	-0.29653700
C	-0.67546500	-1.47724300	0.31169100
C	-2.05047300	-1.92024500	-0.22168300
N	-2.97023700	-0.81127700	-0.06137000
H	-0.16978900	-0.06057700	-1.37345200
H	-1.94942000	-2.22311600	-1.27869300
H	-2.38507700	-2.79059400	0.35000600
N	-2.45573600	1.06048400	-2.92661100
H	-0.20285000	0.73958900	0.31326600
C	-4.33796200	-1.02936200	-0.29392200
C	-4.86519400	-2.31716000	-0.48719600
C	-5.22688800	0.06142500	-0.31974500
C	-6.23315400	-2.49976200	-0.67812800
H	-4.21774400	-3.18507100	-0.50392200
C	-6.58732200	-0.13691800	-0.51315000
H	-4.84203200	1.06555100	-0.18193300
C	-7.10756700	-1.41855500	-0.69167700
H	-6.61142300	-3.50673700	-0.82683000
H	-7.24750400	0.72508500	-0.52493200
H	-8.17079700	-1.56852800	-0.84436700
C	-2.40053600	1.53732700	0.57471900
C	-2.70906900	1.28140900	1.92167500
C	-1.98836900	2.83805700	0.22858000
C	-2.61683000	2.28770600	2.87791700
H	-3.02696400	0.28195000	2.20272100
C	-1.89789900	3.83918200	1.19045100
H	-1.74723200	3.06266700	-0.80830800
C	-2.20889900	3.57318200	2.52393600
H	-2.86640100	2.06403800	3.91115900
H	-1.58095800	4.83547700	0.89371200
H	-2.13599800	4.35483100	3.27268100
C	0.26922100	-2.62129200	-0.00952800
O	0.86138900	-2.76102800	-1.05657400

O	0.32535000	-3.49847400	0.99387700
C	1.13976200	-4.65579400	0.75940500
H	2.17778700	-4.35530100	0.60209900
H	1.05050400	-5.26632100	1.65470500
H	0.78133600	-5.19737800	-0.11706300
P	2.07488900	-0.16020000	-0.10943200
C	3.04524900	-1.36896300	0.90727600
C	4.23474100	-0.81589700	1.69580100
H	3.37172900	-2.14417400	0.20174700
H	2.34331400	-1.85294700	1.59839300
C	5.00339600	-1.92888900	2.40822700
H	4.91611500	-0.27126800	1.03041900
H	3.87771500	-0.09148800	2.43802500
C	6.16879600	-1.38996800	3.23282400
H	4.31277200	-2.48365700	3.05539000
H	5.37255100	-2.64377900	1.66267600
H	6.70662100	-2.19612200	3.73795400
H	6.88154600	-0.85595900	2.59671400
H	5.81418700	-0.69050000	3.99626000
C	2.88399200	-0.14321300	-1.76102200
C	4.38082800	0.17012900	-1.78273800
H	2.33147000	0.58255000	-2.37120000
H	2.68377400	-1.13007400	-2.19490600
C	4.92701200	0.26006100	-3.20787600
H	4.57527200	1.11755100	-1.26165100
H	4.92737400	-0.60838600	-1.23546500
C	6.42439300	0.55285000	-3.23676400
H	4.72021000	-0.68151100	-3.73107400
H	4.38338300	1.04361300	-3.74972300
H	6.79907400	0.61520700	-4.26152200
H	6.64500500	1.50252700	-2.73930500
H	6.98472300	-0.23257800	-2.72015800
C	2.35759100	1.50985200	0.60961400
C	1.86046400	2.62419200	-0.32138100
H	3.41127300	1.66572100	0.86208600
H	1.79493200	1.53257900	1.55296600
C	1.72293200	3.96161000	0.40378400
H	2.55360000	2.73002900	-1.16601700
H	0.88439300	2.36354200	-0.75498900
C	1.24910300	5.07377000	-0.52647700
H	1.00847000	3.84077200	1.22775000
H	2.68525100	4.23181900	0.85558400
H	1.12383500	6.01807300	0.00977500
H	1.96517300	5.23816800	-1.33764400

H	0.28657600	4.81394800	-0.98058000
H	-0.74298500	-1.37211200	1.39800500

P(RR)

C	0.02526600	0.55670900	0.57058600
C	0.19562500	0.38607600	2.04694100
C	-1.42429600	1.01766500	0.29786800
C	-2.22318700	-0.28898100	0.36300200
C	-1.27719000	-1.28884100	-0.31325000
N	0.06228400	-0.73522600	-0.08953800
H	-1.75478900	1.78294200	1.00165200
H	-1.36512200	-2.28611000	0.12900800
H	-1.49795900	-1.35854100	-1.38487500
N	0.29196200	0.21868800	3.18703700
H	-1.45606600	1.41991500	-0.71900000
C	1.18428700	-1.56348700	-0.08965500
C	1.12238700	-2.80686800	-0.74306600
C	2.39021800	-1.19260400	0.52963900
C	2.22733100	-3.65002000	-0.76318500
H	0.21329500	-3.10940600	-1.25028600
C	3.48673200	-2.04806300	0.49730400
H	2.48346800	-0.24010400	1.03744200
C	3.41904100	-3.28202100	-0.14367600
H	2.15055000	-4.60438000	-1.27496500
H	4.40497200	-1.73878600	0.98699300
H	4.27891100	-3.94239700	-0.16149000
C	1.02474100	1.57505600	0.02355900
C	1.37989300	1.51758700	-1.32491700
C	1.52158400	2.59922300	0.82803700
C	2.23046900	2.47891100	-1.86141600
H	0.99373600	0.71364000	-1.94442900
C	2.37145400	3.56183700	0.28644800
H	1.25204000	2.64789900	1.87946700
C	2.72869800	3.50288700	-1.05738500
H	2.50835300	2.42532000	-2.90899300
H	2.75518300	4.35475500	0.91981600
H	3.39581300	4.24874800	-1.47672400
C	-3.54056700	-0.15529900	-0.36736200
O	-3.63779600	-0.01138400	-1.56498200
O	-4.58112400	-0.18395800	0.46479900
C	-5.86493500	-0.02233600	-0.15246200
H	-6.02897800	-0.80969000	-0.88966200
H	-6.59211100	-0.09227300	0.65301600
H	-5.92603000	0.95080400	-0.64263600

H	-2.40892700	-0.56842300	1.40258400
P (RS)			
C	0.08926100	0.41654900	0.86123300
C	0.74202100	0.33272600	2.19474300
C	-1.44898900	0.45018400	1.07492200
C	-1.97843000	-0.24198600	-0.18433000
C	-0.97757700	-1.38950300	-0.35799200
N	0.27584300	-0.81540000	0.11663900
H	-1.81286100	1.46887300	1.21163100
H	-0.88650200	-1.69656300	-1.40462300
H	-1.28467400	-2.25845000	0.23993400
N	1.22788700	0.26753900	3.24148700
H	-1.71494500	-0.15319200	1.94770400
C	1.50707700	-1.41612300	-0.11224200
C	1.56354600	-2.71003600	-0.65961300
C	2.71636700	-0.76088200	0.18385800
C	2.78947500	-3.31828100	-0.90549100
H	0.64985200	-3.24815900	-0.88350700
C	3.93228200	-1.38915400	-0.06117400
H	2.71357700	0.24447800	0.58909100
C	3.98468300	-2.66855000	-0.60882000
H	2.80353600	-4.31817600	-1.32829500
H	4.85031800	-0.86060200	0.17626200
H	4.93790200	-3.14914400	-0.79906500
C	0.56794000	1.67268400	0.12012400
C	0.75875100	1.63486200	-1.26018600
C	0.74818100	2.87259200	0.81082700
C	1.12448100	2.79180000	-1.94554800
H	0.63344700	0.69749900	-1.79395300
C	1.11347900	4.02643400	0.12397200
H	0.60545300	2.90690600	1.88805600
C	1.30242900	3.98809900	-1.25650800
H	1.27527100	2.75386000	-3.01938600
H	1.25354700	4.95468400	0.66798600
H	1.59069600	4.88697500	-1.79140600
C	-3.39089900	-0.74402500	0.01696900
O	-3.71183300	-1.51918500	0.88895000
O	-4.24022700	-0.22972400	-0.87126300
C	-5.60444400	-0.64813800	-0.73217100
H	-5.67836000	-1.73171400	-0.83637000
H	-6.14970100	-0.14800800	-1.52897300
H	-5.99030300	-0.35039200	0.24408900
H	-1.94368000	0.43191500	-1.04300000

R-TS1

C	3.13577200	-1.20639300	0.30404400
C	2.91132400	-2.50738600	0.75144100
C	-0.96907900	-0.68533000	1.18826500
C	-0.09574700	-1.80175700	0.59661400
C	0.83613600	-1.32315400	-0.52333600
N	1.88469600	-0.45877800	0.03123800
H	-1.49014300	-1.05225900	2.07636400
H	1.25650700	-2.19417600	-1.03699900
H	0.25964800	-0.76924700	-1.27358700
N	2.70548100	-3.60720200	1.11950800
H	-0.30682500	0.13248400	1.49787900
C	2.01862500	0.77691300	-0.67566100
C	1.88807800	1.96995100	0.03761400
C	2.28034600	0.82251200	-2.04799900
C	2.06636500	3.19530200	-0.60077100
H	1.69043900	1.91535100	1.10441300
C	2.44141000	2.04744200	-2.69037700
H	2.38676000	-0.10970100	-2.59688800
C	2.34911500	3.23592300	-1.96562100
H	1.98677900	4.11820500	-0.03400100
H	2.65576400	2.07557700	-3.75413500
H	2.48753700	4.19018100	-2.46379900
C	4.48512800	-0.71342200	0.34853300
C	4.94040700	0.60413100	0.04751100
C	5.52796600	-1.61821000	0.73447400
C	6.28397600	0.95897200	0.13129500
H	4.24992500	1.37486000	-0.25903600
C	6.85668500	-1.24754600	0.81180600
H	5.26342500	-2.64252800	0.97823200
C	7.27078500	0.05531400	0.51224500
H	6.55591500	1.98399900	-0.11194000
H	7.58748400	-1.99442200	1.11406700
H	8.31371800	0.34625600	0.57355000
C	-0.86579700	-3.04734300	0.20157100
O	-0.64535200	-3.71797700	-0.77946300
O	-1.81512200	-3.34732000	1.09890000
C	-2.55627000	-4.54664900	0.83350800
H	-1.88444700	-5.40560000	0.81086200
H	-3.27299500	-4.63787300	1.64600500
H	-3.07072100	-4.46619500	-0.12713200
P	-2.26712100	0.05176100	0.12324100
C	-3.62142100	0.60472200	1.20955400

C	-3.17845900	1.23601000	2.53764900
H	-4.24847500	-0.27416000	1.39998500
H	-4.22450500	1.30866300	0.62321400
C	-4.35983500	1.89802700	3.24698600
H	-2.75262800	0.46469100	3.18805300
H	-2.39198400	1.98179100	2.37788200
C	-3.95868100	2.48770300	4.59542000
H	-4.76746100	2.68476800	2.60081000
H	-5.15754200	1.15814900	3.38267800
H	-4.81104800	2.96132200	5.08808000
H	-3.57231900	1.71100100	5.26211900
H	-3.17713100	3.24376000	4.47315900
C	-1.66710600	1.47007400	-0.85516500
C	-1.57475400	2.80616000	-0.11105400
H	-2.36939400	1.56238400	-1.69140200
H	-0.69150100	1.20443200	-1.27933100
C	-1.25726900	3.93990800	-1.08612700
H	-2.52142700	3.03104800	0.39440100
H	-0.79612100	2.75241200	0.66028300
C	-1.05184200	5.26962500	-0.36829600
H	-0.35935000	3.68054100	-1.65765700
H	-2.07871100	4.02618900	-1.80758200
H	-0.83083200	6.07119000	-1.07728400
H	-1.94599800	5.55360500	0.19520400
H	-0.21902800	5.20494200	0.33910300
C	-2.94587500	-1.19216300	-1.02057700
C	-4.14532700	-0.70590400	-1.84282900
H	-3.24267500	-2.04194900	-0.39615700
H	-2.13376400	-1.52985900	-1.67573600
C	-4.68460600	-1.82568200	-2.73413600
H	-4.94329400	-0.36073000	-1.17470800
H	-3.86156700	0.14529800	-2.47128200
C	-5.88265800	-1.36800700	-3.56042400
H	-3.88344600	-2.17307300	-3.39679400
H	-4.96625600	-2.67981600	-2.10695600
H	-6.25706400	-2.17657700	-4.19256200
H	-6.70104700	-1.03894800	-2.91293900
H	-5.61091600	-0.53016800	-4.20952900
H	0.54173300	-2.13645800	1.42483600

R-TS2

C	-3.53850800	0.65255900	0.17718300
C	-0.31760900	0.89566700	-1.00727300
C	-0.88084800	2.09775500	-0.24238700

C	-1.55213200	1.72201600	1.12091000
N	-2.36718000	0.53416000	1.03623100
H	-0.23820900	1.13404500	-2.07423100
H	-0.78196300	1.57317700	1.88048400
H	-2.13220500	2.60301400	1.42484500
H	-1.04772700	0.08402700	-0.91840900
C	-1.90900000	-0.58012400	1.77248100
C	-1.67303400	-0.45155100	3.15083100
C	-1.51431000	-1.77631500	1.14931500
C	-1.05365100	-1.46810600	3.87349600
H	-1.97529500	0.46498300	3.64942400
C	-0.92414400	-2.80506100	1.87986400
H	-1.66652900	-1.89248000	0.08088500
C	-0.68022200	-2.65418100	3.24396700
H	-0.87538500	-1.33591900	4.93621600
H	-0.62907800	-3.71839600	1.37047300
H	-0.19978100	-3.44804200	3.80603600
C	0.13010000	3.16869500	0.06639700
O	1.31761000	2.96770100	0.24459400
O	-0.43842000	4.36021500	0.21690700
C	0.43656200	5.42154900	0.62660600
H	1.21987100	5.56825000	-0.11827200
H	-0.19039600	6.30641300	0.70369300
H	0.88948900	5.18330000	1.59018000
H	-1.66667400	2.53350100	-0.86606600
P	1.32080600	0.16978600	-0.60882300
C	2.56245600	1.06672400	-1.60853700
C	3.99571100	1.08211900	-1.07891100
H	2.18901000	2.08900000	-1.69011900
H	2.51690200	0.61477800	-2.60681200
C	4.87526500	2.02667700	-1.89815200
H	4.00131900	1.40188100	-0.02930200
H	4.42276500	0.07343200	-1.11370400
C	6.31818600	2.03676800	-1.40267300
H	4.84325000	1.72573000	-2.95207600
H	4.45395700	3.03776600	-1.84688700
H	6.93374200	2.72208800	-1.99027200
H	6.36825400	2.35083200	-0.35555800
H	6.76229200	1.03921700	-1.47474200
C	1.61020900	0.07484700	1.20095400
C	2.36755600	-1.13892400	1.76372400
H	0.59366100	0.04717700	1.60615800
H	2.05757900	1.02287400	1.51235600
C	3.89011100	-1.03716000	1.75363700

H	2.04254800	-2.06160700	1.26631300
H	2.03517100	-1.24528000	2.80291300
C	4.53493400	-2.28211800	2.35654600
H	4.26355100	-0.89616300	0.73450400
H	4.19120600	-0.14435800	2.31502900
H	5.62363600	-2.19524700	2.37845500
H	4.18626400	-2.44512200	3.38090900
H	4.27877700	-3.17201000	1.77148000
C	1.21670900	-1.53165000	-1.25906600
C	2.56215000	-2.21417800	-1.52763000
H	0.62881100	-1.47885000	-2.18301900
H	0.62551100	-2.10409200	-0.53464300
C	2.36913900	-3.67907000	-1.91874500
H	3.09122800	-1.68887400	-2.33173100
H	3.20647400	-2.16643800	-0.64184300
C	3.69662200	-4.37633500	-2.19912700
H	1.83987200	-4.19555900	-1.10857200
H	1.72123300	-3.73328900	-2.80167000
H	3.54303900	-5.42167400	-2.47739000
H	4.23092500	-3.88380700	-3.01715000
H	4.34198700	-4.35378400	-1.31529300
C	-4.13430200	-0.33742700	-0.69472900
C	-4.18925000	-1.73154300	-0.44059700
C	-4.82025900	0.09366900	-1.86577600
C	-4.82488200	-2.61404900	-1.31048300
H	-3.78034700	-2.12681500	0.47957200
C	-5.47282200	-0.78808600	-2.71033200
H	-4.81813300	1.15366100	-2.10540100
C	-5.47155600	-2.16395400	-2.45790800
H	-4.83493300	-3.67299100	-1.06376000
H	-5.97213700	-0.39918100	-3.59436200
H	-5.97079100	-2.85594600	-3.12775300
C	-4.09280300	1.92896800	0.15447500
N	-4.52805400	3.02406500	0.11820800

M2 (SR)

C	-2.52199900	0.18273200	-1.00132300
C	0.08337300	-1.75411200	-0.41944200
C	-1.05240600	-1.62244300	0.62825800
C	-1.31980500	-0.21503900	1.15254000
N	-1.78394200	0.69359900	0.11271700
H	0.44420100	-2.78866400	-0.45100000
H	-0.39884400	0.18067700	1.60154400
H	-2.03974700	-0.29385000	1.98299500

H	-0.29968500	-1.52104200	-1.41884900
C	-1.86342100	2.05003300	0.44597000
C	-1.48399100	2.53470200	1.71265600
C	-2.30537000	2.98700100	-0.50952600
C	-1.53236000	3.89976900	1.99448700
H	-1.16888700	1.85816300	2.49729400
C	-2.35037300	4.34071100	-0.21087300
H	-2.61464600	2.62960700	-1.48459500
C	-1.96094800	4.81674100	1.04263300
H	-1.23492900	4.23930400	2.98232900
H	-2.69558700	5.03526100	-0.97136900
H	-1.99754900	5.87665600	1.26954300
C	-0.77116900	-2.54398000	1.80752000
O	-0.31178900	-2.15092300	2.85608100
O	-0.99397300	-3.85686500	1.66133900
C	-1.75737200	-4.37661900	0.56588300
H	-2.77521700	-3.98169700	0.58228000
H	-1.78307700	-5.45334200	0.72011400
H	-1.28707600	-4.16336400	-0.39627600
H	-1.96083400	-1.95842800	0.12162400
P	1.61214900	-0.75185700	-0.26643200
C	2.34143300	-1.05880800	1.37448400
C	3.42112400	-0.08353300	1.85046200
H	1.50496200	-1.05955200	2.08182100
H	2.72107500	-2.08815700	1.33994800
C	3.89113000	-0.43668300	3.26204100
H	3.02120600	0.93772600	1.84939400
H	4.28265700	-0.09392800	1.17367400
C	4.95040000	0.53783200	3.76799500
H	4.29021800	-1.45780200	3.26249500
H	3.02769500	-0.43650000	3.93772500
H	5.27972800	0.27465000	4.77594500
H	4.55810700	1.55893100	3.79709000
H	5.82816800	0.53451200	3.11462300
C	1.24267100	1.00879700	-0.61558800
C	2.26427300	1.80985700	-1.43937400
H	0.30041200	0.95576400	-1.16929800
H	1.01668500	1.50819900	0.33506300
C	3.41962400	2.42756300	-0.65585800
H	2.65048800	1.20159600	-2.26676300
H	1.70147300	2.62119900	-1.91405500
C	4.37037800	3.18845600	-1.57543700
H	3.97987900	1.65708900	-0.11620500
H	3.01168300	3.09979800	0.10865800

H	5.18094500	3.65564000	-1.01165700
H	3.83985700	3.97419500	-2.12181700
H	4.81722500	2.51277600	-2.31294200
C	2.67443800	-1.42696500	-1.58453700
C	4.16806000	-1.10740000	-1.46253700
H	2.52337800	-2.51208000	-1.57683100
H	2.26216400	-1.05504300	-2.53084900
C	4.93714900	-1.57196000	-2.69881900
H	4.57422900	-1.60096600	-0.57154500
H	4.32723200	-0.03153500	-1.33016000
C	6.42864900	-1.27246700	-2.58447100
H	4.52232300	-1.07355300	-3.58332200
H	4.77805000	-2.64742500	-2.84023700
H	6.96776800	-1.60100300	-3.47605400
H	6.86406100	-1.78151400	-1.71927800
H	6.60048500	-0.19830600	-2.46262900
C	-3.89617600	-0.21680400	-0.85655000
C	-4.58453500	-0.03639000	0.36669200
C	-4.62218200	-0.82499700	-1.91088800
C	-5.90481800	-0.44502300	0.52059500
H	-4.07397100	0.44855600	1.19442400
C	-5.93887100	-1.22587400	-1.74516300
H	-4.12846900	-0.97999900	-2.86731500
C	-6.60110300	-1.04607600	-0.52708200
H	-6.39710800	-0.28650100	1.47678700
H	-6.45847600	-1.69052300	-2.57935200
H	-7.63027200	-1.36481600	-0.40151900
C	-1.84213100	0.09579800	-2.21428400
N	-1.21179700	0.02219200	-3.20659100

TS3 (SR)

C	2.51792100	0.59888200	-0.51672800
C	0.48031000	-0.24025500	-0.34621800
C	1.03337800	-1.21000000	0.69034400
C	2.44111300	-1.66855500	0.29080500
N	3.24325200	-0.47698200	0.09201900
H	0.24503700	0.78279100	-0.08311300
H	2.38538900	-2.28897000	-0.61716700
H	2.86167700	-2.28541200	1.09226400
H	0.48630200	-0.51622900	-1.39504600
C	4.62089500	-0.60946400	-0.11763200
C	5.26984600	-1.85121300	-0.01019800
C	5.39876000	0.52130400	-0.43151600
C	6.64719700	-1.94752300	-0.19498400

H	4.70772900	-2.75163400	0.20555900
C	6.77001500	0.40770200	-0.61529000
H	4.91888200	1.48945400	-0.52451300
C	7.41142800	-0.82550900	-0.49749700
H	7.12032500	-2.92106000	-0.10706000
H	7.34377700	1.29787800	-0.85530500
H	8.48280600	-0.90833900	-0.64426400
C	0.14759300	-2.42276100	0.92340300
O	-0.57174600	-2.57408200	1.88581800
O	0.25896700	-3.32542300	-0.05562300
C	-0.42456100	-4.56935400	0.16025900
H	-0.04843800	-5.04360300	1.06808900
H	-0.20481100	-5.17968800	-0.71241900
H	-1.49887400	-4.40735200	0.25574600
H	1.08709700	-0.68769600	1.65026900
P	-1.84349600	-0.46312800	-0.23283800
C	-2.28247600	0.24602100	1.41276500
C	-3.73407600	0.22894400	1.89097900
H	-1.66236800	-0.31058200	2.12603800
H	-1.89516400	1.27386300	1.39591800
C	-3.86492700	0.79160900	3.30712000
H	-4.11543500	-0.79971000	1.87808900
H	-4.36901600	0.81091800	1.21355600
C	-5.30718300	0.76558900	3.80504600
H	-3.48288200	1.81959600	3.32279600
H	-3.22591300	0.21117500	3.98364600
H	-5.38725700	1.16692000	4.81842200
H	-5.69658700	-0.25726400	3.81569400
H	-5.95457500	1.36214000	3.15477800
C	-2.80421400	-2.01194000	-0.58054100
C	-4.09166800	-1.94515700	-1.41631600
H	-2.07624700	-2.64005800	-1.10590700
H	-2.98247000	-2.49167900	0.39007000
C	-5.36009300	-1.60020600	-0.64108800
H	-3.96389200	-1.24381100	-2.25079100
H	-4.23163000	-2.93003700	-1.87832600
C	-6.58167800	-1.54688200	-1.55452100
H	-5.24462300	-0.63825300	-0.13281800
H	-5.51028800	-2.34772700	0.14785900
H	-7.49129000	-1.32133000	-0.99272600
H	-6.72858700	-2.50224200	-2.06789200
H	-6.45805800	-0.77331000	-2.32025500
C	-2.25661600	0.77826100	-1.52615600
C	-3.56815900	1.55781900	-1.41497800

H	-1.41581900	1.48628800	-1.53021600
H	-2.20353500	0.24574000	-2.48447900
C	-3.73857500	2.54597700	-2.56892100
H	-3.59023400	2.10600900	-0.46487500
H	-4.42309500	0.87159400	-1.40456700
C	-5.04867700	3.32234800	-2.47204300
H	-3.69947500	1.99791900	-3.51837100
H	-2.89030700	3.24123400	-2.57523700
H	-5.15775900	4.02746600	-3.29978500
H	-5.09687300	3.88960400	-1.53729900
H	-5.90600600	2.64195300	-2.49347000
C	2.38721500	1.86169700	0.21986100
C	2.74787900	1.94721100	1.57562300
C	1.79592200	2.99024300	-0.37862300
C	2.53696000	3.11843300	2.29590100
H	3.20499500	1.08356800	2.04920300
C	1.58678300	4.15682000	0.34835100
H	1.50630300	2.94667000	-1.42606700
C	1.95574100	4.23230500	1.69109700
H	2.83212900	3.16118100	3.34036400
H	1.13117700	5.01391900	-0.13878600
H	1.79210600	5.14414400	2.25571900
C	2.60506600	0.67465200	-1.93877200
N	2.60156800	0.69625900	-3.10480500

M2 (SS)

C	-2.66505700	-0.62058400	-1.28097800
C	-2.86271800	-0.26500400	-2.61677700
C	0.24885300	0.79751900	-1.68708700
C	-0.85987200	1.65666400	-1.06888800
C	-1.63044200	1.07711200	0.14113300
N	-2.84436700	0.39272800	-0.28475100
H	0.66999800	1.34413700	-2.53424200
H	-1.90090400	1.90790600	0.79338700
H	-0.98021500	0.39975800	0.72482700
N	-3.01301900	0.03098800	-3.74446300
H	-0.18482700	-0.13558500	-2.06419500
C	-3.92785400	0.31327900	0.59843900
C	-3.88730000	0.82239800	1.90909800
C	-5.12460000	-0.29335000	0.16925400
C	-5.01002200	0.75591100	2.73337900
H	-2.97777000	1.25142800	2.31159000
C	-6.23215000	-0.35501000	1.00172700
H	-5.16167200	-0.70935200	-0.83138800

C	-6.19304700	0.17435800	2.29319300
H	-4.94260500	1.15853000	3.73994700
H	-7.14160400	-0.82176700	0.63408900
H	-7.06201400	0.12484700	2.94027200
C	-2.07505400	-1.88108500	-0.92394000
C	-1.53779000	-2.76792000	-1.89351500
C	-1.96353700	-2.28496200	0.43160500
C	-0.90934800	-3.94856800	-1.52784700
H	-1.60590500	-2.49660000	-2.94443400
C	-1.33896100	-3.47786300	0.78267200
H	-2.37623800	-1.64907400	1.20978500
C	-0.78929400	-4.31934600	-0.18437100
H	-0.49719400	-4.58966200	-2.30303100
H	-1.28123100	-3.75232300	1.83338100
H	-0.29594000	-5.24362600	0.09632000
C	-0.35241600	3.07620800	-0.86093600
O	0.73147300	3.47399700	-1.23508600
O	-1.25776500	3.86011300	-0.28213900
C	-0.87476600	5.23280600	-0.11710800
H	0.02862700	5.29782300	0.49102100
H	-1.71156600	5.71428800	0.38277000
H	-0.69214400	5.68933100	-1.09094300
P	1.69528100	0.27281600	-0.67175600
C	1.86293900	1.34825300	0.79906600
C	3.11288400	1.20382900	1.68632500
H	1.80690000	2.37089400	0.41668500
H	0.94732500	1.17368800	1.37456300
C	4.24763700	2.13692900	1.26381400
H	3.46624500	0.16816700	1.72848900
H	2.81754900	1.45130400	2.71194400
C	5.50682500	1.92104900	2.09603000
H	3.90303000	3.17254700	1.36527200
H	4.47694100	1.99438100	0.20190700
H	6.29607500	2.61934100	1.80788300
H	5.89344600	0.90415400	1.96813700
H	5.29808400	2.06604300	3.16043100
C	3.10792200	0.35168000	-1.84438400
C	4.20070800	-0.72353600	-1.74198500
H	2.61841600	0.25769900	-2.81957500
H	3.52192800	1.36516000	-1.80111100
C	5.27012400	-0.48944200	-0.67985100
H	4.69085100	-0.76553500	-2.72086500
H	3.74306800	-1.71052300	-1.60059300
C	6.27125600	-1.63929800	-0.62213100

H	4.80785600	-0.36591300	0.30568700
H	5.79156700	0.45163400	-0.89330700
H	7.04670500	-1.45067000	0.12411900
H	6.75962300	-1.78016400	-1.59111800
H	5.77041200	-2.57705300	-0.36025400
C	1.37299500	-1.46989300	-0.25065200
C	2.23541700	-2.14052500	0.82588800
H	0.31647300	-1.52232000	0.03676000
H	1.43990700	-1.99289900	-1.21281400
C	1.71726300	-1.89307400	2.24344200
H	3.28782100	-1.84089200	0.74690400
H	2.21498900	-3.21862400	0.63082600
C	2.67039500	-2.43867800	3.30137900
H	0.73160600	-2.36312600	2.33510300
H	1.55688300	-0.82171100	2.41215900
H	2.27174000	-2.29690100	4.30852300
H	3.64103300	-1.93328900	3.24735200
H	2.84452000	-3.50887100	3.15281000
H	-1.61090400	1.77315700	-1.86242000

TS3 (SS)

C	-2.38033500	-0.22249300	1.01346700
C	-2.38020000	-0.76908800	2.32952900
C	-0.30343400	-0.54942700	0.38942700
C	-0.73448300	-1.89743600	-0.16978900
C	-2.07958700	-1.73251000	-0.88484200
N	-2.98665900	-1.04006000	0.01406800
H	-0.46519800	0.32968500	-0.21911300
H	-1.92101500	-1.18508000	-1.82693500
H	-2.47792700	-2.72063200	-1.14236200
N	-2.27678400	-1.23781700	3.39294500
H	-0.07509900	-0.41607300	1.44073600
C	-4.34712500	-0.98177100	-0.26801100
C	-4.87769400	-1.54646100	-1.44261800
C	-5.23468800	-0.34752000	0.62310600
C	-6.24612800	-1.49475700	-1.69534400
H	-4.22580900	-2.01654400	-2.16943200
C	-6.59550700	-0.30336300	0.35309900
H	-4.84612100	0.10727400	1.52758800
C	-7.11948900	-0.87807700	-0.80500600
H	-6.62679900	-1.93938100	-2.61019300
H	-7.25578100	0.18854300	1.06138900
H	-8.18373900	-0.83954300	-1.00973000
C	-2.36278100	1.23778400	0.87913300

C	-2.73505300	1.85674300	-0.32722700
C	-1.81655300	2.04602600	1.89395900
C	-2.57506300	3.22863200	-0.50238100
H	-3.15031100	1.25254500	-1.12915200
C	-1.65171700	3.41391900	1.70845200
H	-1.51447500	1.58878400	2.83334200
C	-2.03126800	4.01855000	0.50967200
H	-2.87587200	3.68374500	-1.44197600
H	-1.22321800	4.01278200	2.50709400
H	-1.90363000	5.08678700	0.36683800
C	0.26885300	-2.47233900	-1.15530300
O	0.29932300	-2.21631800	-2.33688100
O	1.12537500	-3.30703500	-0.55534700
C	2.06556800	-3.96818500	-1.41500400
H	2.51309400	-3.26055300	-2.11312700
H	2.81902100	-4.39657300	-0.75748100
H	1.55661800	-4.75467300	-1.97532300
P	1.95732600	-0.26897000	0.12507100
C	2.77060000	-1.14039300	1.52639100
C	4.25018400	-0.84083500	1.77416700
H	2.62332400	-2.21092700	1.33767900
H	2.18014700	-0.89704700	2.41905500
C	4.78204300	-1.58230700	3.00108600
H	4.83933200	-1.13506000	0.89636900
H	4.40204700	0.23741000	1.91169700
C	6.26180300	-1.30315700	3.24819900
H	4.19506900	-1.28939200	3.87986700
H	4.62281900	-2.65894900	2.86519900
H	6.62762000	-1.84210300	4.12572800
H	6.86504100	-1.60996900	2.38812000
H	6.43460200	-0.23504800	3.41267700
C	3.09087800	-0.45638500	-1.32966700
C	4.21335600	0.57896000	-1.46550500
H	2.46942500	-0.46457500	-2.23207700
H	3.51949000	-1.46261400	-1.23743400
C	5.13028500	0.26541400	-2.64833700
H	3.78465400	1.57941200	-1.60054800
H	4.81022400	0.61845700	-0.54682700
C	6.23426500	1.30687500	-2.80956600
H	5.57242200	-0.72838600	-2.50723500
H	4.52979000	0.21298800	-3.56458500
H	6.88135800	1.07232200	-3.65836500
H	5.80941600	2.30198000	-2.97365700
H	6.85873000	1.35408000	-1.91206000

C	1. 98119900	1. 51729600	0. 56577000
C	1. 30459300	2. 40423600	-0. 48955000
H	3. 01795600	1. 83442400	0. 72584400
H	1. 46239500	1. 61919800	1. 52771400
C	1. 59814800	3. 88724700	-0. 26735700
H	1. 63484600	2. 11871200	-1. 49790200
H	0. 21641600	2. 26250900	-0. 46152700
C	1. 01336900	4. 75953800	-1. 37396900
H	1. 18496400	4. 18631600	0. 70431500
H	2. 68404200	4. 03673500	-0. 20973400
H	1. 19582200	5. 82061400	-1. 18487400
H	1. 45838400	4. 50802200	-2. 34206500
H	-0. 06775300	4. 60887800	-1. 45197800
H	-0. 83392200	-2. 60086400	0. 66121800

P (SR)

C	-0. 08926100	0. 41654900	0. 86123300
C	-0. 74202100	0. 33272600	2. 19474300
C	1. 44898900	0. 45018400	1. 07492200
C	1. 97843000	-0. 24198600	-0. 18433000
C	0. 97757700	-1. 38950300	-0. 35799200
N	-0. 27584300	-0. 81540000	0. 11663900
H	1. 81286100	1. 46887300	1. 21163100
H	0. 88650200	-1. 69656300	-1. 40462300
H	1. 28467400	-2. 25845000	0. 23993400
N	-1. 22788700	0. 26753900	3. 24148700
H	1. 71494500	-0. 15319200	1. 94770400
C	-1. 50707700	-1. 41612300	-0. 11224200
C	-1. 56354600	-2. 71003600	-0. 65961300
C	-2. 71636700	-0. 76088200	0. 18385800
C	-2. 78947500	-3. 31828100	-0. 90549100
H	-0. 64985200	-3. 24815900	-0. 88350700
C	-3. 93228200	-1. 38915400	-0. 06117400
H	-2. 71357700	0. 24447800	0. 58909100
C	-3. 98468300	-2. 66855000	-0. 60882000
H	-2. 80353600	-4. 31817600	-1. 32829500
H	-4. 85031800	-0. 86060200	0. 17626200
H	-4. 93790200	-3. 14914400	-0. 79906500
C	-0. 56794000	1. 67268400	0. 12012400
C	-0. 75875100	1. 63486200	-1. 26018600
C	-0. 74818100	2. 87259200	0. 81082700
C	-1. 12448100	2. 79180000	-1. 94554800
H	-0. 63344700	0. 69749900	-1. 79395300
C	-1. 11347900	4. 02643400	0. 12397200

H	-0.60545300	2.90690600	1.88805600
C	-1.30242900	3.98809900	-1.25650800
H	-1.27527100	2.75386000	-3.01938600
H	-1.25354700	4.95468400	0.66798600
H	-1.59069600	4.88697500	-1.79140600
C	3.39089900	-0.74402500	0.01696900
O	3.71183300	-1.51918500	0.88895000
O	4.24022700	-0.22972300	-0.87126300
C	5.60444400	-0.64813700	-0.73217100
H	5.67836000	-1.73171300	-0.83637000
H	6.14970100	-0.14800700	-1.52897300
H	5.99030300	-0.35039100	0.24408900
H	1.94368000	0.43191500	-1.04300000

P(SS)

C	-0.01343200	0.55003500	0.56917500
C	-0.18360300	0.39070100	2.04662200
C	1.44362200	0.98405900	0.29030600
C	2.21910300	-0.33730900	0.35980000
C	1.25408500	-1.32370500	-0.30666400
N	-0.07467300	-0.74502800	-0.08292600
H	1.79023400	1.74693000	0.98890000
H	1.47204300	-1.40442400	-1.37799400
H	1.32509400	-2.31973800	0.14165000
N	-0.28059100	0.23023900	3.18763600
H	1.47789800	1.38125600	-0.72856100
C	-1.21194500	-1.55182400	-0.08140900
C	-1.17359400	-2.79586000	-0.73507600
C	-2.41009800	-1.15929300	0.53998000
C	-2.29405100	-3.61840700	-0.75493100
H	-0.27061100	-3.11464000	-1.24325900
C	-3.52226600	-1.99434100	0.50792600
H	-2.48435900	-0.20597900	1.04945300
C	-3.47818800	-3.22873500	-0.13428800
H	-2.23531900	-4.57355400	-1.26767000
H	-4.43418400	-1.66866600	0.99886200
H	-4.35018500	-3.87302300	-0.15173600
C	-0.99562600	1.58300600	0.01814600
C	-1.34820400	1.52839000	-1.33122200
C	-1.47933100	2.61580600	0.81957300
C	-2.18313100	2.50109900	-1.87151200
H	-0.97271200	0.71736500	-1.94805100
C	-2.31360100	3.58980100	0.27410200
H	-1.21169400	2.66224000	1.87158000

C	-2.66836400	3.53364400	-1.07044800
H	-2.45926800	2.44972300	-2.91966400
H	-2.68704400	4.38955200	0.90503700
H	-3.32331100	4.28854000	-1.49281700
C	3.53856700	-0.22839900	-0.37142100
O	3.64579800	-0.18349500	-1.57561200
O	4.56932100	-0.14904200	0.47025600
C	5.85473700	0.00597500	-0.14540200
H	5.87772700	0.91770200	-0.74424000
H	6.56985600	0.06505600	0.67166100
H	6.07122300	-0.85167000	-0.78434800
H	2.40244000	-0.61070000	1.40154100

React-(S)

C	0.53515400	-0.96477600	0.72277600
C	0.68236500	-0.87193400	2.20504400
C	-1.85472400	-1.27851400	-1.66688700
C	-2.38800300	-0.83194100	-0.53179500
C	-1.65760600	0.04778500	0.46518700
N	-0.22823000	0.14509200	0.19152400
H	-2.41682500	-1.93090200	-2.32608300
H	-1.82446900	-0.35010300	1.47922200
H	-2.07522300	1.05620000	0.47563300
N	0.75121100	-0.78169000	3.35553600
H	-0.84737500	-0.99729300	-1.95470100
C	0.34593400	1.43866700	0.12653200
C	-0.28175700	2.40054500	-0.67832500
C	1.52855800	1.78125300	0.79104100
C	0.24258200	3.68208900	-0.78676800
H	-1.17205600	2.12786000	-1.23845700
C	2.05449600	3.06559000	0.66241900
H	2.04991300	1.05858400	1.40828600
C	1.41613900	4.02464700	-0.11640600
H	-0.26066500	4.41071100	-1.41422800
H	2.97152400	3.31245800	1.18773600
H	1.83032100	5.02270900	-0.20852800
C	1.87437600	-1.20472700	0.03105000
C	2.89683000	-1.88819700	0.68950800
C	2.05624800	-0.80242300	-1.29248800
C	4.08986700	-2.17044300	0.02857900
H	2.76648100	-2.20072200	1.72185300
C	3.25046800	-1.08464000	-1.94978300
H	1.27344600	-0.25001100	-1.80151300
C	4.26984400	-1.76967800	-1.29240300

H	4.87925500	-2.70072100	0.55083800
H	3.38474000	-0.76180800	-2.97694600
H	5.20103100	-1.98541800	-1.80567600
C	-3.76630100	-1.30542700	-0.15796200
O	-4.05345000	-2.47676100	-0.09714900
O	-4.70084300	-0.39231100	0.15220400
C	-4.56704800	0.97885000	-0.23571200
H	-3.86957000	1.09197100	-1.06860300
H	-4.24450600	1.57752200	0.61836200
H	-5.55684200	1.30638900	-0.55139700
H	-0.08023600	-1.85902500	0.55270000

TS1 (S)

C	-3.34614600	0.83580900	-0.34346500
C	-3.63300200	2.24197900	0.02264800
C	-0.16318100	1.16915400	-1.19527500
C	-0.59542300	1.85523500	-0.06791900
C	-1.32621300	1.16654500	1.05633900
N	-2.42001200	0.26512400	0.62431800
H	0.17637000	1.73371600	-2.05636400
H	-0.65379200	0.55215300	1.66698300
H	-1.73729000	1.93306700	1.71897200
N	-3.91963000	3.33148900	0.28134000
H	-0.62294600	0.21208400	-1.43229800
C	-2.09267000	-1.10322600	0.44673200
C	-2.28122000	-1.78832900	-0.76132900
C	-1.58559700	-1.81468200	1.54499600
C	-1.94889600	-3.13812100	-0.86829000
H	-2.68858200	-1.27826000	-1.62811700
C	-1.24152600	-3.15505300	1.42626400
H	-1.47670100	-1.30757800	2.49881300
C	-1.41975600	-3.82822500	0.21744000
H	-2.10389800	-3.64598700	-1.81503500
H	-0.84755400	-3.68188400	2.29007200
H	-1.16010700	-4.87794700	0.12951600
C	-4.68024800	0.09398600	-0.37855300
C	-5.25203900	-0.36864700	0.80670200
C	-5.34736900	-0.08451200	-1.58855500
C	-6.48333000	-1.01540900	0.77757600
H	-4.71850900	-0.22901700	1.74212300
C	-6.58124100	-0.73127600	-1.61593900
H	-4.89944300	0.27555800	-2.51155900
C	-7.15000800	-1.19804900	-0.43363700
H	-6.92271600	-1.37925000	1.70073700

H	-7.09328300	-0.87395000	-2.56187000
H	-8.10872200	-1.70597100	-0.45553300
C	-0.20524100	3.22616000	0.15725200
O	-0.52308000	3.92363400	1.11491500
O	0.60988800	3.71611200	-0.82193900
C	1.03916800	5.05856700	-0.62942300
H	1.59936900	5.15494500	0.30400300
H	1.67901400	5.29545900	-1.47848900
H	0.18706800	5.74147700	-0.59800900
P	1.93209100	0.16577400	-0.78291800
C	2.61678300	1.24160000	0.54116200
C	3.49402900	0.61017000	1.62362200
H	1.73635800	1.70542200	1.00994400
H	3.15012100	2.05368600	0.03032000
C	3.95846700	1.64044800	2.65358800
H	2.93432500	-0.18177200	2.13811900
H	4.37147400	0.13121300	1.17426800
C	4.82825200	1.01799700	3.74183900
H	4.51542900	2.43410300	2.14032100
H	3.08061800	2.11935100	3.10472500
H	5.15982700	1.76606300	4.46644100
H	4.27815900	0.24323600	4.28515900
H	5.71859700	0.55162100	3.30827300
C	1.60094000	-1.48668200	-0.02526400
C	2.75838100	-2.47846800	0.11115100
H	0.79830000	-1.93995400	-0.62410600
H	1.14939900	-1.28659600	0.95577600
C	2.29195700	-3.81517300	0.68782300
H	3.21690700	-2.65293800	-0.87114900
H	3.54286100	-2.06209000	0.75420400
C	3.43463700	-4.81698700	0.82695000
H	1.82495200	-3.63988400	1.66530200
H	1.50475400	-4.22668500	0.04411800
H	3.08453400	-5.76897200	1.23423000
H	3.89785100	-5.01639300	-0.14460100
H	4.21237800	-4.43109500	1.49347600
C	3.27248800	-0.05839400	-2.04177900
C	4.72385900	-0.12880300	-1.55784300
H	3.16582000	0.77910000	-2.74174200
H	3.00900800	-0.96097400	-2.60709300
C	5.70243200	-0.31173200	-2.71831200
H	4.97583600	0.79280300	-1.01746600
H	4.85088700	-0.95299000	-0.84684700
C	7.15303600	-0.36588700	-2.24725100

H	5.45118800	-1.23364800	-3.25723300
H	5.57260000	0.51059100	-3.43270400
H	7.84130700	-0.49745100	-3.08599200
H	7.42832100	0.55708300	-1.72738700
H	7.30605600	-1.19755100	-1.55234900
H	-2.93241500	0.88524800	-1.36509200

M1 (S)

C	-3.31882100	-0.79647600	-0.26645500
C	-3.97852000	-1.25854100	-1.52106200
C	0.43537900	-0.60312700	0.86420400
C	-0.32594700	-1.19021900	-0.28261100
C	-1.11200700	-0.28087900	-1.15894100
N	-2.35194200	0.25465400	-0.50246700
H	0.01488400	0.36069500	1.18709600
H	-0.54644200	0.59716800	-1.47975100
H	-1.40712000	-0.82228400	-2.06918400
N	-4.45835800	-1.61078000	-2.51289800
H	0.45826800	-1.25906500	1.74208800
C	-2.81005100	1.53230300	-0.88941500
C	-1.90677500	2.60944200	-0.84506000
C	-4.13314600	1.80202500	-1.26858000
C	-2.30118700	3.89192200	-1.19921200
H	-0.89168100	2.43744800	-0.50075000
C	-4.52509700	3.09671300	-1.60676400
H	-4.87114900	1.00968000	-1.30382700
C	-3.61665800	4.14848500	-1.58639300
H	-1.57795100	4.70045600	-1.15431000
H	-5.55663200	3.27403900	-1.89563300
H	-3.92675300	5.15212800	-1.85644500
C	-4.31591300	-0.47650900	0.83978500
C	-3.82591000	0.11491500	2.00618600
C	-5.66857000	-0.79943400	0.75045200
C	-4.68177300	0.38172100	3.06943400
H	-2.77169200	0.36916700	2.06389900
C	-6.52553300	-0.53125400	1.81719600
H	-6.06058800	-1.25513500	-0.15476000
C	-6.03557500	0.05989900	2.97766100
H	-4.29197300	0.84232400	3.97161600
H	-7.57810900	-0.78240100	1.73532700
H	-6.70368400	0.27113200	3.80627700
C	-0.52116900	-2.56756000	-0.40601300
O	-1.26927600	-3.16946000	-1.20192600
O	0.22771200	-3.31418000	0.50480800

C	0.04007600	-4.71562200	0.42943900
H	0.29727300	-5.10018700	-0.56123700
H	0.70240400	-5.15207000	1.17844400
H	-0.99571200	-4.99291400	0.64563000
P	2.20063900	-0.27288200	0.47240600
C	2.23819900	0.79045700	-1.00964900
C	3.58314500	1.42308800	-1.41074100
H	1.50515200	1.58443200	-0.81884400
H	1.81748000	0.16576300	-1.80464300
C	3.83444600	2.77683500	-0.74377600
H	4.42010800	0.74669400	-1.20295600
H	3.58097900	1.56393200	-2.49717500
C	5.23166000	3.30956600	-1.04450800
H	3.07576500	3.48665300	-1.09328200
H	3.70015900	2.69918300	0.34168400
H	5.38707400	4.29298700	-0.59491600
H	5.99850800	2.63333000	-0.65098600
H	5.39094500	3.40091600	-2.12340300
C	2.97719600	0.56480400	1.89503900
C	4.50993800	0.58290800	1.92917700
H	2.59089000	0.05124400	2.78436800
H	2.56531900	1.58095300	1.92046500
C	5.03168900	1.47446100	3.05533700
H	4.88395100	-0.43865800	2.06708000
H	4.91957900	0.94053800	0.97678600
C	6.55604800	1.49402500	3.11145600
H	4.65128700	2.49304700	2.90731000
H	4.62326700	1.12419100	4.01083200
H	6.91468800	2.13901500	3.91717800
H	6.95395600	0.48892600	3.28085900
H	6.97419200	1.86563900	2.17046600
C	3.01212800	-1.88331800	0.21057600
C	4.34595400	-1.92345400	-0.55165100
H	2.25779400	-2.50160800	-0.28807900
H	3.11940300	-2.29151500	1.22278300
C	4.18081300	-1.93677800	-2.07136100
H	5.00329500	-1.10006800	-0.25020400
H	4.86693800	-2.83989200	-0.25265700
C	5.52685600	-1.91852100	-2.78866300
H	3.61356400	-2.83115900	-2.35420400
H	3.58196400	-1.08013100	-2.40030100
H	5.40053400	-1.96285100	-3.87293500
H	6.08184900	-1.00489700	-2.55067000
H	6.14208400	-2.77102200	-2.48444500

H	-2.72428500	-1.66184100	0.05331300
TS2 (SR)			
C	-2.90312600	-0.23331300	-1.05302900
C	-2.89555800	0.17212400	-2.43270300
C	0.48647200	-0.45505200	-1.09474500
C	-0.55604800	-0.70048700	-0.02452000
C	-1.19952600	0.51384800	0.58463500
N	-2.47212900	0.78438000	-0.14439900
H	0.59059300	-1.31041900	-1.77034100
H	-1.40619400	0.34312000	1.64956600
H	-0.56542400	1.40792700	0.50557700
N	-2.84807100	0.47699000	-3.55581700
H	0.17717100	0.40120200	-1.70526700
C	-3.27247400	1.84369100	0.24026300
C	-2.87150500	2.72335200	1.26649000
C	-4.51221800	2.08967100	-0.38827100
C	-3.67403200	3.79984300	1.63301300
H	-1.93246400	2.57076100	1.78394700
C	-5.29852800	3.16895600	-0.00820800
H	-4.85486700	1.42500100	-1.17351700
C	-4.89211300	4.03866600	1.00392000
H	-3.33447500	4.45865100	2.42715800
H	-6.24703900	3.32952500	-0.51267600
H	-5.51187600	4.87973800	1.29479000
C	-4.03039700	-1.10684100	-0.63339500
C	-4.22397600	-1.36657500	0.73211100
C	-4.88383000	-1.73171200	-1.55453500
C	-5.23495900	-2.22152300	1.15753400
H	-3.56075400	-0.90347600	1.45738700
C	-5.89299200	-2.58836300	-1.12428300
H	-4.75602400	-1.54034600	-2.61687100
C	-6.07793400	-2.83909800	0.23403200
H	-5.36545200	-2.40775200	2.21966200
H	-6.54347300	-3.05710100	-1.85701000
H	-6.86744600	-3.50414200	0.56836400
C	-0.38405400	-1.84036600	0.85697600
O	-0.98689900	-2.06777000	1.89605200
O	0.53923100	-2.71919800	0.37063500
C	0.73390000	-3.89940600	1.14535600
H	-0.17512100	-4.50453500	1.16058300
H	1.54179300	-4.44584500	0.65956400
H	1.00912000	-3.64696300	2.17150200
P	2.20525400	-0.07525600	-0.53264200

C	3. 17901800	-1. 61517000	-0. 40335200
C	4. 69340500	-1. 47334500	-0. 58235900
H	2. 76655400	-2. 29683000	-1. 15535000
H	2. 93540800	-2. 05046700	0. 57147000
C	5. 38610900	-2. 82786200	-0. 42858100
H	4. 91845200	-1. 06355300	-1. 57466200
H	5. 10824900	-0. 77535400	0. 15406800
C	6. 89628000	-2. 72306900	-0. 61905000
H	5. 16143900	-3. 23320400	0. 56530700
H	4. 96445300	-3. 53123500	-1. 15638800
H	7. 37813500	-3. 69686700	-0. 50373900
H	7. 13750000	-2. 34271100	-1. 61637700
H	7. 33505900	-2. 04014500	0. 11479800
C	2. 93726300	1. 03280400	-1. 78601500
C	4. 12929800	1. 88413600	-1. 33524200
H	2. 12150900	1. 68809300	-2. 11179800
H	3. 20023400	0. 40311500	-2. 64442200
C	4. 63920800	2. 76725000	-2. 47452900
H	3. 82762500	2. 52187800	-0. 49523900
H	4. 94780600	1. 24958200	-0. 97808500
C	5. 80936300	3. 64295400	-2. 03658800
H	4. 94182900	2. 13096000	-3. 31451800
H	3. 81691700	3. 39563500	-2. 83689600
H	6. 16325500	4. 26951800	-2. 85875500
H	5. 51651200	4. 30086000	-1. 21270200
H	6. 64858300	3. 02998600	-1. 69392800
C	2. 15123900	0. 75066800	1. 09137600
C	3. 44741300	0. 69800800	1. 90863700
H	1. 34110000	0. 26132100	1. 64651300
H	1. 84023400	1. 78733900	0. 91488000
C	3. 27869800	1. 41717200	3. 24729300
H	3. 72694900	-0. 34638000	2. 09327000
H	4. 27385100	1. 15763600	1. 35510700
C	4. 55151600	1. 36714200	4. 08713200
H	2. 99469300	2. 45955200	3. 06029100
H	2. 44833400	0. 95898900	3. 79750800
H	4. 41578500	1. 88257200	5. 04087700
H	4. 83719400	0. 33265600	4. 30067400
H	5. 38455500	1. 84361400	3. 56149900
H	-1. 70183100	-0. 92552900	-0. 78436600

TS2 (SS)

C	3. 11290200	-0. 80230200	0. 71838900
C	3. 89574800	-1. 06991300	1. 89518400

C	-0.26781300	-0.97056500	-0.09650300
C	0.56749100	-0.32459000	0.98753400
C	1.33879900	0.92144100	0.64007300
N	2.78435300	0.57285600	0.52214500
H	0.22018900	-0.84003800	-1.06746500
H	0.99964000	1.34840900	-0.31715200
H	1.21712600	1.68980100	1.41348100
N	4.49561300	-1.31052700	2.86338500
H	-0.37826500	-2.04918400	0.06075100
C	3.69968000	1.52616400	0.12155000
C	3.31043200	2.86333900	-0.09942900
C	5.05753900	1.19590400	-0.07776800
C	4.24255400	3.81677700	-0.49856600
H	2.28047100	3.16559200	0.04657400
C	5.97153600	2.16155100	-0.47619600
H	5.38781400	0.17478300	0.07682000
C	5.57955000	3.48260700	-0.69241400
H	3.90934000	4.83842200	-0.65768800
H	7.00862400	1.87279800	-0.62124000
H	6.29946300	4.23123100	-1.00476200
C	3.44993000	-1.60986000	-0.48417100
C	3.05752800	-1.16383600	-1.75544300
C	4.10209200	-2.84930600	-0.39115200
C	3.29581000	-1.93600500	-2.88874700
H	2.57571800	-0.19415400	-1.85100000
C	4.34089900	-3.61626600	-1.52627700
H	4.42425400	-3.21068100	0.58198400
C	3.93766000	-3.16834600	-2.78412000
H	2.98338900	-1.56687100	-3.86123100
H	4.84804400	-4.57156100	-1.42716500
H	4.12763300	-3.76769600	-3.66837400
C	0.06792400	-0.37242700	2.34582700
O	0.54555600	0.19028300	3.31919400
O	-1.03098700	-1.18054200	2.46430600
C	-1.56510400	-1.30135100	3.78120200
H	-1.85924200	-0.32275700	4.16771900
H	-2.43630500	-1.95046500	3.69441800
H	-0.82937200	-1.74285900	4.45617300
P	-1.99889500	-0.34769500	-0.29892800
C	-2.24651600	-0.00929900	-2.07520800
C	-3.69689700	0.04867300	-2.56553000
H	-1.71251400	-0.81041000	-2.60028100
H	-1.71084100	0.92273800	-2.29494100
C	-3.76024800	0.34525000	-4.06399000

H	-4.18993800	-0.91072200	-2.36652300
H	-4.26148400	0.81526500	-2.02368200
C	-5.19541000	0.38093400	-4.58045300
H	-3.26893700	1.30589500	-4.25918700
H	-3.18643600	-0.41644000	-4.60515300
H	-5.22497700	0.59881600	-5.65070300
H	-5.69253200	-0.58024300	-4.41795900
H	-5.77642000	1.15077600	-4.06350900
C	-3.16443400	-1.64910600	0.22881300
C	-4.54199000	-1.16106600	0.68715500
H	-2.65994800	-2.17776600	1.04297400
H	-3.25203100	-2.34743900	-0.61237600
C	-5.41486800	-2.32847900	1.14795900
H	-4.42569800	-0.45124900	1.51625100
H	-5.05273100	-0.62621100	-0.12248400
C	-6.79077900	-1.86419000	1.61605900
H	-5.52168500	-3.04462500	0.32459400
H	-4.90194700	-2.85848100	1.95960300
H	-7.40219400	-2.70790700	1.94480300
H	-6.70224300	-1.16454500	2.45283000
H	-7.32516300	-1.35455300	0.80859700
C	-2.21789600	1.18213200	0.67018600
C	-3.32040600	2.13341900	0.19388700
H	-1.24759900	1.69213500	0.64123800
H	-2.38344900	0.87468700	1.70903000
C	-3.39114300	3.37614400	1.08161900
H	-3.12378500	2.44126600	-0.84026600
H	-4.29467300	1.63100700	0.20041000
C	-4.46876100	4.35017000	0.61479400
H	-3.58747000	3.06785200	2.11539000
H	-2.41298800	3.87182600	1.08252400
H	-4.50678600	5.23433200	1.25549800
H	-4.27534200	4.68373100	-0.40934500
H	-5.45574100	3.87779800	0.63249300
H	1.76928900	-1.04671300	1.02996600

TS2 (R)

C	3.51873000	-0.17044100	-0.73180500
C	-0.72497600	0.15311700	-1.20771700
C	0.35576700	-0.72496300	-0.60908300
C	1.33745600	-0.13898200	0.37512300
N	2.43982000	0.61751900	-0.21516900
H	-0.92342600	-0.08916800	-2.25822800
H	0.81058000	0.50389100	1.08329500

H	1. 76467400	-0. 94140800	0. 98202500
H	-0. 41440900	1. 20473000	-1. 18606900
C	2. 54585700	1. 99935800	-0. 09075500
C	1. 46502300	2. 81623700	0. 30050000
C	3. 76563500	2. 64447100	-0. 38631000
C	1. 60644100	4. 19682000	0. 40088100
H	0. 49445800	2. 38615000	0. 51899800
C	3. 88954800	4. 02363800	-0. 28486200
H	4. 61769500	2. 04658100	-0. 68746300
C	2. 81588800	4. 82053300	0. 11092700
H	0. 74693300	4. 78796000	0. 70330100
H	4. 84744000	4. 48079600	-0. 51644900
H	2. 91916700	5. 89734500	0. 18657600
C	0. 40155200	-1. 95649300	-1. 14601000
O	-0. 06000300	-2. 83080500	-1. 79171700
O	2. 23632700	-2. 63037200	-0. 70485500
C	2. 51946200	-3. 43238100	0. 43111400
H	2. 52961900	-2. 84577700	1. 35682500
H	1. 74353600	-4. 19804900	0. 50204600
H	3. 49242700	-3. 91966200	0. 31392700
H	2. 81797600	-1. 79741600	-0. 73437300
C	3. 76017400	-0. 06784300	-2. 11887100
N	3. 95224100	-0. 01158100	-3. 27206100
C	4. 60747100	-0. 56194100	0. 16103200
C	4. 54265800	-0. 29754200	1. 54440600
C	5. 72768500	-1. 28294300	-0. 30711100
C	5. 54091800	-0. 73871000	2. 40829400
H	3. 70230000	0. 27116800	1. 93342800
C	6. 72065400	-1. 71410100	0. 56172800
H	5. 80647000	-1. 50241300	-1. 36921000
C	6. 63871000	-1. 45178700	1. 93114900
H	5. 45983500	-0. 51533900	3. 46875900
H	7. 57003400	-2. 26412700	0. 16545600
H	7. 41450100	-1. 79412800	2. 60771200
P	-2. 35988700	0. 04894600	-0. 37754900
C	-2. 97752800	-1. 63344100	-0. 70013300
C	-4. 13308000	-2. 14837900	0. 16032200
H	-2. 10716800	-2. 28896400	-0. 58262400
H	-3. 24036300	-1. 64971900	-1. 76567900
C	-4. 53055400	-3. 56560600	-0. 25350300
H	-3. 83636100	-2. 15027700	1. 21581700
H	-5. 00540200	-1. 49164900	0. 07201100
C	-5. 65929900	-4. 11560800	0. 61310200
H	-4. 83561400	-3. 55900900	-1. 30652400

H	-3.65298800	-4.21940800	-0.18543200
H	-5.94024700	-5.12480900	0.30292300
H	-5.35839400	-4.15693600	1.66438400
H	-6.54848500	-3.48146600	0.54433600
C	-2.11943100	0.41262400	1.40118800
C	-3.23212900	1.17781200	2.13660900
H	-1.21071900	1.02184100	1.41916900
H	-1.87561500	-0.53038800	1.90363800
C	-4.41298900	0.33857400	2.61599700
H	-3.58762000	2.01122000	1.51777300
H	-2.76347300	1.64130900	3.01147300
C	-5.44255300	1.19457700	3.34834800
H	-4.89829500	-0.16369000	1.77321200
H	-4.04302000	-0.45570300	3.27562700
H	-6.27150300	0.58686200	3.71792600
H	-4.98873900	1.70622900	4.20244600
H	-5.85552400	1.95862600	2.68111800
C	-3.41067700	1.31048000	-1.16542200
C	-4.92522600	1.15599800	-0.99308700
H	-3.15030900	1.28065900	-2.23041100
H	-3.06535300	2.27919400	-0.78414600
C	-5.67468200	2.31083600	-1.65794800
H	-5.25258000	0.20884600	-1.43815900
H	-5.19394500	1.12214600	0.06940200
C	-7.18509400	2.18253700	-1.48656000
H	-5.32823800	3.25727000	-1.22605700
H	-5.41805500	2.33900900	-2.72349900
H	-7.70939700	3.00866400	-1.97253400
H	-7.54970000	1.24771000	-1.92302800
H	-7.45787100	2.18623600	-0.42655700

TS2 (S)

C	-3.66602400	-0.33168500	-0.80372500
C	0.38120800	0.02595100	0.77896400
C	-0.49934900	-0.78604800	-0.15421500
C	-1.25777900	-0.10345400	-1.27125100
N	-2.51694200	0.52583100	-0.88641300
H	0.34991600	-0.34692900	1.80941300
H	-0.61647900	0.64507200	-1.73992800
H	-1.47440200	-0.82772400	-2.05721700
H	0.04042100	1.06707600	0.81618200
C	-2.62425600	1.89474300	-0.66288400
C	-1.51479000	2.76654800	-0.67436700
C	-3.88751000	2.47155000	-0.40583200

C	-1.66783000	4.13230800	-0.45400700
H	-0.51429200	2.39463300	-0.85873200
C	-4.02256100	3.83555800	-0.18531300
H	-4.76326000	1.83479500	-0.38178500
C	-2.91882600	4.68740700	-0.20657100
H	-0.78482100	4.76433400	-0.47515000
H	-5.01359000	4.23741400	0.00600100
H	-3.03201800	5.75157700	-0.03192400
C	-0.61821000	-2.06730900	0.22348900
O	-0.32252000	-3.02572300	0.84091000
O	-2.28504400	-2.73931800	-0.80226000
C	-2.10150900	-3.44015400	-2.01874400
H	-1.85042100	-2.77006600	-2.85032800
H	-1.27767100	-4.14384600	-1.87601300
H	-3.00251900	-4.00371700	-2.28138400
H	-2.90698600	-1.94535800	-0.91174800
C	-4.49832500	-0.33737800	-1.94944600
N	-5.16368400	-0.38743800	-2.91102500
C	-4.26626600	-0.59734800	0.50275500
C	-3.57579800	-0.29970300	1.69484500
C	-5.53762100	-1.19639900	0.62736500
C	-4.12429400	-0.59684100	2.93794500
H	-2.59678400	0.16725600	1.62964000
C	-6.07757100	-1.49089000	1.87270400
H	-6.09994200	-1.43245800	-0.27265500
C	-5.37846500	-1.19685900	3.04423100
H	-3.56347000	-0.35217000	3.83613800
H	-7.05924900	-1.95361300	1.92980600
H	-5.80353100	-1.42579200	4.01582900
P	2.16111900	0.04683500	0.32313000
C	2.76324400	-1.64871200	0.60406500
C	4.08269900	-2.06138100	-0.05111800
H	1.95652900	-2.30202700	0.25246500
H	2.81133600	-1.76639700	1.69421100
C	4.41373500	-3.51981000	0.26716800
H	4.01282400	-1.93536200	-1.13797600
H	4.90329900	-1.42423600	0.29637500
C	5.71647900	-3.96488200	-0.39029300
H	4.48182400	-3.64237100	1.35453700
H	3.58745300	-4.15719200	-0.06922100
H	5.94420800	-5.00621400	-0.15063500
H	5.65394900	-3.87518900	-1.47910500
H	6.55509600	-3.34923500	-0.05106200
C	2.28868300	0.59575000	-1.41879600

C	3.50627900	1.44202900	-1.82591400
H	1.38808600	1.20100700	-1.56058300
H	2.17725800	-0.28865600	-2.05632800
C	4.78572300	0.66997700	-2.13538700
H	3.70146500	2.20881000	-1.06581300
H	3.21225600	1.99111100	-2.72687000
C	5.91202100	1.60934300	-2.55727700
H	5.10902400	0.09070400	-1.26478800
H	4.58180100	-0.05785700	-2.93007800
H	6.81964200	1.05384300	-2.80343300
H	5.62395400	2.19575100	-3.43496500
H	6.15304800	2.31048500	-1.75119400
C	2.97296500	1.24008900	1.43303500
C	4.49525400	1.12118300	1.56240800
H	2.50138800	1.10410000	2.41347700
H	2.68143500	2.23616300	1.07756900
C	5.06141400	2.22632900	2.45385200
H	4.75171900	0.14363800	1.98763900
H	4.97471900	1.17897200	0.57812900
C	6.57703500	2.12357700	2.59436400
H	4.79111900	3.20041100	2.02888800
H	4.58727400	2.17074000	3.44084200
H	6.96900100	2.91803800	3.23373100
H	6.86452700	1.16365000	3.03393000
H	7.06445600	2.20494100	1.61770700

TS3'(RR)

C	2.48562700	0.46276300	0.84409100
C	2.42846600	0.66658700	2.25529800
C	0.44130900	-0.19273400	0.41206400
C	0.92413900	-1.62137700	0.63380800
C	2.28549400	-1.79798200	-0.04629100
N	3.14849600	-0.73571900	0.43685700
H	0.58404600	0.26880300	-0.55835400
H	2.16238400	-1.77206000	-1.13983800
H	2.70161900	-2.77736400	0.21544700
N	2.27870000	0.80598400	3.40365700
H	0.15935700	0.44200900	1.24442900
C	4.52049800	-0.78623400	0.21270200
C	5.36491400	0.22230700	0.71613100
C	5.10513100	-1.83665400	-0.51848900
C	6.73636100	0.16340700	0.51013300
H	4.93505000	1.05103100	1.26798100
C	6.48330400	-1.88035800	-0.71333700

H	4.48833400	-2.61690800	-0.94874100
C	7.31355000	-0.88776200	-0.20273100
H	7.36262900	0.95361600	0.91370900
H	6.90630700	-2.70414100	-1.28088400
H	8.38573800	-0.92667200	-0.36061600
C	2.52782800	1.65654000	-0.00928700
C	2.94304800	1.56507200	-1.34946400
C	2.03909100	2.89474200	0.44635300
C	2.88230400	2.67094400	-2.19151100
H	3.32098700	0.61839000	-1.72564100
C	1.97625500	3.99447100	-0.40310200
H	1.71059200	2.99074200	1.47828400
C	2.39979200	3.89402100	-1.72787000
H	3.21718400	2.57490400	-3.22022300
H	1.59509100	4.93844900	-0.02452200
H	2.35454900	4.75418900	-2.38731200
C	-0.06273600	-2.68585300	0.18019600
O	-0.89623100	-3.18801600	0.90152900
O	0.08981100	-3.01590600	-1.10462000
C	-0.70699000	-4.11535300	-1.57011000
H	-0.47566100	-5.01057700	-0.99095200
H	-0.43537900	-4.25238300	-2.61420900
H	-1.76947800	-3.88776700	-1.47786800
P	-1.83988400	-0.23947300	0.03731000
C	-2.83418200	-1.30114800	-1.09745900
C	-4.12832700	-0.71622400	-1.67044800
H	-2.16270700	-1.57573700	-1.92036700
H	-3.03536100	-2.22101300	-0.53386600
C	-4.84594000	-1.72157100	-2.57158700
H	-3.89875900	0.18761600	-2.24868700
H	-4.80070900	-0.41021300	-0.86093000
C	-6.12350100	-1.14453700	-3.17474200
H	-5.08088100	-2.62077600	-1.98891900
H	-4.16473300	-2.03775000	-3.37133200
H	-6.62637800	-1.87320800	-3.81545400
H	-5.90271900	-0.25937600	-3.77934200
H	-6.82432200	-0.84582600	-2.38896500
C	-1.97587800	1.49420800	-0.56378400
C	-3.19478400	2.32772400	-0.16152700
H	-1.06444100	2.00068100	-0.21278500
H	-1.88714500	1.44214600	-1.65677100
C	-3.09592600	3.75571100	-0.69941200
H	-3.27544800	2.36061100	0.93254600
H	-4.11643800	1.86481100	-0.53302200

C	-4.29155700	4.61203600	-0.29226000
H	-3.01644000	3.72159100	-1.79290200
H	-2.16704200	4.21178700	-0.33454000
H	-4.20559000	5.62842600	-0.68456500
H	-4.37167400	4.67672000	0.79735200
H	-5.22478900	4.18314500	-0.67039000
C	-2.60281000	-0.34084900	1.71047400
C	-4.12737500	-0.44049800	1.80790100
H	-2.14664800	-1.22534300	2.17256500
H	-2.23621600	0.52970500	2.26987900
C	-4.59435800	-0.54050100	3.26052200
H	-4.47354700	-1.32635100	1.25978300
H	-4.60206200	0.42782900	1.33593300
C	-6.11065400	-0.67215300	3.37007100
H	-4.25618200	0.34762100	3.80827500
H	-4.10925600	-1.40230000	3.73482200
H	-6.43071200	-0.74332100	4.41261100
H	-6.46169000	-1.56749900	2.84754700
H	-6.61038000	0.19265700	2.92253600
H	1.03561700	-1.77175000	1.71179700

TS3'(SR)

C	2.60466800	0.70834600	-0.34249800
C	0.49957000	-0.03276700	-0.22661400
C	1.06595400	-1.23616900	0.51390900
C	2.36630000	-1.69924300	-0.15141000
N	3.25628300	-0.55745400	-0.21198200
H	0.34656000	0.90964400	0.28090200
H	2.13328400	-2.11186300	-1.14649400
H	2.81446100	-2.50252600	0.44461400
H	0.46013200	-0.05288200	-1.31087100
C	4.59021700	-0.73149100	-0.58034000
C	5.11684100	-2.00373800	-0.86426200
C	5.45338400	0.37831200	-0.66241300
C	6.46091500	-2.15383900	-1.19683900
H	4.48190200	-2.88134100	-0.84099200
C	6.78988900	0.21059900	-0.99813900
H	5.06724800	1.36964700	-0.45112900
C	7.31130900	-1.05512400	-1.26676500
H	6.83912700	-3.14892700	-1.41202200
H	7.43213100	1.08493500	-1.04787600
H	8.35625300	-1.17921100	-1.52917900
C	0.11791500	-2.41905200	0.52675900
O	-0.14988100	-3.09193200	-0.44336700

O	-0.38616800	-2.64598300	1.74335800
C	-1.32487700	-3.72655000	1.83267900
H	-2.21769800	-3.49693300	1.24468200
H	-1.57808300	-3.81112600	2.88705000
H	-0.87651800	-4.64970900	1.46394600
H	1.26863100	-0.94022400	1.54676000
P	-1.83361600	-0.21880900	-0.22872300
C	-2.66514600	-0.28600000	1.42373200
C	-4.15075300	-0.63999400	1.49623500
H	-2.08585400	-0.99854300	2.02090400
H	-2.48202900	0.69887100	1.87313500
C	-4.62438200	-0.78447200	2.94320400
H	-4.33935700	-1.58005200	0.96171200
H	-4.74795300	0.13176300	0.99760000
C	-6.10515800	-1.14147300	3.03068000
H	-4.43360800	0.15325400	3.47922500
H	-4.02323700	-1.55605700	3.44054200
H	-6.43135700	-1.23573400	4.06948000
H	-6.30737900	-2.09163300	2.52657000
H	-6.72072400	-0.37264400	2.55331200
C	-2.54649100	-1.45750900	-1.41378200
C	-3.62980100	-1.03239500	-2.41720400
H	-1.66328600	-1.81020100	-1.95695400
H	-2.87961100	-2.31808700	-0.82173700
C	-5.06508600	-1.12262100	-1.90425100
H	-3.43083400	-0.02058900	-2.79218600
H	-3.53988300	-1.68953300	-3.29061400
C	-6.06806600	-0.61644200	-2.93695200
H	-5.17554100	-0.54876100	-0.97909800
H	-5.28462800	-2.16533000	-1.64321300
H	-7.09609800	-0.72960600	-2.58477500
H	-5.97018100	-1.16475800	-3.87916300
H	-5.89953800	0.44466700	-3.15215300
C	-2.15067900	1.46191300	-0.91093700
C	-3.56502700	2.03193700	-0.78732800
H	-1.44333800	2.12974500	-0.40076000
H	-1.83216800	1.43326100	-1.96108900
C	-3.70423700	3.38376800	-1.48780700
H	-3.81878900	2.14895900	0.27386800
H	-4.29888700	1.33772000	-1.21167600
C	-5.11087800	3.95693600	-1.34118100
H	-3.46031200	3.26241500	-2.55027200
H	-2.96768800	4.08375000	-1.07486300
H	-5.20543500	4.92198600	-1.84508800

H	-5.36466200	4.10027000	-0.28632700
H	-5.85272900	3.27727200	-1.77321400
C	2.66199800	1.64903400	0.78168300
C	3.16460100	1.24534500	2.03150000
C	2.12968700	2.94837300	0.67396800
C	3.14142400	2.10877000	3.12184700
H	3.58258500	0.24782500	2.12957400
C	2.10919100	3.80490300	1.76920200
H	1.73627500	3.28430200	-0.28254300
C	2.61381900	3.39398200	3.00270900
H	3.54178800	1.77314900	4.07413800
H	1.69442400	4.80238500	1.65687700
H	2.59678600	4.06382700	3.85587200
C	2.56683400	1.26424800	-1.65274500
N	2.53583800	1.71981800	-2.72593200

TS3'(RS)

C	-2.35054300	0.41940300	-0.26377100
C	-2.28907200	0.65172600	-1.66683600
C	-0.23821200	-0.21117600	0.00034800
C	-0.74669900	-1.28930500	0.94162500
C	-2.04600600	-1.89159700	0.38591800
N	-2.97245300	-0.79670600	0.15989400
H	-0.19037000	-0.43372300	-1.06053000
H	-1.82639400	-2.44959300	-0.53904400
H	-2.46096300	-2.59758200	1.11284500
N	-2.14095900	0.82730900	-2.81166100
H	-0.14618300	0.81435300	0.32891100
C	-4.30036600	-1.07769800	-0.17236900
C	-4.78982700	-2.39408700	-0.21277300
C	-5.19058600	-0.02761500	-0.46536400
C	-6.12724800	-2.64031900	-0.51810000
H	-4.13254500	-3.23334200	-0.01905700
C	-6.51878500	-0.29113500	-0.77122400
H	-4.83065300	0.99584700	-0.44367200
C	-7.00396200	-1.59836900	-0.79845100
H	-6.47671400	-3.66859500	-0.54325200
H	-7.18339500	0.54026800	-0.98916900
H	-8.04226900	-1.79879800	-1.03943500
C	-2.41115200	1.59391400	0.61052200
C	-2.91572600	1.49831700	1.91926500
C	-1.85998400	2.82575500	0.20493500
C	-2.88197000	2.59228400	2.77791800
H	-3.34286200	0.55403200	2.24478100

C	-1.82761900	3.91390700	1.07016200
H	-1.46454700	2.92701000	-0.80377400
C	-2.33805300	3.80802700	2.36428400
H	-3.28733900	2.49355600	3.78004000
H	-1.40135700	4.85321200	0.72887300
H	-2.31328600	4.65803500	3.03623100
C	0.25491700	-2.40058000	1.18263600
O	0.73463300	-2.67833200	2.25657700
O	0.54529200	-3.06058300	0.05390300
C	1.45664800	-4.15814400	0.19908500
H	1.04082600	-4.90333900	0.88011800
H	1.58125600	-4.57471500	-0.79753600
H	2.41394000	-3.80810700	0.59195200
P	2.07816500	-0.21470100	0.06435800
C	3.12058200	-0.61560600	1.54010800
C	4.30686200	0.31196300	1.82152000
H	3.46256800	-1.64981200	1.39805200
H	2.44913400	-0.63738900	2.40551700
C	5.13417700	-0.18069700	3.00851000
H	4.95240100	0.39205900	0.93736800
H	3.94016800	1.32328200	2.03359600
C	6.30504600	0.74813400	3.31889200
H	4.48300000	-0.26681500	3.88801000
H	5.50520100	-1.19070700	2.79529000
H	6.88567000	0.38765800	4.17063000
H	6.97933400	0.82493800	2.45909200
H	5.94975900	1.75730500	3.55566800
C	2.86006000	-1.03058600	-1.38785100
C	4.32695300	-0.68841200	-1.65465600
H	2.24112500	-0.76806600	-2.25482600
H	2.73686100	-2.11069900	-1.24476000
C	4.83966900	-1.33288500	-2.94264700
H	4.45324900	0.40048500	-1.72196500
H	4.94344500	-1.02760400	-0.81205200
C	6.30348200	-0.99711200	-3.21277600
H	4.71236500	-2.42021100	-2.87509100
H	4.21862200	-0.99707900	-3.78261000
H	6.65575000	-1.46270000	-4.13628300
H	6.44316200	0.08442100	-3.30567300
H	6.94106900	-1.34591100	-2.39370100
C	2.25948200	1.59353700	-0.22785300
C	1.64302800	2.04596200	-1.55838600
H	3.31126100	1.89409600	-0.17727200
H	1.74675800	2.08837600	0.60885500

C	1.49936100	3.56527000	-1.63642500
H	2.26609500	1.69387200	-2.39069100
H	0.65124000	1.59985000	-1.70833900
C	0.86075600	4.01080600	-2.94854300
H	0.88613200	3.90341600	-0.79028200
H	2.48349400	4.03282100	-1.51509100
H	0.73674300	5.09581600	-2.98496900
H	1.47462000	3.71146500	-3.80324300
H	-0.12713300	3.55263600	-3.07398700
H	-0.94850200	-0.83847600	1.91742700

TS3'(SS)

C	2.37382400	0.06065700	-0.98210200
C	2.41357000	-0.06559000	-2.40191400
C	0.26783800	-0.41034700	-0.53939500
C	0.69490000	-1.87066900	-0.47913500
C	1.99848400	-1.97409300	0.32181000
N	2.93976300	-1.03465300	-0.26156800
H	0.41780600	0.21289100	0.33548200
H	1.79903100	-1.76028800	1.38338200
H	2.38882300	-2.99662400	0.25753500
N	2.34110700	-0.19350400	-3.55932500
H	0.05485500	0.07096100	-1.48524900
C	4.28640000	-1.08697400	0.07987000
C	4.75994900	-1.99310200	1.04703300
C	5.21661200	-0.22675500	-0.53556100
C	6.11497800	-2.04477500	1.36321600
H	4.07384500	-2.65312000	1.56490400
C	6.56347000	-0.29114500	-0.20574100
H	4.87242100	0.48963500	-1.27331800
C	7.03078100	-1.20071800	0.74339300
H	6.45159600	-2.75487600	2.11292200
H	7.25768300	0.38252500	-0.69957200
H	8.08438900	-1.24412500	0.99671400
C	2.41682800	1.41407800	-0.41881400
C	2.67317300	1.60505800	0.95060200
C	2.09305300	2.54347000	-1.19374100
C	2.61688700	2.87447900	1.51696900
H	2.92512700	0.74607100	1.56678200
C	2.03727700	3.80879100	-0.62009600
H	1.88760300	2.42288800	-2.25445200
C	2.30134300	3.98683300	0.73862200
H	2.82529600	2.99527000	2.57600300
H	1.78221200	4.66439800	-1.23961100

H	2.25969400	4.97678600	1.18136300
C	-0.34533100	-2.81491800	0.09524300
O	-0.96537700	-3.62541700	-0.55277700
O	-0.49400600	-2.66323200	1.41766300
C	-1.41461400	-3.56870700	2.04191100
H	-1.07285700	-4.59681100	1.91271000
H	-1.42889500	-3.29717900	3.09523600
H	-2.40961600	-3.46351800	1.60372100
P	-2.01807900	-0.28315300	-0.16569800
C	-3.20135900	-1.42580300	-1.01705800
C	-4.44248200	-0.79566400	-1.65549700
H	-3.48943300	-2.17417700	-0.26725200
H	-2.62621100	-1.96875100	-1.77486200
C	-5.38760600	-1.86126500	-2.21136900
H	-4.98325000	-0.17840900	-0.92773500
H	-4.13596200	-0.12598700	-2.46808200
C	-6.60900600	-1.25024900	-2.89222000
H	-4.83993700	-2.49190400	-2.92222400
H	-5.70604900	-2.51879000	-1.39317200
H	-7.28033100	-2.02314200	-3.27468300
H	-7.17552600	-0.62887600	-2.19165900
H	-6.30992000	-0.61726900	-3.73332800
C	-2.60707500	-0.10115100	1.57018300
C	-4.06073500	0.34230500	1.74580900
H	-1.92413100	0.61096800	2.05009700
H	-2.43766600	-1.06326600	2.06500600
C	-4.42097700	0.54733300	3.21746700
H	-4.24085400	1.27677100	1.19749500
H	-4.72944000	-0.41180000	1.31197000
C	-5.87133900	0.98417400	3.40138100
H	-4.23935700	-0.38595700	3.76438600
H	-3.74717600	1.29775400	3.64869500
H	-6.11289000	1.12874500	4.45733300
H	-6.06311300	1.92720500	2.88003000
H	-6.55873500	0.23432200	2.99781900
C	-2.25892200	1.37879100	-0.92200400
C	-1.63338600	2.51535000	-0.10325800
H	-3.32669000	1.57192400	-1.06674600
H	-1.80852500	1.33960600	-1.92295200
C	-1.67362200	3.84358800	-0.85984600
H	-2.17952600	2.62112600	0.84325000
H	-0.58843300	2.29222200	0.15651800
C	-1.30802700	5.02747800	0.03026600
H	-0.98285800	3.78445400	-1.71040900

H	-2.67653900	3.99125200	-1.27936000
H	-1.27968200	5.96043200	-0.53896700
H	-2.03959200	5.14585800	0.83580900
H	-0.32518700	4.87776200	0.48677100
H	0.86884500	-2.21552900	-1.50181900