

## Supporting Information

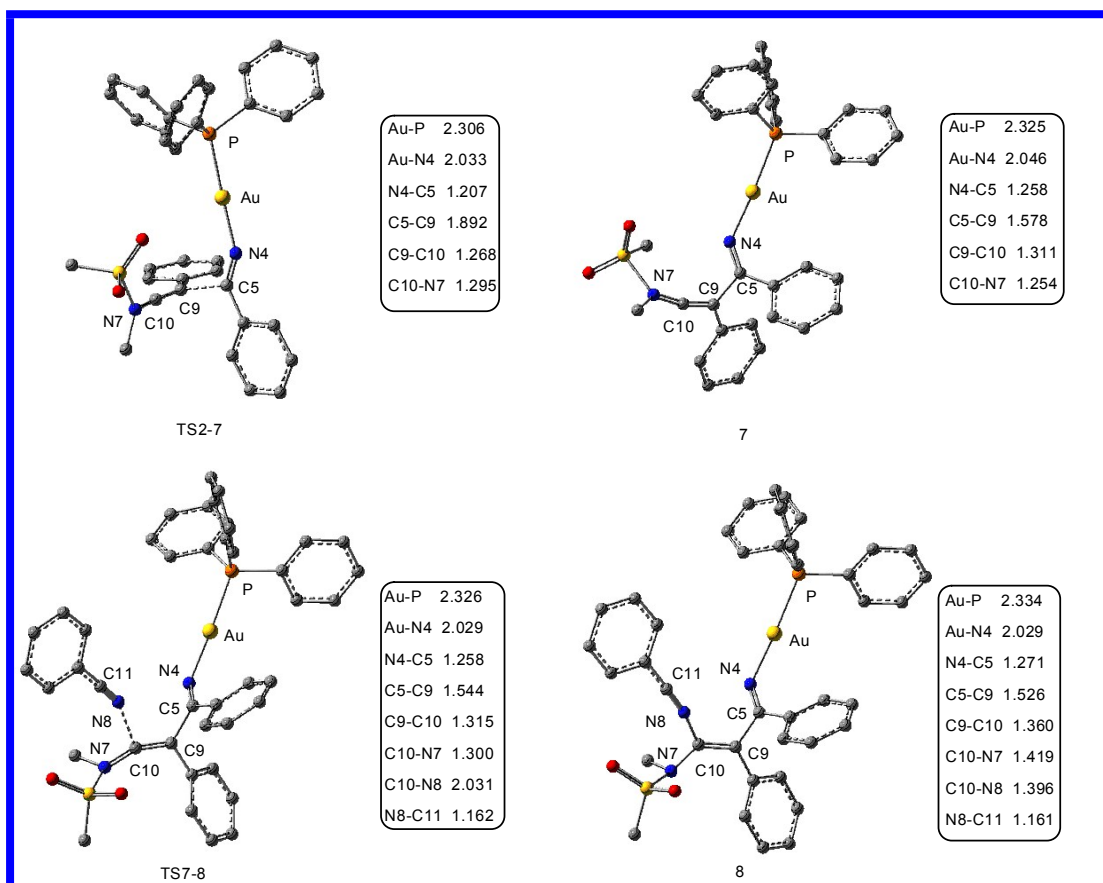
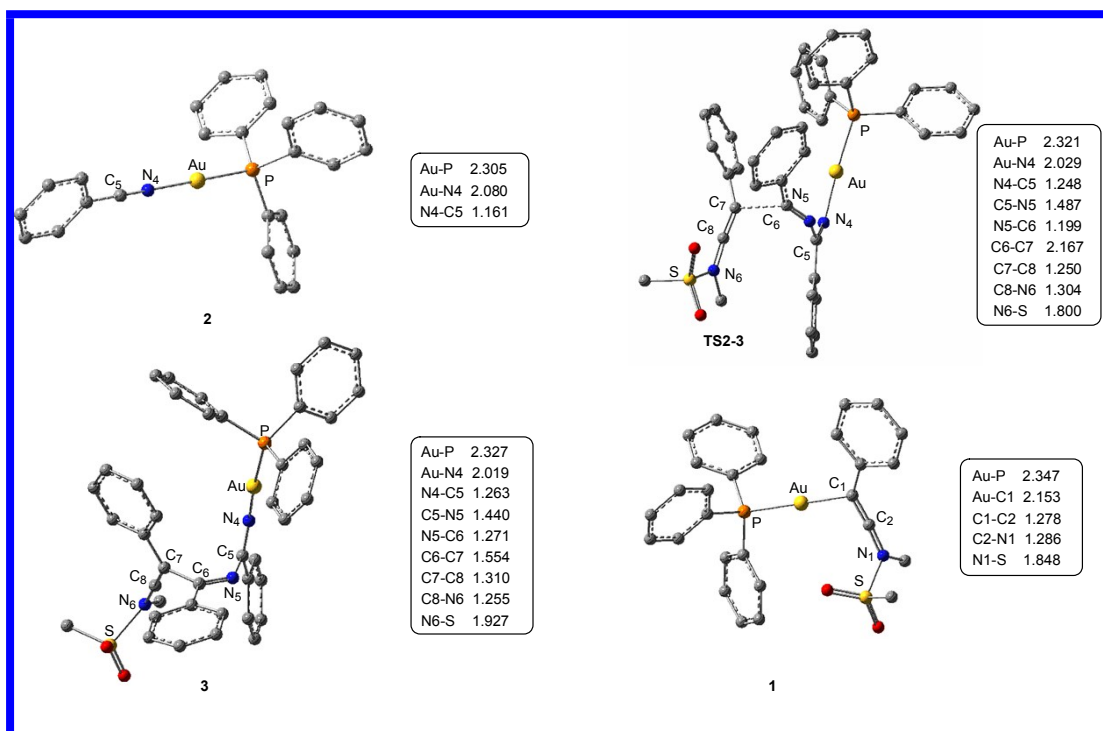
### **Theoretical Study on Au(I)-Catalyzed [2+2+2] Cycloadditions of Ynamides with Two Discrete Nitriles**

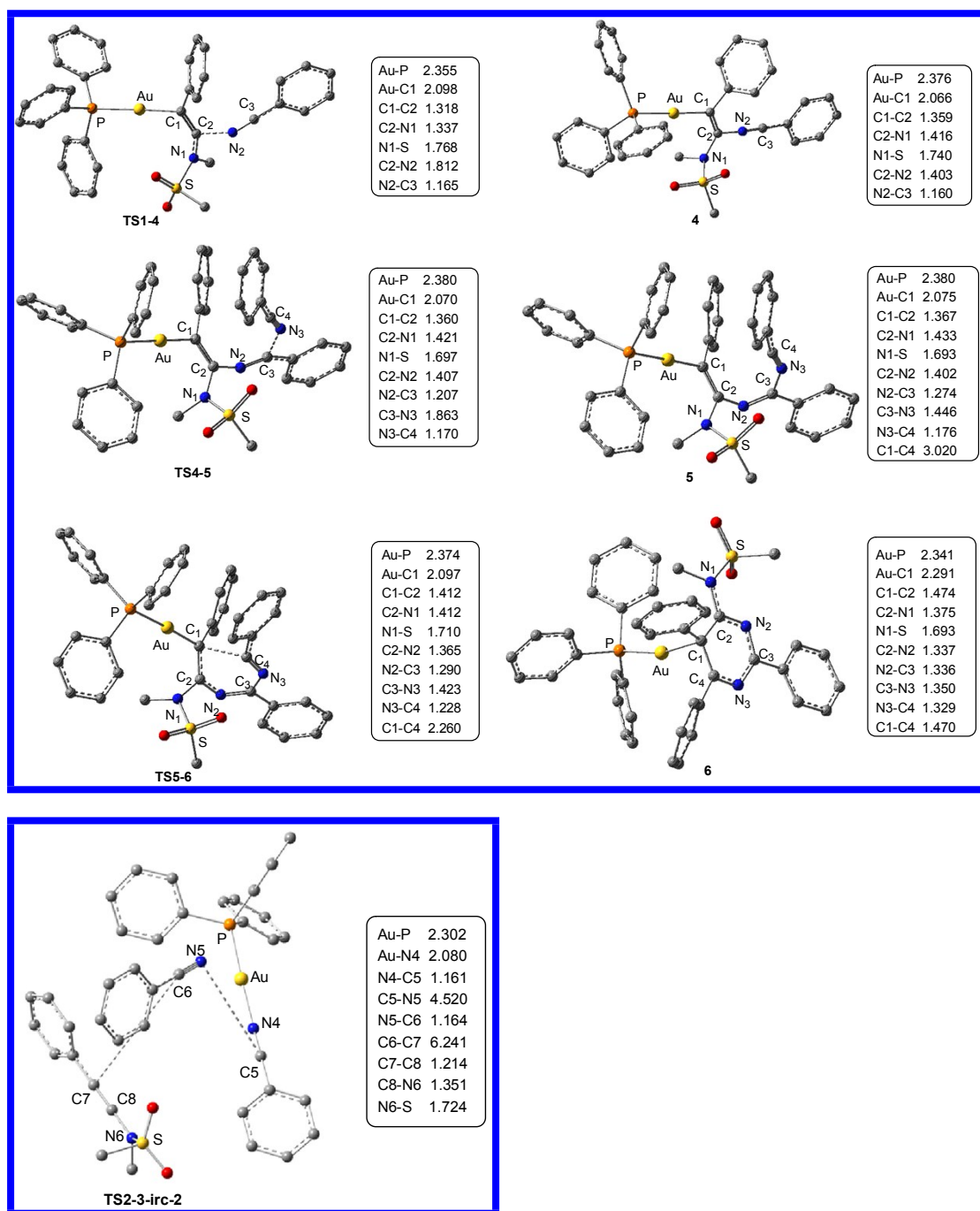
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**Fig. S1.** Structures involved in path a \ path b and path c and TS2-3-irc-2. The bond distances are given in Å.

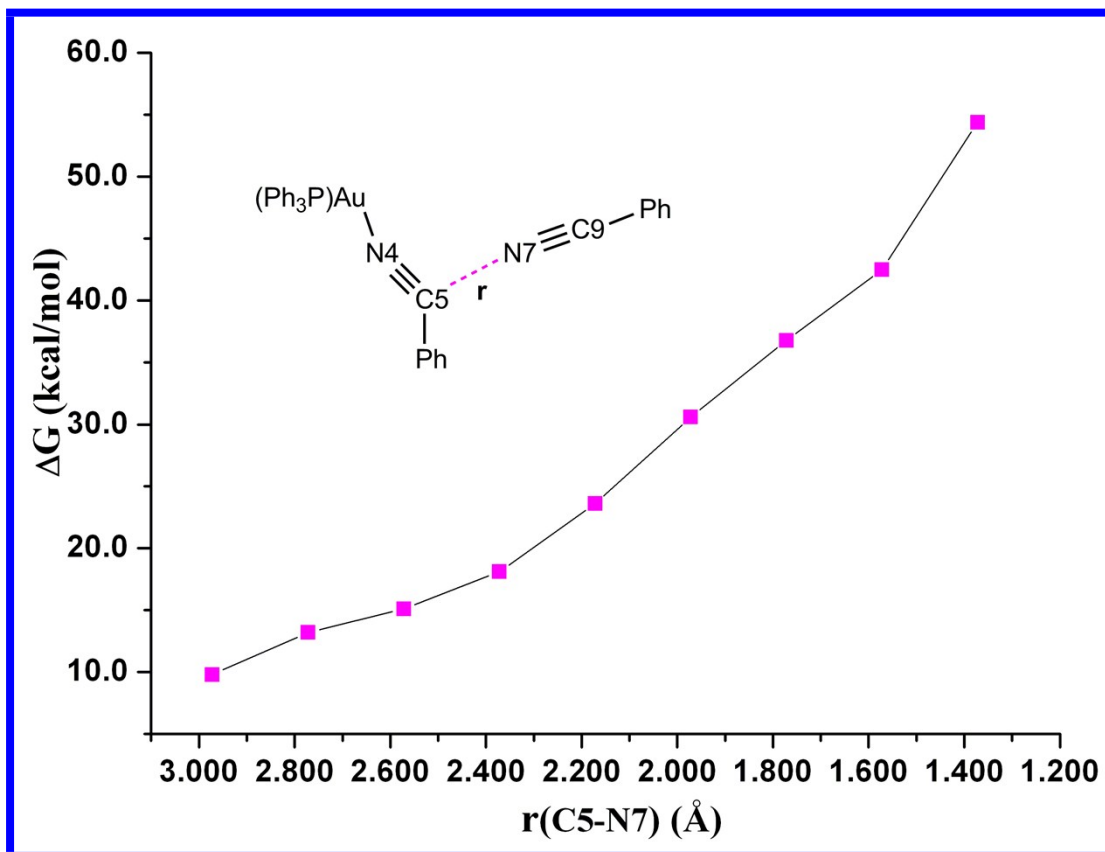


Fig. S2. Gibbs free energy changes with the second nitrile approaching to the C5 atom of the Au-nitrile species. The C5...N7 shortening goes with a decrement of 0.2 Å.

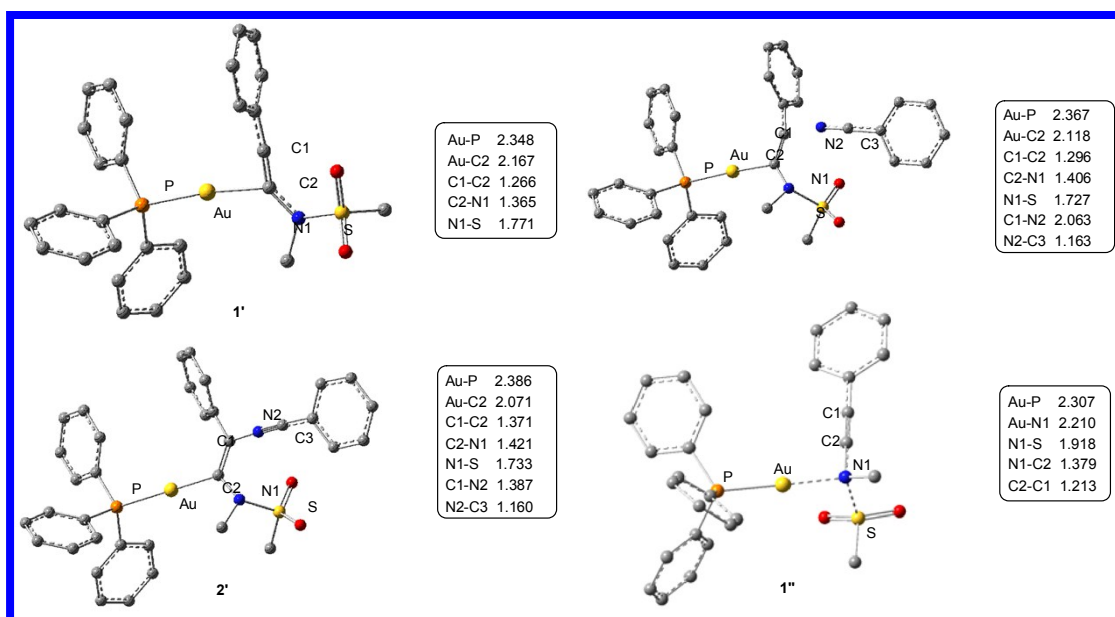
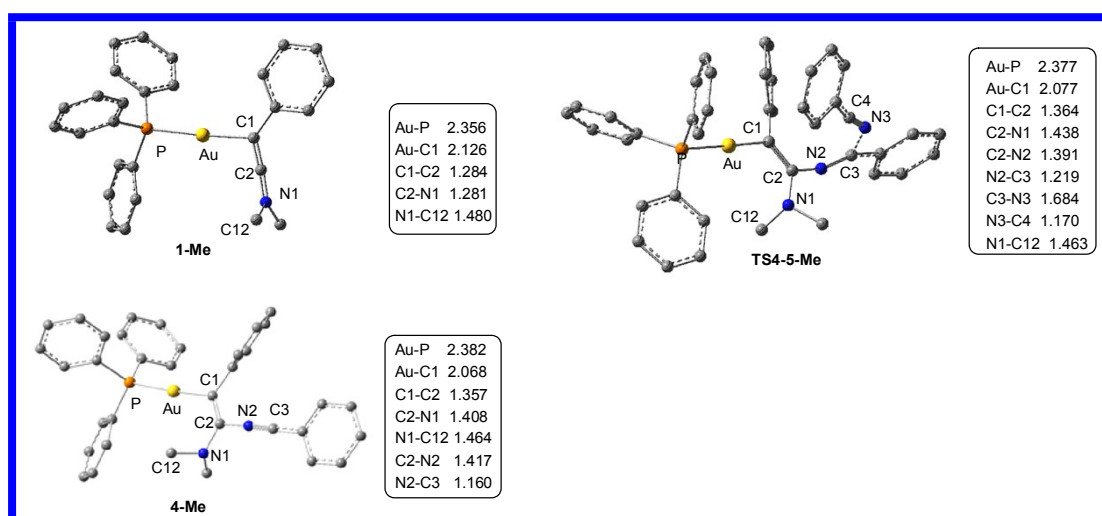


Fig. S3. Structures of intermediates  $1'$ ,  $\text{TS}1'-2'$ ,  $2'$  shown in Fig. 2 and  $1''$ . The bond distances are given in Å.



**Fig. S4.** Structures involved in Fig. 3 (b) where Me is attached on N1 atom. The bond distances are given in Å.

## Cartesian coordinates and electronic energies for all of the calculated structures

	2		
C	3.90622500	-0.00967200	0.00328800
N	2.74510400	-0.01418400	0.00323200
Au	0.66543200	-0.01136100	0.00224700
P	-1.63992500	0.00189500	-0.00010600
C	-2.30930700	-0.04926500	1.70682600
C	-3.41571400	0.72869300	2.07729100
C	-1.71300100	-0.90752800	2.64537400
C	-3.91871300	0.64493000	3.37692100
H	-3.87952100	1.39970400	1.36194000
C	-2.22414700	-0.98871600	3.93917300
H	-0.85343000	-1.51140700	2.36648800
C	-3.32590800	-0.21121800	4.30618400
H	-4.77270800	1.25167200	3.66140700
H	-1.75985100	-1.65312000	4.66119800
H	-3.71858400	-0.27073700	5.31654900
C	-2.29591200	1.51187100	-0.80835000
C	-3.42675600	1.45756400	-1.63620000
C	-1.66632000	2.74348800	-0.56526300
C	-3.92040400	2.62866200	-2.21380700
H	-3.91611700	0.50983900	-1.83529000
C	-2.16773800	3.90855100	-1.14263800
H	-0.78876500	2.79238700	0.07398700
C	-3.29338700	3.85138000	-1.96879900
H	-4.79339400	2.58258200	-2.85733100
H	-1.67772200	4.85834100	-0.95260300
H	-3.67850900	4.75898300	-2.42324500
C	-2.31205400	-1.44652300	-0.90251400
C	-3.43677500	-2.13846000	-0.43017300
C	-1.69903100	-1.84518700	-2.10172100
C	-3.94104900	-3.21961600	-1.15534200
H	-3.91325900	-1.84311900	0.49876500
C	-2.21142000	-2.92259100	-2.82186800
H	-0.82524200	-1.31552900	-2.47209600
C	-3.33119500	-3.61154800	-2.34803400
H	-4.80928400	-3.75559400	-0.78484100
H	-1.73424900	-3.22738600	-3.74801000
H	-3.72487300	-4.45497100	-2.90681900
C	5.32906800	-0.00378700	0.00301400
C	6.02753100	-1.22713700	-0.01130600
C	6.01717100	1.22544000	0.01640500
C	7.41781700	-1.21006200	-0.01229700
H	5.48262200	-2.16498200	-0.02142400
C	7.40754000	1.22030600	0.01518800

H	5.46416900	2.15852100	0.02729200
C	8.10470700	0.00803600	0.00085900
H	7.96674600	-2.14569600	-0.02325900
H	7.94842600	2.16061600	0.02536300
H	9.19019600	0.01263300	0.00007300

TS2-3-irc-2

C	1.22982000	-3.08270000	-0.57571200
N	0.23212600	-2.50714400	-0.43217000
C	4.40300900	1.27386200	2.18815300
C	3.64465800	2.20392800	2.37312800
C	0.16598500	1.21099800	-2.71240800
N	-0.73935800	0.52894400	-2.44927000
N	5.24355900	0.23057600	2.01320400
C	5.97140300	-0.32156700	3.17368300
H	6.53083300	-1.19603500	2.84393400
H	6.64914800	0.41767500	3.61424700
H	5.23475900	-0.62533700	3.91991400
Au	-1.57575600	-1.51598300	-0.15860200
P	-3.61465700	-0.50169000	0.17833200
S	5.89733000	0.02551800	0.43114600
O	6.65970200	-1.23594500	0.46332000
O	4.77974800	0.22556000	-0.51278700
C	7.05128300	1.40236100	0.22543200
H	7.86606500	1.28284600	0.94064700
H	7.43167300	1.35016600	-0.79634400
H	6.50805300	2.33357800	0.39149500
C	-4.71515300	-0.74858200	-1.27113700
C	-6.05944000	-1.11623900	-1.11909600
C	-4.18051300	-0.54950000	-2.55568900
C	-6.86449100	-1.28326000	-2.24763200
H	-6.47677000	-1.27781200	-0.13075200
C	-4.99467500	-0.71657600	-3.67496100
H	-3.13933100	-0.26304500	-2.67708000
C	-6.33422200	-1.08490400	-3.52313700
H	-7.90429700	-1.57146600	-2.12726000
H	-4.58049200	-0.56344500	-4.66685600
H	-6.96259700	-1.21960400	-4.39839200
C	-4.48986500	-1.17325800	1.64816300
C	-5.28326700	-0.35008300	2.46074900
C	-4.38292100	-2.54231800	1.94049900
C	-5.96156800	-0.89488400	3.55235000
H	-5.36687800	0.71095600	2.24998000
C	-5.06734500	-3.08072000	3.02908500
H	-3.76397700	-3.18494000	1.32036700
C	-5.85549300	-2.25728600	3.83681900
H	-6.57031500	-0.25223700	4.18092700
H	-4.97981400	-4.14004200	3.24994400

H	-6.38235400	-2.67662500	4.68853500
C	-3.45536000	1.30947400	0.43077500
C	-4.42562000	2.19371700	-0.06328300
C	-2.36301100	1.80834100	1.15711800
C	-4.30392900	3.56334400	0.17610600
H	-5.26654900	1.81826100	-0.63730500
C	-2.24714700	3.17750700	1.39349300
H	-1.60226300	1.12984400	1.53328400
C	-3.21810700	4.05445300	0.90303300
H	-5.05621800	4.24468200	-0.20947600
H	-1.39570500	3.55914600	1.94846500
H	-3.12570300	5.12126400	1.08374600
C	1.28001200	2.05073300	-3.04072200
C	2.52764300	1.82692100	-2.43218100
C	1.11960900	3.08953900	-3.97487400
C	3.60546500	2.64404900	-2.76359200
H	2.65736100	1.02470300	-1.71445200
C	2.20667600	3.89857400	-4.29435700
H	0.15298600	3.25140400	-4.44002100
C	3.44783000	3.67730000	-3.69090600
H	4.56671500	2.45800300	-2.29692400
H	2.08643100	4.70030500	-5.01597600
H	4.29233800	4.30993300	-3.94723200
C	2.45246400	-3.79316500	-0.73876300
C	3.67421000	-3.09873700	-0.65247600
C	2.41944900	-5.18298200	-0.96798100
C	4.86389900	-3.80778200	-0.78829500
H	3.69074900	-2.02642700	-0.48768200
C	3.61891400	-5.87137700	-1.10872600
H	1.46876100	-5.70153100	-1.03222600
C	4.83550700	-5.18670300	-1.01628200
H	5.80464800	-3.27480100	-0.70300000
H	3.60650500	-6.94151100	-1.28747100
H	5.76760500	-5.73341200	-1.12211500
C	2.75024500	3.29847500	2.56719600
C	2.15953100	3.94029600	1.46035300
C	2.44980100	3.75774600	3.86503500
C	1.29802900	5.01802600	1.65348600
H	2.38672900	3.59117800	0.45796200
C	1.58128300	4.83089900	4.04621100
H	2.90298900	3.26875300	4.72130700
C	1.00428000	5.46759700	2.94413600
H	0.85876100	5.51193800	0.79154100
H	1.36007800	5.17645900	5.05163300
H	0.33842100	6.31282300	3.09021900

**TS2-3**

C	1.56913000	-1.97531300	-0.54699500
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N	0.48554200	-2.14515900	0.04788700
C	3.96517800	0.37318400	0.99083100
C	2.82942700	0.87542900	0.84498400
C	2.15916200	0.41076200	-1.16215500
N	1.83497000	-0.73276700	-1.31940900
N	5.12990100	-0.21242200	1.03307000
C	5.33370300	-1.60716300	1.49668300
H	5.99684800	-2.12391000	0.78883100
H	5.76748800	-1.60415600	2.50854200
H	4.35557000	-2.10701800	1.51090800
Au	-1.28240700	-1.15077800	0.02341700
P	-3.39523400	-0.19025700	0.01507100
S	6.57858600	0.71463200	0.50380500
O	7.47213600	-0.28072500	-0.08705300
O	6.04746500	1.87672800	-0.22318600
C	7.25584000	1.27303400	2.08018300
H	7.51003500	0.40354900	2.68303800
H	8.15697000	1.84023200	1.83963300
H	6.52105400	1.91036600	2.57186100
C	-4.62193100	-1.22236800	-0.88771400
C	-5.96093200	-1.30415700	-0.48307900
C	-4.19631600	-1.93427600	-2.02088500
C	-6.86504000	-2.08444300	-1.20800700
H	-6.29982500	-0.76829400	0.39766100
C	-5.10384200	-2.70982800	-2.74358400
H	-3.15646800	-1.88861300	-2.33488700
C	-6.43802400	-2.78559600	-2.33721100
H	-7.89828400	-2.14656500	-0.88472300
H	-4.76694400	-3.25944700	-3.61714400
H	-7.14181400	-3.39482500	-2.89416500
C	-4.06769100	0.05215300	1.71235500
C	-4.87602300	1.15106100	2.03917400
C	-3.78038500	-0.91032000	2.69322900
C	-5.39197400	1.28105600	3.33086900
H	-5.10029500	1.90611600	1.29250900
C	-4.29937600	-0.77655700	3.98089500
H	-3.15202400	-1.76278700	2.44928100
C	-5.10427200	0.31966200	4.30124900
H	-6.01647900	2.13452600	3.57708700
H	-4.07339700	-1.52619400	4.73314000
H	-5.50465200	0.42437000	5.30511200
C	-3.43120400	1.47227800	-0.78421400
C	-4.42949500	1.83085900	-1.69942100
C	-2.43081100	2.39859100	-0.44910000
C	-4.42730700	3.10504900	-2.27141100
H	-5.20653300	1.12143500	-1.96582800
C	-2.43725400	3.67163900	-1.01953600
H	-1.64934900	2.13029000	0.25559100

C	-3.43592900	4.02700200	-1.93291100
H	-5.20369600	3.37535500	-2.98179300
H	-1.66971800	4.38757300	-0.74352000
H	-3.44137100	5.01787100	-2.37490500
C	2.11893300	1.69936600	-1.81961300
C	3.24383300	2.53624800	-1.90595900
C	0.89796200	2.07078400	-2.41908400
C	3.14800300	3.73017100	-2.61771400
H	4.17714100	2.25254600	-1.43568700
C	0.81411400	3.27819500	-3.10722500
H	0.02959300	1.42596100	-2.32461200
C	1.93809200	4.10206300	-3.21534000
H	4.01885900	4.37162700	-2.70324400
H	-0.14042700	3.57664400	-3.53723100
H	1.87037800	5.03862300	-3.75995700
C	2.70055500	-2.93768700	-0.63093400
C	3.77618000	-2.76550300	-1.51597600
C	2.66463000	-4.07370900	0.19630100
C	4.79931900	-3.71135100	-1.56943900
H	3.80593100	-1.90595400	-2.17746400
C	3.69488600	-5.00893300	0.14627400
H	1.81574700	-4.20129400	0.86015600
C	4.76426100	-4.83102200	-0.73651900
H	5.62164600	-3.57668200	-2.26847400
H	3.65834600	-5.88353400	0.78642100
H	5.56242800	-5.56855800	-0.78235000
C	1.78053100	1.63030600	1.52135800
C	1.72868900	3.03018600	1.42179500
C	0.81158600	0.95059100	2.28218000
C	0.72940500	3.73808700	2.09010400
H	2.47224900	3.55492100	0.83134500
C	-0.18324800	1.66916900	2.94440900
H	0.84340000	-0.13157200	2.34866300
C	-0.22745700	3.06304400	2.85319600
H	0.70560600	4.82155900	2.02057000
H	-0.92487500	1.13621200	3.53153000
H	-0.99900300	3.61878200	3.37402600

### 3

C	1.50030700	1.81779800	0.56417900
N	0.44182100	2.02578400	-0.09179200
C	3.83527400	-0.08189800	-0.73282800
C	2.69012300	-0.64781300	-0.44157400
C	2.19514400	-0.44242900	1.01761600
N	1.69371700	0.66078600	1.40016500
N	4.98035600	0.37408300	-0.97184800
C	5.32094000	1.76802200	-1.35818000
H	6.03566300	2.15691700	-0.63355400
H	5.75887700	1.76018400	-2.35893300

H	4.41098600	2.36614800	-1.34145700
Au	-1.31492500	1.03127100	-0.04922400
P	-3.45669700	0.12081300	-0.03329300
S	6.48868700	-0.77497100	-0.62650900
O	7.47139500	0.11771500	-0.00971600
O	5.88619000	-1.94113000	0.01993400
C	6.98672900	-1.18864300	-2.31208600
H	7.25448900	-0.27278800	-2.83929000
H	7.86250200	-1.83492400	-2.21058300
H	6.16793500	-1.72454300	-2.79237600
C	-4.77141200	1.37553600	-0.33486400
C	-5.93105800	1.08045200	-1.06726600
C	-4.60726000	2.65727600	0.21442100
C	-6.91396300	2.05622700	-1.24260100
H	-6.06482700	0.09731800	-1.50697600
C	-5.59486600	3.62594000	0.03985300
H	-3.70730700	2.89757700	0.77384300
C	-6.74817100	3.32702000	-0.68927000
H	-7.80731200	1.82250200	-1.81390500
H	-5.45967900	4.61501600	0.46673700
H	-7.51324900	4.08456900	-0.82999000
C	-3.69175800	-1.15568700	-1.34724500
C	-4.17658000	-2.44156300	-1.07244400
C	-3.35117100	-0.81433500	-2.66699100
C	-4.32322000	-3.37130400	-2.10619900
H	-4.44260000	-2.71964000	-0.05805800
C	-3.51273500	-1.74020000	-3.69638700
H	-2.96201600	0.17589500	-2.88844400
C	-3.99720900	-3.02180000	-3.41744500
H	-4.70194000	-4.36463900	-1.88441900
H	-3.25990200	-1.46164400	-4.71514600
H	-4.12346800	-3.74266300	-4.21988300
C	-3.89607700	-0.69732700	1.55780200
C	-5.22887400	-0.80350500	1.98476600
C	-2.87263000	-1.23744700	2.35148200
C	-5.52979600	-1.44719400	3.18548200
H	-6.02849900	-0.37594400	1.38834900
C	-3.17945300	-1.88432700	3.54886000
H	-1.83733700	-1.13992300	2.03779500
C	-4.50723400	-1.98910700	3.96736000
H	-6.56272600	-1.52034200	3.51197000
H	-2.38075300	-2.29769200	4.15736200
H	-4.74485600	-2.48548300	4.90344500
C	2.29174000	-1.61324600	1.92355400
C	3.02828900	-2.76000800	1.58726000
C	1.63561200	-1.55819500	3.16839000
C	3.10732700	-3.83078000	2.47765300
H	3.55736800	-2.81712800	0.64291000

C	1. 71666700	-2. 63047300	4. 04982700
H	1. 07655700	-0. 66497500	3. 42480700
C	2. 45185400	-3. 77074500	3. 70755200
H	3. 68572000	-4. 70951600	2. 21008200
H	1. 21080400	-2. 57751100	5. 00922800
H	2. 51526200	-4. 60528500	4. 39925100
C	2. 61244000	2. 82188800	0. 64350700
C	3. 66235600	2. 70536200	1. 56855400
C	2. 57635400	3. 93952800	-0. 20875500
C	4. 65812800	3. 68429400	1. 63679000
H	3. 68415600	1. 86758700	2. 25811500
C	3. 57805400	4. 90574500	-0. 14818200
H	1. 74172100	4. 02867500	-0. 89650500
C	4. 62306500	4. 78245100	0. 77579900
H	5. 45302000	3. 59292800	2. 37152300
H	3. 53799100	5. 76604100	-0. 81026000
H	5. 39394200	5. 54537400	0. 83250500
C	1. 87477500	-1. 39701600	-1. 41710700
C	0. 64450800	-1. 95409400	-1. 02963700
C	2. 31780900	-1. 56595900	-2. 74354000
C	-0. 11949900	-2. 67008500	-1. 95007500
H	0. 28667700	-1. 82919400	-0. 01522800
C	1. 55338800	-2. 28094500	-3. 65590900
H	3. 25921800	-1. 12627500	-3. 06329600
C	0. 33164900	-2. 83681500	-3. 25926800
H	-1. 07244500	-3. 08891500	-1. 64498100
H	1. 90372300	-2. 40398800	-4. 67583600
H	-0. 26886300	-3. 39263000	-3. 97221600

**TS2-7**

C	4. 20061500	-0. 27173900	0. 51881000
N	3. 07133000	-0. 10013200	0. 90741200
Au	1. 06763500	-0. 18971800	0. 57840700
P	-1. 21926200	-0. 30462700	0. 30513200
C	-2. 08841800	1. 13475200	1. 05061100
C	-3. 23652700	1. 68616900	0. 46284900
C	-1. 59514600	1. 67346700	2. 24965500
C	-3. 88301900	2. 76257700	1. 07294400
H	-3. 62144500	1. 28523700	-0. 46919000
C	-2. 24809800	2. 74572900	2. 85571400
H	-0. 70116600	1. 25741700	2. 70611400
C	-3. 39132400	3. 29200400	2. 26732100
H	-4. 76882900	3. 18826600	0. 61150500
H	-1. 86054200	3. 15812500	3. 78218200
H	-3. 89497100	4. 13153400	2. 73677400

C	-1.71930400	-0.35108400	-1.46537000
C	-2.77810300	-1.15586600	-1.90954000
C	-1.03660700	0.46500100	-2.38141900
C	-3.15030000	-1.13908200	-3.25535000
H	-3.30778400	-1.79638300	-1.21190800
C	-1.41625000	0.48086300	-3.72275800
H	-0.21078100	1.08631100	-2.04572300
C	-2.47262400	-0.32180500	-4.16129900
H	-3.97028900	-1.76537300	-3.59346500
H	-0.88604300	1.11709400	-4.42492900
H	-2.76534000	-0.31080900	-5.20691500
C	-1.91875600	-1.81303500	1.09093900
C	-3.16440400	-1.79171300	1.73545800
C	-1.18731100	-3.01072400	1.02656800
C	-3.67400800	-2.95949800	2.30580200
H	-3.73096800	-0.86859100	1.80102000
C	-1.70562600	-4.17301100	1.59658100
H	-0.21675300	-3.03587500	0.53854100
C	-2.94703800	-4.14907200	2.23680700
H	-4.63646800	-2.93625100	2.80766700
H	-1.13480400	-5.09547400	1.54942200
H	-3.34378900	-5.05430500	2.68637900
C	5.53044700	-0.24893600	1.15630800
C	6.73535900	-0.18820200	0.44066000
C	5.56109600	-0.25805000	2.56377100
C	7.95152100	-0.14298000	1.12207700
H	6.72528300	-0.15491100	-0.64258500
C	6.77866600	-0.22316800	3.23567200
H	4.62478100	-0.29801500	3.10960200
C	7.97672700	-0.16570100	2.51756900
H	8.87919100	-0.08412700	0.56129000
H	6.79372200	-0.24047100	4.32100100
H	8.92543900	-0.13538400	3.04455600
C	4.36913500	-0.64625000	-1.32841000
C	4.51086300	-1.90052600	-1.44360000
C	4.23593600	0.50453700	-2.21751900
C	4.23462300	0.30826100	-3.61408600
C	4.13603000	1.81490200	-1.71698400

C	4.13839900	1.39064300	-4.48103200
H	4.31476300	-0.69973500	-4.01015300
C	4.03837700	2.89614700	-2.59141300
H	4.13094100	1.98804700	-0.64755900
C	4.03989500	2.68937400	-3.97157300
H	4.14230700	1.22401100	-5.55380600
H	3.96519200	3.90251100	-2.19130300
H	3.96729600	3.53476400	-4.64886500
N	4.64236100	-3.18302800	-1.32040900
C	5.95898200	-3.86745800	-1.30323100
H	6.66743500	-3.24175800	-0.75912600
H	5.84385600	-4.81799200	-0.78243600
H	6.31362800	-4.03431900	-2.32356000
S	3.15196300	-4.19295700	-1.03430000
O	2.10322700	-3.23393500	-0.66680000
O	3.58852100	-5.29864700	-0.17421600
C	2.83070700	-4.81680100	-2.69765600
H	2.62533800	-3.96987500	-3.35251900
H	3.69439500	-5.39283300	-3.03191300
H	1.95432500	-5.46383800	-2.61783700

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C	3.70626900	-0.59916500	-0.70627900
N	2.60143500	-1.00026800	-1.15366800
Au	0.69864900	-0.74009600	-0.44766200
P	-1.49983000	-0.56961500	0.29058200
C	-1.70374700	0.79781200	1.50709900
C	-2.79163200	1.68005100	1.45777200
C	-0.74144800	0.93872400	2.52079500
C	-2.91445100	2.69109600	2.41367900
H	-3.53846300	1.58401600	0.67671700
C	-0.87426600	1.94482000	3.47625800
H	0.10845900	0.26272100	2.56279800
C	-1.95959800	2.82385200	3.42232500
H	-3.75781800	3.37331500	2.36775200
H	-0.13016200	2.04409900	4.26086600
H	-2.05867600	3.61053200	4.16413000
C	-2.69483100	-0.24019200	-1.06926200

C	-3.98284000	-0.79527700	-1.06956300
C	-2.30428300	0.60624000	-2.11962600
C	-4.86795200	-0.50264700	-2.10874500
H	-4.29329500	-1.45730900	-0.26784000
C	-3.19496000	0.89899600	-3.15150300
H	-1.30499600	1.03339000	-2.13005100
C	-4.47681700	0.34341800	-3.14781500
H	-5.86229600	-0.93859500	-2.10561700
H	-2.88665200	1.55482800	-3.95998800
H	-5.16752600	0.56676000	-3.95523700
C	-2.07196100	-2.09725600	1.14029400
C	-2.95304200	-2.04374400	2.23087600
C	-1.63043600	-3.34273800	0.66607400
C	-3.38987500	-3.22472300	2.83324900
H	-3.29126300	-1.08651000	2.61445000
C	-2.07314900	-4.51881500	1.27025200
H	-0.93938000	-3.39261600	-0.17091300
C	-2.95235300	-4.46084600	2.35412000
H	-4.06916000	-3.17695600	3.67888100
H	-1.72618300	-5.47835200	0.89928700
H	-3.29154100	-5.37724000	2.82750000
C	4.05967700	0.25403800	0.46936100
C	5.28314400	0.08348600	1.13645000
C	3.17247500	1.24249600	0.92678200
C	5.59930700	0.85863200	2.25163600
H	5.98873300	-0.66595500	0.79155300
C	3.49550500	2.02551200	2.03243700
H	2.23484600	1.40440100	0.40415600
C	4.70696600	1.83257600	2.70184400
H	6.54328800	0.70462100	2.76525100
H	2.80370900	2.79275500	2.36699200
H	4.95699200	2.44343600	3.56389100
C	4.94353400	-1.05076300	-1.57462300
C	5.17914700	-2.33900200	-1.50640400
C	5.68054400	-0.09284700	-2.41190700
C	6.88433500	-0.46446800	-3.04308700
C	5.17217200	1.20237000	-2.61278500
C	7.55728000	0.43628800	-3.85986500

H	7.30009200	-1.45447400	-2.87483500
C	5.85121000	2.09964100	-3.43404300
H	4.24662900	1.50213600	-2.13451200
C	7.04142300	1.72143200	-4.05814400
H	8.48690100	0.14192900	-4.33646000
H	5.45034100	3.09686900	-3.58476300
H	7.57010000	2.42583100	-4.69268700
N	5.09573000	-3.58990400	-1.53975200
C	5.90576800	-4.55175600	-0.75437100
H	5.23448700	-5.11420200	-0.10208400
H	6.40307700	-5.23212800	-1.44792800
H	6.63532000	-3.99791400	-0.16491200
S	3.75810600	-4.52287000	-2.59728000
O	2.80405900	-5.00242900	-1.59340100
O	4.56763900	-5.42330400	-3.42367800
C	3.07500400	-3.15719300	-3.54641400
H	2.75321000	-2.37505700	-2.84220900
H	3.83296100	-2.81677200	-4.25255700
H	2.22523500	-3.59670400	-4.07543700

**TS7-8**

C	4.61578000	-0.39107300	1.47611000
N	3.71445900	-0.32282300	0.74570700
C	2.86388400	-0.11293600	-1.08690600
C	1.75362200	0.56663200	-0.89837700
C	1.11931500	0.86204100	0.47794500
N	0.42716500	-0.09554400	0.91068600
N	3.68788200	-0.75848900	-1.85805400
C	3.74370600	-2.23833000	-1.86199600
H	2.72204300	-2.60968000	-1.77988800
H	4.18298300	-2.58645000	-2.79779000
H	4.34376600	-2.59411200	-1.02162900
Au	-0.65958400	-0.32410000	2.60831300
P	-1.91235200	-0.72474400	4.52618900
S	5.22032700	0.09876200	-2.32821700
O	5.01639300	1.49607600	-1.92597300
O	6.32055900	-0.73243200	-1.81177200
C	5.14684600	-0.02720300	-4.12634900



H	4. 20399100	0. 40857700	-4. 45823900
H	5. 99638700	0. 54687700	-4. 50295700
H	5. 23825600	-1. 07288800	-4. 42006900
C	0. 99396400	0. 98718200	-2. 11347900
C	-0. 36377800	0. 65263000	-2. 23152900
C	1. 61940500	1. 73911200	-3. 12109600
C	-1. 07876000	1. 05432800	-3. 35839400
H	-0. 83737700	0. 07332800	-1. 44607800
C	0. 89033400	2. 14785100	-4. 23798800
H	2. 65647200	2. 03745700	-3. 00154100
C	-0. 45641900	1. 80119400	-4. 36212500
H	-2. 12663100	0. 78558400	-3. 45119900
H	1. 37159700	2. 74727600	-5. 00505600
H	-1. 02134500	2. 11850100	-5. 23326200
C	1. 34862500	2. 25074200	0. 99007400
C	2. 50893200	2. 96283300	0. 64350500
C	0. 39702600	2. 87431000	1. 81331300
C	2. 72572700	4. 25022600	1. 13596000
H	3. 25434400	2. 51092000	-0. 00294500
C	0. 60998800	4. 16336200	2. 29580000
H	-0. 52146900	2. 34921200	2. 05718200
C	1. 77880800	4. 85408800	1. 96395000
H	3. 63390100	4. 78200800	0. 86797100
H	-0. 14349300	4. 63657800	2. 91891800
H	1. 94342500	5. 85993100	2. 33883100
C	5. 73675500	-0. 48228200	2. 35408900
C	7. 02374600	-0. 60697600	1. 79676200
C	5. 54815000	-0. 44533600	3. 74754000
C	8. 12059200	-0. 69531200	2. 64836400
H	7. 14403200	-0. 63050200	0. 71831800
C	6. 65813400	-0. 53502900	4. 58128500
H	4. 54830000	-0. 34731200	4. 15688300
C	7. 93892100	-0. 65975100	4. 03407200
H	9. 11780700	-0. 79101600	2. 23152500
H	6. 52594600	-0. 50766100	5. 65789000
H	8. 80003500	-0. 72893700	4. 69159300
C	-3. 47068300	0. 25712700	4. 55420700
C	-3. 96193000	0. 83913000	5. 73176900

C	-4.18954100	0.40464000	3.35708400
C	-5.16021000	1.55568800	5.70977100
H	-3.41027000	0.74103300	6.66118500
C	-5.38782400	1.11708700	3.34243100
H	-3.81031800	-0.03505100	2.43853600
C	-5.87365500	1.69443200	4.51822500
H	-5.53313300	2.00671300	6.62438900
H	-5.93818700	1.22675300	2.41291900
H	-6.80376900	2.25453600	4.50402100
C	-2.41492300	-2.48268500	4.74704200
C	-1.54676200	-3.49180900	4.30164800
C	-3.62698300	-2.83453500	5.35981800
C	-1.88251900	-4.83377100	4.47756800
H	-0.61356100	-3.22624900	3.81242500
C	-3.95994600	-4.17950000	5.52878400
H	-4.31258700	-2.06367300	5.69673300
C	-3.08934700	-5.17888500	5.09023000
H	-1.20655000	-5.60868300	4.12888800
H	-4.90164200	-4.44478800	5.99973600
H	-3.35334700	-6.22413600	5.21988300
C	-0.99531000	-0.25531300	6.05463600
C	-0.22806500	0.92132400	6.03829700
C	-1.05528000	-1.02347100	7.22591500
C	0.45831400	1.32644800	7.18214600
H	-0.16698100	1.51784800	5.13217800
C	-0.36010200	-0.61576300	8.36656800
H	-1.63725400	-1.93889600	7.24989500
C	0.39419200	0.55810500	8.34744600
H	1.04575300	2.23957600	7.16207000
H	-0.41016900	-1.21749900	9.26905800
H	0.93240200	0.87291600	9.23652200

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C	4.18317500	-0.61050900	1.13644700
N	3.52465000	-0.27518800	0.24161300
C	2.96511100	0.06351100	-0.99145300
C	1.78597600	0.74013500	-1.02265200
C	1.03061600	0.96059700	0.28514200

N	0.70786300	-0.10186600	0.90371700
N	3.69339600	-0.43806900	-2.10089800
C	3.62562800	-1.90478800	-2.28514800
H	2.57115700	-2.18293400	-2.32366000
H	4.08393200	-2.17428000	-3.23853900
H	4.12850000	-2.45789000	-1.48422300
Au	-0.33706300	-0.30248700	2.63139800
P	-1.49879600	-0.67717900	4.62060400
S	5.30016100	0.23832900	-2.21496100
O	5.16045400	1.64277900	-1.78767300
O	6.25627800	-0.67025500	-1.53954500
C	5.60566100	0.18377500	-3.99193900
H	4.78449700	0.68994900	-4.49894100
H	6.54631200	0.71632100	-4.14577500
H	5.70524600	-0.85131000	-4.31785200
C	1.16823000	1.20154400	-2.27759300
C	-0.21686200	1.03235100	-2.45882300
C	1.91676000	1.84803900	-3.27909100
C	-0.82986300	1.46238000	-3.63301600
H	-0.80052300	0.54231500	-1.68600000
C	1.29162400	2.29952400	-4.43850800
H	2.97195500	2.03663800	-3.11630300
C	-0.07871000	2.09807600	-4.62424900
H	-1.89581500	1.30980600	-3.77070300
H	1.87155400	2.81889700	-5.19560400
H	-0.56102400	2.44631900	-5.53254300
C	0.77687300	2.39990400	0.62679200
C	1.76043700	3.36178400	0.34288100
C	-0.41401000	2.81372900	1.24236600
C	1.56996700	4.69844400	0.69350300
H	2.68702600	3.06357300	-0.14095000
C	-0.61039700	4.15176500	1.57863200
H	-1.19396500	2.08521100	1.44350500
C	0.38336100	5.09715300	1.31096700
H	2.34665600	5.42723800	0.48176100
H	-1.54389600	4.45956300	2.04086100
H	0.22965900	6.13920400	1.57509100
C	5.01284400	-0.99790100	2.20936300

C	6.39027200	-1.17888400	1.95305400
C	4.46683200	-1.19118100	3.49588100
C	7.21482300	-1.56223600	3.00392300
H	6.77573700	-1.01972300	0.95083300
C	5.31689900	-1.56622400	4.52855700
H	3.40562100	-1.04178500	3.66486600
C	6.68249500	-1.75292300	4.28367600
H	8.27509300	-1.70852700	2.82688200
H	4.91680900	-1.71507100	5.52588300
H	7.33703200	-2.04817200	5.09787200
C	-3.08901400	0.25090000	4.67644400
C	-3.54611700	0.87642500	5.84522500
C	-3.86946300	0.30768700	3.51037500
C	-4.77090300	1.54716900	5.84558300
H	-2.94798100	0.84750900	6.75019900
C	-5.09359700	0.97488300	3.51810200
H	-3.51919800	-0.16961200	2.59898800
C	-5.54480100	1.59660400	4.68516900
H	-5.11745600	2.03199700	6.75323200
H	-5.69212900	1.01358700	2.61298100
H	-6.49572400	2.12075500	4.68826600
C	-1.93288400	-2.43910000	4.93341300
C	-1.08983200	-3.44337200	4.43301900
C	-3.07448300	-2.79735600	5.66690700
C	-1.37848100	-4.78649800	4.67399400
H	-0.21523300	-3.17272000	3.84783000
C	-3.36055800	-4.14289100	5.90167400
H	-3.74305400	-2.03058700	6.04507600
C	-2.51364000	-5.13726300	5.40788300
H	-0.72357900	-5.55805100	4.28050700
H	-4.24779200	-4.41327500	6.46612900
H	-2.74194300	-6.18338500	5.58826600
C	-0.53596600	-0.10655100	6.08569900
C	0.12274500	1.13208200	6.00229900
C	-0.44903400	-0.85726500	7.26614600
C	0.84922400	1.61374400	7.09019800
H	0.06387600	1.71755900	5.08857000
C	0.28669800	-0.37230900	8.35020000

H	-0.95080100	-1.81624100	7.34178800
C	0.93364400	0.86115200	8.26491200
H	1.35084600	2.57428000	7.02000200
H	0.35010300	-0.95957900	9.26138400
H	1.50233200	1.23624600	9.11057700

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C	1.62057100	0.13968100	-0.04753900
C	1.05583600	-0.99950600	-0.17922100
N	2.08653200	1.33231200	0.07381200
C	2.47883400	1.93498300	1.37559900
H	3.19141500	2.73820200	1.19394900
H	1.59825600	2.33965300	1.87959600
H	2.93621700	1.15447400	1.98340200
Au	-1.01446800	-0.46246000	0.06412000
P	-3.28854500	0.09434400	0.23178100
S	1.84442900	2.49678000	-1.34080500
O	0.57219300	2.10461300	-1.95960000
O	2.09104600	3.81893800	-0.75613700
C	3.20636000	2.01920100	-2.42212300
H	3.07949800	0.97198100	-2.69786700
H	3.13036000	2.65887600	-3.30440900
H	4.14538000	2.19706900	-1.89752000
C	1.53245600	-2.34623800	-0.49006200
C	2.89515200	-2.57224500	-0.77205400
C	0.64659200	-3.43744300	-0.50784100
C	3.35233800	-3.85147500	-1.06638900
H	3.59236800	-1.73911500	-0.75341800
C	1.10844800	-4.71847500	-0.80259600
H	-0.40289500	-3.27577600	-0.28218300
C	2.45947700	-4.92822900	-1.08346700
H	4.40422500	-4.01274200	-1.28055800
H	0.41414800	-5.55268500	-0.81080700
H	2.81863500	-5.92669900	-1.31250500
C	-3.49217100	1.88985700	0.56688800
C	-4.47076000	2.36340300	1.45293900
C	-2.65524900	2.79985300	-0.10132000
C	-4.61187200	3.73632500	1.66395100
H	-5.11616300	1.66838500	1.98000200
C	-2.80640800	4.16926600	0.11265400
H	-1.88793500	2.44495600	-0.78466100
C	-3.78282100	4.63844600	0.99545200
H	-5.36914500	4.09819600	2.35259900
H	-2.15844100	4.86853500	-0.40685200
H	-3.89445000	5.70521800	1.16389200
C	-4.19520800	-0.26770100	-1.32418000

C	-3.90106500	-1.45077400	-2.02079800
C	-5.18315200	0.59934200	-1.81318300
C	-4.59353500	-1.76501300	-3.18878100
H	-3.13177500	-2.12400000	-1.65201800
C	-5.87039600	0.28007100	-2.98567600
H	-5.41133700	1.52108200	-1.28815400
C	-5.57762100	-0.89908200	-3.67270000
H	-4.36124700	-2.68065200	-3.72374300
H	-6.63183200	0.95603100	-3.36231300
H	-6.11176300	-1.14185200	-4.58618600
C	-4.14370100	-0.81404400	1.57913500
C	-3.44838300	-1.07296000	2.77139400
C	-5.47768100	-1.22807900	1.44880800
C	-4.08441000	-1.73122200	3.82279300
H	-2.41236300	-0.76189100	2.87643800
C	-6.10686600	-1.89054300	2.50423600
H	-6.02174600	-1.04076600	0.52876000
C	-5.41325700	-2.14159900	3.68938800
H	-3.54166300	-1.92928500	4.74190300
H	-7.13824800	-2.21207900	2.39733400
H	-5.90523400	-2.66015600	4.50655600

**TS1-4**

C	-4.90244500	0.52744600	-0.28707200
N	-3.89333800	1.01078900	0.03871600
C	-2.08454500	1.03078000	-0.06307000
C	-1.57379600	-0.15226400	0.21352800
N	-1.71628800	2.28373800	-0.35038400
C	-2.06048900	2.90913000	-1.63694800
H	-3.13725000	3.10173000	-1.70659900
H	-1.50937400	3.84464800	-1.72757000
H	-1.75743800	2.23736600	-2.44296600
Au	0.50751500	-0.26545100	-0.02631500
P	2.85437600	-0.35840400	-0.19962800
S	-1.09471500	3.31235600	0.94617000
O	-0.50049000	2.40537300	1.93756700
O	-0.32647200	4.36704100	0.26747000
C	-2.58759600	4.04155100	1.65812200
H	-3.23404900	3.23738000	2.01048700
H	-2.26062200	4.66565000	2.49230000
H	-3.07854800	4.65116800	0.89864000
C	-2.28986900	-1.32938700	0.73435800
C	-2.97573700	-1.27147800	1.96183200
C	-2.25349600	-2.54844500	0.03409600
C	-3.61831600	-2.40246600	2.46652200
H	-2.97827200	-0.34483900	2.52711000
C	-2.92172100	-3.66759000	0.52806300
H	-1.70401400	-2.60922400	-0.90055000

C	-3.60219000	-3.60098100	1.74724600
H	-4.12447700	-2.34900800	3.42605000
H	-2.89587900	-4.59826100	-0.03073100
H	-4.09928600	-4.48145000	2.14311900
C	-6.15110800	-0.05427200	-0.63342900
C	-7.01414400	0.61460000	-1.52471200
C	-6.50505700	-1.29980400	-0.07515600
C	-8.23298700	0.03143000	-1.85046600
H	-6.72615500	1.57152100	-1.94664000
C	-7.72874900	-1.86520300	-0.41661700
H	-5.82518900	-1.80165100	0.60525900
C	-8.58914000	-1.20368000	-1.29857500
H	-8.90606200	0.53763900	-2.53434100
H	-8.01308900	-2.82359000	0.00501300
H	-9.54272800	-1.65284700	-1.55804600
C	3.54086300	1.30466100	-0.58311700
C	4.65924100	1.47142600	-1.41340200
C	2.91650200	2.43096100	-0.02238400
C	5.14774800	2.75299600	-1.67378200
H	5.14248400	0.60934300	-1.86206600
C	3.40842500	3.70797100	-0.28935800
H	2.04758500	2.31524900	0.61895400
C	4.52361500	3.86996200	-1.11479400
H	6.01261500	2.87698000	-2.31849200
H	2.90866000	4.57148700	0.13812000
H	4.90248900	4.86532000	-1.32668500
C	3.65165600	-0.91822900	1.36003300
C	3.04592700	-1.95218400	2.09182100
C	4.84731700	-0.34959100	1.82198300
C	3.63626600	-2.41699200	3.26599600
H	2.11331700	-2.38958200	1.74538900
C	5.43072300	-0.81640800	3.00133200
H	5.31718700	0.45770600	1.26970200
C	4.82813300	-1.84855200	3.72234600
H	3.16246200	-3.21621200	3.82770200
H	6.35434100	-0.36983600	3.35677500
H	5.28308700	-2.20637200	4.64101100
C	3.44575600	-1.48894300	-1.52547700
C	2.72486300	-1.54667000	-2.72900100
C	4.59992600	-2.27076700	-1.37204000
C	3.16002900	-2.36765200	-3.76805800
H	1.82422900	-0.95069700	-2.85060700
C	5.02779400	-3.09523500	-2.41464800
H	5.15990000	-2.24208000	-0.44294000
C	4.31134500	-3.14361200	-3.61141800
H	2.59830300	-2.40654700	-4.69646300
H	5.92035400	-3.70044200	-2.28848800
H	4.64613200	-3.78757200	-4.41899600

## 4

C	4.89363000	-0.39119500	-0.37846300
N	3.74917300	-0.57774100	-0.33510100
C	2.35320800	-0.71981900	-0.33714400
C	1.56872500	0.37278200	-0.14502400
N	1.97087800	-2.06449100	-0.56253700
C	1.38263100	-2.40120100	-1.87311400
H	2.07982700	-2.08319900	-2.65201000
H	1.25466300	-3.48259300	-1.95037100
H	0.41310900	-1.91861900	-2.03105000
Au	-0.49389100	0.25555800	-0.15357900
P	-2.86784900	0.20619900	-0.07571700
S	1.29405900	-2.88138000	0.81639400
O	1.68663800	-2.09216400	1.99571000
O	-0.11196700	-3.22859800	0.52619200
C	2.23527300	-4.42524700	0.82714400
H	3.28467800	-4.18993000	1.00187500
H	1.83136000	-5.02397600	1.64568300
H	2.09455100	-4.94502000	-0.12101800
C	2.17357200	1.68422700	0.17721200
C	2.97153200	1.84256200	1.32739600
C	1.91803300	2.80928200	-0.62771200
C	3.50631300	3.09041300	1.65185500
H	3.12829200	0.99370500	1.98726200
C	2.48368200	4.04478400	-0.31826500
H	1.28048700	2.70538300	-1.50061500
C	3.27610400	4.19178200	0.82332900
H	4.09083900	3.20445800	2.56048500
H	2.29086500	4.89934000	-0.95980500
H	3.69367700	5.16161200	1.07589800
C	6.28387700	-0.13600400	-0.39376500
C	7.18025100	-1.12663800	-0.84741000
C	6.74687300	1.12194500	0.05003600
C	8.54158300	-0.84960100	-0.84895400
H	6.80724400	-2.08647100	-1.18794600
C	8.11335300	1.37447000	0.03519200
H	6.03930000	1.86911800	0.39387400
C	9.00701900	0.39506400	-0.41065400
H	9.24186400	-1.60292800	-1.19380600
H	8.48349000	2.33684200	0.37250100
H	10.07237500	0.60255900	-0.41748200
C	-3.59234400	-1.09329400	-1.15969000
C	-4.70507400	-0.84544800	-1.97557900
C	-3.00561900	-2.37014000	-1.14656000
C	-5.22681700	-1.86710300	-2.77195200
H	-5.16205100	0.13842100	-1.99388900
C	-3.53869100	-3.38570300	-1.93984600



H	-2.14211100	-2.57216900	-0.51856400
C	-4.64613900	-3.13597300	-2.75459400
H	-6.08721200	-1.66899900	-3.40400700
H	-3.08619800	-4.37274600	-1.92242100
H	-5.05469000	-3.92835300	-3.37466500
C	-3.49456400	-0.13146800	1.62071000
C	-2.80120700	0.40748100	2.71602600
C	-4.65035100	-0.89531600	1.84021300
C	-3.26482400	0.19159700	4.01310200
H	-1.89906200	0.99158300	2.55537900
C	-5.10712400	-1.11087700	3.14146700
H	-5.18796300	-1.32643300	1.00181700
C	-4.41704400	-0.56848900	4.22696900
H	-2.72219600	0.60963800	4.85542400
H	-6.00042600	-1.70595400	3.30526700
H	-4.77310100	-0.74174100	5.23801700
C	-3.62337400	1.80142400	-0.60069600
C	-3.03960200	2.50204900	-1.66839000
C	-4.76773600	2.32027100	0.02220900
C	-3.59804200	3.70040300	-2.11086900
H	-2.14939700	2.10906700	-2.15244000
C	-5.31890600	3.52406700	-0.42093800
H	-5.22421800	1.79178200	0.85277200
C	-4.73716000	4.21373700	-1.48593300
H	-3.14171500	4.23547700	-2.93822500
H	-6.20232800	3.92225600	0.06886300
H	-5.16776900	5.15063400	-1.82620300

#### TS<sub>4-5</sub>

C	4.41335400	0.38923600	0.13303100
N	3.44040100	0.92841400	0.60053200
C	2.03352400	0.95021700	0.58533200
C	1.25969000	-0.09201600	0.99191600
C	3.05799300	-1.39910000	-1.62162300
N	4.00390600	-0.92204900	-1.12534500
N	1.50746400	2.21500000	0.20701800
C	0.97913000	3.14059600	1.21958100
H	1.78477100	3.58634200	1.81926300
H	0.41015100	3.92732800	0.72187400
H	0.29895400	2.59374100	1.87836100
Au	-0.78268700	0.02439700	0.67406400
P	-3.12410200	0.15303700	0.26870800
S	1.64775200	2.74947700	-1.39718100
O	2.10258600	1.57991500	-2.17775100
O	0.41426500	3.48499000	-1.74101300
C	2.99257400	3.95993200	-1.38850000
H	3.91047200	3.46098800	-1.07709500
H	3.08699500	4.33943000	-2.40738000

H	2. 73524000	4. 77254600	-0. 70644600
C	1. 82512600	-1. 27984900	1. 67207200
C	1. 31421400	-2. 56299000	1. 39162300
C	2. 82155800	-1. 17218800	2. 66303200
C	1. 83389300	-3. 69609100	2. 00993200
H	0. 46667100	-2. 66029100	0. 71324200
C	3. 31547800	-2. 30222900	3. 30985300
H	3. 19199100	-0. 19205500	2. 94901700
C	2. 84084700	-3. 57283000	2. 97335500
H	1. 43065600	-4. 67620200	1. 76770400
H	4. 06926300	-2. 19224200	4. 08561700
H	3. 22926700	-4. 45279900	3. 47479000
C	1. 99068700	-2. 07278100	-2. 27447300
C	1. 95785800	-3. 48182000	-2. 23997500
C	0. 98781500	-1. 33625100	-2. 93833400
C	0. 92033000	-4. 15093800	-2. 87622300
H	2. 73659300	-4. 02948600	-1. 71632800
C	-0. 04681100	-2. 02790200	-3. 56632600
H	1. 03352400	-0. 25389200	-2. 93772700
C	-0. 07500600	-3. 42468500	-3. 53982800
H	0. 88881700	-5. 23509600	-2. 85955600
H	-0. 82346400	-1. 47789100	-4. 08254800
H	-0. 88236200	-3. 95668300	-4. 03813000
C	5. 85061400	0. 42555600	0. 27716900
C	6. 72020600	-0. 36369900	-0. 49116700
C	6. 37106300	1. 31880800	1. 23517100
C	8. 09454600	-0. 25731300	-0. 30224700
H	6. 31300300	-1. 05133900	-1. 22141300
C	7. 74457900	1. 41738100	1. 41581500
H	5. 69271800	1. 92473200	1. 82866500
C	8. 60842900	0. 62769300	0. 64722100
H	8. 76522100	-0. 87061400	-0. 89470100
H	8. 14661100	2. 10554300	2. 15262000
H	9. 68424400	0. 70387600	0. 78968200
C	-3. 65969400	1. 84678200	-0. 21017600
C	-4. 95537800	2. 31720300	0. 05269800
C	-2. 74211800	2. 67412700	-0. 87587800
C	-5. 32548000	3. 60082600	-0. 34910800
H	-5. 66878600	1. 69304000	0. 57696300
C	-3. 11759800	3. 95522100	-1. 27910200
H	-1. 73008400	2. 33530500	-1. 07756500
C	-4. 40793400	4. 42103000	-1. 01732000
H	-6. 32474600	3. 96327600	-0. 14131400
H	-2. 39558700	4. 58223600	-1. 78849500
H	-4. 70138900	5. 42036200	-1. 32479600
C	-3. 63928300	-0. 96584500	-1. 11143900
C	-3. 33680700	-2. 33542100	-1. 00044100
C	-4. 27932900	-0. 48850600	-2. 25807900

C	-3.68672400	-3.21320200	-2.02220700
H	-2.82518300	-2.70996400	-0.11650700
C	-4.62463900	-1.37488200	-3.28433600
H	-4.51787500	0.56526800	-2.35705400
C	-4.33737400	-2.73528800	-3.16490700
H	-3.45486600	-4.27370700	-1.92603700
H	-5.13031200	-0.99970000	-4.16902600
H	-4.61491800	-3.42165000	-3.95859400
C	-4.15387200	-0.34259000	1.71171400
C	-3.65815700	-0.11710800	3.00355600
C	-5.42990400	-0.90902400	1.54528700
C	-4.43314900	-0.43973700	4.11752700
H	-2.66866400	0.30569700	3.13743200
C	-6.19699600	-1.23468100	2.66333300
H	-5.81741300	-1.10555000	0.55166600
C	-5.70395800	-0.99804500	3.94888200
H	-4.04226000	-0.26410500	5.11651200
H	-7.18263300	-1.67137600	2.53070500
H	-6.30189500	-1.25395600	4.81621700

## 5

C	-4.29675100	0.22014000	-0.07101300
N	-3.46358600	0.87625800	-0.77616100
C	-2.06497500	0.81550800	-0.69805500
C	-1.27764400	-0.26638700	-0.97778100
C	-2.82639700	-1.05014900	1.49296800
N	-3.80239000	-0.66032200	0.96457600
N	-1.47370900	2.09715200	-0.44965700
C	-1.02499800	2.92149600	-1.58321700
H	-1.86613000	3.27459100	-2.19249300
H	-0.45930300	3.77174400	-1.19915900
H	-0.36001300	2.31863200	-2.20450800
Au	0.76794800	-0.09213200	-0.67354600
P	3.09880900	0.13912600	-0.25179700
S	-1.77998500	2.87525000	1.02220700
O	-2.21956300	1.81234200	1.95890500
O	-0.61448000	3.72825300	1.32385300
C	-3.19251600	3.97465200	0.75552900
H	-4.04742400	3.37691900	0.43993100
H	-3.39179800	4.46956300	1.70774800
H	-2.92539600	4.71351700	-0.00118800
C	-1.82606100	-1.51968300	-1.54378000
C	-1.27938200	-2.76577800	-1.17106300
C	-2.84856900	-1.52153100	-2.51680000
C	-1.76506700	-3.95836300	-1.70491700
H	-0.45755300	-2.78719100	-0.46128600
C	-3.31675800	-2.71283300	-3.06714800
H	-3.25803200	-0.57794700	-2.86219900

C	-2.78772300	-3.93840600	-2.65583600
H	-1.32773100	-4.90377800	-1.39632700
H	-4.09212300	-2.68349800	-3.82717700
H	-3.15328000	-4.86512500	-3.08747300
C	-1.82779700	-1.67338400	2.26223700
C	-1.79952600	-3.08650600	2.33556800
C	-0.87875900	-0.88126700	2.94820500
C	-0.81687300	-3.69584700	3.10271300
H	-2.53176100	-3.67326700	1.79255400
C	0.09528500	-1.51908200	3.70614800
H	-0.93440100	0.19815700	2.86552600
C	0.12757800	-2.91552600	3.78196300
H	-0.78230000	-4.77799200	3.17176000
H	0.83856600	-0.92880800	4.23091500
H	0.89788700	-3.40110700	4.37268100
C	-5.75398600	0.28931900	-0.18567300
C	-6.58631300	-0.43489500	0.68379200
C	-6.32696200	1.09904300	-1.18403900
C	-7.97066500	-0.34307900	0.56228500
H	-6.15162100	-1.06627600	1.45183700
C	-7.70905800	1.18408500	-1.29990200
H	-5.67743200	1.64782500	-1.85716900
C	-8.53401800	0.46478800	-0.42746700
H	-8.60891800	-0.90317300	1.23800500
H	-8.14773300	1.80842600	-2.07177200
H	-9.61334400	0.53246400	-0.52259700
C	3.56822400	1.87908700	0.12479800
C	4.87438400	2.35354200	-0.07554300
C	2.58939100	2.74334200	0.64019200
C	5.19326200	3.67355500	0.24292100
H	5.63676400	1.70057700	-0.48809000
C	2.91567900	4.06189500	0.96066000
H	1.56929800	2.40315000	0.78747400
C	4.21650300	4.52755300	0.76225600
H	6.20402800	4.03590300	0.08130200
H	2.14452600	4.71573700	1.35559700
H	4.46965700	5.55523200	1.00556900
C	3.62937200	-0.86672300	1.20455900
C	3.46425900	-2.26089200	1.14549000
C	4.14725200	-0.28414600	2.36862500
C	3.82656700	-3.05815300	2.22983800
H	3.06461300	-2.72294000	0.24653500
C	4.49969500	-1.08706600	3.45729500
H	4.28193400	0.79079800	2.42706400
C	4.34390800	-2.47198500	3.38942400
H	3.71251900	-4.13651900	2.16740900
H	4.90726300	-0.62714500	4.35270500
H	4.63229500	-3.09407400	4.23174300

C	4.17885100	-0.41242000	-1.63691800
C	3.70588300	-0.27860600	-2.95164000
C	5.46543500	-0.92845800	-1.41541800
C	4.51348500	-0.64380700	-4.02869400
H	2.70589000	0.10638200	-3.13140000
C	6.26815200	-1.29438700	-2.49672100
H	5.83688200	-1.05330400	-0.40309700
C	5.79466900	-1.15112100	-3.80251900
H	4.13938100	-0.53841600	-5.04249000
H	7.26188500	-1.69373600	-2.31779900
H	6.42061500	-1.43928600	-4.64162700

**TS<sub>5-6</sub>**

C	-4.24856800	0.21330300	0.05812700
N	-3.49218800	0.89476600	-0.73405100
C	-2.12910000	0.85806100	-0.66777300
C	-1.36852600	-0.32833900	-0.75361900
C	-2.43098100	-0.69103800	1.20732200
N	-3.64310900	-0.51097000	1.12232300
N	-1.47064500	2.10208900	-0.55313900
C	-0.81866500	2.68926400	-1.73869300
H	-1.55669500	3.06013900	-2.46164100
H	-0.17301300	3.50172800	-1.41326500
H	-0.20154700	1.92331600	-2.21410700
Au	0.70981000	-0.18296300	-0.51287600
P	3.05226700	0.08239800	-0.23323000
S	-1.81180500	3.11206100	0.78334500
O	-2.21677400	2.19310100	1.86424600
O	-0.65271400	4.01329400	0.91538500
C	-3.24109400	4.12094600	0.32480500
H	-4.07850900	3.46006000	0.10568700
H	-3.46101200	4.76075400	1.18084100
H	-2.97218300	4.72951400	-0.53969600
C	-1.89037400	-1.55949400	-1.40834600
C	-1.32228500	-2.81220200	-1.09039100
C	-2.87112800	-1.52048500	-2.42183400
C	-1.74943200	-3.97758300	-1.72438700
H	-0.54299300	-2.86334300	-0.33964400
C	-3.27511700	-2.68470400	-3.07257400
H	-3.30534900	-0.57152100	-2.71692200
C	-2.72840700	-3.91963600	-2.71905000
H	-1.30389600	-4.92997700	-1.45292100
H	-4.01865400	-2.62474000	-3.86174900
H	-3.04677900	-4.82506300	-3.22752300
C	-1.53223800	-1.39259900	2.08387600
C	-1.84082400	-2.71556800	2.46424700
C	-0.38064500	-0.75377600	2.58583900
C	-0.98870800	-3.39089800	3.33334300
H	-2.73242500	-3.19603900	2.07223100

C	0.46053000	-1.44122700	3.45349200
H	-0.18829700	0.27955400	2.31211200
C	0.16042500	-2.75442700	3.82135100
H	-1.21568900	-4.40819500	3.62834400
H	1.37780600	-0.96933200	3.81371900
H	0.83146100	-3.29154500	4.48965600
C	-5.70201200	0.16938500	-0.03953200
C	-6.45599700	-0.55953800	0.89801300
C	-6.35803700	0.86004500	-1.07864800
C	-7.84448800	-0.58874100	0.80041300
H	-5.95018200	-1.09682600	1.69034300
C	-7.74323100	0.82368300	-1.16928100
H	-5.76941800	1.42093500	-1.79682800
C	-8.48875800	0.10073100	-0.22953900
H	-8.42737200	-1.14895600	1.52672300
H	-8.24765000	1.35810200	-1.96797100
H	-9.57177600	0.07580000	-0.30282900
C	3.51527700	1.86046500	-0.09416300
C	4.79650300	2.31935800	-0.43903700
C	2.56008800	2.77214500	0.38339100
C	5.11364700	3.67079100	-0.30107800
H	5.54098500	1.62945800	-0.82324500
C	2.88404900	4.12230800	0.52268800
H	1.55841000	2.44281700	0.64112300
C	4.16058600	4.57211100	0.18041500
H	6.10505600	4.01975700	-0.57362000
H	2.13032200	4.81169700	0.88970800
H	4.41237300	5.62346400	0.28274300
C	3.65202800	-0.73313000	1.30969100
C	3.54567600	-2.13258700	1.41400400
C	4.15647500	0.00400400	2.38681900
C	3.95571200	-2.77987900	2.57816700
H	3.15413700	-2.71180000	0.58314500
C	4.55320100	-0.65215100	3.55930100
H	4.24723700	1.08231700	2.31792300
C	4.45828200	-2.04025200	3.65432100
H	3.88511700	-3.86096300	2.64390300
H	4.94935100	-0.07306000	4.38882400
H	4.77990600	-2.54825700	4.55835600
C	4.06087300	-0.62876400	-1.59824000
C	3.51929500	-0.64882200	-2.89300400
C	5.36027300	-1.11266000	-1.38485600
C	4.27416600	-1.13903500	-3.96054200
H	2.50991500	-0.28510300	-3.06749700
C	6.10669600	-1.60463700	-2.45344000
H	5.78446900	-1.11653300	-0.38572600
C	5.56757400	-1.61872400	-3.74323700
H	3.84754400	-1.15276300	-4.95881900

H	7.11026900	-1.98162800	-2.28139500
H	6.15002100	-2.00521700	-4.57105700

**6**

C	2.85673600	-0.87294900	0.95569600
N	2.63622700	-1.12939000	-0.33693400
C	2.07809400	-0.19348100	-1.11143600
C	1.69062200	1.12264800	-0.57254100
C	2.06117700	1.28398500	0.84031700
N	2.58848900	0.30211300	1.56420800
N	1.91289800	-0.56125700	-2.42578800
C	1.18071900	0.23953100	-3.41701700
H	1.75495700	1.12089900	-3.69951900
H	1.02135200	-0.38215300	-4.29557600
H	0.20968800	0.54758700	-3.01621800
Au	-0.44261400	0.42634000	-0.10950400
P	-2.59784100	-0.40582200	0.27088400
S	2.09919000	-2.30811800	-2.85772700
O	1.36056600	-3.14184400	-1.89331200
O	1.75056400	-2.34887200	-4.28705000
C	3.87632200	-2.57990800	-2.72487600
H	4.18157500	-2.43580800	-1.69167200
H	4.03427400	-3.60979200	-3.05298100
H	4.36702100	-1.88504100	-3.40662800
C	1.80797200	2.35873200	-1.44617600
C	0.72549700	3.11054700	-1.92102300
C	3.10702900	2.77102100	-1.78555900
C	0.93186000	4.23778600	-2.71612900
H	-0.28943200	2.80872500	-1.67707600
C	3.31588400	3.89660300	-2.58346800
H	3.96201700	2.20707900	-1.42161300
C	2.22767800	4.63371000	-3.05215400
H	0.07882400	4.80584800	-3.07475300
H	4.32861000	4.19693300	-2.83440300
H	2.38754100	5.51019000	-3.67223300
C	1.90962200	2.57610300	1.55985900
C	2.90405700	2.93095400	2.48956200
C	0.81075200	3.43433300	1.38603000
C	2.81586100	4.12457600	3.20050600
H	3.74679900	2.26564300	2.63764600
C	0.71331200	4.61660800	2.11601400
H	0.01550700	3.16903400	0.69899100
C	1.71952700	4.97015700	3.01783500
H	3.60021900	4.39233900	3.90160800
H	-0.14985600	5.26117700	1.98185300
H	1.64601300	5.89659700	3.57921500
C	3.43148000	-1.95165800	1.77465300
C	3.93876000	-1.67570300	3.05765600

C	3.46592800	-3.27131300	1.28448700
C	4.49541100	-2.69624500	3.82201400
H	3.89208800	-0.66115500	3.43528000
C	4.01412900	-4.28845200	2.05968700
H	3.02942500	-3.48789600	0.31568300
C	4.53651900	-4.00233800	3.32474100
H	4.89576100	-2.47678000	4.80688600
H	4.02855800	-5.30662900	1.68332400
H	4.96738800	-4.79763200	3.92573700
C	-2.99699700	-1.73074500	-0.93087800
C	-4.31513100	-1.93635200	-1.36864000
C	-1.96656700	-2.56174300	-1.39891000
C	-4.59433500	-2.97034400	-2.26320000
H	-5.11617900	-1.29162500	-1.02101900
C	-2.25453000	-3.59086700	-2.29449800
H	-0.93909100	-2.41582500	-1.07928600
C	-3.56692300	-3.79571900	-2.72644000
H	-5.61396700	-3.12599500	-2.60198400
H	-1.44628500	-4.21818800	-2.65621600
H	-3.78895900	-4.59368800	-3.42846800
C	-2.74745000	-1.10219800	1.96180300
C	-2.13135600	-0.43253200	3.03192400
C	-3.47961000	-2.27443200	2.20156700
C	-2.25686100	-0.92750900	4.32880300
H	-1.55303000	0.47031500	2.85385500
C	-3.59612000	-2.76606600	3.50286000
H	-3.95090400	-2.80457700	1.38048600
C	-2.98790000	-2.09475700	4.56477200
H	-1.77773700	-0.40690300	5.15209600
H	-4.16035000	-3.67567100	3.68371400
H	-3.07831500	-2.48267800	5.57474000
C	-3.88596600	0.89206600	0.09284000
C	-3.84676600	1.72979700	-1.03434600
C	-4.90631500	1.04915500	1.04070800
C	-4.82218100	2.70862600	-1.21131300
H	-3.06052200	1.61085000	-1.77554500
C	-5.87801200	2.03616600	0.85910700
H	-4.94443100	0.40846100	1.91529400
C	-5.83759800	2.86416600	-0.26291000
H	-4.78998200	3.35078000	-2.08612700
H	-6.66551900	2.15515900	1.59679100
H	-6.59428700	3.63054400	-0.39975600

**P**

C	-1.88091700	0.57417100	0.14844200
N	-1.51102700	-0.70952000	0.28836100
C	-0.20459200	-0.96840900	0.30919300
C	0.78942000	0.02045100	0.19938600
C	0.29376500	1.33544000	-0.01044200



N	-1.02378800	1.58854800	-0.01045200
N	0.17543100	-2.33536500	0.53054000
C	0.00445700	-2.84050500	1.89912500
H	-1.03439900	-2.76553900	2.24543800
H	0.33679500	-3.87866600	1.92544000
H	0.64595600	-2.25496500	2.56377400
S	-0.07299500	-3.42251200	-0.75819000
O	0.31515400	-2.68892000	-1.97934100
O	0.57097000	-4.68742100	-0.36074600
C	-1.85528500	-3.73031600	-0.85782100
H	-2.36220100	-2.77749200	-1.00276900
H	-2.00830600	-4.39944500	-1.70665100
H	-2.17902700	-4.21180800	0.06609000
C	2.23371800	-0.29745700	0.38479200
C	2.90782400	-1.18608000	-0.46794300
C	2.93855500	0.29318100	1.44617700
C	4.25916000	-1.46577000	-0.26351300
H	2.36840100	-1.65571900	-1.28349300
C	4.28713100	0.00385200	1.65148600
H	2.42665900	0.98326600	2.11078100
C	4.95246500	-0.87483700	0.79482500
H	4.76892900	-2.15312100	-0.93246200
H	4.81655500	0.46590900	2.47988700
H	6.00364200	-1.09907400	0.95216400
C	1.15660300	2.52643700	-0.25066500
C	0.76234100	3.76689300	0.27784400
C	2.31286800	2.46543100	-1.04491600
C	1.52003700	4.91175600	0.04219100
H	-0.14356200	3.81774400	0.87200100
C	3.05834100	3.61648300	-1.29491700
H	2.62290700	1.52248500	-1.47989300
C	2.67062200	4.84032300	-0.74638700
H	1.20955600	5.86098300	0.46938200
H	3.94334800	3.55565600	-1.92143600
H	3.25866600	5.73380200	-0.93602600
C	-3.33158000	0.88747700	0.16405100
C	-3.77796200	2.18799900	-0.12010300
C	-4.27492700	-0.10736400	0.46642100
C	-5.13904000	2.48393900	-0.10396700
H	-3.04485000	2.95080100	-0.35580800
C	-5.63511200	0.19300500	0.48385100
H	-3.92759600	-1.10886300	0.69338800
C	-6.07200500	1.48878400	0.19782400
H	-5.47328900	3.49256800	-0.32944800
H	-6.35582700	-0.58395900	0.72248000
H	-7.13306600	1.72140600	0.21014500

1'

C	-1.30502300	1.36609800	0.96233200
C	-1.28820900	2.24032200	0.04625300
N	-2.06698900	0.93878100	2.01099300
C	-1.82593600	-0.37148700	2.64073300
H	-0.79537700	-0.40439700	3.00042500
H	-2.49810800	-0.48772500	3.49071600
H	-2.00553800	-1.19723200	1.94546700
S	-3.73734500	1.52644400	2.03925000
O	-3.82899300	2.50579700	0.94353900
O	-4.60818600	0.34685000	2.14257000
C	-3.77351100	2.41650000	3.60953700
H	-3.05882800	3.23749200	3.55700400
H	-4.79180500	2.79362700	3.72479500
H	-3.53416500	1.72603800	4.41879600
C	-1.18593100	3.15928600	-1.01610200
C	-0.52082700	4.39696500	-0.83337800
C	-1.80298600	2.87413600	-2.25931700
C	-0.47286200	5.31785600	-1.87109000
H	-0.05783700	4.61189600	0.12409400
C	-1.75428900	3.80683600	-3.28660300
H	-2.32221400	1.93037700	-2.38654200
C	-1.08973200	5.02386700	-3.09345900
H	0.03433300	6.26709000	-1.73253600
H	-2.23393100	3.59392000	-4.23629700
H	-1.05524900	5.75016700	-3.90003400
Au	0.59628500	0.49041000	0.40250000
P	2.61249100	-0.64530800	0.00423000
C	3.13224700	-1.55737500	1.51167100
C	3.11141600	-0.88346700	2.74465500
C	3.55176600	-2.89351700	1.45533200
C	3.51295400	-1.54072400	3.90585500
H	2.78831100	0.15333500	2.79454700
C	3.94636100	-3.54737600	2.62476000
H	3.56814700	-3.42369300	0.50903300
C	3.92806500	-2.87438300	3.84687600
H	3.49922400	-1.01496300	4.85559900
H	4.26766000	-4.58321500	2.57741700
H	4.23492000	-3.38700200	4.75333900
C	3.97971200	0.49826900	-0.43419200
C	3.71227800	1.57844900	-1.29046700
C	5.28282400	0.29285200	0.04273800
C	4.74097800	2.43878900	-1.66994700
H	2.70382700	1.74505200	-1.65991400
C	6.30705100	1.16136600	-0.33883200
H	5.49832100	-0.53477100	0.71058700
C	6.03815500	2.23190200	-1.19321000
H	4.53010000	3.27218100	-2.33290700
H	7.31371400	1.00075000	0.03434900

H	6.83697600	2.90662300	-1.48520900
C	2.46280700	-1.86786700	-1.35579400
C	3.54502200	-2.14236700	-2.20577100
C	1.25149700	-2.55787500	-1.52465500
C	3.41268000	-3.10158100	-3.21077700
H	4.48269200	-1.60871600	-2.08981400
C	1.12828000	-3.51756900	-2.52831700
H	0.40667400	-2.34535100	-0.87495500
C	2.20801100	-3.78862300	-3.37246000
H	4.25100500	-3.30866900	-3.86861900
H	0.18945900	-4.04760100	-2.65499100
H	2.10860800	-4.53130900	-4.15806000

**TS1'-2'**

C	-1.63806900	-1.07385600	-0.25350000
C	-2.23804200	0.05420000	0.02397000
N	-2.08166800	-2.35554100	-0.46849600
C	-3.42884500	-2.82192400	-0.09148700
H	-4.18445400	-2.51736600	-0.82051300
H	-3.40665300	-3.90760000	-0.02272200
H	-3.67978200	-2.40334300	0.88399800
S	-1.03927000	-3.51951400	-1.24153300
O	0.34149100	-3.32294900	-0.75568900
O	-1.71714100	-4.81600000	-1.10637200
C	-1.09346600	-3.01833200	-2.97738400
H	-0.71971000	-1.99777800	-3.06693100
H	-0.45064300	-3.71211500	-3.52266400
H	-2.12334700	-3.10065700	-3.32640400
C	-2.06861800	1.41832600	0.49295300
C	-1.77815200	1.67609800	1.84680000
C	-2.20654700	2.49875100	-0.40002400
C	-1.61075700	2.98562300	2.29084100
H	-1.67830300	0.84247700	2.53446800
C	-2.03788400	3.80556200	0.04944500
H	-2.43833000	2.29925600	-1.44166700
C	-1.74028400	4.04991500	1.39416200
H	-1.37927900	3.17740600	3.33390100
H	-2.13927000	4.63398800	-0.64497200
H	-1.61108100	5.07002200	1.74320700
N	-4.19108300	-0.04836100	0.05054000
C	-5.24361700	0.42969000	-0.08395500
C	-6.54528800	0.99019500	-0.23626600
C	-7.15230000	1.64323900	0.85387200
C	-7.21076200	0.88143200	-1.47261500
C	-8.42358800	2.18547200	0.69742800
H	-6.62868700	1.71769200	1.80089700
C	-8.48191000	1.42875200	-1.60974400
H	-6.73229300	0.37445800	-2.30375400

C	-9.08638000	2.07842100	-0.52906000
H	-8.89919400	2.69003700	1.53190000
H	-9.00257500	1.34880900	-2.55825000
H	-10.07916000	2.50239700	-0.64309100
Au	0.44738100	-0.54425500	-0.23514900
P	2.73691100	-0.04183700	-0.20508400
C	3.61375300	-0.92369400	1.15063400
C	2.97803900	-1.05320800	2.39559000
C	4.90261800	-1.44806800	0.97329900
C	3.62888000	-1.68949900	3.45137300
H	1.97376800	-0.66292300	2.53680200
C	5.54766800	-2.08683500	2.03389600
H	5.39851600	-1.36853900	0.01129100
C	4.91373600	-2.20747500	3.27142900
H	3.12996000	-1.78913800	4.41048200
H	6.54359000	-2.49426000	1.88921300
H	5.41635500	-2.70974100	4.09235500
C	3.10956300	1.74629200	0.01236900
C	2.18954800	2.70038100	-0.44795600
C	4.30782900	2.17036900	0.60803600
C	2.47202600	4.06089300	-0.32591000
H	1.25157600	2.37961800	-0.89222600
C	4.58286800	3.53278500	0.73009500
H	5.01963300	1.44144900	0.98209700
C	3.66792700	4.47820200	0.26193800
H	1.75503500	4.79355300	-0.68366000
H	5.51034200	3.85435600	1.19394300
H	3.88447700	5.53766700	0.36048500
C	3.55034800	-0.57398100	-1.76836000
C	4.46222300	0.24268500	-2.45088600
C	3.24468400	-1.85089100	-2.27082000
C	5.06500400	-0.21553800	-3.62466100
H	4.70177400	1.23139000	-2.07410800
C	3.85823600	-2.30283900	-3.43820900
H	2.53183700	-2.48696900	-1.75240400
C	4.76656800	-1.48619200	-4.11750400
H	5.76861900	0.42250100	-4.15070700
H	3.62617000	-3.29315000	-3.81864500
H	5.23895000	-1.83991500	-5.02896700

**2'**

C	-1.64942400	-0.66029500	0.48822000
C	-2.50255600	0.44348600	0.44569000
N	-2.13101900	-1.93190400	0.66860900
C	-3.41538800	-2.25559800	1.32241500
H	-4.24225800	-2.30366300	0.60644400
H	-3.33279300	-3.22855500	1.80406600
H	-3.62010400	-1.49523500	2.07952000

S	-1.03561300	-3.32531400	0.48675500
O	0.23865400	-3.04553200	1.17520300
O	-1.84987400	-4.49601000	0.85248800
C	-0.74856500	-3.35985400	-1.29602500
H	-0.38111600	-2.37885300	-1.62146400
H	0.02419500	-4.12532200	-1.45474900
H	-1.68721100	-3.63683700	-1.78669400
C	-2.05176500	1.86285500	0.53735300
C	-1.24779800	2.27991600	1.61117800
C	-2.45089900	2.81304800	-0.41844400
C	-0.82821000	3.60769700	1.70946600
H	-0.97409200	1.56214100	2.37740100
C	-2.03696800	4.14024700	-0.31368200
H	-3.07287600	2.50797300	-1.25408900
C	-1.22086000	4.53920800	0.74696800
H	-0.21174800	3.91806000	2.54787300
H	-2.34428800	4.86061900	-1.06481300
H	-0.90161400	5.57372800	0.82695300
N	-3.85307900	0.31107300	0.24616900
C	-4.99300500	0.32849900	-0.00867200
C	-6.37349800	0.31296900	-0.32263800
C	-6.80605900	-0.21156800	-1.55981500
C	-7.30660800	0.82571500	0.60536500
C	-8.16416400	-0.23083300	-1.85240000
H	-6.07982200	-0.59861100	-2.26795400
C	-8.65914000	0.81498600	0.28636900
H	-6.96232800	1.22628500	1.55274900
C	-9.08688200	0.28367900	-0.93496700
H	-8.50549000	-0.63916800	-2.79779100
H	-9.38193700	1.21198900	0.99125800
H	-10.14571800	0.27083400	-1.17384500
Au	0.38758200	-0.25420100	0.19083500
P	2.67848100	0.17620600	-0.20558200
C	3.61819700	0.44057500	1.35763900
C	3.04129600	1.24793600	2.35128800
C	4.88288700	-0.12716000	1.57033500
C	3.72829400	1.48862000	3.54074000
H	2.06226200	1.68596900	2.19144900
C	5.56148100	0.11652700	2.76632600
H	5.33246600	-0.75960800	0.81351300
C	4.98825400	0.92254800	3.74914100
H	3.27688900	2.11327300	4.30564600
H	6.53889600	-0.32988700	2.92889000
H	5.51725500	1.10408600	4.67929200
C	2.99290200	1.66612900	-1.24010700
C	2.04113100	2.04458400	-2.19679300
C	4.17185500	2.41331000	-1.10551300
C	2.26924000	3.15068700	-3.01548600

H	1. 11866300	1. 47899700	-2. 29657300
C	4. 39544300	3. 52366200	-1. 92214800
H	4. 91118800	2. 13855900	-0. 35733600
C	3. 44557800	3. 89091300	-2. 88007300
H	1. 52610000	3. 43783400	-3. 75324300
H	5. 30831900	4. 09835700	-1. 81082800
H	3. 62208600	4. 75518200	-3. 51147100
C	3. 49299800	-1. 24026400	-1. 05779600
C	4. 42147200	-1. 05193100	-2. 09266200
C	3. 18061100	-2. 54335800	-0. 63293800
C	5. 03284100	-2. 15360600	-2. 69260600
H	4. 66756300	-0. 05066400	-2. 43038300
C	3. 80320500	-3. 63968700	-1. 23383100
H	2. 45486800	-2. 70362600	0. 15945900
C	4. 72739900	-3. 44594800	-2. 26346800
H	5. 74725500	-2. 00130600	-3. 49520300
H	3. 56402600	-4. 64399500	-0. 89391800
H	5. 20616500	-4. 30274500	-2. 73005200

1"

C	2. 87965800	-0. 74963500	0. 58841300
C	3. 75132900	0. 07203900	0. 39615200
N	1. 90443000	-1. 70553800	0. 78246700
C	2. 03637600	-2. 35092000	2. 13384000
H	1. 21120700	-3. 04803900	2. 28276300
H	2. 99829600	-2. 86501900	2. 20319000
H	1. 98037500	-1. 56372100	2. 88613000
S	2. 15733900	-3. 01223900	-0. 59852500
O	1. 86320100	-2. 26378600	-1. 82651300
O	3. 45006500	-3. 64611500	-0. 31844200
C	0. 81883300	-4. 18948700	-0. 27925800
H	-0. 12713700	-3. 65172400	-0. 20702400
H	0. 81350800	-4. 84501700	-1. 15352400
H	1. 04498500	-4. 76288500	0. 61878500
C	4. 76665900	1. 04745500	0. 17341400
C	4. 54883700	2. 10404800	-0. 73318500
C	5. 99692100	0. 95817100	0. 85455800
C	5. 54626700	3. 04965000	-0. 95050500
H	3. 60311700	2. 16708000	-1. 26179000
C	6. 98490400	1. 91280000	0. 63319400
H	6. 16552000	0. 14010400	1. 54713400
C	6. 76260300	2. 95741900	-0. 26815200
H	5. 37710200	3. 85937900	-1. 65344600
H	7. 93109300	1. 84028200	1. 16007000
H	7. 53783200	3. 69763400	-0. 44086700
Au	-0. 01246000	-0. 67050500	0. 40787500
P	-1. 97485900	0. 46115000	-0. 02744600
C	-2. 80201500	-0. 23127900	-1. 51026000

C	-2.01641000	-0.66582000	-2.59102900
C	-4.20108200	-0.29920900	-1.59043200
C	-2.62989500	-1.15654700	-3.74270400
H	-0.93166600	-0.62460100	-2.53544700
C	-4.80620000	-0.79557600	-2.74623500
H	-4.81511600	0.02755800	-0.75751000
C	-4.02360500	-1.22279100	-3.82048200
H	-2.01958900	-1.49058900	-4.57595100
H	-5.88883400	-0.84952000	-2.80429700
H	-4.49838200	-1.61026700	-4.71662500
C	-1.63967500	2.23510500	-0.35029500
C	-0.71649200	2.91262500	0.46322200
C	-2.30884600	2.92537500	-1.37150700
C	-0.47194100	4.26917000	0.25859200
H	-0.19090200	2.38333500	1.25366500
C	-2.05517700	4.28354200	-1.57207100
H	-3.01854100	2.40923900	-2.00952800
C	-1.13996500	4.95478600	-0.75979400
H	0.24229300	4.78877400	0.88964400
H	-2.57227800	4.81410600	-2.36544000
H	-0.94388200	6.01027100	-0.92131600
C	-3.15967500	0.36829600	1.36914100
C	-3.93808500	1.47777100	1.73057100
C	-3.30905200	-0.84426100	2.06158200
C	-4.85791600	1.36961100	2.77537200
H	-3.82623600	2.42069700	1.20562700
C	-4.23205800	-0.94543200	3.10055800
H	-2.70584400	-1.70602800	1.78873900
C	-5.00563600	0.16199500	3.45912600
H	-5.45594700	2.23136400	3.05470900
H	-4.34411600	-1.88447000	3.63353800
H	-5.71956500	0.08334800	4.27314500

**1-Me**

C	-3.07772300	0.46378600	-0.33481300
C	-2.46842900	-0.66709800	-0.35668900
N	-3.60334100	1.63195500	-0.29041200
C	-3.78195500	2.45311700	-1.50849500
H	-4.83241900	2.74247100	-1.59715000
H	-3.16375900	3.35273900	-1.43356500
H	-3.48419100	1.87026700	-2.37903700
Au	-0.39012300	-0.28215400	-0.12692200
P	1.93610200	0.01755800	0.10177100
C	-3.02343800	-2.02285600	-0.51780200
C	-4.41373700	-2.22040000	-0.63028000
C	-2.17824000	-3.14384100	-0.56565600
C	-4.93834200	-3.49921700	-0.78307400
H	-5.08313500	-1.36497700	-0.59652700

C	-2.70613600	-4.42521800	-0.71991500
H	-1.10392500	-3.00724900	-0.48532900
C	-4.08531600	-4.60663500	-0.82787200
H	-6.01220900	-3.63496600	-0.86741600
H	-2.03914100	-5.28098600	-0.75546900
H	-4.49628900	-5.60461300	-0.94643600
C	2.48157100	1.68527800	-0.45375900
C	3.52196000	1.85561200	-1.37651400
C	1.82881600	2.81210500	0.07387100
C	3.90441200	3.14155600	-1.76576000
H	4.03192500	0.99301200	-1.79188500
C	2.22053500	4.09190400	-0.31266800
H	1.02291400	2.68800300	0.79277700
C	3.25719800	4.25789200	-1.23589900
H	4.70986100	3.26707400	-2.48268200
H	1.71773400	4.95946700	0.10412100
H	3.55816400	5.25560700	-1.53992800
C	2.50165700	-0.15415600	1.84118400
C	1.82728600	-1.04075200	2.69502400
C	3.60997100	0.56227300	2.31929900
C	2.26156900	-1.21344500	4.00897800
H	0.96362600	-1.59301600	2.33525500
C	4.03805300	0.38586600	3.63583400
H	4.13182400	1.25916600	1.67134200
C	3.36595800	-0.50028000	4.48006900
H	1.73470600	-1.89932300	4.66498100
H	4.89431600	0.94383500	4.00156700
H	3.69941700	-0.63175400	5.50497500
C	2.86861600	-1.21118400	-0.89837200
C	2.35965900	-1.59063600	-2.15133300
C	4.07833900	-1.75879400	-0.44619800
C	3.05776900	-2.50131000	-2.94373500
H	1.42074800	-1.17459000	-2.50739400
C	4.76894100	-2.67421800	-1.24217300
H	4.47729900	-1.47914800	0.52318800
C	4.26150500	-3.04533300	-2.48862900
H	2.65917200	-2.79014600	-3.91131300
H	5.70241900	-3.09858600	-0.88539300
H	4.80046100	-3.76014300	-3.10312500
C	-4.02601400	2.25283000	0.98488300
H	-3.45393400	3.17176100	1.14623200
H	-5.09087900	2.49634900	0.93434800
H	-3.84424100	1.55448400	1.80078500

**4-Me**

C	4.91449700	-0.29343800	-0.46997300
N	3.77405100	-0.46464400	-0.34348800



C	2.37652300	-0.69522000	-0.28867900
C	1.56706800	0.33096900	0.07715500
N	2.08599900	-2.01641900	-0.67999200
C	1.59853900	-2.17675900	-2.05179800
H	2.23009200	-1.60862200	-2.74012900
H	1.65511700	-3.23311300	-2.33161000
H	0.55807400	-1.83607900	-2.17414000
Au	-0.49442600	0.19137000	-0.00089100
P	-2.87600700	0.17074000	-0.03558000
C	2.13646700	1.61307600	0.55392300
C	3.01853100	1.65850500	1.65101900
C	1.77923100	2.82512800	-0.06656600
C	3.53774000	2.87388100	2.09965100
H	3.26877400	0.73958400	2.17421700
C	2.32072800	4.03385000	0.36642000
H	1.08138300	2.80937500	-0.89861600
C	3.20008300	4.06458000	1.45216900
H	4.19631300	2.89075900	2.96345500
H	2.04473400	4.95618700	-0.13586900
H	3.60344100	5.01004300	1.80164700
C	6.30368200	-0.05461300	-0.58020800
C	7.15531400	-1.06543400	-1.07327800
C	6.81219000	1.20230200	-0.18711100
C	8.51727800	-0.80763000	-1.16950300
H	6.74707700	-2.02539400	-1.37029000
C	8.17816700	1.43481900	-0.29318900
H	6.13992500	1.96375900	0.19411400
C	9.02724300	0.43634000	-0.78223200
H	9.18319900	-1.57638700	-1.54689500
H	8.58294200	2.39598400	0.00562000
H	10.09259800	0.62827200	-0.86165100
C	-3.58867400	-1.18631400	-1.05677300
C	-4.67215800	-0.97754400	-1.92164600
C	-3.03000700	-2.47008400	-0.94625100
C	-5.18830200	-2.04156300	-2.66466300
H	-5.11079000	0.00992700	-2.01975200
C	-3.55365200	-3.52973600	-1.68494700
H	-2.18942900	-2.64065400	-0.27904400

C	-4.63208000	-3.31591200	-2.54748000
H	-6.02580600	-1.87158500	-3.33440400
H	-3.11875100	-4.52024000	-1.59088500
H	-5.03567900	-4.14055200	-3.12710500
C	-3.59376200	-0.02950700	1.64738200
C	-2.94756700	0.58707600	2.73107700
C	-4.77034100	-0.76068500	1.86843600
C	-3.47780900	0.47996100	4.01621900
H	-2.03175000	1.14953300	2.56976400
C	-5.29317200	-0.86860500	3.15834600
H	-5.27459700	-1.24900500	1.04076400
C	-4.64977600	-0.24924100	4.23126100
H	-2.97295000	0.95997500	4.84900100
H	-6.20244200	-1.43865800	3.32309700
H	-5.05812400	-0.33736200	5.23346700
C	-3.56807800	1.73744100	-0.71296100
C	-2.94860100	2.31491400	-1.83353900
C	-4.69577200	2.35365000	-0.15250800
C	-3.45760400	3.48780600	-2.38930200
H	-2.07144700	1.84559000	-2.27148300
C	-5.19657300	3.53222300	-0.70915000
H	-5.17944500	1.92025300	0.71662700
C	-4.58078300	4.09893800	-1.82601500
H	-2.97521500	3.92690800	-3.25734400
H	-6.06790100	4.00630600	-0.26771000
H	-4.97240300	5.01605200	-2.25550700
C	1.40001500	-2.84938800	0.30742500
H	1.86850500	-2.72395900	1.28635100
H	0.32881300	-2.61264000	0.40496900
H	1.49700400	-3.89905900	0.01221300

**TS4-5-Me**

C	-4.54484200	-0.55523500	-0.47874800
N	-3.60990200	-1.23538400	-0.11759600
C	-2.19918000	-1.26760600	-0.18283700
C	-1.43755300	-0.44040200	0.58884500
C	-2.99408700	1.41856600	-1.58657700
N	-4.03938100	0.92351200	-1.38932100
N	-1.67964300	-2.27149100	-1.03552700

C	-1.33210100	-3.52887800	-0.35761600
H	-2.22197000	-4.10735000	-0.05946300
H	-0.73225300	-4.14652400	-1.03285200
H	-0.73866100	-3.31155600	0.53145500
Au	0.62030000	-0.46760400	0.35134100
P	2.98878200	-0.47327800	0.11716400
C	-2.01412600	0.40331700	1.65923500
C	-1.55973700	1.72555900	1.84117700
C	-2.97235900	-0.09099400	2.56804800
C	-2.07244700	2.53122200	2.85531000
H	-0.79762100	2.11626300	1.17293200
C	-3.46841700	0.70898000	3.59640800
H	-3.30755700	-1.11985900	2.48242800
C	-3.02928400	2.02636200	3.73958200
H	-1.71340500	3.55038800	2.96696600
H	-4.19459900	0.29918000	4.29253500
H	-3.41606500	2.64806500	4.54129900
C	-1.85562300	2.19476200	-1.93788900
C	-1.92539700	3.59558200	-1.78859000
C	-0.69513600	1.58045400	-2.44871700
C	-0.83198100	4.37188800	-2.15625600
H	-2.82576900	4.05344000	-1.39363500
C	0.38629900	2.37477400	-2.81351100
H	-0.64778900	0.50127400	-2.53415800
C	0.31892200	3.76398700	-2.66755800
H	-0.87765100	5.45032000	-2.04569200
H	1.29020700	1.91240400	-3.19515600
H	1.17224800	4.37316400	-2.94770800
C	-5.98721000	-0.57050100	-0.36743000
C	-6.80218200	0.43257500	-0.91437500
C	-6.56937100	-1.65644400	0.32020200
C	-8.18490900	0.34939400	-0.77526500
H	-6.35130700	1.26498900	-1.43987000
C	-7.95043000	-1.72774600	0.45098400
H	-5.93188300	-2.42753600	0.73878000
C	-8.76023500	-0.72616600	-0.09523100
H	-8.81398300	1.12574300	-1.19827000
H	-8.39744400	-2.56371700	0.97921600
H	-9.83907700	-0.78553600	0.01025900
C	3.61843200	-1.88970200	-0.87938600
C	4.94373200	-2.33894800	-0.76777800
C	2.74838700	-2.52435400	-1.77971000
C	5.39040700	-3.40273300	-1.55148400
H	5.62248100	-1.86851200	-0.06359700
C	3.20245400	-3.58494700	-2.56529400
H	1.71561800	-2.19520100	-1.85697900
C	4.52220800	-4.02517100	-2.45163300
H	6.41540100	-3.74781000	-1.45579000

H	2. 52376100	-4. 07176500	-3. 25929000
H	4. 87264000	-4. 85509800	-3. 05779200
C	3. 59523200	1. 05488100	-0. 72529600
C	3. 33860300	2. 29402200	-0. 11443000
C	4. 25210700	1. 02145800	-1. 96264900
C	3. 74882200	3. 47756600	-0. 72563600
H	2. 82732000	2. 33217400	0. 84383500
C	4. 65085700	2. 21206200	-2. 57758100
H	4. 46074800	0. 07214400	-2. 44465700
C	4. 40451000	3. 43915300	-1. 96027700
H	3. 56054700	4. 42898300	-0. 23691300
H	5. 16532800	2. 17563200	-3. 53327100
H	4. 72856100	4. 36132400	-2. 43365200
C	3. 88444300	-0. 53059900	1. 72447100
C	3. 29464300	-1. 22570900	2. 79196200
C	5. 14109900	0. 06970400	1. 90159300
C	3. 95791700	-1. 32813900	4. 01460500
H	2. 31615000	-1. 68146000	2. 66771100
C	5. 79848300	-0. 03348300	3. 12831200
H	5. 60206700	0. 62421000	1. 09022000
C	5. 20951400	-0. 73247200	4. 18392200
H	3. 49377300	-1. 86603400	4. 83557600
H	6. 76914300	0. 43526600	3. 25910400
H	5. 72234500	-0. 80779800	5. 13800000
C	-2. 41045900	-2. 49755600	-2. 28208900
H	-1. 80211600	-3. 12979200	-2. 93479100
H	-3. 38294700	-2. 99641700	-2. 14029200
H	-2. 58137000	-1. 54825700	-2. 79721500

**P1**

C	2. 75569000	-0. 15883600	-0. 70505800
C	2. 42189700	1. 15592400	-0. 35067800
C	2. 46864400	1. 46706100	1. 03505900
N	2. 82894800	0. 55678900	1. 95646300
N	2. 73904200	-0. 61921300	-2. 06324800
C	3. 65509200	-0. 02844500	-3. 05293700
H	4. 60822500	0. 16302100	-2. 55404700
H	3. 82772800	-0. 74251500	-3. 86143600
H	3. 27870900	0. 90291900	-3. 48201300
S	1. 29537300	-1. 31388400	-2. 66907800
O	0. 25551400	-1. 14064100	-1. 63460500
O	1. 11965200	-0. 82404500	-4. 05044000
C	1. 65606300	-3. 08183700	-2. 78062100
H	1. 81864900	-3. 47684700	-1. 77902600
H	0. 78075200	-3. 53809600	-3. 24709500
H	2. 53720600	-3. 22422300	-3. 40636800
C	2. 08877200	2. 18988300	-1. 37586800
C	0. 92596100	2. 10302600	-2. 15573000
C	2. 95973400	3. 27490000	-1. 56546600

C	0.64718900	3.08318500	-3.11011500
H	0.24241400	1.27444800	-2.00824100
C	2.67974300	4.24774800	-2.52368500
H	3.85566700	3.35504500	-0.95687100
C	1.52177000	4.15421700	-3.29910700
H	-0.25585000	3.00349700	-3.70788800
H	3.36422700	5.07969000	-2.66194900
H	1.30223100	4.91295500	-4.04467200
C	2.12619800	2.79686500	1.61715100
C	2.91614200	3.29243100	2.66798600
C	1.00880100	3.53956300	1.20475100
C	2.61333500	4.51136300	3.27085300
H	3.76215800	2.70538600	3.00843800
C	0.70066300	4.75301800	1.81865500
H	0.37014700	3.16422400	0.41373300
C	1.50470800	5.24717000	2.84717000
H	3.24053300	4.88416000	4.07561500
H	-0.17306800	5.31039400	1.49353700
H	1.26544700	6.19590300	3.31916500
C	3.16216700	-1.04400300	0.31914900
N	3.18016700	-0.66800100	1.60770600
C	3.60698800	-2.44716000	0.09077100
C	3.08249100	-3.46582000	0.90151500
C	4.58596100	-2.77521500	-0.86013700
C	3.50280800	-4.78637200	0.74162800
H	2.34817500	-3.20807800	1.65719600
C	5.01571300	-4.09363500	-1.00849200
H	5.02767300	-1.99557100	-1.47125100
C	4.46897500	-5.10477700	-0.21495900
H	3.08049300	-5.56501600	1.37016000
H	5.78317900	-4.33035800	-1.74003700
H	4.80055800	-6.13204500	-0.33559800

**P2**

C	2.83414400	-0.31758600	-0.81403300
C	2.58678800	1.01998300	-0.42030400
N	2.76871600	-0.74214800	-2.17843500
C	3.73926600	-0.20676500	-3.14261300
H	4.73482000	-0.61997900	-2.94695200
H	3.42668700	-0.48147600	-4.14988400
H	3.78683900	0.88469500	-3.09046900
S	1.31334100	-1.41703900	-2.77196800
O	0.29234200	-1.21676300	-1.72422800
O	1.12085100	-0.93204100	-4.15419600
C	1.62168300	-3.19535600	-2.89577500
H	1.77444000	-3.60517000	-1.89891100
H	0.73147700	-3.62063000	-3.36328000
H	2.49582500	-3.35823700	-3.52637500

C	2. 22314200	2. 12131100	-1. 35940500
C	1. 12877100	2. 03500200	-2. 23216600
C	2. 97388400	3. 30793800	-1. 31694400
C	0. 81074900	3. 11050600	-3. 06291100
H	0. 50505800	1. 14967800	-2. 23371000
C	2. 66039700	4. 37316600	-2. 15834000
H	3. 80007500	3. 38464200	-0. 61721500
C	1. 57825900	4. 27546100	-3. 03678500
H	-0. 04394300	3. 03436500	-3. 72844100
H	3. 25581300	5. 28108800	-2. 12382900
H	1. 33003900	5. 10701400	-3. 69024800
C	3. 20052600	-1. 21607200	0. 21100700
N	3. 23953700	-0. 83478300	1. 49382500
C	3. 55563300	-2. 64551700	-0. 02772000
C	2. 93899000	-3. 63800400	0. 74913700
C	4. 53647800	-3. 02186500	-0. 95644400
C	3. 27013300	-4. 98157900	0. 57352600
H	2. 20006900	-3. 34377400	1. 48718800
C	4. 88111000	-4. 36410400	-1. 11690000
H	5. 05030300	-2. 26241100	-1. 53582300
C	4. 24194800	-5. 34857400	-0. 36034500
H	2. 77551600	-5. 74078600	1. 17242900
H	5. 65311800	-4. 64008400	-1. 82953400
H	4. 50604200	-6. 39398500	-0. 49101900
N	2. 71861700	1. 39424400	0. 85907900
C	3. 00828500	0. 45617600	1. 77238700
C	3. 08568100	0. 87971100	3. 19260900
C	2. 79563400	2. 20496300	3. 55466100
C	3. 44993300	-0. 03951400	4. 18953300
C	2. 86909300	2. 60071300	4. 88821500
H	2. 51296800	2. 90723600	2. 77880200
C	3. 52250400	0. 36101300	5. 52165300
H	3. 67407900	-1. 06023300	3. 90141400
C	3. 23273500	1. 68130500	5. 87546500
H	2. 64073200	3. 62771900	5. 15869600
H	3. 80649800	-0. 35712000	6. 28568600
H	3. 28942600	1. 99185900	6. 91506600

**P3**

C	3. 15797300	-0. 95867500	1. 04321700
N	2. 89361300	-1. 18703200	-0. 25069200
C	2. 57395900	-0. 18103700	-1. 06021000
C	2. 50382200	1. 14769600	-0. 57153600
N	2. 35893000	-0. 51291700	-2. 41703700
C	3. 02511200	0. 19929400	-3. 51781000
H	3. 83871000	0. 79423600	-3. 09959200
H	3. 44590900	-0. 51878100	-4. 22578900
H	2. 34104400	0. 85913100	-4. 05514400

S	1. 43721800	-1. 90300700	-2. 80724200
O	0. 39822100	-2. 04927500	-1. 77455300
O	1. 10793600	-1. 75145600	-4. 23717900
C	2. 59114200	-3. 28671300	-2. 65658300
H	2. 95586700	-3. 30460800	-1. 63065000
H	2. 03177100	-4. 19102100	-2. 90475900
H	3. 40434500	-3. 14025300	-3. 36902600
C	2. 03675600	2. 32300500	-1. 35369400
C	0. 93607100	2. 23421400	-2. 22220400
C	2. 64927700	3. 57132400	-1. 16025500
C	0. 47306500	3. 36655900	-2. 89192500
H	0. 43233000	1. 28238800	-2. 35570100
C	2. 19266100	4. 69766100	-1. 84115000
H	3. 47867500	3. 64624600	-0. 46496500
C	1. 10386700	4. 59891900	-2. 71088600
H	-0. 38615800	3. 28479300	-3. 55122000
H	2. 68322400	5. 65489400	-1. 68913400
H	0. 74522400	5. 47800400	-3. 23855900
C	3. 48720300	-2. 17621700	1. 83500300
C	4. 59138300	-2. 23156200	2. 69926100
C	2. 70424200	-3. 32857500	1. 65576900
C	4. 89858000	-3. 41147100	3. 37550900
H	5. 21496200	-1. 35422500	2. 83455400
C	3. 00639400	-4. 50291400	2. 34369800
H	1. 85744100	-3. 28611600	0. 97730100
C	4. 10491100	-4. 54798500	3. 20500200
H	5. 76165300	-3. 44361000	4. 03419700
H	2. 38480900	-5. 38309900	2. 20617800
H	4. 34329800	-5. 46401900	3. 73792300
C	3. 14302800	0. 37246500	1. 53270500
C	3. 38732000	0. 76967500	2. 94836700
C	2. 79205800	0. 08797300	4. 02150400
C	4. 16911100	1. 90348400	3. 21847700
C	2. 98833700	0. 52259200	5. 33160500
H	2. 16335200	-0. 77494800	3. 82985700
C	4. 37450100	2. 32937700	4. 52962800
H	4. 60789000	2. 44864300	2. 38916900
C	3. 78528500	1. 63943900	5. 59114500
H	2. 51231800	-0. 00958900	6. 15013500
H	4. 99012900	3. 20343700	4. 72225500
H	3. 94014900	1. 97371000	6. 61300900
N	2. 84105300	1. 38130700	0. 70268900