

Electronic supplementary information (ESI)

**Mechanistic insight into difunctionalization of aryl chlorides via
palladium/phosphine ligand/norbornene cooperative catalysis**

Xuexiang Ma,^{a*} Chao Shan,^a Tingting Zhang,^a Yusheng Liu,^b Aili Feng,^{c*} and Dongju
Zhang^{d*}

^a Heze University, Heze 274015, P. R. China

^b Heze Medical College, Heze 274000, P. R. China

^c Shandong Institute of Petroleum and Chemical Technology, Carbon Neutrality
Research Institute, Dongying 257061, P. R. China

^d Key Lab of Colloid and Interface Chemistry, Ministry of Education, Institute of
Theoretical Chemistry, School of Chemistry and Chemical Engineering, Shandong
University, Jinan 250100, P. R. China

Corresponding author:

E-mail: maxuexiang_hezeu@163.com, aili1678@163.com, zhangdj@sdu.edu.cn

Table of Contents

I. Another form of oxidative addition of Ar-Cl to Pd ⁰	S3
II. Analysis of C-H··· π interaction in TS2 and the 2,1-insertion mode of NBE.....	S3
III. Comparison between C(sp ³)-Br oxidative addition vs. C-C _{norbornene} reductive elimination.....	S4
IV. Cartesian coordinates of all the structures.....	S5

I. Another form of oxidative addition of Ar–Cl to Pd⁰.

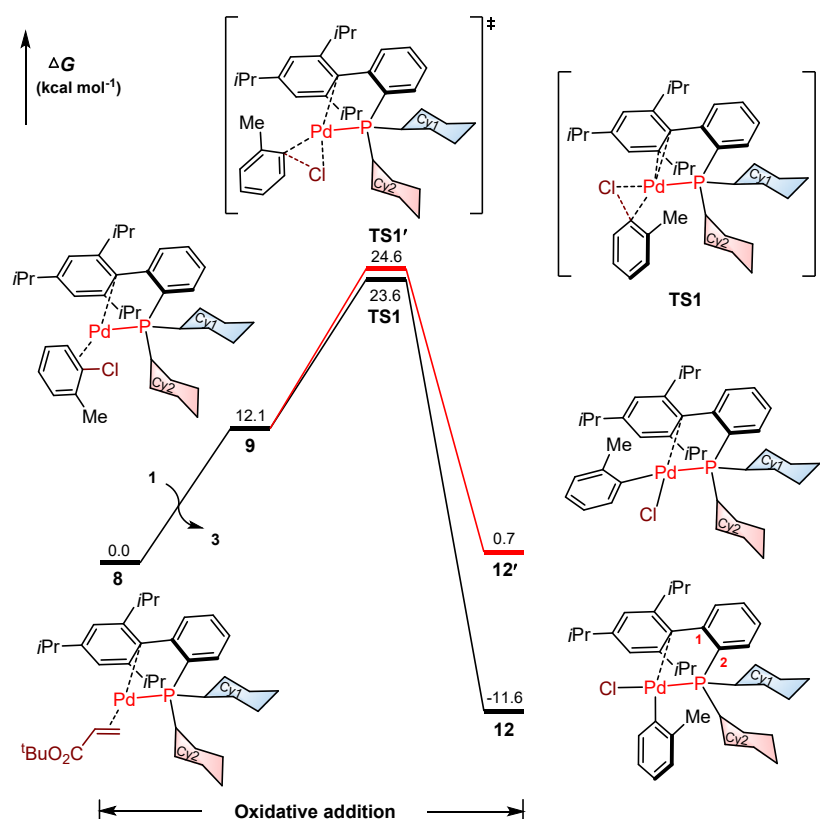


Fig. S1 Calculated Gibbs free energy profiles for oxidative addition of Ar–Cl to Pd⁰ with the Cl atom and P atom in a *cis* orientation.

II. Analysis of C–H⋯π interaction in TS2 and the 2,1-insertion mode of NBE.

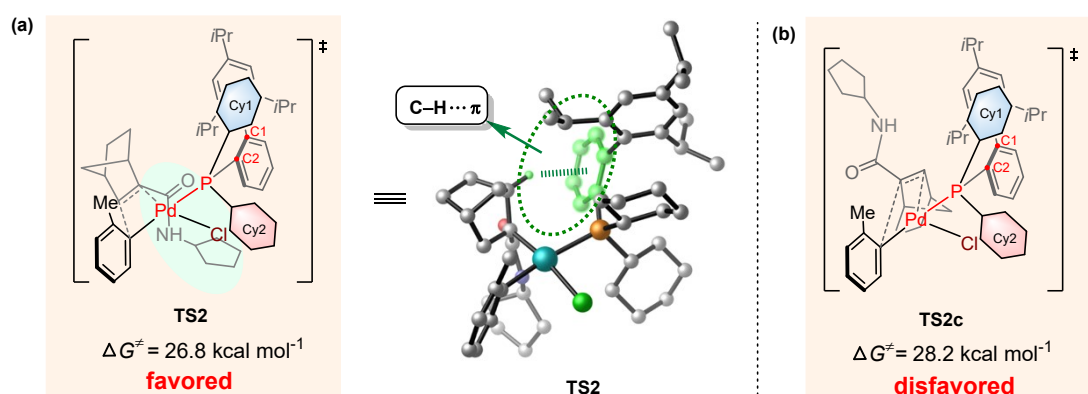


Fig. S2 (a) Analysis of C–H⋯π interaction in TS2, and (b) calculated Gibbs energy for 2,1-insertion of NBE.

III. Comparison between C(sp³)–Br oxidative addition vs. C–C_{norbornene} reductive elimination.

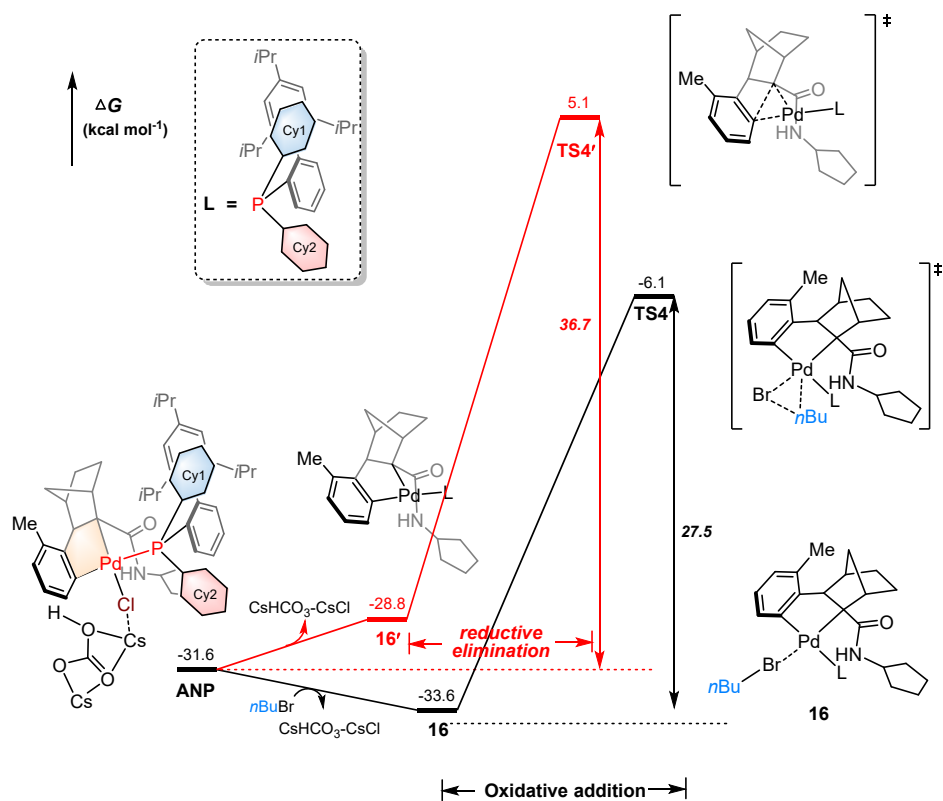


Fig. S3 Calculated Gibbs energy profiles for C(sp³)–Br oxidative addition vs. C–C_{norbornene} reductive elimination.

IV. Cartesian coordinates of all the structures.

1

C	-2.37429100	0.06017600	-0.00002600
C	-1.88670100	-1.24563100	0.00000400
C	-0.51130800	-1.47096100	0.00003200
C	0.35804200	-0.38297400	0.00007500
C	-0.09713600	0.94269600	0.00011200
C	-1.48493400	1.13305500	-0.00002300
H	-3.44382100	0.24451400	-0.00018800
H	-2.56904400	-2.08955800	-0.00004000
H	-0.10928600	-2.47751000	0.00004700
H	-1.86671900	2.14999000	-0.00009200
C	0.84907900	2.11254800	0.00001800
H	0.29735300	3.05520800	0.00075900
H	1.50275500	2.09402900	0.87805600
H	1.50150900	2.09485700	-0.87901000
Cl	2.09239700	-0.70382300	-0.00004000

2

C	-3.00707543	-0.05896226	0.00000000
H	-2.65042100	-1.06777227	0.00000000
H	-2.65040259	0.44543593	-0.87365150
H	-4.07707543	-0.05894908	0.00000000
C	-2.49373321	0.66699401	1.25740497
H	-1.42373502	0.66528694	1.25838332
H	-2.85200217	0.16372601	2.13105517
C	-3.00474919	2.11973648	1.25599826
H	-4.07474697	2.12144243	1.25464336
H	-2.64617323	2.62311289	0.38253649
C	-2.49184940	2.84553739	2.51367344
H	-1.42185179	2.84375823	2.51506962
H	-2.85049347	2.34220954	3.38713524
Br	-3.12552007	4.64735818	2.51185435

3

C	-2.26813600	0.75144100	0.00007600
C	-3.48349000	0.20283300	-0.00012800
H	-2.11214900	1.82531400	0.00013200
H	-4.38394300	0.80776900	-0.00024000
H	-3.59137400	-0.87744200	-0.00017600
C	-1.05225000	-0.10565800	0.00025700
O	-1.06637700	-1.32260800	-0.00000100
O	0.05138000	0.66843500	0.00018900

C	1.39881600	0.07529900	-0.00003300
C	2.30582600	1.30448600	0.00041200
H	2.12280300	1.91634400	0.88783600
H	3.35479300	0.99539800	0.00028100
H	2.12277400	1.91700200	-0.88655200
C	1.60222200	-0.75193600	1.27076100
H	1.39719600	-0.14147200	2.15526000
H	0.94827800	-1.62341600	1.28132200
H	2.64225500	-1.08860500	1.32266500
C	1.60225800	-0.75103200	-1.27141400
H	1.39728200	-0.13993100	-2.15548500
H	2.64228800	-1.08768400	-1.32351800
H	0.94830300	-1.62249200	-1.28262300

4

C	4.05729600	-2.31197900	-0.13432300
C	3.81817500	-1.00519200	-0.53993700
C	2.52999300	-0.45692700	-0.52085100
C	1.44986800	-1.26341900	-0.08649000
C	1.69150100	-2.60801100	0.30223500
C	2.99260900	-3.10732000	0.28528300
H	5.06549100	-2.71468700	-0.15286900
H	4.64168200	-0.38731300	-0.88765600
H	3.17108700	-4.13126400	0.60073100
C	0.56334100	-3.50037300	0.76341800
H	0.94900800	-4.46681800	1.09608100
H	0.00457400	-3.05479200	1.59260800
H	-0.15810100	-3.69289900	-0.04001000
C	2.80037700	4.46253800	0.76892400
H	2.57631200	5.48388600	0.44593600
H	3.86882900	4.41370400	1.00717000
H	2.24615600	4.27729400	1.69561900
C	2.42763800	3.44034100	-0.30632400
H	2.96736500	3.66545500	-1.23597000
H	1.35949100	3.52964300	-0.54460300
C	2.72624100	1.99945400	0.11318300
H	2.17720200	1.76372600	1.03374700
H	3.78832100	1.89698100	0.37123800
C	2.37417800	0.97430900	-0.98078900
H	3.03955700	1.14255300	-1.83619000
H	1.35694400	1.15569400	-1.33687400
O	-2.24468900	1.87222900	0.62203300
O	-2.64094600	-0.25258000	-0.11021600
C	-4.67143700	0.19553800	1.19853100

C	-4.54956800	-1.48102300	-0.67500300
C	-4.45899100	0.97727300	-1.21042100
C	-4.10052800	-0.10379000	-0.18906200
C	-1.85110700	0.76587700	0.29346400
C	-0.41806900	0.40421200	0.30029000
C	0.05444100	-0.80259500	-0.05747700
H	-4.34735900	-0.56755000	1.91258800
H	-5.76485000	0.17836800	1.15390300
H	-4.34739900	1.17351100	1.55305200
H	-4.10319100	-1.70925600	-1.64678900
H	-5.63812900	-1.50729900	-0.77678300
H	-4.24747000	-2.25549200	0.03549800
H	-4.12809800	1.95873700	-0.87239100
H	-5.54369900	0.99797700	-1.35430600
H	-3.99108700	0.75539800	-2.17424400
H	0.21950000	1.20702400	0.64636000
H	-0.69278600	-1.54325500	-0.32828200

toluene

C	-1.20424100	1.20254500	0.00038700
C	-1.90297300	-0.00381600	0.00181400
C	-1.19528100	-1.20725300	0.00040400
C	0.19809200	-1.20014200	-0.00186400
C	0.91276900	0.00523800	-0.00231000
C	0.19136400	1.20382900	-0.00182700
H	-1.74438000	2.14473500	0.00027400
H	-2.98866300	-0.00759900	0.00294600
H	-1.72962900	-2.15283600	0.00023600
H	0.73011800	2.14772100	-0.00363300
C	2.42200700	0.00265000	0.00196700
H	2.82210700	-0.57345200	-0.83975900
H	2.82243100	1.01737300	-0.06558300
H	2.81619200	-0.45236900	0.91788300
H	0.74140300	-2.14188600	-0.00378800

NBE

C	2.55523700	1.26398500	-0.16272100
C	2.00859800	-0.82055600	0.67259600
C	3.78247300	0.38928600	-0.01814400
C	1.49014800	0.55249300	0.24768200
C	3.39280400	-0.42776600	1.23626000
H	4.04762400	-1.28695800	1.41744200
H	3.32411700	0.18446200	2.13882400
C	2.42771800	-1.55302800	-0.64448000

H	2.71283900	-2.58856700	-0.43463400
H	1.61349600	-1.57074700	-1.37351300
C	3.65252700	-0.71597800	-1.12549900
H	4.56104600	-1.32531600	-1.15769700
H	3.50665300	-0.28178900	-2.11716100
H	1.36515400	-1.40431800	1.33537100
H	4.74608300	0.90075500	-0.00696000
C	0.08468000	0.99974200	0.09131100
O	-0.20698700	2.15213700	-0.22464400
H	2.51203200	2.23900100	-0.63271800
N	-0.86117600	0.03588300	0.32806100
H	-0.55594900	-0.91107200	0.49618200
C	-2.27594100	0.26436500	0.12238500
C	-2.84897400	-0.32850800	-1.17659000
C	-3.16277200	-0.35601700	1.21894500
H	-2.39785800	1.35037000	0.10024600
C	-4.36412300	-0.24316400	-0.95015500
H	-2.52876500	-1.37575700	-1.26735900
H	-2.50254900	0.20497500	-2.06575200
C	-4.56126100	-0.52268900	0.56835000
H	-3.17542800	0.25083800	2.12796700
H	-2.75328200	-1.33616800	1.49600700
H	-4.71012000	0.76806400	-1.19094900
H	-4.92990900	-0.93308600	-1.58216400
H	-5.29126400	0.16665300	1.00152400
H	-4.94647900	-1.53261500	0.73642500

Cs₂CO₃

C	-0.00002600	1.23040000	0.00009800
O	-1.12543700	1.85575900	-0.00004900
O	-0.00004400	-0.10956000	0.00037200
O	1.12544400	1.85572800	-0.00004100
Cs	-2.86909100	-0.32907300	-0.00002600
Cs	2.86909900	-0.32906900	-0.00002600

CsCl

Cs	0.00000000	0.00000000	0.74644800
Cl	0.00000000	0.00000000	-2.41497800

5

C	0.56899300	-0.21857200	3.02372400
C	-0.41423000	-0.36045100	3.99879600
C	-1.75467600	-0.38117700	3.61954000
C	-2.08882900	-0.25822400	2.27308400

C	-1.11229500	-0.11729600	1.27110100
C	0.25087700	-0.10096200	1.66096900
C	1.44121800	0.02810500	0.73325400
C	2.06593700	1.30404300	0.57674800
C	3.36206900	1.37492300	0.05696600
C	4.08547900	0.24037100	-0.31769000
C	3.46667100	-1.00405800	-0.16995300
C	2.17895600	-1.14476200	0.36480300
C	1.62527400	-2.53917700	0.63199600
C	1.35278400	2.57646200	1.00940900
P	-1.54403300	-0.02392200	-0.53886700
C	-2.70547700	-1.46970900	-0.85451700
C	-2.64098400	1.48823300	-0.77708100
Pd	0.54305200	-0.08251000	-1.39324500
C	2.34320500	-3.19393000	1.82516600
C	1.68904300	-3.43817600	-0.61210800
C	1.45703400	3.69161000	-0.04250200
C	1.86869000	3.06754300	2.37349200
C	-4.15576000	-1.42018100	-0.34665400
C	-4.94844300	-2.64023000	-0.84366400
C	-4.27654100	-3.95305100	-0.42385000
C	-2.82205600	-4.00658400	-0.90691100
C	-2.02602400	-2.78300700	-0.43530500
C	-1.78719900	2.66801700	-1.27514200
C	-2.64649100	3.87738700	-1.65949900
C	-3.53459900	4.32163000	-0.49180900
C	-4.38631000	3.15433900	0.01894000
C	-3.52154900	1.94229700	0.40032400
H	1.61605200	-0.20249800	3.31014400
H	-0.13406700	-0.45520500	5.04364000
H	-2.53753700	-0.49173300	4.36394400
H	-3.13457500	-0.26836300	1.99933000
H	3.82977600	2.34911200	-0.05590700
H	4.00724900	-1.90224500	-0.45335500
H	0.57193000	-2.43043000	0.90160600
H	0.29334700	2.32956500	1.12641700
H	-2.74845100	-1.46060300	-1.95360700
H	-3.29909500	1.17894900	-1.60371600
H	2.23860300	-2.58525800	2.72789800
H	1.92567000	-4.18518300	2.03308100
H	3.41290800	-3.31250600	1.62136700
H	1.19647000	-2.95163100	-1.46077600
H	1.19020700	-4.39427500	-0.42055400
H	2.72189900	-3.65757500	-0.90220600

H	1.14768600	3.32963300	-1.02648700
H	0.81804300	4.53756300	0.23316500
H	2.48016600	4.07167000	-0.12676300
H	1.71796800	2.31153200	3.14846400
H	1.34545200	3.97968800	2.68107700
H	2.93984200	3.29127000	2.32250300
H	-4.17031500	-1.42260400	0.74911300
H	-4.65137500	-0.50162700	-0.67546900
H	-5.97583100	-2.59630000	-0.46327100
H	-5.01724200	-2.60157900	-1.93972600
H	-4.29542500	-4.03079700	0.67247800
H	-4.84042800	-4.81041400	-0.80917500
H	-2.33621100	-4.92519900	-0.55761400
H	-2.80686900	-4.04129900	-2.00511100
H	-1.93472600	-2.80400200	0.65859400
H	-1.01036000	-2.80994500	-0.83943400
H	-1.09583800	2.95862200	-0.47702200
H	-1.16550600	2.34275200	-2.11544100
H	-2.00291200	4.70207800	-1.98752600
H	-3.28069000	3.61254900	-2.51744000
H	-2.89779100	4.68676400	0.32624700
H	-4.17500300	5.15977300	-0.79033300
H	-4.98676500	3.46570900	0.88203600
H	-5.09635400	2.85510600	-0.76500100
H	-2.87516400	2.20843300	1.24547000
H	-4.16914000	1.13194100	0.74479600
C	5.48356100	0.36241100	-0.89483400
H	5.76124800	1.42353700	-0.84806500
C	5.51319700	-0.06202700	-2.37376100
H	6.51071900	0.08017600	-2.80388400
H	5.24952600	-1.11989500	-2.48093600
H	4.79788000	0.52085000	-2.96241600
C	6.51819600	-0.42623400	-0.07531600
H	7.52667400	-0.28038200	-0.47737200
H	6.51540500	-0.10857500	0.97172300
H	6.30473100	-1.50024000	-0.09848300

6

C	-0.31176600	-0.83794100	3.20655300
C	0.77699400	-1.12296000	4.01976400
C	2.05652500	-1.07655700	3.46739100
C	2.21077900	-0.73397000	2.13130100
C	1.12292600	-0.38858600	1.29906000
C	-0.17501500	-0.46805900	1.85440400

C	-1.46322600	-0.31427800	1.10497800
C	-1.97899100	-1.43520100	0.41712400
C	-3.22757100	-1.33045300	-0.20539800
C	-3.97450500	-0.15420500	-0.17228600
C	-3.45871200	0.93325900	0.53831700
C	-2.22730200	0.87296900	1.19632200
C	-1.77219700	2.05871300	2.04528600
C	-1.23413000	-2.76510800	0.39568300
P	1.64853200	-0.18534000	-0.47799800
C	0.58259300	0.92309000	-1.56036400
C	3.17751000	0.93519000	-0.36981200
Pd	1.93080900	-2.19186300	-1.39741700
C	-2.33126500	1.95179000	3.47811500
C	-2.17038200	3.42780800	1.46652600
C	-1.30988000	-3.48776300	-0.95693000
C	-1.74762600	-3.67301200	1.52773400
C	0.21308700	2.30051600	-0.99872000
C	-0.49209500	3.16931500	-2.05258500
C	-1.70535600	2.45543400	-2.65647300
C	-1.29278800	1.10539300	-3.25332700
C	-0.62314200	0.21862800	-2.19642800
C	4.50645400	0.17207600	-0.51814800
C	5.67473500	1.14711200	-0.72043900
C	5.74980600	2.18341200	0.40883600
C	4.41541300	2.92131000	0.57791100
C	3.25853900	1.93510200	0.79982800
H	-1.31641300	-0.93154700	3.60478400
H	0.62669100	-1.40640000	5.05683200
H	2.92858700	-1.32637600	4.06410800
H	3.20553200	-0.77217900	1.70584300
H	-3.62719400	-2.18667100	-0.74000600
H	-4.03777300	1.84907600	0.59071300
H	-0.67916200	2.01979900	2.11098400
H	-0.17522300	-2.56396200	0.58005000
H	1.30580500	1.07782100	-2.37636300
H	3.06649300	1.52802500	-1.28816300
H	-1.97801700	1.05486700	3.98774400
H	-2.02660900	2.81994700	4.07269100
H	-3.42603300	1.92268700	3.45606600
H	-1.91370200	3.52894300	0.41035300
H	-1.66258200	4.22486700	2.01857800
H	-3.24640600	3.60482600	1.56615500
H	-0.95480400	-2.84137200	-1.76459000
H	-0.67397000	-4.37911900	-0.93221600

H	-2.32545100	-3.82118100	-1.19658800
H	-1.61865600	-3.19837000	2.50403700
H	-1.20244400	-4.62310700	1.53702900
H	-2.81308500	-3.89250100	1.39530300
H	-0.44493300	2.16133900	-0.14139900
H	1.10248100	2.82429100	-0.64009600
H	-0.78872200	4.12517100	-1.60368000
H	0.22166100	3.41035900	-2.85308000
H	-2.45104200	2.28325900	-1.87016500
H	-2.18058300	3.08654700	-3.41662900
H	-2.16553000	0.58615700	-3.66703400
H	-0.60064600	1.27392500	-4.09097300
H	-1.35822900	-0.02862900	-1.43342600
H	-0.28678500	-0.72695000	-2.63620700
H	4.69481300	-0.43506500	0.37682600
H	4.43132800	-0.53239500	-1.35275300
H	6.61762800	0.59277900	-0.79400200
H	5.54160000	1.66802300	-1.67916300
H	5.99588600	1.67199900	1.35012700
H	6.55972900	2.89727900	0.21906600
H	4.47197500	3.62336700	1.41817700
H	4.21453300	3.52184500	-0.32051700
H	3.42695200	1.40026600	1.73876600
H	2.31500700	2.47295700	0.92614400
C	-5.31269000	-0.06246600	-0.88453100
H	-5.50694800	-1.04468000	-1.33407400
C	-5.27316600	0.97193300	-2.02176700
H	-6.22634500	0.99498300	-2.56076500
H	-5.08544000	1.97764600	-1.63100900
H	-4.47853000	0.73985400	-2.73670500
C	-6.45840100	0.23781400	0.09617500
H	-7.42301200	0.23965700	-0.42244300
H	-6.49852700	-0.50835000	0.89536100
H	-6.33003500	1.22028300	0.56287000

7

C	0.28451700	-0.08452800	3.33141600
C	-0.80442600	-0.28410200	4.16944800
C	-2.06654100	-0.44803000	3.59981300
C	-2.20521800	-0.39196700	2.21994300
C	-1.12120100	-0.13778000	1.35061600
C	0.16211200	-0.00553600	1.93061800
C	1.45733100	0.10303100	1.18529700
C	2.13191500	1.33897800	1.07040600

C	3.37153000	1.37017900	0.42104300
C	3.97569100	0.21842800	-0.08208800
C	3.31734400	-1.00075900	0.09407000
C	2.06970400	-1.08346600	0.71635200
C	1.41977300	-2.44577000	0.92970500
C	1.57853500	2.62213000	1.68798200
P	-1.60648800	-0.33307100	-0.43878700
C	-3.22277000	0.65272800	-0.58061300
C	-0.59327200	0.62758400	-1.69807900
Pd	-1.72149700	-2.49767400	-0.94320000
C	1.92570900	-3.07114200	2.24213300
C	1.62261800	-3.41439400	-0.24397300
C	1.87004200	3.88775500	0.86258600
C	2.13656000	2.82685200	3.11067500
C	-3.42270000	1.86001200	0.35722700
C	-4.64708900	2.67750300	-0.08116500
C	-5.91161200	1.80996800	-0.11382300
C	-5.71706000	0.57411700	-1.00306900
C	-4.48068800	-0.23487400	-0.58769800
C	0.66857400	-0.09724100	-2.18526400
C	1.29129800	0.62219600	-3.38749900
C	1.61193300	2.08201400	-3.04634900
C	0.34893800	2.81429300	-2.57884000
C	-0.32022200	2.10408100	-1.39158300
H	1.28100200	-0.01633000	3.75408400
H	-0.66548300	-0.34072000	5.24458400
H	-2.93596600	-0.63920100	4.22154900
H	-3.18208000	-0.58915000	1.79758700
H	3.88892500	2.31793900	0.30844400
H	3.78017300	-1.90937500	-0.27552700
H	0.34033500	-2.29508600	1.02209900
H	0.49164900	2.50966800	1.76826300
H	-3.13072200	1.05345900	-1.59955400
H	-1.30795600	0.58421900	-2.53490900
H	1.71032700	-2.42537400	3.09722800
H	1.44449800	-4.03943500	2.41812400
H	3.00910900	-3.23105700	2.20151200
H	1.28768300	-2.96673900	-1.18359900
H	1.03506000	-4.32269100	-0.07367900
H	2.66822500	-3.72184800	-0.35623000
H	1.60215700	3.77452200	-0.18944200
H	1.30472200	4.73229100	1.26903500
H	2.92967400	4.15928600	0.90925700
H	1.85736500	2.01288700	3.78053000

H	1.75776100	3.76131800	3.53877500
H	3.23001700	2.88460600	3.08330900
H	-3.57792600	1.51525600	1.38363700
H	-2.53094500	2.49176400	0.38575600
H	-4.78689600	3.52946500	0.59465300
H	-4.46630900	3.09575600	-1.08139800
H	-6.14608800	1.48320600	0.90913300
H	-6.76971900	2.39811400	-0.45936900
H	-6.60917100	-0.06229800	-0.97322700
H	-5.59709100	0.89658500	-2.04707200
H	-4.64698900	-0.66090400	0.41015200
H	-4.32211800	-1.08532000	-1.25857800
H	1.40548900	-0.14045100	-1.38604900
H	0.40743000	-1.13090500	-2.43780400
H	2.19846900	0.09301500	-3.70072700
H	0.59752500	0.59219500	-4.23989700
H	2.36110800	2.10462500	-2.24369600
H	2.05080100	2.59494300	-3.91037100
H	0.58127500	3.85084700	-2.30551300
H	-0.36540700	2.86577700	-3.41263600
H	0.32737100	2.16119700	-0.51707500
H	-1.24637400	2.62679100	-1.14048400
C	5.30350100	0.29604800	-0.81525900
H	5.65362800	1.33399000	-0.74359200
C	5.12601800	-0.03477200	-2.30723200
H	6.07655000	0.05715500	-2.84372400
H	4.76288800	-1.05983400	-2.43811100
H	4.40062000	0.63770200	-2.77400400
C	6.37186200	-0.60239200	-0.17196400
H	7.33541200	-0.48003300	-0.67775200
H	6.50573300	-0.36022000	0.88658900
H	6.09421800	-1.65943100	-0.24024000

8

C	-1.50617200	-2.07735900	2.87888100
C	-2.75529000	-2.15048400	3.48911900
C	-3.81983400	-1.41693600	2.96742600
C	-3.61734500	-0.61710700	1.84596400
C	-2.36299200	-0.53028300	1.21799200
C	-1.28497500	-1.28117300	1.74273700
C	0.11453100	-1.33171500	1.17717700
C	1.13070600	-0.49041200	1.70907600
C	2.47461400	-0.80070700	1.45688900
C	2.85595600	-1.91052800	0.70623100

C	1.84831000	-2.70376100	0.15289500
C	0.49303100	-2.43690100	0.36021300
C	-0.55183700	-3.36890300	-0.23431100
C	0.78529700	0.66872500	2.63288800
P	-2.04437800	0.46649000	-0.30216700
C	-3.36381300	-0.00371300	-1.54818300
C	-2.42274000	2.27011800	0.07299200
Pd	0.15660700	0.09223600	-0.91215300
C	-0.61712100	-4.69626200	0.54072300
C	-0.31189300	-3.61735300	-1.73181900
C	1.61964000	1.92519100	2.34392500
C	0.92781000	0.25027900	4.10776600
C	-4.81459700	0.45482700	-1.32604300
C	-5.69903400	0.07095000	-2.52344100
C	-5.64728700	-1.43606100	-2.80079600
C	-4.20296100	-1.90437000	-3.01213400
C	-3.30654300	-1.51294500	-1.83070700
C	-1.12648000	3.03584000	0.39569900
C	-1.37832500	4.54192700	0.52730900
C	-2.44796000	4.83827700	1.58465500
C	-3.73975000	4.06948300	1.28534900
C	-3.48513100	2.56024600	1.14658600
H	-0.67472400	-2.64999800	3.27779500
H	-2.89545400	-2.77813400	4.36400600
H	-4.80124800	-1.46506300	3.42949600
H	-4.44950500	-0.04816600	1.45424900
H	3.24539800	-0.16270100	1.87508900
H	2.12174800	-3.55981300	-0.45500500
H	-1.52274200	-2.87898300	-0.13345800
H	-0.26682600	0.91663600	2.46390800
H	-2.99071500	0.51210700	-2.44596400
H	-2.79665300	2.64177600	-0.89346700
H	-0.86756400	-4.52745400	1.59163400
H	-1.37769800	-5.35745400	0.11151600
H	0.34557300	-5.21715300	0.50204600
H	-0.19454800	-2.66922700	-2.26535500
H	-1.15380200	-4.16619200	-2.16711900
H	0.59093300	-4.21251500	-1.90256300
H	1.61609900	2.17662300	1.28115100
H	1.22248900	2.77646300	2.90714700
H	2.66039000	1.79284700	2.65504100
H	0.27028500	-0.58838700	4.35091000
H	0.67402300	1.08529200	4.76974500
H	1.95846500	-0.05184900	4.32309700

H	-5.22042400	-0.02112200	-0.42584100
H	-4.86091600	1.53649300	-1.16944000
H	-6.73087600	0.39309500	-2.34101100
H	-5.35241500	0.61493000	-3.41313800
H	-6.07966700	-1.97437600	-1.94552500
H	-6.26312600	-1.68491500	-3.67261800
H	-4.16880800	-2.98992200	-3.16103900
H	-3.80499000	-1.44882500	-3.92958100
H	-3.63055600	-2.05622200	-0.93295200
H	-2.27308700	-1.80655300	-2.02754000
H	-0.72814900	2.66113800	1.34396700
H	-0.36087900	2.83362900	-0.35820400
H	-0.43989700	5.05067700	0.77457800
H	-1.70488700	4.94118100	-0.44350400
H	-2.07089300	4.53510300	2.57156400
H	-2.64960600	5.91426700	1.64150700
H	-4.48486200	4.24752200	2.06983600
H	-4.17475900	4.44543200	0.34848700
H	-3.13865600	2.15838000	2.10673600
H	-4.42722800	2.05475600	0.91909600
C	1.88625400	0.51677200	-2.20507300
C	0.66950300	0.98890800	-2.74838600
H	2.34399700	-0.40037300	-2.55941300
H	0.19948100	0.44251700	-3.56228000
H	0.45731400	2.05373500	-2.70914600
C	2.76053100	1.46443600	-1.49937800
O	2.42688700	2.57436800	-1.10070700
O	4.01908500	0.96205500	-1.36500700
C	5.12098700	1.80301800	-0.88997200
C	6.33567700	0.88055000	-0.99742300
H	6.45979700	0.52721100	-2.02465300
H	7.24089800	1.41864700	-0.70112000
H	6.22110800	0.01096400	-0.34599200
C	5.28775900	3.01091600	-1.81718700
H	5.40088800	2.67588400	-2.85291100
H	4.42631500	3.67482600	-1.75189900
H	6.18810000	3.56741800	-1.53767300
C	4.89536200	2.22466500	0.56285700
H	4.74809700	1.34238800	1.19166900
H	5.77694200	2.76046700	0.92993600
H	4.02240600	2.86925600	0.64833500
C	4.31999500	-2.25076100	0.49889000
H	4.90528900	-1.41764900	0.90821500
C	4.67706100	-2.38775800	-0.98949500

H	5.74896500	-2.57889900	-1.11091500
H	4.14049500	-3.22464200	-1.44906400
H	4.42509000	-1.47317700	-1.52939200
C	4.70101600	-3.51963800	1.28174300
H	5.76814600	-3.74087800	1.17160500
H	4.48074200	-3.40699500	2.34786500
H	4.13890200	-4.38561900	0.91498300

9

C	0.39561300	3.37294500	1.89126500
C	-0.59302400	4.08451200	2.56518700
C	-1.90188000	3.60714200	2.56419500
C	-2.20413500	2.43900200	1.86901500
C	-1.22378800	1.71452800	1.16801600
C	0.11451700	2.18158700	1.20068100
C	1.31461600	1.50910700	0.57694600
C	1.70895900	1.82606100	-0.75054900
C	2.98433400	1.44537900	-1.19151900
C	3.88849700	0.77457700	-0.36932600
C	3.47294100	0.43810200	0.92137900
C	2.20975400	0.78412200	1.40980900
C	1.83922400	0.41670300	2.84064200
C	0.82494100	2.67034200	-1.65719800
P	-1.60368000	0.19223400	0.18988100
C	-2.34777300	-1.05592600	1.37276800
C	-3.02282400	0.57027200	-0.99068700
Pd	0.38188300	-0.63731900	-0.66106100
C	2.54380400	1.33649800	3.85314500
C	2.13450500	-1.05784400	3.15688600
C	0.77467700	2.13666700	-3.09577300
C	1.27365400	4.14245000	-1.62498200
C	-3.59845200	-0.68111000	2.17989500
C	-4.10192700	-1.88074700	2.99949400
C	-3.00663100	-2.43468000	3.91919200
C	-1.74716900	-2.79353700	3.12110900
C	-1.24877500	-1.60266100	2.29638200
C	-2.44790800	0.87330100	-2.38657100
C	-3.54612200	0.97417600	-3.44996800
C	-4.59889800	2.02117600	-3.06950200
C	-5.17294900	1.73301900	-1.67827800
C	-4.06856700	1.63282500	-0.61382400
H	1.41892100	3.73487700	1.89665500
H	-0.33937900	5.00028000	3.09067200
H	-2.68498800	4.14055200	3.09456200

H	-3.22578000	2.08664400	1.86901500
H	3.28901600	1.70380400	-2.20121500
H	4.15334300	-0.10027900	1.57385400
H	0.76239200	0.56913200	2.94980000
H	-0.19075500	2.63014300	-1.25479100
H	-2.61942600	-1.86669500	0.67951700
H	-3.53330300	-0.40415400	-1.04650600
H	2.27229100	2.38372500	3.69772500
H	2.27011000	1.06286300	4.87799900
H	3.63204900	1.25229200	3.76013400
H	1.72566100	-1.71682800	2.38925700
H	1.69779600	-1.33157200	4.12324000
H	3.21164400	-1.24581900	3.22192900
H	0.51368600	1.07516400	-3.10575000
H	0.02618700	2.68503200	-3.67716200
H	1.73513400	2.25869700	-3.60697100
H	1.23260500	4.54497200	-0.60878700
H	0.62786400	4.75732400	-2.26123800
H	2.30255000	4.24240400	-1.98733900
H	-3.35377100	0.13926400	2.86538600
H	-4.39781100	-0.32657000	1.52146000
H	-4.98234500	-1.58941600	3.58446400
H	-4.42966500	-2.67183900	2.31072800
H	-2.75089000	-1.67415300	4.67030600
H	-3.37708000	-3.30774900	4.46890900
H	-0.95210100	-3.14137200	3.79100600
H	-1.97083500	-3.62677100	2.44048000
H	-0.92214000	-0.80193900	2.97221100
H	-0.38380800	-1.88822700	1.69171700
H	-1.90305400	1.82380700	-2.34037800
H	-1.71668300	0.10847300	-2.65873500
H	-3.09989200	1.21200200	-4.42253800
H	-4.03134900	-0.00612800	-3.55930800
H	-4.13229400	3.01637700	-3.06664600
H	-5.40211600	2.05225000	-3.81476800
H	-5.89155000	2.50945900	-1.39027200
H	-5.72940900	0.78557900	-1.70611700
H	-3.57210400	2.60578100	-0.51430000
H	-4.52527700	1.41145900	0.35444100
C	5.28711300	0.44422300	-0.86135400
H	5.35424900	0.78993900	-1.90092300
C	5.56744100	-1.06695400	-0.85643600
H	6.56979400	-1.27622300	-1.24480900
H	5.51517700	-1.47375900	0.15938000

H	4.84426100	-1.60757600	-1.47355200
C	6.35130800	1.20059200	-0.04730600
H	7.35451800	1.00985100	-0.44340300
H	6.17048200	2.27933300	-0.07135500
H	6.33941500	0.88362300	1.00110800
C	1.53789300	-3.76854600	0.48283700
C	2.29209300	-2.83711500	-0.20462600
C	1.77895500	-2.20432100	-1.37022700
C	0.44724000	-2.53047500	-1.77336500
C	-0.32193700	-3.52273600	-1.08555100
C	0.24265000	-4.10898900	0.03448400
H	1.94172800	-4.24893000	1.36850600
H	3.29549100	-2.58976500	0.12107700
H	2.44128400	-1.67455400	-2.04625700
H	-0.33923800	-4.84190800	0.58652800
C	-1.70510200	-3.87793900	-1.55283400
H	-2.19125200	-4.55173500	-0.84278100
H	-2.32126500	-2.97778000	-1.65874700
H	-1.68810700	-4.36407100	-2.53436300
Cl	-0.01838900	-2.14414700	-3.46430400

10

C	0.18547000	-1.88227700	3.19356000
C	1.27516700	-1.99493400	4.05163200
C	2.49825500	-1.44354500	3.67699700
C	2.61487500	-0.81197200	2.44163700
C	1.53172100	-0.70305300	1.55057100
C	0.27891600	-1.23113100	1.95119800
C	-1.01313300	-1.14077700	1.18454700
C	-1.34825700	-2.11933500	0.21533800
C	-2.64752400	-2.14250300	-0.29948300
C	-3.63352300	-1.24475900	0.11940200
C	-3.27540500	-0.27442800	1.05158400
C	-1.98452900	-0.19986100	1.58747500
C	-1.67217500	0.89436800	2.59975700
C	-0.36198100	-3.21093300	-0.17466900
P	1.69754400	0.08835700	-0.11580900
C	2.24847200	1.85400300	0.20597000
C	3.18729400	-0.68317300	-0.98403200
Pd	-0.23147400	0.11636200	-1.36199900
C	-2.26243900	0.56669500	3.98240700
C	-2.15480100	2.27491600	2.12371200
C	-0.38247000	-3.52450800	-1.67645900
C	-0.61306800	-4.47972700	0.65983700

C	3.54247300	2.13032400	0.98460500
C	3.84234700	3.63782900	1.03362300
C	2.67286100	4.42700400	1.63420400
C	1.37130700	4.14306300	0.87515800
C	1.07654600	2.64090600	0.81275000
C	2.69695300	-1.78778500	-1.93932700
C	3.81524600	-2.29554700	-2.85604800
C	5.01856200	-2.79139100	-2.04672000
C	5.51178900	-1.70294100	-1.08831100
C	4.38586100	-1.19910100	-0.17032800
H	-0.77426500	-2.29920000	3.48185500
H	1.16595400	-2.50277700	5.00525700
H	3.35873000	-1.50693000	4.33640900
H	3.57270100	-0.39718600	2.16483600
H	-2.90677000	-2.89476400	-1.03885100
H	-4.01170700	0.45073100	1.37599300
H	-0.58541200	0.94338700	2.70744800
H	0.64003600	-2.85020100	0.07096400
H	2.38816900	2.21909900	-0.82259600
H	3.53593800	0.15647300	-1.60558900
H	-1.85151500	-0.36447800	4.38084500
H	-2.04384500	1.36784300	4.69715000
H	-3.35066700	0.45581300	3.92131100
H	-1.84407700	2.46801600	1.09572500
H	-1.74783600	3.06162900	2.76801600
H	-3.24636100	2.35424200	2.16227400
H	-0.26179000	-2.60502600	-2.25718600
H	0.43269400	-4.20903800	-1.93299600
H	-1.31834000	-4.00544700	-1.97925800
H	-0.51964900	-4.27232700	1.72966000
H	0.10671900	-5.26385900	0.40037200
H	-1.62100600	-4.86817300	0.47728700
H	3.43720900	1.75784400	2.01036500
H	4.38932500	1.60522200	0.53218500
H	4.75979500	3.81645300	1.60691500
H	4.03446300	3.99758500	0.01299100
H	2.54573400	4.13523100	2.68630900
H	2.89577800	5.50038900	1.63061900
H	0.53071600	4.66910000	1.34280500
H	1.45294100	4.53323100	-0.14910200
H	0.88701900	2.26714300	1.82711400
H	0.17550900	2.45043300	0.22429300
H	2.31342600	-2.62513100	-1.34281800
H	1.85127000	-1.41027500	-2.52258600

H	3.43263400	-3.09313300	-3.50383600
H	4.13572300	-1.47911800	-3.51886500
H	4.72130100	-3.67485500	-1.46429000
H	5.82862400	-3.11073800	-2.71269600
H	6.34420800	-2.07523900	-0.47936000
H	5.90331800	-0.85734100	-1.67125900
H	4.05531400	-2.01977900	0.47776700
H	4.78494600	-0.42042700	0.48466400
C	-5.04562900	-1.38217500	-0.43248300
H	-4.95321500	-1.52580800	-1.51896100
C	-5.93627500	-0.15647700	-0.19871200
H	-6.89834400	-0.28740100	-0.70330000
H	-6.14273000	-0.01454800	0.86769900
H	-5.47797700	0.76242700	-0.57604200
C	-5.71932600	-2.64332700	0.14209300
H	-6.71517900	-2.78840200	-0.29066400
H	-5.12509000	-3.53935700	-0.05778600
H	-5.82879300	-2.55172900	1.22827900
C	-0.65682900	1.59230400	-3.06214700
C	-1.77123500	0.72541600	-2.88717200
C	-2.87916600	1.18840100	-2.13458900
C	-2.88479200	2.45794500	-1.58634500
C	-1.78968200	3.33721500	-1.77025900
C	-0.69997300	2.89745400	-2.50788500
H	0.11953500	1.34741100	-3.77950000
H	-1.85809400	-0.18730900	-3.47061700
H	-3.73586700	0.53849500	-2.00844900
H	0.14309100	3.56456700	-2.66918700
C	-1.81174200	4.71031800	-1.14722800
H	-0.95927800	5.31166200	-1.47463400
H	-2.72875800	5.25364100	-1.40190100
H	-1.77017000	4.64660000	-0.05286500
H	-3.74239300	2.79232900	-1.00828600

11

C	1.49849100	-2.09745000	-2.98532800
C	2.81080800	-2.42453700	-3.31077700
C	3.84929100	-1.92178500	-2.53027600
C	3.55271600	-1.11153900	-1.43842900
C	2.23319700	-0.77452700	-1.08505700
C	1.18135200	-1.27728500	-1.88769900
C	-0.28834500	-1.03371000	-1.68565600
C	-0.93995100	-0.03457600	-2.43883100
C	-2.33800900	0.01996700	-2.42271000

C	-3.10853100	-0.87360100	-1.68066300
C	-2.44361700	-1.83789800	-0.91782100
C	-1.04979900	-1.94256600	-0.91040800
C	-0.38193700	-3.10115600	-0.17815300
C	-0.15909100	0.95015400	-3.30207500
P	1.87523500	0.21587900	0.44709100
C	3.06673100	-0.44088000	1.75470100
C	2.52597100	1.95061800	0.09980400
Pd	-0.22451500	0.07869600	1.13923600
C	-0.48839200	-4.38968900	-1.01398200
C	-0.93193400	-3.32319300	1.23761800
C	-0.74843700	2.37015100	-3.27457900
C	-0.05769500	0.46079000	-4.75880200
C	4.55781700	-0.06240000	1.74145800
C	5.24813100	-0.56189300	3.02119500
C	5.07928700	-2.07726900	3.18813700
C	3.59779300	-2.47414800	3.17740700
C	2.88279800	-1.95879200	1.92142800
C	1.35695900	2.86703100	-0.29823700
C	1.79670800	4.32418300	-0.47605100
C	2.94569900	4.44102600	-1.48408200
C	4.11840500	3.54097800	-1.07888700
C	3.67639300	2.07938200	-0.91070900
H	0.68138700	-2.48629200	-3.58457800
H	3.01730200	-3.06497100	-4.16308000
H	4.88297200	-2.15845400	-2.76458800
H	4.37199000	-0.73060900	-0.84628100
H	-2.84611400	0.77436900	-3.01614300
H	-3.02378000	-2.54329100	-0.33122300
H	0.67859600	-2.85819100	-0.07567500
H	0.85869900	1.00346900	-2.90106300
H	2.63298300	0.03196400	2.64666700
H	2.88771000	2.28160800	1.08490800
H	-0.02652800	-4.26374800	-1.99708500
H	0.01199600	-5.22255300	-0.50765000
H	-1.53736800	-4.66613300	-1.16780500
H	-0.85429700	-2.40208900	1.82390700
H	-0.36027300	-4.10950800	1.74265300
H	-1.98046600	-3.64033800	1.22239400
H	-0.93852400	2.70886000	-2.25392300
H	-0.05608600	3.07446200	-3.74789300
H	-1.69223600	2.42410000	-3.82696400
H	0.46289300	-0.49670100	-4.82389100
H	0.48747700	1.18606700	-5.37319400

H	-1.05732100	0.33471400	-5.18895000
H	5.06701400	-0.51535300	0.88390400
H	4.68228800	1.02127500	1.65100900
H	6.31139000	-0.29445600	3.00106700
H	4.81065400	-0.04948100	3.88933800
H	5.59531200	-2.58748700	2.36228100
H	5.55979800	-2.41475500	4.11395400
H	3.49401200	-3.56346200	3.24746100
H	3.10540200	-2.05353400	4.06526000
H	3.27932800	-2.47150000	1.03550500
H	1.81349000	-2.18914000	1.97236500
H	0.93323500	2.50145900	-1.23821900
H	0.56186300	2.78005900	0.44776100
H	0.94333100	4.93470700	-0.79577800
H	2.12420100	4.72523100	0.49386900
H	2.58486100	4.13537600	-2.47650600
H	3.27580800	5.48248300	-1.57554000
H	4.92340900	3.60233400	-1.82095100
H	4.53884800	3.90188800	-0.12941900
H	3.34649800	1.68782100	-1.88081100
H	4.53245700	1.47076400	-0.60773400
C	-4.35368500	-0.58766900	2.96134500
C	-4.06057000	-1.85543300	3.26096300
H	-5.34071500	-0.16393000	3.11428800
H	-4.80381300	-2.52523600	3.68026600
H	-3.06273500	-2.24326800	3.08352400
C	-3.32602400	0.31350100	2.38805900
O	-2.16952200	-0.04023900	2.19898400
O	-3.83930500	1.52086600	2.13667600
C	-3.04831400	2.65367800	1.60306700
C	-4.07155100	3.78906400	1.62504000
H	-4.42348200	3.97264000	2.64404500
H	-3.61530300	4.70636400	1.24288700
H	-4.93323600	3.54192300	0.99865800
C	-1.87258100	2.95974300	2.53200700
H	-2.21993200	3.06538800	3.56458100
H	-1.10599700	2.18212200	2.48178500
H	-1.42007200	3.90834900	2.22597000
C	-2.60502500	2.35266200	0.17378400
H	-3.45905600	2.07011000	-0.44634100
H	-2.15615200	3.25474300	-0.25336900
H	-1.85580700	1.55550700	0.13035900
C	-4.62546500	-0.83856300	-1.76840200
H	-4.89353100	0.03718500	-2.37409100

C	-5.30060600	-0.68340200	-0.39841300
H	-6.39051900	-0.65631900	-0.50676200
H	-5.05381900	-1.51903500	0.26293900
H	-4.98643200	0.23680300	0.10025400
C	-5.15240500	-2.08703200	-2.49856400
H	-6.24002400	-2.03984700	-2.62185100
H	-4.69643000	-2.18418500	-3.48843200
H	-4.91689600	-2.99512700	-1.93305900

TS1

C	1.41892600	3.13872100	2.16249900
C	0.56703300	4.09438300	2.70924000
C	-0.79553600	4.04143500	2.42228600
C	-1.28290000	3.03117500	1.59736900
C	-0.44008300	2.05607800	1.03556300
C	0.94663000	2.11712500	1.32267800
C	1.96232500	1.13555000	0.81204300
C	2.75234700	1.44425500	-0.31362800
C	3.73836600	0.53520500	-0.71770900
C	3.96296500	-0.66447300	-0.04667700
C	3.17921100	-0.94728900	1.07620300
C	2.18838100	-0.06894400	1.52616700
C	1.46198100	-0.35316900	2.83541400
C	2.58216200	2.75243600	-1.07616400
P	-1.13038000	0.66785100	0.02168400
C	-2.67377500	0.07199800	0.91468900
C	-1.76063600	1.46450100	-1.55728400
Pd	0.25074500	-1.11869300	-0.31261300
C	2.31765100	0.12189400	4.02408300
C	1.06390700	-1.82490200	3.00767200
C	2.75814900	2.59291300	-2.59565000
C	3.55448500	3.82697900	-0.55403200
C	-4.00534800	0.82733900	0.77541400
C	-5.14036700	0.04093900	1.45071200
C	-4.83162100	-0.22794800	2.92795200
C	-3.49929300	-0.97037900	3.08022400
C	-2.35048600	-0.22432000	2.38897800
C	-0.62488000	1.51789800	-2.59227100
C	-1.12663000	1.96401600	-3.96866500
C	-1.82393600	3.32703700	-3.88660200
C	-2.93747100	3.31317000	-2.83262400
C	-2.41788100	2.85224400	-1.46110000
H	2.47882600	3.16544900	2.39371900
H	0.96479400	4.86940400	3.35753400

H	-1.47681900	4.77676500	2.83988600
H	-2.34374600	2.99871800	1.38750100
H	4.35117600	0.76521600	-1.58403300
H	3.34631200	-1.87047300	1.62063200
H	0.54111000	0.23457800	2.83595200
H	1.56495800	3.11269100	-0.88966800
H	-2.81407900	-0.89575100	0.42036400
H	-2.51058600	0.73966600	-1.90926200
H	2.53828100	1.19038300	3.95130800
H	1.79676200	-0.05421800	4.97158700
H	3.27029900	-0.41823300	4.05255500
H	0.49606800	-2.16941200	2.13748600
H	0.44159300	-1.94522200	3.90075300
H	1.93624600	-2.47575400	3.12777000
H	2.19125600	1.74307900	-2.98227900
H	2.41958200	3.49793600	-3.11083500
H	3.80931000	2.44482400	-2.86313600
H	3.38385600	4.04413600	0.50243000
H	3.43661900	4.76035300	-1.11561600
H	4.59070800	3.49044900	-0.66792200
H	-3.94361000	1.81826000	1.24109300
H	-4.24833200	0.98242900	-0.27998000
H	-6.08534300	0.58749300	1.34800200
H	-5.26671400	-0.91627000	0.92719900
H	-4.77859200	0.72986000	3.46507900
H	-5.64397400	-0.80159400	3.38940900
H	-3.26156300	-1.11901400	4.14028600
H	-3.59132300	-1.96748900	2.63228900
H	-2.15196200	0.71698600	2.91738600
H	-1.43601600	-0.82086100	2.44369500
H	0.12595300	2.23087300	-2.23732300
H	-0.12405500	0.54689400	-2.64570700
H	-0.29029300	2.00393000	-4.67649900
H	-1.83155000	1.21457900	-4.35574100
H	-1.08232900	4.09083600	-3.61336200
H	-2.22679300	3.61520600	-4.86454000
H	-3.39057000	4.30757700	-2.74243600
H	-3.73698800	2.63305600	-3.15906000
H	-1.67352300	3.56988500	-1.09541300
H	-3.23769300	2.85919400	-0.74026600
C	5.02595000	-1.63647100	-0.52599500
H	5.55498900	-1.15280800	-1.35742500
C	4.39201800	-2.93041200	-1.06410600
H	5.16122500	-3.61976800	-1.42904400

H	3.82315000	-3.44103100	-0.28014400
H	3.70198800	-2.71432300	-1.88448700
C	6.06061500	-1.94103000	0.56964000
H	6.85415600	-2.58927300	0.18300600
H	6.51973600	-1.02140000	0.94504900
H	5.59860000	-2.45483500	1.41936900
C	-3.68786800	-3.30245400	-0.45319600
C	-2.77851600	-3.69763300	0.52906900
C	-1.40852300	-3.59475900	0.29970100
C	-0.95214400	-3.04480900	-0.91001700
C	-1.84646200	-2.71776300	-1.95661600
C	-3.21008800	-2.82207100	-1.67765700
H	-4.75584700	-3.38776300	-0.28151300
H	-3.12968100	-4.10133500	1.47385000
H	-0.69101500	-3.91853500	1.04389100
H	-3.91482900	-2.53319000	-2.45334900
C	-1.35292900	-2.25152800	-3.29631200
H	-2.18130300	-1.89522400	-3.91395300
H	-0.62718700	-1.44144900	-3.17986500
H	-0.84607300	-3.06021900	-3.83549600
Cl	0.81775700	-3.39969200	-1.33844300

12

C	1.29025300	2.92784500	2.13950600
C	0.47629500	3.80905200	2.84498600
C	-0.91033400	3.68094600	2.76777300
C	-1.46070500	2.68103300	1.97236800
C	-0.64913700	1.79450700	1.24258900
C	0.75514000	1.90593100	1.33559700
C	1.76654300	0.98951900	0.69301100
C	2.45429600	1.39969300	-0.48013600
C	3.61821300	0.72700100	-0.85544300
C	4.14648700	-0.32336500	-0.10734100
C	3.46749300	-0.71283300	1.04841600
C	2.29121700	-0.09068400	1.46039900
C	1.63072800	-0.53363800	2.75709600
C	1.99735300	2.60071700	-1.29249300
P	-1.39424900	0.48460300	0.19631800
C	-2.67573000	-0.41186200	1.21417400
C	-2.32025400	1.34897800	-1.18048200
Pd	0.28804300	-0.86620700	-0.60832600
C	2.42251900	-0.02974500	3.97623300
C	1.43862100	-2.05720000	2.81554000
C	1.96767800	2.30271600	-2.80012900

C	2.87590500	3.82970900	-0.99779700
C	-4.07537000	0.19434700	1.40168800
C	-4.98901400	-0.80720100	2.12763800
C	-4.39798400	-1.24357100	3.47305500
C	-2.99201400	-1.82606000	3.29044200
C	-2.07093000	-0.84007700	2.56160500
C	-1.35451000	1.73842300	-2.31148800
C	-2.10772000	2.24619000	-3.54512800
C	-3.00562400	3.43814100	-3.19506300
C	-3.94202500	3.09681900	-2.03038100
C	-3.16475200	2.58235000	-0.80754200
H	2.36971000	3.01089100	2.21449000
H	0.92306100	4.58429200	3.45995100
H	-1.55859700	4.35198000	3.32262100
H	-2.53745100	2.58515600	1.91875300
H	4.13120600	1.02856800	-1.76304500
H	3.85440800	-1.53715900	1.63611300
H	0.64207800	-0.07194200	2.79790600
H	0.98123600	2.84719600	-0.97298200
H	-2.80694000	-1.32117100	0.61719300
H	-2.98489000	0.55464100	-1.55203500
H	2.49612300	1.06152700	3.97602400
H	1.93500100	-0.33819000	4.90736900
H	3.43918400	-0.43668200	3.97461000
H	0.95294900	-2.42539300	1.90786300
H	0.82762800	-2.33158700	3.68228300
H	2.39451000	-2.58155600	2.90875500
H	1.45865000	1.35891700	-3.00744500
H	1.45383100	3.10662200	-3.33782700
H	2.97906000	2.22950400	-3.21178700
H	2.83248600	4.10554400	0.05939100
H	2.54392500	4.69098000	-1.58762900
H	3.92152400	3.62682500	-1.25145500
H	-4.02434800	1.11921000	1.98960200
H	-4.51656400	0.44672000	0.43377900
H	-5.98203400	-0.36519800	2.26845600
H	-5.12261900	-1.69018800	1.48823300
H	-4.34523800	-0.37439000	4.14384800
H	-5.05555000	-1.97452200	3.95684200
H	-2.55682300	-2.09348100	4.26013100
H	-3.05396600	-2.75173900	2.70313600
H	-1.90895500	0.04748700	3.18653400
H	-1.09204400	-1.29563100	2.40005200
H	-0.69975200	2.53547500	-1.94526700

H	-0.71049100	0.89602800	-2.56625800
H	-1.39067800	2.52043000	-4.32705700
H	-2.72278800	1.43298900	-3.95491300
H	-2.37413000	4.29056200	-2.90831400
H	-3.58454100	3.75538300	-4.06972500
H	-4.53493100	3.97376100	-1.74586500
H	-4.65617200	2.32543300	-2.35052600
H	-2.49325400	3.37152000	-0.44885200
H	-3.86296500	2.37051100	0.00325300
C	5.44903500	-0.98059800	-0.52366700
H	5.61643100	-0.71750600	-1.57549500
C	5.40780200	-2.51217000	-0.42673200
H	6.32467500	-2.94051700	-0.84514000
H	5.34015500	-2.84499700	0.61501300
H	4.54650400	-2.91063700	-0.96701500
C	6.61570400	-0.40175400	0.29870600
H	7.57007800	-0.83200700	-0.02324900
H	6.67534900	0.68621600	0.19341100
H	6.48538400	-0.62797000	1.36297500
C	-2.92773200	-4.33211400	-1.44185800
C	-2.30986600	-4.18530900	-0.20093100
C	-1.37738300	-3.16261700	-0.01294800
C	-1.06061700	-2.28093300	-1.05198400
C	-1.63635400	-2.44706900	-2.31991300
C	-2.58045500	-3.47500800	-2.48322900
H	-3.65674900	-5.12033500	-1.60514000
H	-2.54063400	-4.86202500	0.61730900
H	-0.90035900	-3.05626400	0.95485800
H	-3.03449900	-3.60909300	-3.46251500
C	-1.26434600	-1.59421900	-3.50637200
H	-1.43995400	-2.13690200	-4.43983200
H	-1.86088100	-0.67658700	-3.54838500
H	-0.20872300	-1.31853100	-3.46044100
Cl	1.90562200	-2.19829500	-1.71134800

13

C	2.31668600	1.83317000	2.72135500
C	1.30896300	2.55122600	3.35273700
C	0.07576200	2.67873200	2.71879900
C	-0.11312400	2.06442200	1.48975600
C	0.88470600	1.30876800	0.83735200
C	2.14974900	1.20939500	1.46704800
C	3.41382000	0.58944100	0.93882500
C	4.34485600	1.42501800	0.28132300

C	5.58640100	0.89937500	-0.09401600
C	5.94384400	-0.41876100	0.17875100
C	5.02161800	-1.22058200	0.85672700
C	3.77095600	-0.74283000	1.25535000
C	2.83900800	-1.64439500	2.06085100
C	4.05985100	2.90190900	0.02721200
P	0.15649100	0.56165200	-0.70524000
C	-0.27232300	2.06708800	-1.75542100
C	1.31588700	-0.35616000	-1.83984800
Pd	-1.84219800	-0.96748800	-0.55486600
C	3.02087200	-1.42881000	3.57550500
C	2.99807200	-3.13916800	1.74287200
C	4.46720500	3.37215300	-1.37832100
C	4.75174000	3.77168600	1.09341700
C	0.65807700	3.27475800	-1.56634900
C	0.35373400	4.36325100	-2.60546000
C	-1.11708300	4.79403900	-2.55111700
C	-2.05199400	3.58709600	-2.69781300
C	-1.74271900	2.50337300	-1.65685600
C	1.71139600	-1.73207000	-1.29342500
C	2.41193400	-2.57322600	-2.36701700
C	3.62321500	-1.82961800	-2.94050400
C	3.20732900	-0.46817700	-3.50739100
C	2.51138300	0.39212400	-2.44140800
H	3.28900900	1.74938100	3.19525300
H	-0.74784800	3.20870100	3.18294600
H	-1.08711400	2.14555800	1.02613900
H	6.30150600	1.53876800	-0.60326100
H	5.29152100	-2.24443700	1.08888900
H	1.81563300	-1.35449700	1.81032400
H	2.98364000	3.05604500	0.12859600
H	-0.13444700	1.67156700	-2.76883300
H	0.60070800	-0.54019200	-2.65117200
H	2.79771400	-0.40229800	3.86903200
H	2.35242400	-2.09170700	4.13620500
H	4.05030000	-1.65498300	3.87379900
H	2.93999600	-3.34471900	0.67140000
H	2.21016000	-3.71160200	2.23994100
H	3.95289500	-3.52807900	2.11100200
H	-1.31048800	5.28454300	-1.58635300
H	4.11483600	4.39526000	-1.54490200
H	5.55453000	3.38005000	-1.50449700
H	4.40856800	3.51733000	2.09894700
H	4.54058800	4.83250900	0.92069100

H	5.83758200	3.63138100	1.06064300
H	0.51869400	3.68542700	-0.55950400
H	1.70413500	2.97288300	-1.63523000
H	1.01240000	5.22466400	-2.44307300
H	0.58243200	3.97703100	-3.60847200
H	4.04496300	2.73618100	-2.15964700
H	-1.32585900	5.53776600	-3.32874100
H	-3.09883000	3.90034600	-2.60977800
H	-1.93892300	3.15399000	-3.70064200
H	-1.95075400	2.89923600	-0.65599200
H	-2.38972900	1.63824100	-1.81397500
H	2.38915500	-1.60266800	-0.45140700
H	0.82115000	-2.25542300	-0.93211500
H	2.71912400	-3.53595300	-1.94055800
H	1.69981600	-2.79612700	-3.17301900
H	4.35588600	-1.67273300	-2.13884600
H	4.11468200	-2.43283300	-3.71277800
H	4.08142600	0.06871200	-3.89491900
H	2.52528300	-0.61960500	-4.35518800
H	3.23214900	0.63574900	-1.66087500
H	2.18290900	1.33236800	-2.89388500
C	7.31081000	-0.95426200	-0.21233200
H	7.84355400	-0.14055000	-0.72105900
C	7.20763500	-2.13163700	-1.19553400
H	8.20390800	-2.48600200	-1.48048900
H	6.66970300	-2.97385600	-0.74721100
H	6.67356800	-1.84240700	-2.10482300
C	8.13034100	-1.34372800	1.02990800
H	9.13728100	-1.66643500	0.74495700
H	8.22117100	-0.50093400	1.72162600
H	7.65564100	-2.16967600	1.57021800
C	-5.36331200	-4.05872200	-1.83542300
C	-5.68762700	-2.75103200	-1.47957200
C	-4.67854700	-1.88026400	-1.05984400
C	-3.35210400	-2.30542000	-1.00522200
C	-3.00536000	-3.61198100	-1.37854500
C	-4.03363600	-4.47564300	-1.78314600
H	-6.13741200	-4.74948000	-2.15614300
H	-6.71716800	-2.40606000	-1.52244000
H	-4.94427400	-0.86705500	-0.76908900
H	-3.77672200	-5.49206600	-2.07300200
C	-1.57058000	-4.07733800	-1.41762900
H	-1.50699900	-5.14051500	-1.66735100
H	-1.01626200	-3.51086600	-2.17300100

H	-1.06237100	-3.92485100	-0.46075700
Cl	-1.81718900	-0.80282200	-2.95100300
C	-2.73820300	-1.78374000	1.42853000
C	-0.85908200	-1.04527700	2.58975900
C	-1.98260100	-2.93567000	2.04564400
C	-2.04551400	-0.61039500	1.73107300
C	-0.53337800	-2.42247100	1.98070100
H	0.14614300	-3.00497300	2.60711000
H	-0.13762300	-2.36862600	0.96503000
C	-1.47653100	-1.49468000	3.95447600
H	-0.66564700	-1.72394100	4.65269800
H	-2.09138800	-0.70728700	4.38771100
C	-2.27302100	-2.78040500	3.57797100
H	-1.90565000	-3.65989900	4.11516700
H	-3.34378400	-2.69396700	3.78272500
H	-0.05177300	-0.32494500	2.68119500
H	-2.20221900	-3.91972100	1.63242400
C	-2.79909500	0.66365300	1.99111800
O	-2.74142800	1.21914600	3.08931100
H	-3.80839000	-1.82004900	1.29075600
N	-3.58666900	1.11404900	0.98069700
H	-3.51954200	0.65172600	0.08168300
C	-4.51631900	2.21665600	1.15244000
C	-4.96973800	2.81976900	-0.19675900
C	-5.82612600	1.83829300	1.86620500
H	-4.00695200	2.97593600	1.75572000
C	-6.43604400	3.28745400	0.02218400
H	-4.31103100	3.63275300	-0.51019000
C	-6.74625900	3.01097900	1.51230100
H	-5.67851100	1.68388900	2.93762200
H	-6.21032500	0.90409100	1.43556400
H	-6.57921100	4.33888000	-0.24115200
H	-7.11145500	2.70710400	-0.61426500
H	-6.47920400	3.88285100	2.12186100
H	-7.80429400	2.80191500	1.69322900
H	1.48711900	3.00349900	4.32331600
H	-4.92081200	2.05761200	-0.98306400
TS2			
C	2.22737100	1.79037300	2.76062000
C	1.19794000	2.47541300	3.39331000
C	-0.02813200	2.59666400	2.74464600
C	-0.18788500	2.01365600	1.49642500
C	0.83518200	1.29674100	0.83992000

C	2.08987500	1.19741800	1.48817400
C	3.36720000	0.60022600	0.96781200
C	4.30562100	1.45881000	0.35236700
C	5.55869700	0.95128900	-0.00935100
C	5.91896900	-0.37120300	0.23733500
C	4.98704300	-1.19717700	0.87186900
C	3.72392500	-0.73918400	1.25398200
C	2.77530500	-1.67202000	2.00395000
C	4.01282700	2.93913800	0.12803100
P	0.16157900	0.58558000	-0.74134300
C	-0.28712300	2.09814100	-1.76672700
C	1.34562800	-0.29313200	-1.87449100
Pd	-1.72275900	-0.90584700	-0.54070900
C	2.89881000	-1.49305400	3.52915100
C	2.96587500	-3.15636000	1.65503900
C	4.44128000	3.44564800	-1.25845100
C	4.67790600	3.78929100	1.22669000
C	0.59754900	3.32973000	-1.52068400
C	0.27515500	4.44150500	-2.52944600
C	-1.21125300	4.81768700	-2.49255600
C	-2.09831900	3.58480500	-2.70472600
C	-1.77482200	2.47674400	-1.69449100
C	1.74316100	-1.67888700	-1.35803200
C	2.45998000	-2.48665100	-2.44561500
C	3.67372600	-1.72044100	-2.98440900
C	3.25794100	-0.34452000	-3.51624700
C	2.54431100	0.48113600	-2.43463100
H	3.19254400	1.70698300	3.24899000
H	-0.86844100	3.09734400	3.21119000
H	-1.15716500	2.08833900	1.02195100
H	6.28010900	1.60797400	-0.48668600
H	5.25841900	-2.22552900	1.08105700
H	1.75715600	-1.39086900	1.72233700
H	2.93338400	3.08185000	0.21366100
H	-0.10946400	1.73258000	-2.78552500
H	0.64129200	-0.46286400	-2.69911400
H	2.65467700	-0.47670300	3.84048500
H	2.21662000	-2.17612200	4.04726100
H	3.91891400	-1.71755800	3.85921900
H	2.95109800	-3.33470600	0.57724400
H	2.16648400	-3.74970800	2.10668100
H	3.91102800	-3.54346600	2.04934100
H	-1.44317900	5.26396100	-1.51492100
H	4.08710800	4.47110900	-1.40590800

H	5.53052900	3.46123300	-1.36595800
H	4.32063700	3.50732000	2.21988300
H	4.45921700	4.85196500	1.07622000
H	5.76552000	3.66026800	1.20893700
H	0.42579700	3.70175900	-0.50392200
H	1.65501200	3.06510300	-1.57865100
H	0.89886100	5.31957100	-2.32420200
H	0.53757400	4.09845700	-3.53980500
H	4.03514100	2.82725000	-2.06204900
H	-1.42980200	5.58230500	-3.24682900
H	-3.15757700	3.85749000	-2.63145700
H	-1.94678900	3.19230800	-3.71913700
H	-2.02157500	2.82953300	-0.68615100
H	-2.38117000	1.59132200	-1.89822100
H	2.41076700	-1.56582300	-0.50613200
H	0.85033300	-2.21252100	-1.01927500
H	2.76885100	-3.45859600	-2.04176800
H	1.75791800	-2.69131500	-3.26492300
H	4.39743200	-1.58413400	-2.17068100
H	4.17636400	-2.29814100	-3.76892400
H	4.13411300	0.20746600	-3.87688200
H	2.58695700	-0.47453200	-4.37617900
H	3.25288700	0.70410100	-1.63683200
H	2.21688400	1.43364100	-2.86203600
C	7.29868200	-0.88709000	-0.13475300
H	7.83360800	-0.06008000	-0.61921300
C	7.22792400	-2.04927900	-1.13855700
H	8.23354600	-2.38836200	-1.40889900
H	6.69047800	-2.90449800	-0.71500000
H	6.70908700	-1.75087400	-2.05372100
C	8.09611800	-1.28822900	1.11814100
H	9.11166900	-1.59768700	0.84947500
H	8.16487600	-0.45525000	1.82415500
H	7.61768700	-2.12627500	1.63615600
C	-5.18751600	-3.84009800	-2.19345500
C	-5.54478100	-2.60880400	-1.64472400
C	-4.60356800	-1.88862200	-0.91352700
C	-3.29647500	-2.36250900	-0.75084700
C	-2.91954800	-3.59578500	-1.31374700
C	-3.89111500	-4.31943700	-2.02042500
H	-5.91257000	-4.42468600	-2.75168800
H	-6.55077400	-2.21825100	-1.76851000
H	-4.90358100	-0.95682000	-0.44294600
H	-3.60697100	-5.27063900	-2.46382600

C	-1.50123200	-4.10569900	-1.30258100
H	-1.45882500	-5.14864000	-1.62904500
H	-0.90099600	-3.50602300	-1.99490000
H	-1.03533500	-4.03902100	-0.31876600
Cl	-1.74985500	-0.89802000	-2.98280100
C	-2.81963300	-1.94193600	1.30691600
C	-0.91833500	-1.20669700	2.49603400
C	-2.06710100	-3.08310900	1.95941600
C	-2.06404500	-0.74587800	1.58701600
C	-0.60730100	-2.59248800	1.90226500
H	0.05335400	-3.18400200	2.54109300
H	-0.19279600	-2.54823100	0.89391300
C	-1.54623500	-1.63012000	3.85766400
H	-0.74414400	-1.88033700	4.55965000
H	-2.14296100	-0.82831900	4.28766600
C	-2.37333800	-2.89595600	3.48182400
H	-2.04247800	-3.78070200	4.03383900
H	-3.44455000	-2.77645800	3.66984700
H	-0.09640700	-0.50114000	2.58817400
H	-2.29491500	-4.07568900	1.57189800
C	-2.83188500	0.50626600	1.92703100
O	-2.77637300	1.02854800	3.04199500
H	-3.89539900	-1.92351100	1.39993900
N	-3.63723900	1.00043100	0.94479300
H	-3.50734900	0.64734400	0.00487000
C	-4.48626300	2.16134100	1.15659800
C	-5.00890800	2.75244400	-0.17500000
C	-5.75305600	1.87513100	1.98216900
H	-3.89549400	2.91169200	1.69577300
C	-6.45293700	3.24621100	0.11780800
H	-4.35909000	3.55499100	-0.53136100
C	-6.65055800	3.06862300	1.63983700
H	-5.52978000	1.76117600	3.04495100
H	-6.20506700	0.94062200	1.62491500
H	-6.61402400	4.27770500	-0.20703100
H	-7.17488600	2.62645000	-0.42388400
H	-6.29692500	3.95958100	2.17335300
H	-7.69767500	2.91892300	1.91783000
H	1.35293100	2.90499400	4.37807300
H	-5.01214200	1.98318300	-0.95559600
14			
C	2.08358600	1.43963600	2.97084900
C	1.01866500	2.00500300	3.66161000

C	-0.19590700	2.18122000	3.00414000
C	-0.31023400	1.77078700	1.68460500
C	0.74855300	1.17148800	0.97049200
C	1.99203300	1.01565700	1.62942200
C	3.29651100	0.52973100	1.06246800
C	4.21974500	1.49425100	0.59877600
C	5.49544500	1.07951000	0.20021700
C	5.89148100	-0.25435200	0.26054300
C	4.97163900	-1.18944000	0.74373800
C	3.68775900	-0.82691700	1.15958200
C	2.75765800	-1.88445200	1.75029200
C	3.88697400	2.98308000	0.57607100
P	0.13604900	0.65452600	-0.70088300
C	-0.34703400	2.26471300	-1.54241100
C	1.35086600	-0.05430900	-1.91915800
Pd	-1.64517400	-0.81815300	-0.75060100
C	2.83238400	-1.90105400	3.28891200
C	3.01820000	-3.30292500	1.21956200
C	4.31537100	3.68575000	-0.72275800
C	4.51686500	3.69162500	1.78961500
C	0.50012500	3.47565000	-1.11879500
C	0.17348600	4.69745100	-1.98926800
C	-1.32193300	5.03353300	-1.94145300
C	-2.17116300	3.81814000	-2.33200600
C	-1.84574300	2.59554000	-1.46448500
C	1.74791900	-1.49616200	-1.58938400
C	2.53494700	-2.12907900	-2.74203300
C	3.75960700	-1.27860600	-3.09600200
C	3.34162900	0.14984400	-3.45919900
C	2.55319700	0.81103800	-2.31802400
H	3.03935000	1.31772200	3.46971900
H	-1.06182900	2.58929500	3.51179300
H	-1.26967500	1.88107300	1.19810200
H	6.20559800	1.81921800	-0.15784800
H	5.26944900	-2.22970700	0.80787400
H	1.73573600	-1.61037700	1.47601600
H	2.80310000	3.08555400	0.66445500
H	-0.13624600	2.03103700	-2.59334000
H	0.67086700	-0.10849900	-2.77922600
H	2.52983100	-0.94618400	3.72004800
H	2.17036200	-2.67528100	3.69122500
H	3.85344100	-2.12008600	3.61971300
H	3.06434800	-3.33772100	0.12830400
H	2.21679300	-3.97127900	1.54486000

H	3.95610300	-3.71172700	1.60992000
H	-1.58631600	5.34643600	-0.92129100
H	3.94322500	4.71542900	-0.72862300
H	5.40478700	3.73474900	-0.81806300
H	4.15461900	3.26865500	2.72950600
H	4.27364300	4.75954100	1.78100300
H	5.60742300	3.59125600	1.77190000
H	0.29270400	3.71174300	-0.06891200
H	1.56560000	3.24590300	-1.18004100
H	0.77187800	5.55522800	-1.66051100
H	0.46587400	4.48834700	-3.02755500
H	3.92590200	3.17870400	-1.60856200
H	-1.54285100	5.88288500	-2.59800800
H	-3.23860900	4.05481200	-2.25355300
H	-1.98492900	3.56327000	-3.38376400
H	-2.12956100	2.80282700	-0.42617100
H	-2.42088700	1.73130600	-1.80315100
H	2.36448900	-1.50345700	-0.69328100
H	0.84578000	-2.07902700	-1.37909000
H	2.84051400	-3.14560400	-2.46558100
H	1.88051300	-2.22063900	-3.61892000
H	4.43146800	-1.24538500	-2.22958500
H	4.31966700	-1.73438100	-3.92084800
H	4.22244300	0.76051700	-3.69090600
H	2.72211300	0.12752200	-4.36591200
H	3.21598700	0.94928600	-1.46483700
H	2.21661100	1.80144300	-2.63837800
C	7.29077600	-0.67155400	-0.15953100
H	7.82475900	0.24107500	-0.45375600
C	7.26595500	-1.61064600	-1.37674200
H	8.28349100	-1.88323700	-1.67614000
H	6.72495700	-2.53535000	-1.14897200
H	6.77200900	-1.13835300	-2.23032000
C	8.06140000	-1.30638200	1.01046800
H	9.08970400	-1.54014800	0.71535500
H	8.09521900	-0.63295800	1.87210900
H	7.58784400	-2.23938500	1.33383700
C	-4.52554000	-2.79966300	-2.94624400
C	-5.10415900	-1.97439700	-1.98510400
C	-4.52397900	-1.90015700	-0.72806600
C	-3.35085100	-2.61502000	-0.37106700
C	-2.77413500	-3.46507400	-1.36076500
C	-3.39152100	-3.52973200	-2.62055100
H	-4.95263600	-2.87639000	-3.94084100

H	-6.00178500	-1.40515200	-2.20545200
H	-4.99735800	-1.29614400	0.03783100
H	-2.94078400	-4.16655600	-3.37509500
C	-1.52361600	-4.30450000	-1.20680800
H	-1.50121300	-5.06699000	-1.98891600
H	-0.62620600	-3.69251500	-1.33415500
H	-1.44863300	-4.80877900	-0.24648300
Cl	-1.71980800	-0.59504600	-3.19336100
C	-2.92763800	-2.40835200	1.10486900
C	-0.92395200	-1.54618800	2.20329200
C	-2.05486800	-3.46531000	1.82049700
C	-2.07506500	-1.08816900	1.29054800
C	-0.61815900	-2.93803700	1.62360500
H	0.11200000	-3.49343500	2.21998800
H	-0.27974700	-2.90496600	0.58901600
C	-1.43355500	-1.94550100	3.61648800
H	-0.56598800	-2.14599500	4.25515600
H	-2.02365800	-1.15769600	4.07453800
C	-2.23616600	-3.25099000	3.34297600
H	-1.82592400	-4.10190200	3.89624000
H	-3.29230300	-3.16333300	3.61749600
H	-0.09871500	-0.84020700	2.24115900
H	-2.26428200	-4.49001000	1.51034400
C	-2.88969100	0.09739600	1.78749600
O	-2.87273000	0.49918400	2.95504500
H	-3.86981600	-2.31287400	1.65611500
N	-3.69683200	0.71551300	0.87409700
H	-3.60113600	0.46910100	-0.10165500
C	-4.55611000	1.82864100	1.23699900
C	-5.13732100	2.54342100	-0.00400900
C	-5.79153700	1.44057300	2.06798600
H	-3.96242400	2.53305300	1.83332800
C	-6.54281700	3.05390000	0.42192400
H	-4.48441900	3.35035300	-0.34412200
C	-6.69403300	2.66890200	1.91276500
H	-5.52819200	1.19422500	3.09811900
H	-6.26313100	0.55865900	1.61424300
H	-6.66009400	4.12882600	0.25924800
H	-7.31656700	2.55849000	-0.17328600
H	-6.32208500	3.47956600	2.55121200
H	-7.73306900	2.48358000	2.19952000
H	1.13841200	2.30068200	4.69915500
H	-5.22017200	1.83416100	-0.83596400

15

C	3.78493000	-0.58728500	3.30538900
C	2.75968900	-0.74775100	4.22924400
C	1.45680100	-0.44032900	3.84986400
C	1.21620600	-0.00072800	2.55592000
C	2.23791700	0.14965700	1.59355900
C	3.56927800	-0.13890400	1.98666100
C	4.84415900	0.05055400	1.21121900
C	5.56598500	1.25140100	1.39848300
C	6.82258100	1.39376300	0.79951500
C	7.39520100	0.38042100	0.03522500
C	6.67997300	-0.81056400	-0.11401800
C	5.42511700	-1.00625600	0.46942100
C	4.73907800	-2.36462100	0.34094000
C	5.03806000	2.37705600	2.28220100
P	1.47371700	0.64317400	-0.02783400
C	0.73455800	2.33737500	0.30823000
C	2.61802100	1.00291600	-1.45202400
Pd	-0.22494900	-0.68593400	-0.91374600
C	5.04640900	-3.26241200	1.55466800
C	5.09854700	-3.12283100	-0.94629600
C	5.22441100	3.77461900	1.66903900
C	5.69695900	2.32384800	3.67326000
C	1.52108300	3.20736200	1.30065100
C	0.93595900	4.62646600	1.35893100
C	-0.55828900	4.61130000	1.70812200
C	-1.33946900	3.70022800	0.75308500
C	-0.74416400	2.28877500	0.71513500
C	3.21559500	-0.26849900	-2.06218000
C	3.91138700	0.03284500	-3.39365100
C	4.97835500	1.11880300	-3.21717800
C	4.35970400	2.39535500	-2.63810300
C	3.65429700	2.12390900	-1.30005000
H	4.80672000	-0.80551500	3.59815700
H	0.62407800	-0.57744000	4.52958900
H	0.19132300	0.18822400	2.26565000
H	7.37619000	2.31775200	0.93917300
H	7.11991400	-1.61449100	-0.69289200
H	3.66131200	-2.18800100	0.32861400
H	3.96703800	2.21667100	2.42158500
H	0.78464100	2.79659800	-0.68873300
H	1.85524000	1.35041700	-2.15965300
H	4.69194800	-2.82076300	2.48655200
H	4.55673700	-4.23492900	1.43765800

H	6.12560100	-3.43141300	1.64087000
H	4.97191800	-2.50781700	-1.84073800
H	4.45522400	-4.00108500	-1.04645900
H	6.13223800	-3.48377100	-0.92583200
H	-0.68373900	4.23551600	2.73289100
H	4.70390600	4.52102900	2.27813400
H	6.27946400	4.06470900	1.63354300
H	5.49692700	1.37283700	4.17184800
H	5.31526900	3.12857300	4.31114700
H	6.78291700	2.44182300	3.59027000
H	1.46513300	2.74857800	2.29483900
H	2.57837400	3.25251300	1.03704000
H	1.49288200	5.22751000	2.08769100
H	1.07508600	5.11100400	0.38173800
H	4.82913800	3.82960500	0.65196700
H	-0.96319600	5.63048300	1.69378500
H	-2.39413800	3.64239800	1.04643900
H	-1.30539000	4.13781300	-0.25852400
H	-0.83984300	1.85184100	1.71394000
H	-1.32424200	1.64055200	0.05876500
H	3.94182600	-0.69443200	-1.37273100
H	2.42134900	-1.00515700	-2.20749100
H	4.36071600	-0.88519900	-3.79199200
H	3.16135600	0.36401300	-4.12403900
H	5.75052400	0.75111900	-2.52962400
H	5.47328700	1.33340300	-4.17195500
H	5.12903500	3.16363900	-2.49299200
H	3.63361700	2.80213300	-3.35551700
H	4.40102600	1.85153000	-0.55543200
H	3.16910000	3.04326800	-0.95943700
C	8.77163300	0.55370200	-0.58387800
H	9.12188800	1.55903400	-0.31641900
C	8.72639000	0.46769700	-2.11816400
H	9.72360900	0.62054300	-2.54471800
H	8.36925900	-0.51413600	-2.44674800
H	8.05434100	1.22211100	-2.53651000
C	9.77405500	-0.45900400	-0.00424600
H	10.77823100	-0.28561500	-0.40566600
H	9.82134500	-0.38541900	1.08640000
H	9.48605500	-1.48500300	-0.25702600
C	-3.47728500	-1.57453500	-3.69465500
C	-3.87951300	-1.58210300	-2.36250900
C	-3.00927800	-2.07448100	-1.39583000
C	-1.72997400	-2.58764500	-1.70841700

C	-1.30968800	-2.54243100	-3.07433400
C	-2.20762200	-2.03727300	-4.02643200
H	-4.14086100	-1.21146900	-4.47681500
H	-4.84415700	-1.19955600	-2.04774100
H	-3.35975400	-2.06503200	-0.36858400
H	-1.88387100	-2.00155200	-5.06239400
C	0.04736300	-2.93221000	-3.62370000
H	-0.02032300	-3.04357700	-4.70889200
H	0.77358500	-2.13627600	-3.43228600
H	0.44468400	-3.85980500	-3.21918400
Cl	-0.36837000	0.85980400	-2.93601800
C	-1.03024700	-3.26394300	-0.49371400
C	1.08368400	-2.93134500	0.67588000
C	0.05826400	-4.32577300	-0.77045800
C	-0.28891600	-2.24956200	0.45927800
C	1.36338900	-3.50324600	-0.72530200
H	2.25790000	-4.13310100	-0.75613300
H	1.44128300	-2.73940200	-1.49579400
C	0.98585000	-4.26175000	1.47424900
H	2.00625400	-4.63397700	1.62653900
H	0.50938300	-4.13070900	2.43860400
C	0.20356900	-5.19120700	0.50536200
H	0.75617300	-6.11094300	0.28570500
H	-0.77247700	-5.48379100	0.90553100
H	1.82519300	-2.25720100	1.09510500
H	-0.13376800	-4.91904100	-1.66586400
C	-1.03675900	-1.89079500	1.74900400
O	-0.76872400	-2.50465500	2.79578500
H	-1.84783600	-3.73069800	0.06508100
N	-1.94683300	-0.89190000	1.75881600
H	-2.36671400	-0.42003900	0.91868100
C	-2.61121800	-0.59933900	3.02710000
C	-3.19583700	0.84151800	3.08728700
C	-3.79356400	-1.54349400	3.34370000
H	-1.85663000	-0.72642800	3.80840000
C	-4.65384300	0.68541700	3.57808200
H	-2.61082700	1.45604400	3.78132800
C	-4.70076700	-0.70032900	4.24746400
H	-3.45179400	-2.47840500	3.79450700
H	-4.30250700	-1.74580900	2.39766300
H	-4.97879900	1.50053500	4.23452100
H	-5.30085400	0.67093000	2.69673400
H	-4.29001600	-0.64147500	5.26476800
H	-5.71897400	-1.10200100	4.33627400

H	2.97903800	-1.11103700	5.22850700
H	-3.16538800	1.30482200	2.10145400
C	-4.56881500	0.33956300	-0.03605100
O	-4.98541600	-0.74437300	0.52880400
O	-5.40957800	1.14292500	-0.62490700
O	-3.29717600	0.63202900	-0.03375800
Cs	-7.70783700	0.00948500	0.82293900
Cs	-3.33233100	2.40093500	-2.36457000

TS3

C	-3.85590100	0.32737400	3.29455600
C	-2.83074600	0.32667800	4.23243900
C	-1.54095600	0.01347200	3.81610300
C	-1.31740900	-0.29148100	2.48041200
C	-2.33970900	-0.29755400	1.50721600
C	-3.65485900	0.02807100	1.93204200
C	-4.92356200	0.08110900	1.12419700
C	-5.77421000	-1.04652600	1.10130300
C	-7.01161300	-0.95697000	0.45345100
C	-7.44561700	0.22024500	-0.15183300
C	-6.61248600	1.33950300	-0.07669700
C	-5.37199100	1.30273900	0.56536400
C	-4.58159600	2.59696300	0.73532100
C	-5.41349300	-2.33405400	1.83334600
P	-1.57763500	-0.72658400	-0.14503500
C	-1.08406300	-2.52844500	0.06483900
C	-2.71898500	-0.76223400	-1.61318000
Pd	0.35256600	0.44546900	-0.96204100
C	-5.02932000	3.32918400	2.01528700
C	-4.67885300	3.55948300	-0.45789300
C	-5.72723300	-3.60748800	1.03174000
C	-6.12275500	-2.38669300	3.19972800
C	-2.03695100	-3.38779700	0.90517000
C	-1.61504000	-4.86453000	0.87671900
C	-0.16432300	-5.04793800	1.33895700
C	0.78751400	-4.15994900	0.52718600
C	0.35653000	-2.68872300	0.57568200
C	-3.16356800	0.65479800	-1.99794000
C	-3.87352100	0.66197900	-3.35633200
C	-5.04765800	-0.32334200	-3.36660500
C	-4.57443700	-1.73872000	-3.01888800
C	-3.86913700	-1.77384400	-1.65440200
H	-4.86564900	0.56891100	3.60979000
H	-0.70330200	0.04156300	4.50380200

H	-0.30106700	-0.49307800	2.16885400
H	-7.66337200	-1.82564100	0.43080000
H	-6.94785600	2.27399800	-0.51379700
H	-3.53075600	2.33226100	0.86124600
H	-4.33917500	-2.31526600	2.02544100
H	-1.09607500	-2.87872500	-0.97482200
H	-1.98242900	-1.07579800	-2.36396700
H	-4.87391700	2.71594800	2.90436200
H	-4.45966000	4.25576500	2.14197200
H	-6.09302500	3.58572500	1.95692600
H	-4.42399200	3.07644900	-1.40362100
H	-3.98777900	4.39416200	-0.30875200
H	-5.68270700	3.98681100	-0.55336000
H	-0.08702900	-4.77012700	2.39917800
H	-5.31886900	-4.48328600	1.54698800
H	-6.80568500	-3.76617800	0.92973700
H	-5.84007900	-1.53831800	3.82727800
H	-5.86166000	-3.30661700	3.73461600
H	-7.21050300	-2.36516000	3.07127800
H	-2.02835700	-3.02561900	1.94043400
H	-3.06199700	-3.29100900	0.54799300
H	-2.29150800	-5.45866000	1.50275800
H	-1.71936900	-5.24649100	-0.14872900
H	-5.29884900	-3.57309700	0.02730500
H	0.13143400	-6.10149200	1.26566000
H	1.81379400	-4.26329600	0.90646000
H	0.78464300	-4.50349100	-0.51923500
H	0.42332800	-2.34514400	1.61280900
H	1.03020200	-2.05369300	-0.00265400
H	-3.84778200	1.03502200	-1.24001600
H	-2.29277000	1.31717400	-2.02025900
H	-4.22279000	1.67597400	-3.58700100
H	-3.15462800	0.38736500	-4.14002400
H	-5.78752500	-0.00151100	-2.62349900
H	-5.54783400	-0.31643100	-4.34273900
H	-5.42194500	-2.43529000	-3.01095400
H	-3.88012500	-2.08935000	-3.79490000
H	-4.59753100	-1.54960000	-0.87591200
H	-3.48803900	-2.78353300	-1.47185100
C	-8.80723800	0.29792600	-0.82174900
H	-9.26576900	-0.69611900	-0.73956300
C	-8.69660800	0.63926200	-2.31642100
H	-9.68889100	0.68086300	-2.77851800
H	-8.21786000	1.61330500	-2.46296000

H	-8.10035000	-0.10624700	-2.84923300
C	-9.72550800	1.29623900	-0.09590900
H	-10.72616400	1.29904000	-0.54134900
H	-9.82045600	1.04412000	0.96456400
H	-9.32752100	2.31438900	-0.16210700
C	3.21467900	2.20658300	-3.86489200
C	2.52555000	1.23407700	-3.15277200
C	2.04907900	1.49864000	-1.85475500
C	2.19904700	2.79375100	-1.31090300
C	2.96686100	3.75754000	-1.99581800
C	3.46466100	3.44244300	-3.26417300
H	3.58491300	2.00349300	-4.86672200
H	2.35639200	0.24848100	-3.57293100
H	2.37527900	0.53891000	-1.10955900
H	4.05862200	4.18647000	-3.79188600
C	3.30336800	5.10790000	-1.40059800
H	4.29650000	5.42838500	-1.73238100
H	2.59652200	5.88909200	-1.70419500
H	3.30516700	5.08266700	-0.30806900
Cl	0.40003300	-1.38525200	-2.80788900
C	1.46657000	3.12235400	-0.03888100
C	-0.85377900	2.64593500	0.58385700
C	0.43490200	4.27931100	-0.26412800
C	0.53194400	1.95273400	0.50145100
C	-0.82263200	3.50863800	-0.69218200
H	-1.70391000	4.15002900	-0.79377800
H	-0.68416100	2.93395000	-1.61148200
C	-0.94434400	3.75697800	1.66054700
H	-1.97578600	4.13041500	1.67968600
H	-0.67648400	3.40078500	2.64972100
C	0.02246200	4.84452500	1.11342300
H	-0.47412400	5.81498400	1.00489700
H	0.89057600	4.98624300	1.76513900
H	-1.66684600	1.93284700	0.66299100
H	0.78304700	5.03512100	-0.96650400
C	1.12297300	1.42797600	1.81528400
O	0.93271500	1.99184600	2.90182300
H	2.17847600	3.42290600	0.74112800
N	1.90661700	0.32373700	1.73411700
H	2.27292000	0.02550700	0.81893900
C	2.67010000	-0.13243800	2.88069200
C	3.14171200	-1.60609300	2.69312500
C	3.96145600	0.68351700	3.13800500
H	2.02099100	-0.04634200	3.75637800

C	4.65992500	-1.62067900	2.98980300
H	2.59242100	-2.27219300	3.36643900
C	4.90677500	-0.33017300	3.79485800
H	3.76132700	1.57002100	3.74468200
H	4.34552100	1.00530400	2.16278700
H	4.98326400	-2.52274900	3.52033500
H	5.19044100	-1.58884300	2.03102500
H	4.62767400	-0.48581100	4.84497200
H	5.96072200	-0.01418100	3.80451700
H	-3.03898800	0.58018500	5.26746800
H	2.94832800	-1.93335600	1.67048300
C	4.46058200	-0.20060600	-0.35338400
O	4.76210800	1.00017700	-0.07219600
O	5.32463600	-1.15974500	-0.44392200
O	3.17985900	-0.52684200	-0.54368300
Cs	7.40529300	0.47671800	0.89150400
Cs	3.36518000	-2.97319000	-2.03998900

ANP

C	-4.31763300	-0.78529800	3.31240300
C	-3.42628200	-1.34895700	4.21612700
C	-2.20121700	-1.81120600	3.74338100
C	-1.90161400	-1.69044900	2.39316600
C	-2.79164700	-1.12752300	1.45326300
C	-4.04272000	-0.66850400	1.93426000
C	-5.16858400	-0.05327000	1.15593200
C	-6.27119600	-0.85484500	0.78155900
C	-7.37217300	-0.24714600	0.16749000
C	-7.42501900	1.12663300	-0.06307500
C	-6.34035700	1.90478800	0.34721800
C	-5.21193500	1.34488500	0.95131100
C	-4.07037500	2.24755000	1.41091300
C	-6.30552000	-2.35593100	1.06781600
P	-1.96241700	-0.97651800	-0.21200300
C	-1.39175900	-2.73912300	-0.59476000
C	-3.10866200	-0.70505600	-1.65447600
Pd	-0.04457900	0.63664700	-0.65552900
C	-4.28014800	2.67216800	2.87692200
C	-3.87521200	3.49316300	0.53359400
C	-6.95394100	-3.18924900	-0.05098600
C	-7.03856500	-2.64118900	2.39298100
C	-2.15245200	-3.89917200	0.06427800
C	-1.67033500	-5.24558600	-0.49869300
C	-0.15328600	-5.41631900	-0.33623900

C	0.60862200	-4.24181100	-0.96567200
C	0.12407500	-2.90332100	-0.39752300
C	-3.49237100	0.76599900	-1.85951800
C	-4.14383000	0.96888800	-3.23208600
C	-5.35167800	0.04069000	-3.41247500
C	-4.94871500	-1.42616800	-3.22074700
C	-4.29737000	-1.64865900	-1.84721100
H	-5.27022800	-0.40512500	3.66603600
H	-1.46374900	-2.23702100	4.41660900
H	-0.90788200	-1.96888400	2.07773800
H	-8.21528100	-0.85851900	-0.14011100
H	-6.36981800	2.97577300	0.18148500
H	-3.14459800	1.66647700	1.36219100
H	-5.26989100	-2.69386700	1.17845600
H	-1.57095000	-2.79124900	-1.67673100
H	-2.38415400	-0.92135600	-2.44743800
H	-4.30839900	1.80927000	3.54495900
H	-3.46766500	3.32830200	3.20525200
H	-5.22382400	3.21920300	2.98279200
H	-3.77862200	3.23538400	-0.52351600
H	-2.96560100	4.01689500	0.83687000
H	-4.70562600	4.19966100	0.63973100
H	0.08876700	-5.46100200	0.73479900
H	-6.81574000	-4.25523600	0.15748700
H	-8.03278700	-3.01185300	-0.11224300
H	-6.54488400	-2.16154000	3.23935800
H	-7.07390700	-3.71889000	2.58740000
H	-8.06863900	-2.27119200	2.34435200
H	-1.98794400	-3.88031400	1.14666200
H	-3.23161300	-3.79079200	-0.08264100
H	-2.19771800	-6.06976500	-0.00357200
H	-1.92754300	-5.30346400	-1.56586200
H	-6.52221400	-2.97627800	-1.03070900
H	0.17245500	-6.36729200	-0.77475200
H	1.68844300	-4.35999500	-0.79389900
H	0.45326900	-4.25332900	-2.05495800
H	0.38622800	-2.83682000	0.66269200
H	0.62276400	-2.05948900	-0.88023400
H	-4.19579700	1.07818200	-1.08943300
H	-2.59575700	1.38867800	-1.77089000
H	-4.44944200	2.01627100	-3.34572800
H	-3.39970300	0.76482600	-4.01299200
H	-6.11600600	0.29561300	-2.66606900
H	-5.80601600	0.18538400	-4.40052100

H	-5.82348800	-2.08075400	-3.32648200
H	-4.24006800	-1.71398400	-4.00968300
H	-5.03908700	-1.46132300	-1.07375200
H	-3.98246400	-2.69326200	-1.75574200
C	-8.63967300	1.76065400	-0.71867000
H	-9.31482200	0.94485000	-1.00846400
C	-8.26886000	2.53500400	-1.99417100
H	-9.16565100	2.94395600	-2.47215200
H	-7.60117300	3.37315700	-1.76825300
H	-7.75846400	1.88970700	-2.71435400
C	-9.39497800	2.66259300	0.27266500
H	-10.29987800	3.07583700	-0.18618800
H	-9.68623500	2.10524400	1.16821400
H	-8.76767400	3.50182600	0.59210400
C	2.10194300	3.77081100	-2.74299900
C	1.25992700	2.69350700	-2.46138600
C	1.17516700	2.17359900	-1.15675800
C	1.92869600	2.79081600	-0.13590300
C	2.82542100	3.84625700	-0.42120500
C	2.89434300	4.32923000	-1.73537500
H	2.15665600	4.16752500	-3.75412100
H	0.67586700	2.23906200	-3.25427900
H	4.08438200	2.34962900	-1.55538200
H	3.57540300	5.14536500	-1.96586000
C	3.74301600	4.40669400	0.64074000
H	4.32409100	5.24655000	0.24732100
H	3.19833600	4.75850600	1.52165000
H	4.44341500	3.63000300	0.96876800
Cl	-0.24896900	-0.17654300	-3.12072200
C	1.70116600	2.28670200	1.25405700
C	-0.32640800	1.38719400	2.27305800
C	0.90925200	3.27425300	2.16793300
C	0.77714900	1.01159700	1.26295700
C	-0.55023600	2.86587400	1.91421400
H	-1.25095700	3.37286100	2.58615400
H	-0.86480400	3.00522800	0.87788500
C	0.26799400	1.50723900	3.70112100
H	-0.54058100	1.59269300	4.43518200
H	0.85594100	0.62758800	3.96840500
C	1.10705300	2.82170700	3.63010100
H	0.72440400	3.57689900	4.32538400
H	2.16551300	2.66522900	3.86814200
H	-1.19801300	0.74322700	2.23494600
H	1.15109900	4.32298400	1.98361600

C	1.48678000	-0.26518600	1.55773400
O	0.99419300	-1.17773900	2.23643000
H	2.66509200	2.08460200	1.74411400
N	2.77737300	-0.43640700	1.04479300
H	3.26334400	0.40184500	0.73956200
C	3.61561700	-1.45465100	1.65169700
C	4.48138900	-2.26833800	0.67447600
C	4.64516700	-0.90630900	2.65674300
H	2.92770100	-2.12570200	2.17049200
C	5.54016900	-2.94597500	1.57324500
H	3.88634700	-2.99943400	0.11554900
C	5.60591900	-2.08898300	2.88034700
H	4.17417100	-0.55394600	3.57815600
H	5.13957300	-0.04678600	2.18933600
H	5.24965500	-3.97197900	1.81548700
H	6.51234600	-3.02515700	1.06971700
H	5.26777900	-2.68787000	3.73072400
H	6.62705800	-1.77343500	3.13370200
H	-3.68220600	-1.41144400	5.26971100
H	4.96142700	-1.59376000	-0.04316200
C	5.29949200	0.94749100	-1.04494600
O	5.34503100	1.42380800	0.12350200
O	5.88029600	-0.09154800	-1.46935500
O	4.51717700	1.58159500	-1.97566100
Cs	7.88785900	-0.02077000	0.72259000
Cs	2.96466000	-1.03140500	-2.56801200

15'

C	3.37457600	-1.32481900	3.18507100
C	2.52462300	-1.59617500	4.25053500
C	1.16450900	-1.32241200	4.11883800
C	0.69075400	-0.77015800	2.93576600
C	1.54895600	-0.45226200	1.85842800
C	2.92304200	-0.75321800	1.97864100
C	3.99016300	-0.55093300	0.94472500
C	4.89281700	0.52632000	1.07792800
C	5.95798600	0.63797700	0.17563700
C	6.16923000	-0.29467000	-0.83695700
C	5.28150300	-1.37093600	-0.93321400
C	4.20228800	-1.52717200	-0.06019800
C	3.31731300	-2.76846700	-0.15882400
C	4.77628600	1.54111100	2.21070300
P	0.55127700	0.34752900	0.51990800
C	0.08929100	1.99415600	1.32954300

C	1.38775500	0.96498700	-1.03010000
Pd	-1.43619300	-0.43191300	-0.31562700
C	3.77181100	-3.84289300	0.84872000
C	3.26361200	-3.39027800	-1.56248100
C	4.89918900	2.99936800	1.73820800
C	5.82545700	1.25509000	3.30115200
C	1.13551500	2.55499600	2.30316500
C	0.74606200	3.96014900	2.78253500
C	-0.64474700	3.96357800	3.42857300
C	-1.69382800	3.38175600	2.47441900
C	-1.30523200	1.98501900	1.97448700
C	1.77739600	-0.16104300	-1.99307900
C	2.09128300	0.39783900	-3.38517600
C	3.18828600	1.46701200	-3.31048500
C	2.80133700	2.58825700	-2.33953800
C	2.48406500	2.03229800	-0.94268300
H	4.42942300	-1.56639400	3.26437400
H	0.46223200	-1.56269400	4.91027700
H	-0.38353300	-0.65302200	2.82795600
H	6.65259600	1.46765000	0.27357000
H	5.44269700	-2.11445300	-1.70537000
H	2.29914500	-2.47529200	0.11319700
H	3.79020100	1.42043500	2.66522400
H	0.03609500	2.66322200	0.45963400
H	0.49386700	1.43812000	-1.46228000
H	3.72790100	-3.47996300	1.87643300
H	3.12825100	-4.72547300	0.77453000
H	4.80119200	-4.15208500	0.63614000
H	3.02123400	-2.65728800	-2.33599100
H	2.49803900	-4.16964700	-1.58737400
H	4.21473300	-3.86284200	-1.82980900
H	-0.61659000	3.35105400	4.33961900
H	4.69766400	3.68040700	2.57176100
H	5.90637800	3.22287800	1.37212000
H	5.70597300	0.25176000	3.71658900
H	5.73514000	1.97525200	4.12155000
H	6.83874400	1.33111100	2.89242600
H	1.21035100	1.88815400	3.16896000
H	2.12474200	2.57542600	1.84220500
H	1.49769200	4.33693100	3.48589700
H	0.75126100	4.65068600	1.92421500
H	4.19525800	3.22722400	0.93456800
H	-0.92304900	4.97762000	3.73927900
H	-2.67943400	3.34468000	2.95095800

H	-1.79579700	4.06080300	1.61049100
H	-1.32424400	1.28388100	2.81555700
H	-2.03539300	1.61965000	1.25240400
H	2.66151700	-0.66756700	-1.60852300
H	0.96695700	-0.89210000	-2.04851100
H	2.39828700	-0.41541700	-4.05325100
H	1.17714300	0.83166500	-3.81431300
H	4.11340300	0.99911500	-2.95105400
H	3.40060200	1.87654400	-4.30515100
H	3.60501600	3.33129900	-2.27001900
H	1.91609800	3.11407700	-2.73168800
H	3.39052400	1.59874200	-0.51780100
H	2.17701300	2.85209200	-0.28536400
C	7.36213600	-0.17455800	-1.77055300
H	7.88197400	0.75762600	-1.51366400
C	6.94161000	-0.08248300	-3.24589400
H	7.81927900	0.02658700	-3.89182000
H	6.40625400	-0.98390500	-3.56224700
H	6.28348900	0.77390900	-3.41771100
C	8.34959000	-1.33420500	-1.55202000
H	9.23907600	-1.21119700	-2.17900100
H	8.66902400	-1.38670000	-0.50696000
H	7.88892700	-2.29405500	-1.80860000
C	-3.12893000	-1.66909000	-4.49753100
C	-1.83850000	-1.69233200	-3.97440500
C	-1.62312000	-2.22797400	-2.70707100
C	-2.67067700	-2.73532900	-1.92483100
C	-3.97029700	-2.74169700	-2.47260300
C	-4.17441300	-2.20341100	-3.74877100
H	-3.32151400	-1.24795700	-5.48019200
H	-1.00160000	-1.29340600	-4.54140500
H	-0.61581700	-2.24087600	-2.31391900
H	-5.18203000	-2.19592900	-4.15644600
C	-5.15659100	-3.31031000	-1.72722700
H	-6.06875600	-3.19544200	-2.31870200
H	-5.03099900	-4.37893800	-1.51628000
H	-5.31935100	-2.81429500	-0.76580500
C	-2.40987200	-3.28161900	-0.52895300
C	-0.58376800	-3.15837600	1.08417900
C	-1.43001000	-4.49428000	-0.52462900
C	-1.76537100	-2.32244100	0.55589400
C	-0.07298800	-3.84916900	-0.18680800
H	0.70515600	-4.59321400	0.01836100
H	0.29930900	-3.15313500	-0.93800400

C	-1.12887300	-4.37734800	1.87902300
H	-0.30902600	-4.86174400	2.42122900
H	-1.87371600	-4.07564900	2.61535700
C	-1.69201000	-5.30854000	0.76131100
H	-1.15662800	-6.26390500	0.72935200
H	-2.75542500	-5.53430700	0.89100900
H	0.14980000	-2.59482500	1.64778700
H	-1.47898200	-5.07949400	-1.44628200
C	-2.68405300	-1.82034100	1.63819300
O	-2.31040900	-1.65778400	2.81315000
H	-3.36740400	-3.61984600	-0.13117700
N	-3.97654100	-1.54265200	1.25483100
H	-4.07627600	-1.27091700	0.27898400
C	-4.86285300	-0.81872500	2.14789300
C	-4.65736400	0.72140300	2.15305200
C	-6.33991800	-0.98915300	1.76778500
H	-4.68910900	-1.21182700	3.15291800
C	-6.06036000	1.34095300	2.39607700
H	-3.92246500	1.01094800	2.90792400
C	-7.02835400	0.14024400	2.54230500
H	-6.72341400	-1.98695400	2.00127500
H	-6.45335600	-0.82872800	0.68711100
H	-6.08820300	1.99240100	3.27561400
H	-6.35262000	1.95346900	1.53652200
H	-7.11648900	-0.14456200	3.59826400
H	-8.03735900	0.36128900	2.18129700
H	2.91855700	-2.03765600	5.16103300
H	-4.26724100	1.01524700	1.17524500
C	-3.06378600	1.18880400	-1.47007300
O	-3.82521400	2.06295800	-1.92695700
O	-1.75301900	1.43248500	-1.30379100
O	-3.42847800	0.00321400	-1.07043900
Cs	-1.96816500	4.32384400	-1.61338000

TS3'

C	3.37457600	-1.32481900	3.18507100
C	2.52462300	-1.59617500	4.25053500
C	1.16450900	-1.32241200	4.11883800
C	0.69075400	-0.77015800	2.93576600
C	1.54895600	-0.45226200	1.85842800
C	2.92304200	-0.75321800	1.97864100
C	3.99016300	-0.55093300	0.94472500
C	4.89281700	0.52632000	1.07792800
C	5.95798600	0.63797700	0.17563700

C	6.16923000	-0.29467000	-0.83695700
C	5.28150300	-1.37093600	-0.93321400
C	4.20228800	-1.52717200	-0.06019800
C	3.31731300	-2.76846700	-0.15882400
C	4.77628600	1.54111100	2.21070300
P	0.55127700	0.34752900	0.51990800
C	0.08929100	1.99415600	1.32954300
C	1.38775500	0.96498700	-1.03010000
Pd	-1.43619300	-0.43191300	-0.31562700
C	3.77181100	-3.84289300	0.84872000
C	3.26361200	-3.39027800	-1.56248100
C	4.89918900	2.99936800	1.73820800
C	5.82545700	1.25509000	3.30115200
C	1.13551500	2.55499600	2.30316500
C	0.74606200	3.96014900	2.78253500
C	-0.64474700	3.96357800	3.42857300
C	-1.69382800	3.38175600	2.47441900
C	-1.30523200	1.98501900	1.97448700
C	1.77739600	-0.16104300	-1.99307900
C	2.09128300	0.39783900	-3.38517600
C	3.18828600	1.46701200	-3.31048500
C	2.80133700	2.58825700	-2.33953800
C	2.48406500	2.03229800	-0.94268300
H	4.42942300	-1.56639400	3.26437400
H	0.46223200	-1.56269400	4.91027700
H	-0.38353300	-0.65302200	2.82795600
H	6.65259600	1.46765000	0.27357000
H	5.44269700	-2.11445300	-1.70537000
H	2.29914500	-2.47529200	0.11319700
H	3.79020100	1.42043500	2.66522400
H	0.03609500	2.66322200	0.45963400
H	0.49386700	1.43812000	-1.46228000
H	3.72790100	-3.47996300	1.87643300
H	3.12825100	-4.72547300	0.77453000
H	4.80119200	-4.15208500	0.63614000
H	3.02123400	-2.65728800	-2.33599100
H	2.49803900	-4.16964700	-1.58737400
H	4.21473300	-3.86284200	-1.82980900
H	-0.61659000	3.35105400	4.33961900
H	4.69766400	3.68040700	2.57176100
H	5.90637800	3.22287800	1.37212000
H	5.70597300	0.25176000	3.71658900
H	5.73514000	1.97525200	4.12155000
H	6.83874400	1.33111100	2.89242600

H	1.21035100	1.88815400	3.16896000
H	2.12474200	2.57542600	1.84220500
H	1.49769200	4.33693100	3.48589700
H	0.75126100	4.65068600	1.92421500
H	4.19525800	3.22722400	0.93456800
H	-0.92304900	4.97762000	3.73927900
H	-2.67943400	3.34468000	2.95095800
H	-1.79579700	4.06080300	1.61049100
H	-1.32424400	1.28388100	2.81555700
H	-2.03539300	1.61965000	1.25240400
H	2.66151700	-0.66756700	-1.60852300
H	0.96695700	-0.89210000	-2.04851100
H	2.39828700	-0.41541700	-4.05325100
H	1.17714300	0.83166500	-3.81431300
H	4.11340300	0.99911500	-2.95105400
H	3.40060200	1.87654400	-4.30515100
H	3.60501600	3.33129900	-2.27001900
H	1.91609800	3.11407700	-2.73168800
H	3.39052400	1.59874200	-0.51780100
H	2.17701300	2.85209200	-0.28536400
C	7.36213600	-0.17455800	-1.77055300
H	7.88197400	0.75762600	-1.51366400
C	6.94161000	-0.08248300	-3.24589400
H	7.81927900	0.02658700	-3.89182000
H	6.40625400	-0.98390500	-3.56224700
H	6.28348900	0.77390900	-3.41771100
C	8.34959000	-1.33420500	-1.55202000
H	9.23907600	-1.21119700	-2.17900100
H	8.66902400	-1.38670000	-0.50696000
H	7.88892700	-2.29405500	-1.80860000
C	-3.12893000	-1.66909000	-4.49753100
C	-1.83850000	-1.69233200	-3.97440500
C	-1.62312000	-2.22797400	-2.70707100
C	-2.67067700	-2.73532900	-1.92483100
C	-3.97029700	-2.74169700	-2.47260300
C	-4.17441300	-2.20341100	-3.74877100
H	-3.32151400	-1.24795700	-5.48019200
H	-1.00160000	-1.29340600	-4.54140500
H	-0.61581700	-2.24087600	-2.31391900
H	-5.18203000	-2.19592900	-4.15644600
C	-5.15659100	-3.31031000	-1.72722700
H	-6.06875600	-3.19544200	-2.31870200
H	-5.03099900	-4.37893800	-1.51628000
H	-5.31935100	-2.81429500	-0.76580500

C	-2.40987200	-3.28161900	-0.52895300
C	-0.58376800	-3.15837600	1.08417900
C	-1.43001000	-4.49428000	-0.52462900
C	-1.76537100	-2.32244100	0.55589400
C	-0.07298800	-3.84916900	-0.18680800
H	0.70515600	-4.59321400	0.01836100
H	0.29930900	-3.15313500	-0.93800400
C	-1.12887300	-4.37734800	1.87902300
H	-0.30902600	-4.86174400	2.42122900
H	-1.87371600	-4.07564900	2.61535700
C	-1.69201000	-5.30854000	0.76131100
H	-1.15662800	-6.26390500	0.72935200
H	-2.75542500	-5.53430700	0.89100900
H	0.14980000	-2.59482500	1.64778700
H	-1.47898200	-5.07949400	-1.44628200
C	-2.68405300	-1.82034100	1.63819300
O	-2.31040900	-1.65778400	2.81315000
H	-3.36740400	-3.61984600	-0.13117700
N	-3.97654100	-1.54265200	1.25483100
H	-4.07627600	-1.27091700	0.27898400
C	-4.86285300	-0.81872500	2.14789300
C	-4.65736400	0.72140300	2.15305200
C	-6.33991800	-0.98915300	1.76778500
H	-4.68910900	-1.21182700	3.15291800
C	-6.06036000	1.34095300	2.39607700
H	-3.92246500	1.01094800	2.90792400
C	-7.02835400	0.14024400	2.54230500
H	-6.72341400	-1.98695400	2.00127500
H	-6.45335600	-0.82872800	0.68711100
H	-6.08820300	1.99240100	3.27561400
H	-6.35262000	1.95346900	1.53652200
H	-7.11648900	-0.14456200	3.59826400
H	-8.03735900	0.36128900	2.18129700
H	2.91855700	-2.03765600	5.16103300
H	-4.26724100	1.01524700	1.17524500
C	-3.06378600	1.18880400	-1.47007300
O	-3.82521400	2.06295800	-1.92695700
O	-1.75301900	1.43248500	-1.30379100
O	-3.42847800	0.00321400	-1.07043900
Cs	-1.96816500	4.32384400	-1.61338000
9'			
C	0.35767600	-3.24260300	2.07663600
C	-0.65746800	-4.06894200	2.55038800

C	-1.98735100	-3.73043100	2.30736600
C	-2.27984200	-2.56913500	1.59747900
C	-1.26962600	-1.72214100	1.10965600
C	0.08216600	-2.07008000	1.35210900
C	1.30384100	-1.30329200	0.89849800
C	1.91681300	-0.36561600	1.77295500
C	3.22620100	0.05744600	1.51282000
C	3.95586100	-0.40478800	0.41802000
C	3.32696300	-1.29139200	-0.45878400
C	2.02094600	-1.74446200	-0.24961300
C	1.41355300	-2.74311800	-1.22371900
C	1.19432100	0.13659800	3.01455300
P	-1.60835500	-0.20312000	0.11388400
C	-2.73241900	-0.71115000	-1.29594300
C	-2.70706200	0.94936900	1.12001500
Pd	0.43767100	0.64680100	-0.53354900
C	2.02547600	-4.14215100	-1.03675600
C	1.54612800	-2.27436200	-2.68158100
C	1.38317600	1.64659900	3.22630700
C	1.62722900	-0.65253500	4.26252800
C	-4.16317500	-1.18332100	-0.99430300
C	-4.94946200	-1.40034300	-2.29690400
C	-4.23725200	-2.39757000	-3.21913500
C	-2.79854200	-1.95172400	-3.50770200
C	-2.01094600	-1.70765500	-2.21483700
C	-1.85726400	2.09939900	1.68981100
C	-2.72248300	3.16911600	2.36298100
C	-3.59873300	2.56153000	3.46411900
C	-4.44450000	1.40741100	2.91415200
C	-3.58035000	0.33783500	2.22724900
H	1.39570100	-3.50130600	2.26144200
H	-0.40984900	-4.97005800	3.10337400
H	-2.79260600	-4.36338100	2.66797000
H	-3.31560600	-2.31453200	1.42155900
H	3.69349200	0.76669500	2.18919000
H	3.86633200	-1.64988000	-1.32992600
H	0.34774700	-2.81655600	-0.99642900
H	0.12605900	-0.04649100	2.86354600
H	-2.80554900	0.23911800	-1.84703200
H	-3.37204000	1.37507300	0.35310400
H	1.86558200	-4.51027500	-0.01940800
H	1.57395400	-4.85745900	-1.73265700
H	3.10466400	-4.12342100	-1.22383000
H	1.17697500	-1.25168500	-2.79908800

H	0.97366700	-2.93071600	-3.34552100
H	2.58788400	-2.29658700	-3.01865900
H	1.16582700	2.20193700	2.31040400
H	0.71851100	2.00350700	4.02026500
H	2.40721600	1.88430400	3.53268000
H	1.41436000	-1.71895900	4.14986200
H	1.09881300	-0.29135900	5.15164300
H	2.70262900	-0.53755900	4.43670800
H	-4.12965500	-2.13184500	-0.44601400
H	-4.68868500	-0.46081800	-0.36160100
H	-5.96381400	-1.74720200	-2.06695500
H	-5.05589100	-0.43765300	-2.81616100
H	-4.21936200	-3.38376400	-2.73371700
H	-4.79640600	-2.51814500	-4.15417600
H	-2.28230100	-2.69765600	-4.12322800
H	-2.81616700	-1.02128300	-4.09169100
H	-1.88080100	-2.65694500	-1.67762200
H	-1.01455200	-1.32630600	-2.44784000
H	-1.16138900	1.68600000	2.42724700
H	-1.24154300	2.53727500	0.90043000
H	-2.08320600	3.96023900	2.77213700
H	-3.36490200	3.64370300	1.60716700
H	-2.95225000	2.18279800	4.26836300
H	-4.24406900	3.32562100	3.91291700
H	-5.03290200	0.94667700	3.71648000
H	-5.16582500	1.80454400	2.18581100
H	-2.93023900	-0.14041100	2.97053100
H	-4.22886400	-0.44729500	1.82939400
C	5.39093600	0.03774500	0.19290200
H	5.61607500	0.80441000	0.94587100
C	5.59847000	0.66890500	-1.19394200
H	6.63182300	1.01182200	-1.31137300
H	5.39742700	-0.05351700	-1.99193400
H	4.93631800	1.52570000	-1.34652900
C	6.36562200	-1.13290800	0.41204800
H	7.40455100	-0.80396100	0.30121800
H	6.24443700	-1.56258100	1.41096400
H	6.18562300	-1.92971600	-0.31775500
C	1.62535000	3.95233800	-0.04963500
C	2.37036800	2.88404200	-0.50733700
C	1.86251500	2.02390800	-1.51935800
C	0.54010900	2.26812800	-2.00618400
C	-0.21707200	3.40056600	-1.56326600
C	0.34427100	4.20729700	-0.58852100

H	2.02376900	4.60645400	0.71956600
H	3.36308800	2.69323600	-0.11420900
H	2.52783500	1.35346700	-2.05210900
H	-0.23255100	5.05073900	-0.21871700
C	-1.59663100	3.65701400	-2.09953400
H	-2.05694300	4.50746600	-1.59037500
H	-1.58398300	3.86120600	-3.17522500
H	-2.23508000	2.77791500	-1.95125600
Cl	0.08777900	1.53589600	-3.58512100

TS1'

C	-0.31630600	-2.80273500	2.60441300
C	-1.45579100	-3.35410600	3.18134100
C	-2.71216700	-2.90318700	2.78107300
C	-2.80221200	-1.89799800	1.82366300
C	-1.66142100	-1.31921400	1.23730200
C	-0.38611800	-1.79352600	1.62622700
C	0.95994100	-1.37694200	1.08904500
C	1.74576200	-0.44385500	1.80028700
C	3.11304700	-0.35733600	1.52697100
C	3.73057000	-1.15500600	0.56396100
C	2.92491600	-2.01913000	-0.17960800
C	1.55369900	-2.14328900	0.06024700
C	0.74649200	-3.14008400	-0.75658600
C	1.14454500	0.45203100	2.87134600
P	-1.80343700	0.01847900	-0.01905600
C	-3.00430000	-0.57134900	-1.33697700
C	-2.70774000	1.46046700	0.78770900
Pd	0.18599400	0.79782000	-1.01077000
C	1.04101400	-4.58513400	-0.31929900
C	0.97613100	-2.95804200	-2.26558000
C	1.52781800	1.92505500	2.64828400
C	1.53586400	-0.01873600	4.28190500
C	-4.50376700	-0.68922400	-1.02088100
C	-5.30144200	-1.04384800	-2.28578000
C	-4.78559400	-2.33597500	-2.93001600
C	-3.28648100	-2.23549500	-3.23482000
C	-2.47841000	-1.86164200	-1.98580900
C	-1.69483900	2.47537900	1.34796500
C	-2.37708900	3.76578700	1.81499700
C	-3.46358300	3.47386200	2.85650400
C	-4.46865200	2.44712900	2.32367500
C	-3.77410900	1.15869200	1.85426500
H	0.66521700	-3.15927800	2.90059500

H	-1.36154200	-4.13376000	3.93125500
H	-3.61515900	-3.32579400	3.21107200
H	-3.78198500	-1.54995200	1.52955000
H	3.71983800	0.34998700	2.08462700
H	3.37396700	-2.63294600	-0.95314000
H	-0.31049400	-2.94939500	-0.55957300
H	0.05602500	0.37265800	2.79319800
H	-2.88701600	0.23432600	-2.07714900
H	-3.20414100	1.92899500	-0.07624100
H	0.80845500	-4.73139100	0.73958300
H	0.44298800	-5.29498800	-0.90111000
H	2.09796600	-4.83080300	-0.46984400
H	0.82785700	-1.91621100	-2.56482300
H	0.28256900	-3.58671500	-2.83422400
H	1.99125600	-3.24731800	-2.55700700
H	1.31674800	2.23641000	1.62195900
H	0.97055900	2.57420300	3.33242200
H	2.59314600	2.09380500	2.83199200
H	1.19618200	-1.04293700	4.46218100
H	1.09025700	0.62827700	5.04544500
H	2.62323300	0.00420800	4.41188500
H	-4.66889400	-1.47548100	-0.27506700
H	-4.88539300	0.24523900	-0.59944700
H	-6.36575400	-1.13508500	-2.03907100
H	-5.21497700	-0.21905900	-3.00666300
H	-4.95985100	-3.17519100	-2.24156200
H	-5.34871800	-2.55771600	-3.84382800
H	-2.91437400	-3.18032800	-3.64766000
H	-3.12248800	-1.47025500	-4.00557300
H	-2.53572700	-2.67825100	-1.25340500
H	-1.42579000	-1.73582300	-2.24873700
H	-1.17345200	2.01896700	2.19632900
H	-0.92882400	2.69369800	0.59749700
H	-1.62783800	4.45418700	2.22291500
H	-2.82794200	4.26922200	0.94810700
H	-2.99162000	3.07611300	3.76576300
H	-3.97800600	4.39714100	3.14685100
H	-5.21339000	2.20590400	3.09115700
H	-5.01921600	2.88449100	1.47887400
H	-3.29254400	0.67213700	2.71091900
H	-4.52736400	0.46128900	1.48100100
C	5.24013700	-1.11548800	0.38975300
H	5.59161400	-0.17708400	0.83876500
C	5.69852200	-1.13513900	-1.07580300

H	6.78849500	-1.04982100	-1.13301700
H	5.41988000	-2.07141200	-1.56986700
H	5.26508800	-0.31247800	-1.65081400
C	5.88517600	-2.27459700	1.17298700
H	6.97795400	-2.23345300	1.10752200
H	5.60042100	-2.24124800	2.22884500
H	5.55619000	-3.23824900	0.76883100
C	3.57748400	3.54202800	-0.41315300
C	3.85987400	2.20738200	-0.70313600
C	2.91509000	1.42558300	-1.36841000
C	1.67650900	1.98955300	-1.67780800
C	1.37891300	3.35376400	-1.47008100
C	2.35585100	4.09994400	-0.80050200
H	4.31156400	4.15680100	0.09836100
H	4.81139600	1.77039500	-0.41750300
H	3.10557600	0.38765200	-1.60811000
H	2.15177100	5.14730000	-0.59149400
C	0.11239300	4.00231900	-1.97166200
H	0.01519500	5.01473400	-1.57030400
H	0.13010700	4.06078500	-3.06550400
H	-0.77866800	3.43207900	-1.70091500
Cl	0.73865500	1.12453800	-3.43662600

13'

C	-2.25556700	2.35453200	1.85172500
C	-1.38010200	2.99011400	2.72397800
C	-0.07767700	2.50904700	2.84040100
C	0.30490100	1.39460400	2.10479900
C	-0.59865600	0.67297700	1.29401300
C	-1.90429200	1.19578600	1.13385300
C	-2.95285700	0.69256500	0.18717800
C	-4.03457000	-0.09158100	0.64395200
C	-5.01373800	-0.48933300	-0.27377900
C	-4.97745800	-0.10285800	-1.61414700
C	-3.94063900	0.73802800	-2.02542600
C	-2.93356000	1.15305500	-1.15051800
C	-1.91337800	2.18545900	-1.62088900
C	-4.21335900	-0.42298100	2.12220500
P	0.22704500	-0.90926800	0.75459700
C	0.32377700	-1.83700600	2.38419800
C	-0.67125700	-2.10019700	-0.36567100
Pd	2.42386900	-0.74344700	-0.40641800
C	-2.53789900	3.59148000	-1.54135500
C	-1.36250300	1.93346700	-3.03253900

C	-4.66725300	-1.86536200	2.39766400
C	-5.21579700	0.55929500	2.75966400
C	-0.93723300	-1.72470000	3.25647700
C	-0.85389900	-2.68094300	4.45488600
C	0.40709300	-2.42564600	5.28970100
C	1.66904800	-2.46918200	4.41884300
C	1.56676600	-1.50348100	3.22960300
C	-0.87034800	-1.52138400	-1.77354800
C	-1.37245000	-2.58191600	-2.75995800
C	-2.64970000	-3.25287900	-2.24365500
C	-2.41674100	-3.86525300	-0.85955300
C	-1.93054000	-2.80911600	0.14326600
H	-3.25288600	2.75542000	1.70648400
H	0.63995200	3.00262800	3.48755600
H	1.33435700	1.05798800	2.16661000
H	-5.83957600	-1.10734400	0.06649000
H	-3.92156100	1.09158100	-3.05080900
H	-1.07020900	2.17819300	-0.92707100
H	-3.25000800	-0.27424900	2.61534100
H	0.44075100	-2.87277000	2.04420900
H	0.13114300	-2.85090800	-0.43114000
H	-2.83635900	3.83410400	-0.51813600
H	-1.82192600	4.34910900	-1.87603800
H	-3.42643400	3.65614800	-2.17848100
H	-0.96169800	0.92300000	-3.14150000
H	-0.55606300	2.64270000	-3.24395800
H	-2.12970200	2.07386800	-3.80074700
H	0.32908300	-1.43441500	5.75853200
H	-4.67450300	-2.05123500	3.47636800
H	-5.68317700	-2.04578100	2.03189300
H	-4.88790100	1.59590800	2.65383200
H	-5.33412100	0.34826200	3.82782200
H	-6.19809100	0.46803600	2.28395200
H	-1.02735400	-0.69402800	3.61995300
H	-1.83822700	-1.93197900	2.67909000
H	-1.75270600	-2.57714000	5.07459900
H	-0.84384900	-3.71613500	4.08655900
H	-4.00919300	-2.60200800	1.93311400
H	0.47794200	-3.15417900	6.10566200
H	2.55381400	-2.22544000	5.01799100
H	1.82064000	-3.48669400	4.03525300
H	1.48427700	-0.48021400	3.61554600
H	2.46584800	-1.56527400	2.61410000
H	-1.59978200	-0.71192000	-1.72770900

H	0.07340300	-1.09817900	-2.13071000
H	-1.55130600	-2.11705300	-3.73683200
H	-0.59332000	-3.34228400	-2.90689200
H	-3.44389800	-2.49929800	-2.16779400
H	-2.99460400	-4.01741700	-2.94950300
H	-3.33739900	-4.32686900	-0.48344600
H	-1.66893000	-4.66648800	-0.93570000
H	-2.72118900	-2.07363800	0.29509700
H	-1.73143200	-3.28997800	1.10431200
C	-6.09196600	-0.50939100	-2.56420100
H	-6.64415800	-1.32655600	-2.08252700
C	-5.57298100	-1.02727300	-3.91393800
H	-6.40692700	-1.35817700	-4.54126300
H	-5.03970300	-0.24514900	-4.46442300
H	-4.88915400	-1.87020100	-3.78271800
C	-7.07059200	0.66206000	-2.76640100
H	-7.90803700	0.36625100	-3.40719300
H	-7.47355400	1.00767500	-1.80967800
H	-6.56412600	1.50963300	-3.24092100
C	7.13242100	-0.95386700	-1.38503900
C	6.60622200	-0.12619600	-0.39606300
C	5.22117600	-0.06979600	-0.20676900
C	4.38231000	-0.85171600	-0.99375700
C	4.88454300	-1.68328700	-2.00273000
C	6.27522800	-1.71676300	-2.17876700
H	8.20579400	-1.00451900	-1.54353200
H	7.26067400	0.48004500	0.22405300
H	4.80835700	0.59862000	0.54165500
H	6.68759300	-2.36050400	-2.95242300
C	3.98639900	-2.51694200	-2.88083800
H	4.57116500	-3.18801500	-3.51623800
H	3.30563300	-3.11493300	-2.27003400
H	3.37586400	-1.88872500	-3.54107300
Cl	2.77420700	-2.98422100	0.37325700
C	2.44169500	0.48556500	-2.26680700
C	1.76298200	1.21746300	-1.30766600
C	2.40716600	2.42565300	-0.71945100
O	3.60690000	2.61221700	-0.65775300
H	3.45386000	0.75996700	-2.53198000
C	1.81211500	4.66760600	0.08378300
H	-1.70222000	3.86452600	3.28094800
H	1.90787200	-0.16325000	-2.95157900
H	0.68523500	1.18351900	-1.24915200
O	1.45549100	3.29968200	-0.33984500

C	2.52919900	5.38396000	-1.06247100
H	3.50154300	4.93459900	-1.26336400
H	1.92161200	5.34345300	-1.97178200
H	2.67445500	6.43554400	-0.79705900
C	2.66044100	4.62073400	1.35541600
H	2.81393300	5.63933100	1.72523700
H	2.14453000	4.05004600	2.13044300
H	3.63046200	4.16410800	1.16212100
C	0.44971300	5.30291500	0.35174100
H	-0.09635500	4.73665500	1.10841500
H	0.58110000	6.33066100	0.70245000
H	-0.15015900	5.32257500	-0.56176200

TS2'

C	-2.37662200	2.37444400	1.82481400
C	-1.58690700	3.02892200	2.76189300
C	-0.27855900	2.59317100	2.96153700
C	0.19773400	1.51018300	2.23407000
C	-0.62273600	0.76650700	1.35866100
C	-1.93656300	1.23531400	1.12432000
C	-2.91726700	0.68235300	0.13478600
C	-4.00218400	-0.11542400	0.56053200
C	-4.93072700	-0.55412100	-0.39049200
C	-4.84084500	-0.19820900	-1.73640700
C	-3.79975500	0.65003100	-2.12164700
C	-2.84208400	1.10643400	-1.21271100
C	-1.81825100	2.14510900	-1.65968200
C	-4.23552600	-0.43216300	2.03501400
P	0.28099500	-0.78146900	0.85741900
C	0.38256800	-1.69835000	2.49086000
C	-0.54261400	-2.02238500	-0.26773900
Pd	2.36169600	-0.56633300	-0.31116200
C	-2.45674600	3.54576300	-1.59930900
C	-1.23132700	1.89599500	-3.05718900
C	-4.64361100	-1.88832400	2.31120500
C	-5.30554000	0.51517800	2.61263700
C	-0.88086100	-1.58891100	3.36043900
C	-0.79288400	-2.54535100	4.55842900
C	0.46777100	-2.28391500	5.39228900
C	1.73055800	-2.32582700	4.52229200
C	1.62800300	-1.36279900	3.33097200
C	-0.67901400	-1.51588000	-1.71107400
C	-1.06798800	-2.65183000	-2.66449900
C	-2.34750500	-3.35187200	-2.19328400

C	-2.18363100	-3.87635200	-0.76341300
C	-1.80677200	-2.74549200	0.20536700
H	-3.37752500	2.73780100	1.61876700
H	0.37152200	3.09853700	3.66785800
H	1.23429200	1.21465800	2.35500800
H	-5.75834500	-1.18149200	-0.07247000
H	-3.73896000	0.97663400	-3.15425200
H	-0.99244900	2.14463900	-0.94491900
H	-3.30161300	-0.23905300	2.56844400
H	0.50272000	-2.73448400	2.15388700
H	0.27732500	-2.75526400	-0.26352000
H	-2.78338900	3.78778000	-0.58471800
H	-1.73909800	4.30887400	-1.91700000
H	-3.32919000	3.60033600	-2.25935000
H	-0.82091300	0.88802100	-3.15558600
H	-0.42596200	2.61188300	-3.24985900
H	-1.97987400	2.03091900	-3.84455300
H	0.38636700	-1.29189900	5.85892800
H	-4.70152500	-2.05734700	3.39119000
H	-5.62988300	-2.11676300	1.89470800
H	-5.01833100	1.56360400	2.50573600
H	-5.46274000	0.31336300	3.67754300
H	-6.26094900	0.37541300	2.09562200
H	-0.97702700	-0.55917500	3.72417600
H	-1.78076500	-1.79967900	2.78064300
H	-1.69146600	-2.44570200	5.17906700
H	-0.77802100	-3.58047000	4.19011200
H	-3.93121500	-2.60280800	1.89549400
H	0.54048600	-3.01035700	6.20999600
H	2.61435700	-2.07976600	5.12194000
H	1.88412300	-3.34367200	4.14030300
H	1.55106700	-0.33793300	3.71388300
H	2.52295200	-1.42939100	2.70984700
H	-1.44603100	-0.74154300	-1.75399700
H	0.26757800	-1.06817100	-2.03244800
H	-1.19961300	-2.25235800	-3.67717400
H	-0.24771000	-3.38069600	-2.71354900
H	-3.17557000	-2.63163400	-2.21185200
H	-2.61321500	-4.16849800	-2.87462200
H	-3.10867200	-4.35567200	-0.42165000
H	-1.40068800	-4.64653700	-0.74401200
H	-2.63266600	-2.03678600	0.26138700
H	-1.65489300	-3.16317200	1.20390200
C	-5.90164800	-0.64772900	-2.72766400

H	-6.48337400	-1.44074000	-2.24050600
C	-5.30639000	-1.22951800	-4.01865200
H	-6.10364600	-1.57883400	-4.68278000
H	-4.72857900	-0.47792000	-4.56660000
H	-4.64321200	-2.07255000	-3.80742600
C	-6.86320700	0.51304700	-3.04185600
H	-7.66353200	0.18634300	-3.71422900
H	-7.31893200	0.90503600	-2.12763800
H	-6.32843000	1.33652100	-3.52762800
C	6.77006200	-1.60513800	-1.92045900
C	6.56326700	-0.58557400	-0.99129400
C	5.26553100	-0.13983500	-0.73561000
C	4.18538600	-0.74560900	-1.37891300
C	4.36809300	-1.76389800	-2.32759100
C	5.68258000	-2.17575100	-2.58287600
H	7.77621900	-1.95169400	-2.13750400
H	7.40431100	-0.12732000	-0.47880100
H	5.08936400	0.69193700	-0.06088300
H	5.84966000	-2.97030600	-3.30605200
C	3.21287400	-2.44509900	-3.01586900
H	3.56868800	-3.17420000	-3.74881200
H	2.59785300	-2.96598500	-2.27621000
H	2.56431800	-1.73582700	-3.54351800
Cl	2.80062100	-2.83310700	0.44468800
C	2.82003900	0.81026900	-2.11014500
C	1.90607000	1.34801500	-1.17154400
C	2.39630800	2.52139700	-0.40077100
O	3.56686200	2.70330800	-0.10972800
H	3.76044600	1.32361100	-2.24325200
C	1.67763400	4.75372000	0.31968500
H	-1.97912800	3.88107400	3.30825500
H	2.43885300	0.28026500	-2.97366300
H	0.84464000	1.31438300	-1.37341100
O	1.39263900	3.38365700	-0.15103200
C	2.50737600	5.47684000	-0.74352500
H	3.49922700	5.03332600	-0.83619600
H	2.00173800	5.43192000	-1.71295000
H	2.61925700	6.52923000	-0.46541600
C	2.38249900	4.73538400	1.67710500
H	2.44759400	5.75878600	2.06015000
H	1.81056500	4.14057300	2.39036900
H	3.38565300	4.32065900	1.59423000
C	0.28412100	5.36738000	0.43243600
H	-0.33570000	4.78782800	1.11927300

H	0.35874000	6.39424700	0.80202900
H	-0.20781300	5.38483000	-0.54328300
14'			
C	-2.32998500	2.34457200	1.87586500
C	-1.56517400	3.01461000	2.82265600
C	-0.24427400	2.62016700	3.02599100
C	0.26804200	1.55434000	2.29805500
C	-0.52702800	0.79458500	1.41377300
C	-1.85172200	1.22555600	1.16868700
C	-2.80310500	0.65190900	0.16253500
C	-3.88090800	-0.16722100	0.56691500
C	-4.77503000	-0.63291500	-0.40398800
C	-4.66222400	-0.28049000	-1.74902300
C	-3.63449200	0.59267800	-2.11284600
C	-2.70850300	1.07513300	-1.18441300
C	-1.70475300	2.13999100	-1.61428600
C	-4.15047400	-0.47646200	2.03688400
P	0.39056900	-0.75195900	0.95128700
C	0.46556800	-1.64906600	2.59363400
C	-0.37233700	-2.01527400	-0.19109500
Pd	2.43683500	-0.50159200	-0.03007100
C	-2.39084800	3.51908600	-1.58104400
C	-1.07826100	1.89750100	-2.99557200
C	-4.52388600	-1.94125000	2.31703800
C	-5.26664600	0.44398200	2.56906300
C	-0.83746000	-1.56010200	3.40678400
C	-0.78434100	-2.51938400	4.60409400
C	0.43107500	-2.23348300	5.49514800
C	1.73249100	-2.24131600	4.68249900
C	1.66239200	-1.27967200	3.48770400
C	-0.50597900	-1.50993700	-1.63363700
C	-0.84629700	-2.65709300	-2.59222400
C	-2.11347300	-3.39126600	-2.14030600
C	-1.95779000	-3.90913700	-0.70729300
C	-1.62458600	-2.76915300	0.26743800
H	-3.33913500	2.68101400	1.66525200
H	0.38899600	3.14744300	3.73164700
H	1.31135300	1.28728700	2.42332900
H	-5.59547700	-1.27754100	-0.10228500
H	-3.55859200	0.91929600	-3.14441300
H	-0.89363800	2.17098300	-0.88419200
H	-3.24095100	-0.24895600	2.59775800
H	0.62752400	-2.68328200	2.26780300

H	0.46849300	-2.72413800	-0.17226100
H	-2.74565600	3.76025000	-0.57543300
H	-1.69308500	4.30262400	-1.89291500
H	-3.25155900	3.53890200	-2.25836600
H	-0.64696600	0.89706000	-3.07843700
H	-0.27944200	2.62574500	-3.16706100
H	-1.80768300	2.01731900	-3.80333400
H	0.30523400	-1.24629800	5.96196100
H	-4.61408400	-2.10005100	3.39638100
H	-5.48765700	-2.20412900	1.86945300
H	-5.01100600	1.49951400	2.45208000
H	-5.44721900	0.25393000	3.63240700
H	-6.20207000	0.26518900	2.02824200
H	-0.96321800	-0.53313300	3.76868500
H	-1.70866300	-1.78255700	2.78997400
H	-1.71259300	-2.44063100	5.18250500
H	-0.73046300	-3.55227000	4.23338700
H	-3.77694900	-2.63903800	1.93481700
H	0.48412300	-2.96268000	6.31183100
H	2.58148800	-1.97377600	5.32181500
H	1.92938600	-3.25387000	4.30656300
H	1.54234600	-0.25624800	3.86297100
H	2.58575400	-1.32836500	2.90836100
H	-1.29774300	-0.76212200	-1.68600700
H	0.42777800	-1.02578000	-1.93399300
H	-0.97317500	-2.26150900	-3.60713400
H	-0.00588200	-3.36348500	-2.62772900
H	-2.96076600	-2.69458400	-2.17391900
H	-2.34531800	-4.21638800	-2.82364400
H	-2.87535900	-4.41096000	-0.37823000
H	-1.15592000	-4.65898200	-0.67439200
H	-2.46879100	-2.08124000	0.31178600
H	-1.47600900	-3.18565000	1.26677900
C	-5.69015000	-0.75815700	-2.76149100
H	-6.25680800	-1.56999900	-2.28770200
C	-5.05506600	-1.31685300	-4.04367100
H	-5.82998600	-1.68933000	-4.72143000
H	-4.49288000	-0.54583900	-4.58067500
H	-4.36899700	-2.13907300	-3.82359800
C	-6.68012800	0.37481900	-3.08881400
H	-7.45728700	0.02783500	-3.77805200
H	-7.16475300	0.74803600	-2.18164200
H	-6.16109300	1.21658300	-3.56005800
C	5.72840200	-2.18638600	-1.54516000

C	5.74952300	-0.99713200	-0.83202500
C	4.80254900	-0.00457700	-1.11256600
C	3.82283200	-0.19794400	-2.11443000
C	3.80722900	-1.41703600	-2.84016400
C	4.76675500	-2.38286200	-2.54091400
H	6.44681900	-2.97032700	-1.32852600
H	6.48623700	-0.83134900	-0.05281900
H	4.83847200	0.95565300	-0.60681700
H	4.75464700	-3.31953600	-3.09119600
C	2.79111600	-1.68387000	-3.92383800
H	2.95142300	-2.67061400	-4.36485500
H	1.76835300	-1.66027800	-3.53531800
H	2.84905600	-0.94474700	-4.73096000
Cl	3.01677500	-2.75265900	0.69633700
C	2.81863900	0.92503100	-2.37848700
C	2.00909600	1.24291900	-1.09890400
C	2.48721500	2.48483000	-0.43521200
O	3.66286600	2.78018600	-0.26713600
H	3.35144800	1.81407900	-2.73646300
C	1.72047100	4.68792100	0.32978700
H	-1.98563300	3.85201100	3.37078300
H	2.12440800	0.62591200	-3.16424800
H	0.94315100	1.30589900	-1.28826600
O	1.45984800	3.30634200	-0.10770400
C	2.47029100	5.44189100	-0.77242100
H	3.48108000	5.05583300	-0.89903900
H	1.93157300	5.35154500	-1.72100600
H	2.52583800	6.50378600	-0.51300000
C	2.48583100	4.70276800	1.65486800
H	2.55398400	5.73154500	2.02314100
H	1.95693800	4.10781000	2.40188700
H	3.49058200	4.30210500	1.52945900
C	0.31593100	5.26316900	0.50123200
H	-0.25966600	4.67004600	1.21293500
H	0.37691600	6.29324000	0.86497500
H	-0.21585500	5.26403000	-0.45332100
TS2_1			
C	-1.88871400	2.93981000	-1.58550600
C	-0.82961800	3.83263400	-1.66491700
C	0.31176500	3.58208200	-0.90680700
C	0.37186800	2.43360300	-0.12843400
C	-0.69041600	1.50929900	-0.03031800
C	-1.86805100	1.78988300	-0.76740300

C	-3.18767000	1.07114700	-0.74503000
C	-4.19628800	1.55050000	0.12094100
C	-5.47450900	0.98605700	0.04967400
C	-5.79147200	-0.01550300	-0.86567600
C	-4.78810000	-0.45135300	-1.73583000
C	-3.49513500	0.07693000	-1.70210900
C	-2.45668200	-0.38920200	-2.71954500
C	-3.94569400	2.70964400	1.08200100
P	-0.17765600	0.08823200	1.06668700
C	0.20674100	0.90096000	2.71466900
C	-1.50363700	-1.13672200	1.50911800
Pd	1.69986400	-1.31756500	0.43727800
C	-2.46617400	0.50545000	-3.97355400
C	-2.62609300	-1.85642200	-3.14412200
C	-4.55898400	2.50314000	2.47647700
C	-4.46715100	4.02688200	0.47636600
C	-0.64203700	2.13326300	3.06349500
C	-0.36410800	2.59110600	4.50298000
C	1.12891600	2.86322100	4.72660600
C	1.97966000	1.64362600	4.34955900
C	1.70718500	1.19111100	2.90935700
C	-1.84430200	-2.06378500	0.33752700
C	-2.70188200	-3.24598300	0.80033700
C	-3.96538300	-2.75406500	1.51537900
C	-3.60274400	-1.85859400	2.70515300
C	-2.74766100	-0.65974800	2.26499800
H	-2.79465900	3.13380300	-2.14973600
H	1.15153300	4.26693800	-0.92371900
H	1.28701500	2.23185200	0.41073900
H	-6.25042900	1.34468800	0.71944900
H	-5.02395700	-1.21950400	-2.46384000
H	-1.47448800	-0.28700300	-2.24886800
H	-2.86489900	2.80991200	1.20842400
H	-0.04085200	0.09065800	3.41165900
H	-0.90660000	-1.73737000	2.20607600
H	-2.24200100	1.54565300	-3.73197100
H	-1.71870800	0.15756200	-4.69535500
H	-3.44739200	0.47089500	-4.45897000
H	-2.70038300	-2.52965100	-2.28718200
H	-1.77106500	-2.17157500	-3.74852800
H	-3.51996200	-1.99385700	-3.76100800
H	1.43278000	3.71942900	4.10724000
H	-4.23946200	3.31011600	3.14372800
H	-5.65302800	2.52373000	2.44577300

H	-3.98354400	4.25000300	-0.47720100
H	-4.27802200	4.86416000	1.15671200
H	-5.54696300	3.96810400	0.30204700
H	-0.40062400	2.94940500	2.37190300
H	-1.70684600	1.92226500	2.93529600
H	-0.95591800	3.48626200	4.72887800
H	-0.69798300	1.80879600	5.19844500
H	-4.25320700	1.55413700	2.92113300
H	1.31024700	3.15041700	5.76883900
H	3.04552500	1.86697400	4.47215200
H	1.75228200	0.81246200	5.03025100
H	2.03418100	1.98375800	2.22414200
H	2.28880400	0.29801700	2.67010100
H	-2.39423600	-1.50682300	-0.41826200
H	-0.91910800	-2.42787000	-0.11866500
H	-2.96705300	-3.87214700	-0.06051200
H	-2.11250100	-3.87381100	1.48168300
H	-4.57270500	-2.17665600	0.80664500
H	-4.57541500	-3.60230500	1.84766000
H	-4.51053700	-1.49538800	3.20192900
H	-3.04788400	-2.44833800	3.44717000
H	-3.35002300	-0.01405600	1.62824300
H	-2.45494900	-0.07941100	3.14521200
C	-7.19993300	-0.57945000	-0.94527500
H	-7.78048600	-0.11340900	-0.13884100
C	-7.23201300	-2.10037300	-0.72447600
H	-8.26126600	-2.47236500	-0.75964200
H	-6.66233200	-2.62516500	-1.49876900
H	-6.80266900	-2.36957100	0.24434000
C	-7.86771900	-0.20204300	-2.27915200
H	-8.90283500	-0.55835500	-2.31006800
H	-7.87215800	0.88241000	-2.42452200
H	-7.33402300	-0.64999300	-3.12422900
C	4.62487300	-5.13978900	0.84284100
C	5.11359300	-3.85434200	1.08456300
C	4.34530500	-2.74767900	0.73079100
C	3.07940100	-2.92302400	0.16543800
C	2.55726500	-4.20535800	-0.06107100
C	3.36327400	-5.30358800	0.27558000
H	5.22154700	-6.01108100	1.09701900
H	6.09235700	-3.71196700	1.53402900
H	4.72231000	-1.73959700	0.86969000
H	2.97370300	-6.30515200	0.10792100
C	1.14140100	-4.44592900	-0.51790000

H	1.01392700	-5.46652400	-0.89120000
H	0.46230600	-4.30405700	0.33011700
H	0.82880700	-3.75333800	-1.30070000
Cl	1.30836300	-2.44862900	2.56551900
C	3.02195000	-1.51705800	-1.51941500
C	1.50055500	0.04805900	-2.40892300
C	2.31013400	-2.04152300	-2.74685500
C	2.47426000	-0.21985600	-1.25384600
C	0.93076100	-1.36386300	-2.64975100
H	0.36253500	-1.43407700	-3.58098300
H	0.32126900	-1.72215900	-1.81938900
C	2.36960900	0.21370800	-3.69523800
H	1.73802900	0.52038300	-4.53489900
H	3.15498800	0.96465400	-3.57994200
C	2.94637700	-1.21911700	-3.91410100
H	2.63137700	-1.63579100	-4.87518000
H	4.03915700	-1.24578900	-3.88652400
H	0.77157500	0.84033900	-2.24374100
H	2.34392300	-3.12090100	-2.88885400
C	3.44466700	0.77720900	-0.69645900
O	4.35113500	0.44110400	0.07094700
H	4.08557300	-1.66618800	-1.42614700
N	3.31967200	2.07291400	-1.10832600
H	2.61029700	2.31341400	-1.78365900
C	4.33522600	3.05641300	-0.76927200
C	5.62142700	2.96791900	-1.60823300
C	3.87655100	4.50742700	-0.97703400
H	4.59799400	2.88883600	0.28000600
C	6.33177900	4.28949400	-1.28224500
H	6.20456400	2.07621400	-1.36935300
C	5.18812800	5.32891400	-1.08938300
H	3.22176100	4.85889300	-0.17448300
H	3.30996300	4.57382600	-1.91525700
H	6.89868700	4.18077300	-0.35146900
H	7.04401400	4.58888800	-2.05571200
H	5.35513700	5.93212800	-0.19284500
H	5.13495700	6.02568800	-1.93061400
H	-0.90043400	4.71242900	-2.29693400
H	5.34762700	2.92364800	-2.67091900
TS2_2			
C	2.66041300	-1.33660500	3.02462500
C	1.87409400	-2.10838000	3.86968200
C	0.61033300	-2.50062700	3.43704500

C	0.17410900	-2.09978600	2.18156900
C	0.96122800	-1.33134300	1.29569200
C	2.25102300	-0.94004800	1.73463400
C	3.29968900	-0.16551100	0.98544900
C	3.32457100	1.24751300	1.03327900
C	4.37124500	1.92215400	0.39419000
C	5.40658700	1.25205500	-0.25747500
C	5.39818900	-0.14223400	-0.23310800
C	4.37423900	-0.86472200	0.38511300
C	4.48485500	-2.38472600	0.43359800
C	2.27765100	2.04002400	1.80950100
P	0.03355600	-1.15180300	-0.31523500
C	0.84383500	-0.19687700	-1.69342400
C	0.03600300	-2.92198500	-0.94911400
Pd	-2.29382900	-0.42184800	-0.32408000
C	5.48902500	-2.81743000	1.51823100
C	4.87764400	-3.00810400	-0.91655100
C	2.09413500	3.48014800	1.31001200
C	2.60933100	2.08047500	3.31392100
C	2.16990000	-0.70223500	-2.27887600
C	2.59593800	0.14715300	-3.48653800
C	2.65737800	1.63785400	-3.13770200
C	1.30560300	2.12315900	-2.60477400
C	0.87434000	1.30451700	-1.38335900
C	-1.15674100	-3.76589800	-0.47011800
C	-1.20621100	-5.09481200	-1.23449200
C	0.09968800	-5.88342400	-1.06808200
C	1.31565700	-5.03559700	-1.46231000
C	1.33950200	-3.69597200	-0.71121800
H	3.64450900	-1.02132400	3.35390000
H	-0.03893400	-3.09755400	4.06991700
H	-0.82130000	-2.38724200	1.87129800
H	4.38684400	3.00644900	0.40772200
H	6.21150800	-0.68527600	-0.70338000
H	3.50851000	-2.78365700	0.71318000
H	1.31317900	1.53535100	1.70967800
H	0.06641200	-0.35423000	-2.45378500
H	-0.10502900	-2.76477500	-2.02424200
H	5.19034800	-2.46035100	2.50665800
H	5.56385300	-3.90951200	1.55979800
H	6.48542800	-2.41672900	1.30304800
H	4.24663000	-2.64692900	-1.73193300
H	4.78309300	-4.09775300	-0.86811500
H	5.91702900	-2.78424600	-1.17763300

H	3.41978400	1.79556600	-2.36447900
H	1.19789100	3.89905000	1.77032100
H	2.94655700	4.11312200	1.58049500
H	2.64994600	1.08166800	3.75050400
H	1.83800800	2.64813500	3.84327400
H	3.57659600	2.56746800	3.48189900
H	2.95529800	-0.66047400	-1.52435300
H	2.06778000	-1.74475600	-2.59360500
H	3.57117600	-0.20164800	-3.84648500
H	1.88196600	-0.00309400	-4.30789300
H	1.97674900	3.52795000	0.22329000
H	2.95875500	2.22285400	-4.01467700
H	1.35746800	3.18567800	-2.33642400
H	0.54546900	2.03062300	-3.39294400
H	1.57372100	1.49219900	-0.57024300
H	-0.11284400	1.62129700	-1.04432300
H	-1.05403000	-3.98085600	0.60063700
H	-2.08404400	-3.21233800	-0.61443200
H	-2.05830400	-5.69196500	-0.88874300
H	-1.38000100	-4.88205100	-2.29740300
H	0.20289200	-6.18778500	-0.01678300
H	0.07032100	-6.80543300	-1.66020900
H	2.24479900	-5.58506000	-1.26872200
H	1.28695500	-4.83805500	-2.54271100
H	1.45652800	-3.88056600	0.36376100
H	2.20354300	-3.11215000	-1.02414400
C	6.52471200	2.01997700	-0.94063600
H	6.27669000	3.08660500	-0.86757200
C	6.63411200	1.66537500	-2.43294500
H	7.41308900	2.26441300	-2.91629600
H	6.89409100	0.61022900	-2.56943000
H	5.68957400	1.84600300	-2.95359100
C	7.86764600	1.80099800	-0.22301200
H	8.65909400	2.39922200	-0.68695000
H	7.79971200	2.07926000	0.83295700
H	8.17030100	0.74943400	-0.27253300
C	-6.73984900	-0.00400000	-2.24883700
C	-5.91748700	1.12019200	-2.17454000
C	-4.77019800	1.07544700	-1.38874400
C	-4.40118800	-0.08588900	-0.69724900
C	-5.21523100	-1.22907000	-0.78116100
C	-6.38565500	-1.15495500	-1.55250300
H	-7.64993400	0.01683500	-2.84061600
H	-6.17353700	2.03120000	-2.70747800

H	-4.17658300	1.97973300	-1.29969700
H	-7.01623700	-2.03833600	-1.61942300
C	-4.83977400	-2.56506100	-0.19494500
H	-5.72825000	-3.17009300	0.01018100
H	-4.21962500	-3.10970300	-0.91504800
H	-4.26504600	-2.47397400	0.72457700
Cl	-2.32604300	-1.26864800	-2.60800600
C	-3.75807200	0.60087000	1.24730000
C	-2.12987200	0.00095300	2.84370200
C	-4.32296800	-0.27577700	2.34866300
C	-2.34868200	0.72161000	1.51570800
C	-3.11955900	-1.17006800	2.71495900
H	-3.26869400	-1.71250200	3.65331600
H	-2.84981600	-1.87350400	1.92581600
C	-2.84603200	0.85832200	3.93054000
H	-2.61896800	0.45493900	4.92229200
H	-2.50819500	1.89420100	3.90632200
C	-4.35469800	0.68079600	3.58418600
H	-4.90703500	0.20657600	4.40088000
H	-4.85712800	1.62561700	3.35671600
H	-1.09492300	-0.22592800	3.07695000
H	-5.27340900	-0.75812100	2.12245800
C	-1.64346000	2.02374200	1.29391200
O	-0.85660400	2.47757600	2.12715900
H	-4.31768400	1.47835500	0.95871500
N	-1.97085600	2.70107500	0.15176900
H	-2.38488300	2.15246400	-0.59011000
C	-1.29840200	3.93281600	-0.23004100
C	-1.63558900	4.34869400	-1.66559200
C	-1.69873300	5.16598500	0.59018200
H	-0.21620200	3.79158900	-0.13415200
C	-1.19881300	5.83006100	-1.73690500
H	-1.15248900	3.71812700	-2.41708300
C	-1.16756400	6.33579800	-0.26071600
H	-1.29717700	5.13765300	1.60465400
H	-2.79315400	5.19515600	0.65984000
H	-0.20763400	5.91504600	-2.19285800
H	-1.88164900	6.41473600	-2.35909000
H	-0.13972500	6.57387400	0.03199400
H	-1.75526200	7.24680300	-0.11950200
H	2.24326500	-2.39320100	4.84995400
H	-2.72066800	4.26329000	-1.80962900

TS2_3

C	2.49950800	1.74270900	2.30479600
C	1.71950700	2.06577200	3.40784800
C	0.51060200	1.39742600	3.59209700
C	0.10630600	0.46797900	2.64191400
C	0.86486000	0.13999500	1.49845500
C	2.12618800	0.77577300	1.34828900
C	3.20680900	0.46334300	0.34783400
C	3.34412800	1.18713500	-0.85654600
C	4.38998100	0.86054100	-1.72775600
C	5.33526000	-0.11694100	-1.42508500
C	5.24366100	-0.74667000	-0.18350100
C	4.20598100	-0.47439400	0.71044100
C	4.22068700	-1.16006700	2.07165800
C	2.47472300	2.39884700	-1.17558500
P	-0.09591300	-1.10572400	0.48509100
C	0.71788400	-1.70062900	-1.07421200
C	-0.14501200	-2.63524000	1.57797300
Pd	-2.40490800	-0.68473100	-0.35118500
C	5.17000500	-0.41925300	3.03239600
C	4.60814400	-2.64664700	1.99760300
C	2.20177100	2.60582700	-2.67552900
C	3.16906600	3.65990400	-0.61813700
C	2.04447100	-2.46710600	-1.01347100
C	2.38900400	-3.03459200	-2.40005700
C	2.41107800	-1.93531900	-3.46930600
C	1.07342100	-1.18711000	-3.51880600
C	0.71317900	-0.60536700	-2.14697900
C	-1.43097900	-2.74462300	2.41520200
C	-1.49700600	-4.10273100	3.12629700
C	-0.25546900	-4.35141200	3.99194400
C	1.02867200	-4.21393600	3.16540800
C	1.09293300	-2.85576500	2.45282300
H	3.46195300	2.22585400	2.17625500
H	-0.11234100	1.59519700	4.45945200
H	-0.83740800	-0.04223900	2.78350300
H	4.47698600	1.39267100	-2.66920000
H	5.99380700	-1.47917000	0.09413500
H	3.21621600	-1.09688200	2.49303800
H	1.51337000	2.27760200	-0.66358800
H	-0.05280800	-2.42312700	-1.36625100
H	-0.19764000	-3.43103300	0.82606100
H	4.85955600	0.61773000	3.18148200
H	5.18884600	-0.91182100	4.01066100
H	6.19054300	-0.41210400	2.63479800

H	4.04296800	-3.17658300	1.22656600
H	4.41588800	-3.13359800	2.95892800
H	5.67266400	-2.77639000	1.77697900
H	3.21046500	-1.22153100	-3.23286500
H	1.45472900	3.39194000	-2.81377200
H	3.10497400	2.92593100	-3.20509600
H	3.27183700	3.62238300	0.46825800
H	2.60810300	4.56193600	-0.87559000
H	4.17226100	3.75312000	-1.04688400
H	2.85349800	-1.81723400	-0.68635400
H	1.97169800	-3.28871100	-0.29268700
H	3.35966700	-3.54293100	-2.35429500
H	1.64446500	-3.79287300	-2.67736000
H	1.82779600	1.70309800	-3.16113700
H	2.64442500	-2.36564800	-4.45051700
H	1.11107100	-0.38475000	-4.26569800
H	0.27747200	-1.87486100	-3.83332300
H	1.43728400	0.16120200	-1.87671900
H	-0.27202700	-0.12665900	-2.18712500
H	-1.46080300	-1.94633800	3.16898600
H	-2.29684200	-2.62286800	1.76167500
H	-2.40640900	-4.15941700	3.73596400
H	-1.57869600	-4.89061700	2.36584800
H	-0.23388300	-3.61903400	4.81178400
H	-0.30552800	-5.34238800	4.45768200
H	1.91240900	-4.34128800	3.80208600
H	1.06382400	-5.01434600	2.41365700
H	1.15854500	-2.05675100	3.20179900
H	1.99678900	-2.79451000	1.84837300
C	6.44529700	-0.46205800	-2.40167400
H	6.28152800	0.14027600	-3.30433900
C	6.39443500	-1.94358700	-2.81088000
H	7.17283600	-2.16870600	-3.54747400
H	6.55494200	-2.59591500	-1.94583000
H	5.42463000	-2.19930000	-3.24632100
C	7.82588200	-0.09105600	-1.83452700
H	8.61427000	-0.29618500	-2.56636300
H	7.87040500	0.96937700	-1.56852300
H	8.04892400	-0.67111300	-0.93252500
C	-5.45986300	-1.01941300	-4.05196300
C	-4.34960100	-0.17256400	-4.05610500
C	-3.62279000	0.01336700	-2.88065000
C	-3.98516100	-0.67587400	-1.72001400
C	-5.09432200	-1.52632900	-1.68805400

C	-5.82425900	-1.67499900	-2.87873200
H	-6.04381100	-1.16188200	-4.95656400
H	-4.06126000	0.35750500	-4.95942600
H	-2.80397700	0.72654800	-2.85014000
H	-6.68734500	-2.33743500	-2.87815400
C	-5.49687700	-2.32876000	-0.47622500
H	-6.57234400	-2.24294000	-0.28144900
H	-5.26259500	-3.38539200	-0.63378100
H	-4.94913300	-2.01687900	0.41170200
Cl	-2.29869300	-3.04292800	-0.99576500
C	-4.05497000	0.97171900	-0.08832200
C	-3.13567500	1.27625500	2.03490300
C	-5.05565300	0.68178100	1.00446500
C	-2.82194100	1.29599900	0.52667400
C	-4.15887400	0.12860600	2.12873800
H	-4.66564700	0.09004800	3.09794200
H	-3.72784600	-0.84775100	1.89934200
C	-4.06034200	2.50755000	2.28676400
H	-4.22002300	2.64026800	3.36136300
H	-3.62968000	3.43514700	1.90134200
C	-5.38142200	2.10559300	1.56442700
H	-6.22016100	2.04475000	2.26402600
H	-5.66264300	2.80388600	0.77161900
H	-2.28913100	1.22390200	2.71302500
H	-5.92910600	0.10319500	0.71127000
C	-2.02678900	2.39324500	-0.12051000
O	-2.22815600	2.73431400	-1.28561800
H	-4.35402700	1.47337200	-0.99412700
N	-1.13448200	3.03452500	0.69903900
H	-1.04402600	2.66521800	1.63506900
C	-0.80676400	4.45273900	0.55922500
C	0.34845300	4.84671700	1.48923800
C	-0.31741700	4.90207000	-0.82174700
H	-1.69729200	5.05053500	0.81771100
C	0.85953700	6.19403500	0.93252900
H	0.04867800	4.90043000	2.54126500
C	0.35411600	6.26069000	-0.53974500
H	-1.12057000	4.94848300	-1.55543000
H	0.40669900	4.17031400	-1.18197200
H	0.46501000	7.03319100	1.51342100
H	1.94961900	6.25315500	0.99563400
H	-0.37490100	7.07028200	-0.64990300
H	1.16029300	6.46988200	-1.24890700
H	2.06001900	2.81251700	4.11809300

H	1.12063300	4.07627200	1.41175700
TS2a			
C	3.01055700	-3.39544000	-0.11837500
C	2.17722800	-4.50071500	-0.01323900
C	0.81589700	-4.29693300	0.19848900
C	0.33542600	-3.00108400	0.31388700
C	1.16995400	-1.86247800	0.25689700
C	2.54499600	-2.07103700	0.00732500
C	3.59334000	-1.02682400	-0.22787400
C	4.43624300	-0.60354400	0.82010000
C	5.44700900	0.32342100	0.54084400
C	5.65776200	0.82289600	-0.74329600
C	4.83929000	0.35531200	-1.77452700
C	3.81219400	-0.56377400	-1.54827700
C	2.97281000	-1.06316700	-2.71679900
C	4.28338000	-1.14878200	2.23542200
P	0.15447700	-0.33553300	0.60944600
C	0.03246200	-0.26504700	2.49376000
C	0.73891600	1.38277300	0.12926200
Pd	-1.93094400	-0.68951300	-0.54574400
C	3.61273300	-2.31212500	-3.35249200
C	2.73673500	-0.00205200	-3.80232900
C	4.61117400	-0.11618600	3.32682300
C	5.15392200	-2.40282600	2.44215500
C	1.05903300	0.60982900	3.22995900
C	0.75992100	0.66313200	4.73545300
C	0.71951400	-0.73649700	5.35306900
C	-0.31010100	-1.60813700	4.62882900
C	-0.02822600	-1.66874500	3.12119700
C	0.32970200	1.75586900	-1.30749700
C	0.61584600	3.23451500	-1.61312900
C	2.06083400	3.63863100	-1.30230800
C	2.40582200	3.28584600	0.14667500
C	2.19951100	1.78557000	0.38266700
H	4.06594900	-3.53746300	-0.32522800
H	0.12728700	-5.13431400	0.25275900
H	-0.73175500	-2.85584800	0.43376900
H	6.08788600	0.67240800	1.34448200
H	4.99882200	0.72298300	-2.78251800
H	1.99104900	-1.35240800	-2.33558300
H	3.23871300	-1.45439600	2.35727700
H	-0.93150000	0.22997600	2.63717700
H	0.09569900	1.95978000	0.81347600

H	3.70167200	-3.13007100	-2.63464400
H	3.00004900	-2.66389600	-4.18891200
H	4.61444600	-2.08156600	-3.73356200
H	2.42197200	0.95450200	-3.37714100
H	1.94789400	-0.34320800	-4.47815900
H	3.63591400	0.17778900	-4.40259900
H	1.71216000	-1.20143100	5.26620100
H	4.28604200	-0.48660500	4.30446500
H	5.68858100	0.06641200	3.39312300
H	4.86604800	-3.20640000	1.76231400
H	5.05505700	-2.77433100	3.46809000
H	6.20887500	-2.16709000	2.26550500
H	2.06572000	0.21613500	3.07821800
H	1.04052100	1.62778200	2.83600800
H	1.51420400	1.28322600	5.23397900
H	-0.20902900	1.15732600	4.88641300
H	4.12270300	0.84527200	3.14650600
H	0.49015500	-0.67934100	6.42330800
H	-0.31633400	-2.62441000	5.03985400
H	-1.31280000	-1.19280600	4.80049800
H	0.92508200	-2.18419600	2.95608900
H	-0.79074100	-2.27778700	2.62867400
H	0.85771300	1.11192200	-2.01325200
H	-0.73152000	1.54197900	-1.45992400
H	0.37377200	3.43815500	-2.66295700
H	-0.05241900	3.86222200	-1.00927800
H	2.74827800	3.10180100	-1.96945500
H	2.20465800	4.70891000	-1.49132600
H	3.44635500	3.54564400	0.37200800
H	1.77584300	3.87145600	0.83221400
H	2.83355400	1.25076800	-0.31798600
H	2.53232600	1.50689500	1.37949500
C	6.74928900	1.84336300	-1.01509700
H	7.24321500	2.05476600	-0.05786400
C	6.16314100	3.16446900	-1.54108400
H	6.95252100	3.90843900	-1.69254900
H	5.65590000	3.01502100	-2.49999700
H	5.43141600	3.57659600	-0.84023200
C	7.81188200	1.28881400	-1.97847000
H	8.61834700	2.01473100	-2.12768400
H	8.24893800	0.36327700	-1.59183800
H	7.37585900	1.06760800	-2.95835700
C	-4.81066300	-1.45814300	-4.37331500
C	-4.54957900	-0.15764000	-3.94563200

C	-3.96094600	0.04140600	-2.69923800
C	-3.59922300	-1.03224800	-1.87822100
C	-3.83257900	-2.35087400	-2.31536900
C	-4.44990000	-2.53118600	-3.56150600
H	-5.28140800	-1.63794600	-5.33505500
H	-4.80569600	0.69448300	-4.56834900
H	-3.78062700	1.06360800	-2.37488300
H	-4.62463800	-3.54633700	-3.90906700
C	-3.36131300	-3.57036100	-1.56189100
H	-3.48730000	-4.46696900	-2.17434600
H	-2.29824600	-3.47338400	-1.32553100
H	-3.90873600	-3.72956800	-0.62921300
Cl	-0.61692900	-1.35253100	-2.46674000
C	-4.19436400	-0.42910300	0.11054800
C	-3.37548700	-0.90076800	2.27300500
C	-4.90851100	-1.59653700	0.76357900
C	-3.19082400	0.00048700	1.04897200
C	-3.78968200	-2.22724700	1.61807300
H	-4.16874200	-2.96013100	2.33667300
H	-2.99131200	-2.67534400	1.02571600
C	-4.71886900	-0.45637800	2.92010300
H	-4.85929900	-0.96639100	3.87822700
H	-4.73680200	0.61790700	3.11216000
C	-5.77696600	-0.92104000	1.87416900
H	-6.46787200	-1.65675500	2.29614500
H	-6.37935500	-0.09788500	1.47884400
H	-2.54493900	-0.92984200	2.96829200
H	-5.46719500	-2.23967300	0.08501800
C	-2.85773300	1.43864800	1.27155100
O	-2.40338300	1.83634600	2.35021100
H	-4.79541300	0.30192900	-0.41146100
N	-3.09689700	2.29545800	0.23483300
H	-3.24240500	1.89015900	-0.67740800
C	-2.67954200	3.68700200	0.28084700
C	-2.87822300	4.38393600	-1.06838500
C	-3.48849400	4.56953800	1.24363100
H	-1.62098200	3.73405500	0.57307000
C	-2.74562600	5.88034400	-0.72452400
H	-2.17252600	4.05144800	-1.83490600
C	-3.18585500	6.00815700	0.76739000
H	-3.22900000	4.38250100	2.28625600
H	-4.55066200	4.32986100	1.11372900
H	-1.70444600	6.19793900	-0.84224300
H	-3.34341700	6.50453100	-1.39384700

H	-2.38119900	6.45033200	1.36280200
H	-4.05633300	6.65933800	0.88437100
H	2.58227000	-5.50240400	-0.11898000
H	-3.89230800	4.16072700	-1.42609000

TS2a_1

C	3.09454800	-1.81849400	2.93112000
C	2.35951600	-2.29370300	4.00910300
C	0.97496500	-2.13836700	4.00294800
C	0.37276200	-1.47721600	2.94173700
C	1.11097100	-0.91966000	1.87493900
C	2.50702200	-1.14211400	1.84253300
C	3.46161500	-0.82492200	0.72712800
C	4.37947600	0.23957100	0.85305400
C	5.33468500	0.43915200	-0.15114900
C	5.41726000	-0.38812300	-1.26799800
C	4.52387300	-1.46025500	-1.35622800
C	3.56405200	-1.71521300	-0.37344900
C	2.72041200	-2.98430400	-0.44974900
C	4.39004900	1.16374400	2.06410000
P	-0.02001700	0.09697900	0.81094700
C	-0.27838100	1.60730000	1.89157800
C	0.59952000	0.73822500	-0.82990700
Pd	-2.02990800	-1.09180700	0.10339600
C	3.36713600	-4.10644500	0.38702600
C	2.48144700	-3.50871000	-1.87376100
C	4.47456100	2.65126800	1.68125400
C	5.54343100	0.80377700	3.01864800
C	0.98836100	2.30703500	2.40898800
C	0.63201100	3.62491200	3.11207700
C	-0.35172700	3.40183900	4.26684300
C	-1.58875800	2.62107400	3.80367200
C	-1.18628400	1.31732600	3.10154800
C	0.68097900	-0.41390300	-1.84601100
C	0.83140000	0.11798700	-3.27345500
C	2.06287200	1.02054400	-3.39080800
C	1.98649800	2.17410900	-2.38515200
C	1.81641100	1.66721200	-0.94335500
H	4.16466200	-1.99208600	2.89497100
H	0.36428700	-2.54742700	4.80162200
H	-0.70797400	-1.41057700	2.91408700
H	6.03854100	1.26140300	-0.05860000
H	4.59043900	-2.13187800	-2.20522500
H	1.74011500	-2.77744500	-0.01468500

H	3.45590800	1.00926500	2.60734200
H	-0.80696200	2.29229800	1.21604100
H	-0.27519200	1.33373200	-1.10646600
H	3.46631000	-3.82650100	1.43673000
H	2.74987800	-5.00911600	0.33771500
H	4.36358800	-4.34881700	-0.00019200
H	2.14408100	-2.72811000	-2.56000900
H	1.70613900	-4.27890300	-1.84274700
H	3.38465100	-3.96286100	-2.29743500
H	0.15161500	2.82907100	5.05758300
H	4.30419300	3.27909200	2.56229800
H	5.46209100	2.90868300	1.28488400
H	5.45630500	-0.22309300	3.38170300
H	5.54911100	1.47140000	3.88743100
H	6.50932300	0.89992200	2.51134700
H	1.48611400	1.63664900	3.11895600
H	1.69914300	2.49484200	1.60751900
H	1.54476200	4.10962600	3.47765900
H	0.18650000	4.31136400	2.37772500
H	3.73567000	2.91812200	0.92187000
H	-0.64596400	4.35955900	4.71115700
H	-2.24326000	2.40226600	4.65527600
H	-2.17395400	3.24632900	3.11285400
H	-0.63220600	0.69517500	3.81240700
H	-2.06428800	0.74024900	2.80628100
H	1.54182100	-1.03126000	-1.59631000
H	-0.20171500	-1.05330700	-1.77030300
H	0.90896100	-0.72566100	-3.96956200
H	-0.07628800	0.67234500	-3.54256300
H	2.96091200	0.42735200	-3.18123900
H	2.16594100	1.41132200	-4.41015600
H	2.88780100	2.79668600	-2.44143500
H	1.13930300	2.82294000	-2.64750200
H	2.72101900	1.14249100	-0.64060300
H	1.70356700	2.52775200	-0.27973600
C	6.46983300	-0.14616900	-2.33634900
H	7.07847200	0.70456700	-2.00283900
C	5.83614900	0.23615100	-3.68388600
H	6.60899200	0.44339800	-4.43197600
H	5.20837500	-0.57527800	-4.06710000
H	5.20684200	1.12535700	-3.58528000
C	7.40690900	-1.35562600	-2.49081300
H	8.20222600	-1.14046900	-3.21241200
H	7.87060100	-1.61857900	-1.53536400

H	6.86116000	-2.23439900	-2.84966000
C	-4.17970300	-4.60990500	-2.41128400
C	-3.52036700	-3.55250600	-3.03886900
C	-3.12202000	-2.44936300	-2.28558200
C	-3.35228600	-2.41287600	-0.90728300
C	-3.99537800	-3.47460800	-0.25292500
C	-4.41078700	-4.56111200	-1.03783600
H	-4.51040400	-5.46998000	-2.98614000
H	-3.32829900	-3.57628500	-4.10785100
H	-2.64639500	-1.60056300	-2.76970600
H	-4.90504600	-5.39601300	-0.54656300
C	-4.14806600	-3.54576800	1.24544000
H	-4.71641900	-4.43387600	1.53579100
H	-3.15650500	-3.60294900	1.70529900
H	-4.65546600	-2.67325500	1.66182000
Cl	-0.77087400	-3.12830500	0.39668700
C	-4.16660200	-0.34559000	-0.61250600
C	-3.95377900	1.29536800	1.05135500
C	-5.28834000	-0.40719900	0.39852200
C	-3.28668300	0.69196600	-0.19306200
C	-4.58165700	0.04359600	1.69385400
H	-5.28106800	0.28298800	2.50050500
H	-3.83663000	-0.67220100	2.04902100
C	-5.23190900	2.03201800	0.54315200
H	-5.69236000	2.59243000	1.36283200
H	-5.01139200	2.74073700	-0.25908500
C	-6.14524000	0.85903300	0.07649300
H	-7.07969500	0.82723200	0.64409100
H	-6.40592500	0.91835100	-0.98364000
H	-3.32075500	1.90184600	1.69596200
H	-5.85387000	-1.33692200	0.41725600
C	-2.64198300	1.52575100	-1.24624200
O	-2.41409200	1.10846200	-2.38447000
H	-4.37179900	-0.47705100	-1.66276200
N	-2.29319200	2.79056100	-0.85591200
H	-2.58937000	3.11503100	0.05207800
C	-1.66575700	3.74643200	-1.74624200
C	-2.62497900	4.72894000	-2.43828100
C	-0.67651800	4.67475100	-1.02833700
H	-1.14955800	3.15707400	-2.50925100
C	-1.68844800	5.82848700	-2.97598200
H	-3.22592800	4.24404100	-3.21163000
C	-0.44386500	5.82467000	-2.03155000
H	0.24305500	4.16392500	-0.73359200

H	-1.14813200	5.05474300	-0.11103900
H	-1.38220600	5.59301200	-3.99989200
H	-2.18020000	6.80421900	-3.01029600
H	0.46911600	5.64403300	-2.60677200
H	-0.31029000	6.78175600	-1.52040900
H	2.85855200	-2.80962800	4.82370700
H	-3.31393000	5.13728900	-1.68711600

TS2a_2

C	3.41145900	0.09196300	-3.28162400
C	2.72700800	0.25984000	-4.47754200
C	1.36378200	0.53690400	-4.43518100
C	0.73087000	0.64995300	-3.20558400
C	1.41561200	0.54193300	-1.97660300
C	2.79317600	0.22930800	-2.02317100
C	3.68692100	-0.08698800	-0.86424200
C	3.67483400	-1.40190500	-0.34622600
C	4.57595200	-1.73395200	0.67056800
C	5.47885200	-0.80703700	1.19001200
C	5.49213000	0.47893200	0.64315600
C	4.62798900	0.85569000	-0.38881300
C	4.75832000	2.24911600	-1.00076000
C	2.71598600	-2.45047700	-0.89117000
P	0.24090700	0.71118200	-0.53813100
C	0.98140100	1.23723100	1.10093600
C	-0.70888700	2.29149800	-0.97360700
Pd	-1.38185300	-1.12261200	-0.36350800
C	5.82079100	2.26179800	-2.11780700
C	5.11223900	3.34467400	0.02093200
C	2.17806400	-3.40742800	0.18044800
C	3.37443100	-3.24709600	-2.03176400
C	1.73944800	2.57214200	1.11827800
C	2.13038500	2.97374800	2.55009400
C	2.91398800	1.87293600	3.27136500
C	2.11895600	0.56371100	3.26742100
C	1.78108400	0.14862900	1.83015600
C	-2.07503900	2.06135000	-1.64918000
C	-2.85236500	3.38230100	-1.75364200
C	-2.05314100	4.46565000	-2.48640100
C	-0.68554400	4.67383200	-1.82626200
C	0.09224300	3.35287500	-1.75564200
H	4.45942400	-0.18619300	-3.29742100
H	0.78414900	0.63114400	-5.34778000
H	-0.33887100	0.79550600	-3.20141600

H	4.56604200	-2.73909700	1.08080300
H	6.20097400	1.20536100	1.02630300
H	3.79471800	2.50256200	-1.45667300
H	1.85062700	-1.94420800	-1.32202300
H	0.03930700	1.39823400	1.64303600
H	-0.93014300	2.68835900	0.02403200
H	5.55815700	1.59216800	-2.93709200
H	5.93139600	3.27121100	-2.52890000
H	6.79207400	1.94916800	-1.71933500
H	4.47738100	3.31455700	0.90848800
H	5.00562200	4.33099200	-0.44154500
H	6.15180900	3.25776700	0.35356000
H	3.87002300	1.70686100	2.75961100
H	1.36044300	-3.99649300	-0.24227200
H	2.94328500	-4.10618100	0.53664500
H	3.69686500	-2.58684400	-2.84046000
H	2.66075100	-3.96499200	-2.44834500
H	4.25050200	-3.79680500	-1.66801600
H	2.63229800	2.48602700	0.49764500
H	1.12511600	3.36843000	0.69520900
H	2.70979800	3.90460900	2.52136200
H	1.21398700	3.19333800	3.11494300
H	1.79315700	-2.86217900	1.04650900
H	3.14844900	2.18146600	4.29685900
H	2.69207100	-0.23720500	3.74914900
H	1.20288200	0.69754100	3.85980300
H	2.71690100	-0.02047500	1.30975600
H	1.24264800	-0.80092700	1.81326900
H	-1.94397300	1.64880400	-2.65556300
H	-2.65422300	1.32368300	-1.08968500
H	-3.81006500	3.21033800	-2.25856300
H	-3.08440300	3.73914100	-0.74220300
H	-1.90367800	4.16157900	-3.53178600
H	-2.61782000	5.40497000	-2.50894900
H	-0.10223900	5.41802700	-2.38105100
H	-0.82576000	5.07349000	-0.81207600
H	0.27459200	2.99759200	-2.77354000
H	1.07852100	3.51320600	-1.31450100
C	6.42305400	-1.18583400	2.31794800
H	6.23771300	-2.24126000	2.55524700
C	6.13912200	-0.36463900	3.58689200
H	6.79622700	-0.67414100	4.40673300
H	6.30610300	0.70300500	3.40902400
H	5.10186900	-0.48836100	3.91172700

C	7.89529800	-1.05348600	1.89388200
H	8.56222700	-1.38166700	2.69828400
H	8.10469900	-1.65612300	1.00508700
H	8.14453000	-0.01339200	1.65817500
C	-4.88852700	-3.97421000	-2.10314300
C	-5.01902500	-2.58637900	-2.01980500
C	-4.07137800	-1.85375600	-1.30889100
C	-2.97729800	-2.48875300	-0.70601000
C	-2.81477600	-3.87754500	-0.81143600
C	-3.79785600	-4.60052900	-1.50511000
H	-5.62851700	-4.56380000	-2.63602000
H	-5.85405200	-2.07968300	-2.49551800
H	-4.17710000	-0.77430100	-1.23404200
H	-3.68371900	-5.67861000	-1.59234200
C	-1.58381700	-4.59786000	-0.32815400
H	-1.81055800	-5.62618800	-0.02888200
H	-0.85388800	-4.62253700	-1.14340300
H	-1.10077400	-4.08598700	0.50230800
Cl	-0.56406100	-2.06690000	-2.42071400
C	-2.93094200	-1.74602500	1.37631800
C	-1.29266400	-0.82733800	2.77818600
C	-2.40520200	-2.75149900	2.37797500
C	-2.20363200	-0.53379200	1.57951700
C	-0.94060000	-2.30710700	2.54870400
H	-0.45269300	-2.77118000	3.41080300
H	-0.33642700	-2.46747500	1.65342700
C	-2.24013500	-0.93702600	4.00807800
H	-1.65049700	-1.01692900	4.92635700
H	-2.88378800	-0.05975100	4.10734200
C	-3.02472000	-2.25280300	3.72561900
H	-2.85469000	-3.00199800	4.50427100
H	-4.10589000	-2.10142500	3.65054700
H	-0.47760500	-0.13224200	2.92236900
H	-2.60865800	-3.79631700	2.15009200
C	-2.83088900	0.82037300	1.52134200
O	-2.23240300	1.82137200	1.93092400
H	-3.99194500	-1.76467800	1.18111300
N	-4.09756200	0.89790700	1.01998800
H	-4.58402900	0.04781300	0.78192000
C	-4.86653000	2.12661000	1.02324800
C	-5.94023800	2.15849800	-0.07000200
C	-5.67307000	2.38428600	2.30793500
H	-4.15416500	2.94350400	0.88555400
C	-6.87320000	3.31334700	0.35395300

H	-5.52242500	2.28133200	-1.07180000
C	-6.67079500	3.48393800	1.89373900
H	-5.03140700	2.66227300	3.14766300
H	-6.20172000	1.46192500	2.58128200
H	-6.59723200	4.23367700	-0.16958500
H	-7.91426200	3.10351900	0.09475200
H	-6.25380900	4.47242300	2.11024100
H	-7.61136400	3.41103100	2.44613600
H	3.24474400	0.14442900	-5.42484700
H	-6.48563100	1.20435800	-0.05722600

TS2a_3

C	-3.35150500	-1.43751800	3.02930600
C	-2.74472700	-1.68213200	4.25415200
C	-1.40911300	-1.33033300	4.42227500
C	-0.72294300	-0.73535000	3.37233700
C	-1.33389600	-0.42459600	2.13919300
C	-2.68143900	-0.81254200	1.96064700
C	-3.48043800	-0.71790100	0.69952000
C	-3.29831400	-1.70411500	-0.29660700
C	-4.11634200	-1.67115700	-1.43089700
C	-5.09407600	-0.69326700	-1.61205800
C	-5.26969800	0.25901300	-0.60491400
C	-4.49460100	0.25851100	0.55837600
C	-4.79023400	1.28631500	1.64914600
C	-2.24433000	-2.79251700	-0.14331500
P	-0.12794700	0.29522800	0.92078400
C	-0.85712400	1.45705600	-0.35302500
C	0.85814700	1.53163600	1.95625600
Pd	1.60235700	-1.19954300	0.04069400
C	-5.92524500	0.80167800	2.57302800
C	-5.16668900	2.67556300	1.10267300
C	-1.64306500	-3.25003700	-1.47821000
C	-2.81160600	-4.00161600	0.62207900
C	-1.61807900	2.68989200	0.15441500
C	-1.94054500	3.65481400	-0.99999200
C	-2.65166200	2.96814000	-2.17121500
C	-1.84648100	1.75859400	-2.65784800
C	-1.61922700	0.78098900	-1.49960400
C	2.21629700	0.99945100	2.45637900
C	3.06831200	2.13766900	3.03544200
C	2.32658000	2.92394500	4.12272000
C	0.96496900	3.42180700	3.62112700
C	0.11413900	2.25617600	3.09525000

H	-4.37226300	-1.76164600	2.86060300
H	-0.88776800	-1.54476600	5.34954000
H	0.32941100	-0.53983800	3.50569300
H	-3.98046000	-2.41764100	-2.20708000
H	-6.03461800	1.01887200	-0.72666700
H	-3.88665900	1.39294000	2.25923400
H	-1.42050500	-2.40103000	0.45712700
H	0.08696200	1.82241200	-0.77323200
H	1.09070800	2.28346400	1.19487100
H	-5.66594200	-0.12412100	3.08731000
H	-6.14902400	1.55867700	3.33249700
H	-6.83658300	0.62438400	1.99176300
H	-4.46893500	3.03160400	0.34234300
H	-5.18143800	3.40412500	1.91941900
H	-6.16732300	2.67219000	0.65841200
H	-3.64112200	2.61871500	-1.84998100
H	-0.76098600	-3.86673600	-1.28735200
H	-2.34646300	-3.85280800	-2.06358400
H	-3.17689400	-3.71086700	1.60948500
H	-2.03040300	-4.75519600	0.76236200
H	-3.64109500	-4.45660000	0.06819800
H	-2.53742800	2.36945500	0.64815300
H	-1.02772200	3.23115500	0.89565400
H	-2.54207000	4.48972700	-0.62154200
H	-0.99817300	4.09111200	-1.36212300
H	-1.33768300	-2.39942300	-2.09411000
H	-2.81527200	3.68223100	-2.98658900
H	-2.37045400	1.24896200	-3.47425500
H	-0.88646900	2.10565400	-3.07086300
H	-2.59360400	0.45939100	-1.15035700
H	-1.09563500	-0.11972800	-1.82798400
H	2.07064000	0.22469300	3.21714800
H	2.75228800	0.53244000	1.63013000
H	4.00323800	1.72612700	3.43275300
H	3.35281300	2.81248500	2.21872000
H	2.16626400	2.27327100	4.99384500
H	2.93739600	3.76606600	4.46875700
H	0.42774000	3.93961900	4.42445700
H	1.11654600	4.15757900	2.81857100
H	-0.07446600	1.56084400	3.91730000
H	-0.86804600	2.60944700	2.77317900
C	-5.93785200	-0.65999700	-2.87423900
H	-5.62170200	-1.50614800	-3.49770500
C	-5.69296700	0.62932600	-3.67615300

H	-6.26995400	0.62618000	-4.60712800
H	-5.99135700	1.51219500	-3.10075600
H	-4.63409000	0.74004500	-3.92842100
C	-7.43296300	-0.84125500	-2.56364300
H	-8.02083500	-0.87036100	-3.48720000
H	-7.61012800	-1.76989500	-2.01318000
H	-7.81178800	-0.01427100	-1.95358800
C	5.40452000	-4.03869800	0.99524200
C	5.40731300	-2.67266200	1.27650000
C	4.39185100	-1.86674500	0.76506900
C	3.35739500	-2.41847800	0.00248100
C	3.32944900	-3.79444300	-0.27931100
C	4.37818500	-4.57975700	0.22407700
H	6.19583400	-4.67992500	1.37218500
H	6.20037100	-2.23083700	1.87315800
H	4.41789300	-0.79412000	0.93464400
H	4.36658300	-5.64787300	0.02047400
C	2.18443100	-4.47697000	-0.98270800
H	2.42374600	-5.52377300	-1.18992400
H	1.30214900	-4.44192900	-0.33674100
H	1.91961400	-3.99871700	-1.92617800
Cl	0.94500900	-2.77323300	1.73889500
C	3.21928100	-0.97790500	-1.69078200
C	1.43774200	-0.14196800	-2.96942000
C	2.97474000	-1.79741700	-2.93729400
C	2.23798400	0.05912700	-1.66927100
C	1.44653000	-1.67625200	-3.09563100
H	1.08495400	-2.02705200	-4.06691700
H	0.89183500	-2.16654200	-2.29501700
C	2.39020800	0.24282800	-4.14578000
H	1.83710600	0.22189200	-5.09005900
H	2.81964500	1.24107000	-4.03659100
C	3.46892800	-0.87855800	-4.09837400
H	3.50152800	-1.44736200	-5.03204300
H	4.47513000	-0.49178100	-3.91436600
H	0.46121200	0.33354000	-3.01370400
H	3.41610600	-2.79203300	-2.93731600
C	2.69264000	1.40871100	-1.20966400
O	3.58206600	1.56474600	-0.36682200
H	4.22532500	-0.75754100	-1.37062700
N	2.08429700	2.46924600	-1.82255400
H	1.41693700	2.26628900	-2.54879300
C	2.48996800	3.86561700	-1.65476400
C	2.20889300	4.42724800	-0.23997800

C	4.00515400	4.13871100	-1.92075200
H	1.89241800	4.41553500	-2.38736700
C	3.33714100	5.43445500	0.01334500
H	1.20149500	4.84572800	-0.15084500
C	4.55607000	4.73829900	-0.61452500
H	4.10071900	4.85573200	-2.74340300
H	4.52789400	3.22673200	-2.21310800
H	3.13204700	6.38239700	-0.50129100
H	3.46777200	5.65978300	1.07626500
H	5.40146600	5.41284600	-0.77917300
H	4.88673400	3.92586600	0.03940900
H	-3.29910300	-2.16767300	5.05143300
H	2.30273400	3.60927000	0.47328800

TS2b

C	-2.26790400	-0.46451700	-3.12971900
C	-1.29948900	-0.45701500	-4.12703300
C	-0.00611500	-0.05913000	-3.80271900
C	0.28513600	0.31987100	-2.49771300
C	-0.69056600	0.34608900	-1.47552100
C	-2.00489600	-0.06612300	-1.80366900
C	-3.20810700	-0.13037000	-0.90808900
C	-4.06695700	0.98332900	-0.80335100
C	-5.26032200	0.85260500	-0.08243100
C	-5.63691900	-0.34994100	0.51298600
C	-4.78052400	-1.44720200	0.38004900
C	-3.57523700	-1.36594100	-0.32010100
C	-2.68669500	-2.60279400	-0.44422000
C	-3.76145200	2.28979700	-1.52781100
P	0.02642500	1.16029300	0.04623300
C	-0.27599800	2.97823400	-0.31210600
C	-0.91186600	0.96634700	1.67717400
Pd	2.41876300	0.50526300	0.15818600
C	-3.08546500	-3.45838800	-1.66136000
C	-2.68346300	-3.48657300	0.81381400
C	-4.15465200	3.54860200	-0.74032800
C	-4.44085000	2.30400600	-2.91014500
C	-0.13307000	3.43853600	-1.77285900
C	-0.48454900	4.92886500	-1.88922400
C	0.37567400	5.78834300	-0.95512400
C	0.23276400	5.32360300	0.49886100
C	0.58092500	3.83596900	0.63884800
C	-1.35536000	-0.47087900	1.97298700
C	-1.85828600	-0.63137200	3.41339400

C	-3.02409300	0.32103200	3.68702500
C	-2.60629700	1.76367400	3.39351800
C	-2.08177000	1.92841800	1.95850500
H	-3.28023300	-0.77329600	-3.36858300
H	0.77851100	-0.03965800	-4.55245300
H	1.29095800	0.65925000	-2.27543500
H	-5.92446500	1.70699500	0.00575800
H	-5.05939400	-2.39165300	0.83516500
H	-1.66304400	-2.25034000	-0.60244900
H	-2.68349800	2.32966600	-1.69678300
H	-1.32812100	3.12371900	-0.05029500
H	-0.10461300	1.22975500	2.37549700
H	-2.99988900	-2.90396400	-2.59737400
H	-2.44210200	-4.34237600	-1.73066200
H	-4.12084900	-3.80212400	-1.56299200
H	-2.51628200	-2.90806100	1.72283200
H	-1.88015700	-4.22476100	0.74943100
H	-3.62742200	-4.03126000	0.92238400
H	1.42757200	5.70344400	-1.25689200
H	-3.79899300	4.43968500	-1.26643900
H	-5.24078200	3.64442500	-0.64265200
H	-4.10270400	1.46931900	-3.52805600
H	-4.21209300	3.23412500	-3.44136400
H	-5.52856900	2.22996800	-2.80358300
H	0.88904800	3.26936200	-2.11215300
H	-0.79016600	2.85337800	-2.42212800
H	-0.35954300	5.25187900	-2.92913300
H	-1.54510700	5.07781000	-1.63902200
H	-3.72524100	3.55515000	0.26440700
H	0.09975800	6.84557200	-1.04621700
H	0.87609900	5.91783500	1.15816200
H	-0.80183200	5.49064200	0.83298100
H	1.63397900	3.67474800	0.39005800
H	0.44096100	3.51704500	1.67911900
H	-2.18079600	-0.70280400	1.30563300
H	-0.57409000	-1.19672300	1.77259300
H	-2.15722900	-1.67225100	3.57923800
H	-1.04517100	-0.42728800	4.12399800
H	-3.86269900	0.05034900	3.03326800
H	-3.37529800	0.22401800	4.72096900
H	-3.44761800	2.44950700	3.54782900
H	-1.82110800	2.06618900	4.10115100
H	-2.89294600	1.71863900	1.25742600
H	-1.78514000	2.96991700	1.81953400

C	-6.95866400	-0.47275600	1.25234700
H	-7.44007300	0.51305700	1.22084200
C	-6.76056800	-0.85003200	2.72945400
H	-7.72493200	-0.92008700	3.24363300
H	-6.25970300	-1.81915500	2.82495700
H	-6.14900100	-0.10716100	3.24907600
C	-7.89323600	-1.47211400	0.54926500
H	-8.86644400	-1.51222400	1.04976000
H	-8.05442300	-1.19192400	-0.49601100
H	-7.46849800	-2.48149000	0.56249700
C	6.97807600	-0.00292300	-1.41281100
C	5.98111800	-0.89203600	-1.81122400
C	4.75007600	-0.87253300	-1.15839000
C	4.49010600	0.04379300	-0.13445500
C	5.47977900	0.95921800	0.26605500
C	6.71956500	0.90438300	-0.38742200
H	7.94860600	-0.01008200	-1.89968500
H	6.15955700	-1.60340000	-2.61247600
H	3.99045000	-1.59579900	-1.44255500
H	7.48880300	1.61505500	-0.09520100
C	5.24318800	2.04300600	1.28926600
H	6.03635600	2.79323200	1.23685400
H	4.29240400	2.54367500	1.09278700
H	5.22100400	1.65874700	2.31304400
Cl	3.01556800	2.27655300	-1.39955500
C	3.52522600	-1.20085500	1.41476700
C	1.85622800	-0.76218900	3.00073100
C	4.10032200	-0.77397100	2.74516600
C	2.09959000	-1.16737100	1.53712700
C	3.02460500	0.21024200	3.24705600
H	3.14344400	0.46407600	4.30460300
H	2.96236100	1.12702800	2.65647800
C	2.29713000	-1.96196300	3.89114700
H	2.05472100	-1.74074800	4.93552300
H	1.78827900	-2.87946300	3.60381100
C	3.83718100	-2.00448600	3.67414200
H	4.38864700	-1.88030800	4.61072900
H	4.17738600	-2.93870600	3.21740700
H	0.86235800	-0.39601700	3.22707000
H	5.13784200	-0.44620500	2.72042900
C	1.32436200	-2.29999300	0.91423800
O	0.68154700	-3.09810000	1.60278900
H	4.00215600	-1.99221000	0.85612500
N	1.42663300	-2.43798300	-0.43493300

H	1.80717000	-1.66607000	-0.96701100
C	0.85477400	-3.57662100	-1.13188800
C	0.52055000	-3.28062600	-2.59844000
C	1.77019700	-4.80832400	-1.21363500
H	-0.05148000	-3.86044000	-0.58964200
C	0.43183500	-4.67405000	-3.26992300
H	-0.38861100	-2.68916600	-2.70843200
C	1.06346000	-5.68089000	-2.26245500
H	1.89730500	-5.29554600	-0.24345700
H	2.75992000	-4.49232500	-1.56842600
H	-0.60672200	-4.94027000	-3.48693200
H	0.96282500	-4.67840100	-4.22603700
H	0.27568600	-6.26834900	-1.77788600
H	1.73898300	-6.39241100	-2.74488400
H	-1.55567200	-0.75959400	-5.13775000
H	1.33568800	-2.69425900	-3.03993300

TS2b_1

C	-2.12977600	2.06327300	2.21278900
C	-1.20599100	2.38360400	3.19950400
C	-0.00547700	1.67848000	3.25346400
C	0.23643200	0.67951700	2.32115600
C	-0.71047100	0.29911700	1.34300200
C	-1.92877700	1.01850500	1.28786600
C	-3.09516200	0.76563300	0.37650800
C	-4.21744100	0.06450500	0.87940100
C	-5.32989200	-0.11422400	0.05546400
C	-5.37727200	0.37154100	-1.25258000
C	-4.28293300	1.10522800	-1.71238800
C	-3.15672100	1.33741500	-0.91360200
C	-2.08571700	2.31167100	-1.39306300
C	-4.26500500	-0.47439900	2.30385900
P	-0.05065400	-1.21230000	0.46949400
C	-0.12037200	-2.51044400	1.87122400
C	-1.04090700	-1.94377200	-0.92824300
Pd	2.33395200	-0.93509500	-0.24499000
C	-2.42506800	3.72945100	-0.89227100
C	-1.89029700	2.36034600	-2.91654000
C	-4.75818300	-1.92851200	2.38088900
C	-5.13862300	0.42824300	3.19403900
C	-0.39676500	-3.95365900	1.39399000
C	-0.12287100	-4.94413200	2.53384800
C	-0.99536100	-4.64160000	3.75623300
C	-0.82604000	-3.18571400	4.20227800

C	-1.06000800	-2.19773600	3.04841100
C	-0.88877400	-1.13845500	-2.22305100
C	-1.41210100	-1.92484100	-3.43170700
C	-2.86497300	-2.36648000	-3.22575600
C	-3.02261900	-3.15068600	-1.91764900
C	-2.51171300	-2.33034400	-0.72491400
H	-3.06488300	2.61123000	2.15845000
H	0.74853300	1.90977600	3.99840600
H	1.19444300	0.16987700	2.35255900
H	-6.18984700	-0.65497400	0.44088800
H	-4.31317300	1.53206500	-2.70663400
H	-1.14073700	2.01169600	-0.92787000
H	-3.25052400	-0.44875900	2.70505100
H	0.91325400	-2.49455600	2.23387000
H	-0.45374600	-2.86483500	-1.05583600
H	-2.47933200	3.76955500	0.19621600
H	-1.66936200	4.45048000	-1.22307500
H	-3.39231700	4.04856500	-1.29411200
H	-1.71315600	1.37457600	-3.35263300
H	-1.03317000	2.99600100	-3.16074300
H	-2.76093100	2.79722500	-3.41537300
H	-2.04949000	-4.81638900	3.49684900
H	-4.65581300	-2.30572600	3.40349000
H	-5.81445500	-2.01502800	2.10592500
H	-4.76147700	1.45381000	3.21461100
H	-5.15716100	0.05246300	4.22257500
H	-6.16946000	0.45687000	2.82464000
H	-1.44602100	-4.05072500	1.09669000
H	0.22660600	-4.20343900	0.53911300
H	-0.30128500	-5.96633900	2.18041800
H	0.93904800	-4.88536000	2.80504300
H	-4.18740600	-2.58363000	1.71848700
H	-0.75807200	-5.32347700	4.58135400
H	-1.51027000	-2.95365500	5.02747200
H	0.19241200	-3.04070300	4.58804000
H	-2.09829500	-2.27718100	2.71002100
H	-0.92225600	-1.18080300	3.41734200
H	-1.45407900	-0.20962700	-2.12193400
H	0.15615400	-0.87543600	-2.37705400
H	-1.32176000	-1.31450800	-4.33882400
H	-0.77641500	-2.80808800	-3.58232500
H	-3.50101800	-1.47292900	-3.17892400
H	-3.21055800	-2.96300500	-4.07813400
H	-4.07503100	-3.41204700	-1.75733200

H	-2.46588100	-4.09568500	-1.98399400
H	-3.11319500	-1.42924900	-0.64546400
H	-2.65028500	-2.88475600	0.20368100
C	-6.60270500	0.08156800	-2.10698300
H	-7.47636900	0.20551300	-1.45213700
C	-6.59312700	-1.38369200	-2.58376800
H	-7.51928200	-1.62551500	-3.11588700
H	-5.75427100	-1.56124500	-3.26393200
H	-6.49092000	-2.07433300	-1.74179800
C	-6.77570800	1.03310600	-3.29546600
H	-7.72626900	0.83760000	-3.80090400
H	-6.76757500	2.08053300	-2.97857900
H	-5.98022000	0.89646700	-4.03636800
C	7.04658100	-1.92872400	0.16902000
C	6.34983800	-1.16843700	1.10857500
C	5.04581400	-0.75875500	0.83005000
C	4.42928900	-1.13735100	-0.36550600
C	5.10516300	-1.91049900	-1.32064000
C	6.42628300	-2.28403000	-1.02703000
H	8.06872900	-2.24060900	0.36304500
H	6.82022100	-0.87671800	2.04347300
H	4.51580600	-0.11043700	1.52242900
H	6.96677400	-2.88621300	-1.75387200
C	4.45778000	-2.43820300	-2.57580500
H	5.21162800	-2.79427700	-3.28421100
H	3.79552100	-3.26939300	-2.31621400
H	3.84306000	-1.69125100	-3.07850000
Cl	2.47870500	-3.32992300	0.01814700
C	3.61023900	0.86914000	-1.15226500
C	1.57613400	1.50420300	-2.11372700
C	3.69026800	0.90933800	-2.65836300
C	2.28784900	1.21736800	-0.78112200
C	2.26428700	0.49347500	-3.05762700
H	2.03714000	0.68054300	-4.11146400
H	2.04952400	-0.54766800	-2.81373500
C	2.17998300	2.83241100	-2.67338300
H	1.64431200	3.12473800	-3.58217900
H	2.11741600	3.66413600	-1.96950700
C	3.65332900	2.43712800	-2.99126100
H	3.89477200	2.59164100	-4.04677800
H	4.37969000	3.00305000	-2.40140700
H	0.49046400	1.47269600	-2.09313100
H	4.52813100	0.37523700	-3.10224700
C	2.18398400	2.06871400	0.44551300

O	2.94634800	1.92091300	1.40518400
H	4.44485900	1.17850700	-0.54460000
N	1.26666100	3.07695500	0.41897500
H	0.68379100	3.19539600	-0.39437600
C	1.31667100	4.15076500	1.39771700
C	2.52455100	5.09414000	1.25663200
C	0.12502100	5.10612600	1.31137000
H	1.35114200	3.68735800	2.38727500
C	2.13634300	6.30045300	2.13259900
H	3.45799700	4.61226800	1.55246300
C	0.57573400	6.33990800	2.12427300
H	-0.80162300	4.65936100	1.67573700
H	-0.03271600	5.38266700	0.26050700
H	2.50310500	6.15723100	3.15394800
H	2.57779000	7.23162900	1.76739700
H	0.18740700	6.28482800	3.14607900
H	0.18768300	7.26584600	1.69122700
H	-1.41810000	3.17859200	3.90801500
H	2.61510500	5.39202000	0.20382600

TS2b_2

C	2.66028600	-1.33653000	3.02471200
C	1.87394300	-2.10828100	3.86977200
C	0.61021800	-2.50059800	3.43708900
C	0.17404400	-2.09983600	2.18157100
C	0.96118700	-1.33141400	1.29569800
C	2.25095500	-0.94006700	1.73467100
C	3.29963800	-0.16556500	0.98545700
C	3.32461200	1.24747300	1.03323600
C	4.37133700	1.92199800	0.39408200
C	5.40660900	1.25179600	-0.25759400
C	5.39810500	-0.14248700	-0.23318200
C	4.37412200	-0.86486500	0.38509700
C	4.48465900	-2.38486000	0.43363300
C	2.27779700	2.04011500	1.80952900
P	0.03352800	-1.15180000	-0.31522000
C	0.84385500	-0.19689600	-1.69340400
C	0.03582600	-2.92195600	-0.94914800
Pd	-2.29387700	-0.42175100	-0.32408400
C	5.48871800	-2.81758400	1.51836100
C	4.87755400	-3.00825700	-0.91647700
C	2.09423400	3.48023900	1.31002600
C	2.60966800	2.08066900	3.31390100
C	2.16993800	-0.70223800	-2.27884000

C	2.59600300	0.14715800	-3.48648700
C	2.65742800	1.63785300	-3.13763700
C	1.30563900	2.12314200	-2.60474100
C	0.87434900	1.30448800	-1.38334000
C	-1.15697100	-3.76576300	-0.47011000
C	-1.20659200	-5.09467300	-1.23448800
C	0.09923800	-5.88340500	-1.06812400
C	1.31526400	-5.03568900	-1.46240500
C	1.33926600	-3.69606400	-0.71131800
H	3.64435000	-1.02119200	3.35402500
H	-0.03906200	-3.09751200	4.06995900
H	-0.82134800	-2.38732200	1.87127400
H	4.38704900	3.00628600	0.40758300
H	6.21136600	-0.68561700	-0.70345700
H	3.50827000	-2.78373600	0.71313800
H	1.31329200	1.53547500	1.70987100
H	0.06644500	-0.35424600	-2.45378000
H	-0.10525200	-2.76470200	-2.02426600
H	5.18982900	-2.46070100	2.50679400
H	5.56369300	-3.90966200	1.55977300
H	6.48509800	-2.41671000	1.30339500
H	4.24684200	-2.64681600	-1.73197600
H	4.78264700	-4.09787900	-0.86814300
H	5.91707300	-2.78470300	-1.17729700
H	3.41981200	1.79555800	-2.36439200
H	1.19797100	3.89912700	1.77031300
H	2.94662900	4.11324300	1.58052300
H	2.64980900	1.08191800	3.75064700
H	1.83870600	2.64882400	3.84325300
H	3.57720400	2.56719100	3.48167900
H	2.95532500	-0.66049700	-1.52430500
H	2.06782100	-1.74474800	-2.59359100
H	3.57124900	-0.20163400	-3.84642000
H	1.88204600	-0.00308200	-4.30785600
H	1.97686900	3.52803200	0.22330500
H	2.95882800	2.22286300	-4.01459900
H	1.35748700	3.18565900	-2.33638300
H	0.54552700	2.03060300	-3.39293100
H	1.57369200	1.49216800	-0.57018900
H	-0.11285300	1.62123500	-1.04434400
H	-1.05423800	-3.98072600	0.60064400
H	-2.08422600	-3.21211400	-0.61439300
H	-2.05872600	-5.69174800	-0.88870900
H	-1.38040000	-4.88189600	-2.29739300

H	0.20245400	-6.18776400	-0.01682600
H	0.06976600	-6.80541700	-1.66024100
H	2.24436400	-5.58524000	-1.26885600
H	1.28653500	-4.83814500	-2.54280400
H	1.45633400	-3.88066400	0.36365600
H	2.20334000	-3.11232500	-1.02429300
C	6.52478400	2.01960400	-0.94080200
H	6.27684900	3.08625300	-0.86776500
C	6.63413600	1.66494600	-2.43310200
H	7.41309300	2.26397000	-2.91650400
H	6.89411500	0.60979700	-2.56956000
H	5.68958000	1.84555200	-2.95372400
C	7.86770900	1.80053500	-0.22319200
H	8.65919600	2.39869600	-0.68714600
H	7.79980700	2.07881300	0.83277400
H	8.17028500	0.74894700	-0.27270400
C	-6.73987800	-0.00386700	-2.24880700
C	-5.91749400	1.12031100	-2.17451200
C	-4.77016800	1.07553500	-1.38876700
C	-4.40116200	-0.08583800	-0.69734100
C	-5.21522200	-1.22899300	-0.78122700
C	-6.38568300	-1.15484400	-1.55251000
H	-7.64998600	0.01700000	-2.84054800
H	-6.17355800	2.03133800	-2.70741100
H	-4.17652600	1.97980200	-1.29969700
H	-7.01629700	-2.03820600	-1.61940100
C	-4.83977900	-2.56496900	-0.19497300
H	-5.72827900	-3.16981900	0.01060200
H	-4.22000600	-3.10982200	-0.91524000
H	-4.26466500	-2.47383300	0.72430700
Cl	-2.32601100	-1.26850200	-2.60800100
C	-3.75796000	0.60092900	1.24741200
C	-2.12969700	0.00096300	2.84372100
C	-4.32282600	-0.27573400	2.34876500
C	-2.34860500	0.72170200	1.51579500
C	-3.11941200	-1.17004200	2.71498700
H	-3.26851500	-1.71249600	3.65333800
H	-2.84972200	-1.87346200	1.92581400
C	-2.84580500	0.85827400	3.93064000
H	-2.61872200	0.45480600	4.92235400
H	-2.50793700	1.89414400	3.90648600
C	-4.35448900	0.68081700	3.58431000
H	-4.90683200	0.20660800	4.40100500
H	-4.85688200	1.62566500	3.35686500

H	-1.09473600	-0.22594700	3.07689000
H	-5.27328000	-0.75806900	2.12258600
C	-1.64344700	2.02386500	1.29398200
O	-0.85654900	2.47768900	2.12718700
H	-4.31757800	1.47838400	0.95876500
N	-1.97089200	2.70118800	0.15182700
H	-2.38466100	2.15242600	-0.59009800
C	-1.29826700	3.93281900	-0.23007900
C	-1.63557900	4.34871000	-1.66560400
C	-1.69828200	5.16606800	0.59016300
H	-0.21607200	3.79144000	-0.13432000
C	-1.19897000	5.83014800	-1.73699100
H	-1.15247700	3.71818300	-2.41712600
C	-1.16677100	6.33567700	-0.26076300
H	-1.29674400	5.13764200	1.60463900
H	-2.79269900	5.19554600	0.65978300
H	-0.20814100	5.91536200	-2.19365800
H	-1.88235800	6.41482300	-2.35857200
H	-0.13863400	6.57297600	0.03154800
H	-1.75377700	7.24706700	-0.11916000
H	2.24306800	-2.39303400	4.85008200
H	-2.72065600	4.26319200	-1.80956100

TS2b_3

C	-2.51197600	1.64592800	-2.50120400
C	-1.64600200	2.00298000	-3.52744000
C	-0.38017300	1.42283400	-3.56578000
C	-0.01508900	0.54704100	-2.55118800
C	-0.86016300	0.18812700	-1.48273000
C	-2.16973500	0.73739800	-1.47795800
C	-3.30497200	0.41191200	-0.54809300
C	-3.68515700	1.30940800	0.47530100
C	-4.78606900	0.99083100	1.27966500
C	-5.53582000	-0.16643900	1.09241100
C	-5.18576100	-1.00547200	0.03303800
C	-4.09855100	-0.73657800	-0.79947500
C	-3.83109200	-1.65157500	-1.98952700
C	-2.97893800	2.64031800	0.71113700
P	0.05795000	-0.98063300	-0.34412300
C	-0.63576600	-1.06374800	1.38776600
C	0.02425600	-2.67426400	-1.20003200
Pd	2.47726100	-0.68106400	0.25196200
C	-4.44709200	-1.07166500	-3.27818000
C	-4.34471100	-3.08644400	-1.79579600

C	-2.86773200	3.01445600	2.19943000
C	-3.71005700	3.77735200	-0.03050100
C	-2.04421000	-1.57384800	1.73183000
C	-2.14692700	-1.77240900	3.25132300
C	-1.90336100	-0.45166200	3.98856000
C	-0.54660000	0.15588800	3.60527900
C	-0.36530300	0.28447200	2.08555000
C	-0.07215900	-2.60442600	-2.73298400
C	0.11351100	-3.99689500	-3.35389100
C	-0.88297600	-5.00933700	-2.78191500
C	-0.76477000	-5.07800700	-1.25632800
C	-0.94818800	-3.70010200	-0.60476200
H	-3.51740700	2.05116600	-2.49142500
H	0.31617200	1.64955900	-4.36805300
H	0.97189600	0.10838200	-2.56685300
H	-5.06784800	1.66404600	2.08228000
H	-5.77625100	-1.89611700	-0.14466800
H	-2.74896100	-1.69821800	-2.13365200
H	-1.96718900	2.56166900	0.30025200
H	0.07667600	-1.78594000	1.80166300
H	1.02656400	-3.03313700	-0.95383000
H	-4.03484800	-0.09149500	-3.52108400
H	-4.25613400	-1.73916800	-4.12552800
H	-5.53160900	-0.96816400	-3.16462000
H	-4.05009000	-3.50707100	-0.83107000
H	-3.94789600	-3.73259200	-2.58425200
H	-5.43685900	-3.13239300	-1.86133100
H	-2.70929500	0.24703800	3.72571000
H	-2.22386900	3.88840400	2.32063400
H	-3.84350400	3.27811800	2.61838900
H	-3.70937000	3.63024500	-1.11172600
H	-3.23522200	4.74011400	0.17900700
H	-4.75214400	3.83487500	0.30110700
H	-2.79701700	-0.85282500	1.42795400
H	-2.27166900	-2.50825300	1.22120000
H	-3.13689300	-2.17139700	3.50169500
H	-1.41054700	-2.51940800	3.57740900
H	-2.45267500	2.20377300	2.79925500
H	-1.95599000	-0.59832000	5.07381400
H	-0.41874500	1.13884400	4.07440900
H	0.25606200	-0.48479100	3.99333500
H	-1.04674800	1.03996600	1.68540600
H	0.65015500	0.63560900	1.87426500
H	-1.03786400	-2.19164800	-3.04616400

H	0.69345800	-1.93369700	-3.13305400
H	0.01417100	-3.92857800	-4.44369300
H	1.13549300	-4.34408400	-3.14971800
H	-1.90301800	-4.70718700	-3.05719400
H	-0.71853000	-5.99849600	-3.22462700
H	-1.49964600	-5.77915100	-0.84370500
H	0.22672200	-5.46504400	-0.98689200
H	-1.97925200	-3.36666900	-0.73779400
H	-0.76156900	-3.78675300	0.46756000
C	-6.68221700	-0.50936700	2.02635200
H	-6.83219400	0.35499700	2.68598300
C	-6.31727100	-1.71439900	2.91075300
H	-7.12524600	-1.94308800	3.61390600
H	-6.13913800	-2.60544900	2.29905000
H	-5.40689800	-1.51651500	3.48409300
C	-7.99792600	-0.75334600	1.27065000
H	-8.81868300	-0.92825400	1.97389100
H	-8.25859400	0.10491200	0.64406600
H	-7.92757500	-1.63256500	0.62161000
C	5.99415300	-1.35343900	3.48533400
C	4.99309200	-0.39638700	3.66105100
C	4.12397200	-0.10985300	2.60934400
C	4.23484900	-0.80212800	1.40037400
C	5.22097500	-1.77681100	1.20486300
C	6.10223900	-2.02416200	2.26935100
H	6.68997200	-1.57373500	4.28959100
H	4.89966500	0.14031400	4.60086700
H	3.38479000	0.67988700	2.70971100
H	6.87471800	-2.77866600	2.13790500
C	5.30258800	-2.63488600	-0.03152700
H	6.32139500	-3.00057800	-0.19439100
H	4.63663500	-3.49545000	0.08588300
H	4.97526100	-2.10596400	-0.92656000
Cl	2.15336400	-2.89159000	1.25710100
C	4.21883900	0.85836100	-0.14981300
C	3.22670400	1.26465800	-2.22272700
C	5.15098300	0.53695000	-1.29246100
C	2.97201600	1.24732300	-0.70325400
C	4.17404100	0.06261400	-2.38801200
H	4.63606100	0.01444500	-3.37880700
H	3.69020600	-0.89032100	-2.15793100
C	4.20674500	2.45234200	-2.47245700
H	4.32041600	2.62095100	-3.54792600
H	3.84344100	3.38329700	-2.02970300

C	5.53560600	1.95157600	-1.83382600
H	6.33093200	1.85937600	-2.57924100
H	5.90120600	2.60778800	-1.03968200
H	2.36097600	1.29457300	-2.87588400
H	6.00085400	-0.09750400	-1.04866000
C	2.24825200	2.35058600	0.01143300
O	2.55211700	2.68634400	1.15853200
H	4.58467600	1.36238400	0.72938200
N	1.29102100	2.99734400	-0.71294200
H	1.08254500	2.64787400	-1.63684400
C	0.85756800	4.35340700	-0.40189400
C	-0.26531600	4.81906700	-1.33499600
C	0.26161100	4.56008800	0.99891000
H	1.71828900	5.03213600	-0.51292300
C	-0.78600900	6.09440100	-0.65121800
H	0.07020100	4.98562700	-2.36421500
C	-0.56567600	5.86284600	0.87360400
H	1.03167100	4.59742400	1.76762700
H	-0.37546000	3.70226400	1.22677500
H	-0.20678400	6.96035800	-0.98870300
H	-1.83070300	6.29603900	-0.90263000
H	-0.03297100	6.70971000	1.31610000
H	-1.51535300	5.78207600	1.41029100
H	-1.96496400	2.70429700	-4.29202400
H	-1.04200200	4.04637100	-1.36182800

TS2c

C	3.53251300	0.18749300	2.94820000
C	3.21103500	1.17464800	3.87075300
C	2.24342500	2.11990800	3.53570300
C	1.63553500	2.05343700	2.28865000
C	1.98201900	1.08760600	1.31661000
C	2.94733200	0.11705600	1.66768400
C	3.41587100	-1.03991300	0.83512100
C	4.63809100	-0.95975300	0.13449600
C	5.09978100	-2.09083700	-0.54913800
C	4.40750900	-3.30100300	-0.53269100
C	3.22234800	-3.37084300	0.20528500
C	2.71440900	-2.26816200	0.89542800
C	1.45976100	-2.41771400	1.75088600
C	5.50167700	0.29709800	0.17568400
P	1.02387100	1.43133200	-0.24078700
C	1.72429100	3.09189400	-0.76292600
C	1.29016300	0.36706600	-1.74889500

Pd	-1.35214700	1.35119000	-0.12247300
C	1.83152100	-2.85814700	3.17971000
C	0.41290900	-3.38102100	1.17018000
C	6.11146800	0.68260800	-1.18177500
C	6.62545300	0.13356900	1.21709900
C	3.24468500	3.23070900	-0.57774000
C	3.75106300	4.51840600	-1.24503800
C	3.01561000	5.75653700	-0.71665700
C	1.49447200	5.59706000	-0.83692500
C	1.01045000	4.31184700	-0.15254500
C	0.71458600	-1.04349100	-1.56531800
C	0.66722800	-1.80733100	-2.89199500
C	2.05363200	-1.85690300	-3.54240700
C	2.60647600	-0.44313800	-3.74822700
C	2.66512400	0.33704500	-2.42576500
H	4.26275700	-0.57124700	3.20835200
H	1.94764200	2.88992800	4.24142800
H	0.84625800	2.76011300	2.05878500
H	6.03482500	-2.03311600	-1.09872800
H	2.68137400	-4.30991600	0.24780900
H	1.00277300	-1.42768600	1.82684300
H	4.86754400	1.12481500	0.50253100
H	1.48598600	3.09808500	-1.83305600
H	0.60389100	0.91502400	-2.41214000
H	2.50029000	-2.14235500	3.66257900
H	0.93084200	-2.95035500	3.79639600
H	2.33133900	-3.83270800	3.16063900
H	0.17938500	-3.16241300	0.12674100
H	-0.52400400	-3.30464300	1.72841200
H	0.74841200	-4.42153800	1.23432500
H	3.27779700	5.90218900	0.34105700
H	6.62299200	1.64685000	-1.09731300
H	6.85464700	-0.04949800	-1.51390800
H	6.22433500	-0.05596300	2.21530600
H	7.24084900	1.03842200	1.26473900
H	7.27575000	-0.70649900	0.95044600
H	3.47432400	3.25952200	0.49444100
H	3.77576800	2.36951300	-0.98621300
H	4.83167000	4.61754500	-1.08639500
H	3.59852500	4.44076800	-2.33035100
H	5.35433400	0.76848200	-1.96355800
H	3.35213300	6.65363000	-1.24935600
H	0.98558400	6.46430700	-0.40041700
H	1.20504800	5.56301200	-1.89537900

H	1.24236400	4.38097700	0.91717300
H	-0.06940000	4.20240100	-0.26577800
H	1.34274900	-1.59684500	-0.86821700
H	-0.28665500	-0.98614200	-1.13136600
H	0.28655900	-2.82048800	-2.71713800
H	-0.04176400	-1.31512100	-3.57160100
H	2.73496000	-2.41118500	-2.88425400
H	2.01529200	-2.39591500	-4.49639400
H	3.60871600	-0.48277900	-4.19144400
H	1.96687900	0.09800300	-4.45893400
H	3.38726700	-0.13969200	-1.76155400
H	3.01413500	1.35373800	-2.62473700
C	4.96698500	-4.52469200	-1.23973000
H	5.83298900	-4.19200900	-1.82625900
C	3.95968400	-5.15926400	-2.21112100
H	4.40869800	-6.01719300	-2.72245600
H	3.06986000	-5.51774600	-1.68330500
H	3.63178500	-4.44292000	-2.96889000
C	5.46521100	-5.55842300	-0.21387200
H	5.91832500	-6.41970800	-0.71618300
H	6.20945100	-5.11943000	0.45736900
H	4.63597300	-5.92468100	0.40091900
C	-5.88792900	1.93185700	-1.64943500
C	-5.50595500	2.56979500	-0.47065000
C	-4.30159000	2.21580600	0.14163400
C	-3.47507900	1.23329100	-0.41088300
C	-3.83958700	0.60113700	-1.62064200
C	-5.04977600	0.97120900	-2.21733400
H	-6.82584800	2.18797500	-2.13316100
H	-6.13340600	3.33845600	-0.02878600
H	-4.00744100	2.72008700	1.05498900
H	-5.33149900	0.49956800	-3.15537100
C	-2.94137700	-0.38220600	-2.32458800
H	-3.49575000	-0.94737600	-3.07899400
H	-2.13871900	0.16931000	-2.82435000
H	-2.48145000	-1.09302700	-1.63581900
Cl	-1.33720000	2.77902100	-2.12246000
C	-1.41895200	-0.05893800	1.44108200
C	-3.42226500	0.58054300	2.50422400
C	-1.19340800	0.47523100	2.84926100
C	-2.83961000	-0.04367100	1.23233900
C	-2.30117800	1.54244800	2.94485600
H	-2.45264400	1.92332600	3.95964100
H	-2.14370600	2.37768900	2.25665700

C	-3.27736300	-0.53666900	3.58615800
H	-3.79357300	-0.21486700	4.49540900
H	-3.72633000	-1.48161500	3.27365200
C	-1.73907200	-0.62434000	3.80627800
H	-1.46725600	-0.40193200	4.84305700
H	-1.33528200	-1.61062400	3.56188700
H	-4.43067400	0.98142600	2.42025300
H	-0.17918300	0.79091700	3.07298800
C	-3.50480100	-1.29821700	0.69370900
O	-2.85143000	-2.30260600	0.41502300
H	-0.87782700	-0.93720600	1.11088800
N	-4.86222100	-1.26320700	0.66663600
H	-5.30090300	-0.35155000	0.66382300
C	-5.64639500	-2.39029900	0.19416300
C	-7.10936800	-2.31383800	0.65880600
C	-5.76676200	-2.52720400	-1.33294400
H	-5.16502700	-3.29107000	0.58811100
C	-7.88826800	-3.23544600	-0.31508400
H	-7.22981500	-2.58987600	1.70990500
C	-6.91261500	-3.53764600	-1.49100700
H	-4.82845300	-2.84237200	-1.79410600
H	-6.04116800	-1.55313800	-1.75312000
H	-8.20420800	-4.15926200	0.17782300
H	-8.79804500	-2.74196000	-0.66838500
H	-6.52005100	-4.55626500	-1.39769800
H	-7.39997600	-3.47309600	-2.46765000
H	3.69675900	1.19414800	4.84138200
H	-7.45546100	-1.27715100	0.55475300

16

C	3.36612400	1.14351600	3.12541600
C	2.59777800	1.87972800	4.01888900
C	1.37650800	2.39499500	3.59034400
C	0.95554700	2.16525500	2.28662600
C	1.73743200	1.44549000	1.35567100
C	2.97271800	0.91506600	1.79212600
C	3.93549700	0.08918000	0.99189200
C	5.08639800	0.69584500	0.43843700
C	6.03017500	-0.10953200	-0.20945000
C	5.88334800	-1.49309200	-0.30186500
C	4.75428000	-2.07451700	0.27921700
C	3.77336400	-1.31401300	0.92115200
C	2.57917900	-2.01301100	1.56643900
C	5.33931600	2.19777300	0.56402800

P	0.78442500	1.15391400	-0.20683500
C	0.23415600	2.86982700	-0.78725200
C	1.74002800	0.66859600	-1.74079600
Pd	-0.85091200	-0.67364200	-0.02000500
C	2.88469500	-2.32846200	3.04315500
C	2.14943800	-3.29553000	0.83776400
C	5.97410100	2.82981700	-0.68665300
C	6.23035500	2.49921200	1.78464700
C	1.04530800	4.06959100	-0.27234200
C	0.60625500	5.35560400	-0.98864100
C	-0.90088200	5.59719000	-0.83000800
C	-1.71140000	4.39005300	-1.31929500
C	-1.27496200	3.09955800	-0.61474500
C	1.99720000	-0.83683800	-1.87300200
C	2.51192300	-1.18640600	-3.27437700
C	3.76345300	-0.36859100	-3.61724000
C	3.48583600	1.13512900	-3.50587600
C	2.96994900	1.50057200	-2.10676100
H	4.30383200	0.70841700	3.45468100
H	0.73299200	2.94574900	4.26895800
H	-0.04237300	2.48676300	2.01576100
H	6.90835900	0.35111500	-0.65141500
H	4.62935600	-3.14982500	0.22270600
H	1.72689900	-1.32585100	1.54021300
H	4.37089700	2.68207300	0.72875900
H	0.41520100	2.80612700	-1.86814500
H	0.95670700	0.90032200	-2.47435300
H	3.06040500	-1.41720200	3.61850800
H	2.04818400	-2.86367400	3.50130500
H	3.77688100	-2.95974200	3.12035900
H	2.00381600	-3.12869200	-0.23167400
H	1.20321900	-3.65598300	1.24819900
H	2.88306000	-4.09907400	0.96244700
H	-1.12517300	5.77223800	0.23134400
H	5.99663200	3.91874400	-0.57740000
H	7.00890800	2.49967700	-0.82382700
H	5.76596700	2.17026900	2.71538800
H	6.42159100	3.57484800	1.86343100
H	7.19485400	1.98908500	1.68668900
H	0.89243100	4.19027400	0.80423500
H	2.11836200	3.89902300	-0.41177300
H	1.17268000	6.20966300	-0.59918100
H	0.85061200	5.27735200	-2.05749700
H	5.42294400	2.59273300	-1.59895400

H	-1.19923300	6.50382900	-1.36922300
H	-2.78226500	4.56182400	-1.15508300
H	-1.57411900	4.27626100	-2.40430900
H	-1.52992700	3.15048300	0.44717200
H	-1.81843100	2.24007500	-1.01844800
H	2.73506300	-1.15195400	-1.13740700
H	1.07337800	-1.39306800	-1.66023300
H	2.72858400	-2.25946600	-3.33099800
H	1.72566200	-0.98163300	-4.01480300
H	4.56548300	-0.63252800	-2.91567500
H	4.12014100	-0.61854700	-4.62328400
H	4.39351200	1.70889800	-3.72897400
H	2.73774900	1.42477400	-4.25732000
H	3.75122100	1.30260900	-1.37556400
H	2.74124400	2.56961700	-2.05941800
C	6.93550900	-2.34626700	-0.98966000
H	7.68557200	-1.66224800	-1.40748700
C	6.34780700	-3.16133600	-2.15350100
H	7.13233100	-3.73683400	-2.65626200
H	5.59180900	-3.87010800	-1.79921600
H	5.87315200	-2.51067200	-2.89331900
C	7.64823500	-3.26315900	0.01916400
H	8.44262000	-3.83694600	-0.46993800
H	8.09272800	-2.68235200	0.83286900
H	6.94493900	-3.97561300	0.46348700
C	-2.75467600	-4.24014700	-1.43336400
C	-1.88858100	-3.15241900	-1.29340300
C	-1.99673300	-2.30850200	-0.18051500
C	-2.95592400	-2.59259800	0.80995700
C	-3.86182800	-3.66102600	0.65610900
C	-3.74441300	-4.47529200	-0.47658100
H	-2.67284200	-4.89393100	-2.29818900
H	-1.15153000	-2.95149800	-2.06788100
H	-4.43409100	-5.30568800	-0.60601000
C	-4.93990600	-3.93149600	1.67839400
H	-5.65102900	-4.67683200	1.31146600
H	-4.52605600	-4.30371100	2.62223100
H	-5.50091300	-3.02170900	1.92212700
C	-2.89880300	-1.71580100	2.02110300
C	-0.90505900	-0.64796100	2.95378400
C	-2.28582400	-2.41010000	3.27581800
C	-1.90432500	-0.51311300	1.79148900
C	-0.78035300	-2.17791300	3.07156200
H	-0.18426200	-2.49077200	3.93459600

H	-0.39242200	-2.64728300	2.16688000
C	-1.61885700	-0.31024300	4.29288300
H	-0.87178600	-0.25250200	5.09147000
H	-2.12992700	0.65085600	4.25088400
C	-2.57730600	-1.52296800	4.50445800
H	-2.34759900	-2.05749600	5.43193400
H	-3.63059400	-1.22585800	4.55178900
H	0.01554200	-0.08910100	2.81282100
H	-2.60145600	-3.44957800	3.38498900
C	-2.56617500	0.82958100	1.65042900
O	-2.13169000	1.85947600	2.18349500
H	-3.89798400	-1.34396500	2.28836700
N	-3.71723800	0.85615000	0.90631800
H	-4.05352900	-0.01691800	0.52579500
C	-4.56847500	2.02279700	0.81664800
C	-5.07358600	2.34789800	-0.59574900
C	-5.87259500	1.91636900	1.63481600
H	-3.96763700	2.85501300	1.19141300
C	-6.17608800	3.38633400	-0.33846500
H	-4.28085100	2.70805500	-1.25631000
C	-6.82040900	2.97556600	1.02001600
H	-5.69493700	2.05537300	2.70450000
H	-6.28532400	0.90809600	1.50359300
H	-5.72435100	4.38084700	-0.25242600
H	-6.90448200	3.43735800	-1.15234000
H	-6.92686300	3.84469100	1.67537700
H	-7.82452100	2.56601800	0.87740600
H	2.93997900	2.02900500	5.03841900
H	-5.49903000	1.44118600	-1.04539400
C	-6.15052500	-2.63003100	-2.70304700
H	-7.02105700	-2.79158700	-2.05953300
H	-5.54796600	-3.54294500	-2.68660600
H	-6.51188500	-2.47673000	-3.72596500
C	-5.32082700	-1.43819600	-2.22225700
H	-4.98368000	-1.62956900	-1.19608200
H	-5.94579000	-0.53535000	-2.19591900
C	-4.08508700	-1.19926400	-3.10339600
H	-4.38155400	-1.02377300	-4.14414400
H	-3.46854300	-2.09980400	-3.08300800
C	-3.27527100	-0.02673400	-2.58732300
H	-3.06678500	-0.09853600	-1.52216900
H	-3.71381300	0.94146400	-2.82148900
Br	-1.45306800	0.03029700	-3.38967300

TS4

C	3.33758800	1.03835100	3.12815300
C	2.46201200	1.59814000	4.04922000
C	1.15621100	1.86934100	3.64980100
C	0.77251200	1.59271400	2.34446400
C	1.65621800	1.06089200	1.37910400
C	2.97527300	0.75618900	1.79433900
C	4.09152100	0.14694600	0.99802300
C	5.11832500	0.98387100	0.50880500
C	6.23587800	0.40403000	-0.10246700
C	6.37230300	-0.97562300	-0.23355200
C	5.35529900	-1.78794900	0.27730100
C	4.22465100	-1.25999200	0.90606000
C	3.19339000	-2.20154600	1.52913200
C	5.06036000	2.50042200	0.66294900
P	0.75518900	0.90681600	-0.24851700
C	0.46045200	2.70091100	-0.71480800
C	1.73307500	0.24321200	-1.69199200
Pd	-1.45602200	-0.50576300	-0.59574000
C	3.45173200	-2.38922100	3.03675500
C	3.13039900	-3.58142600	0.85574900
C	5.42826900	3.25561700	-0.62495600
C	5.96820800	2.96442900	1.81706400
C	1.60213600	3.68576600	-0.41979800
C	1.28549100	5.07204800	-1.00375400
C	-0.05546800	5.61495100	-0.49209400
C	-1.19279400	4.61116700	-0.72704800
C	-0.84776200	3.24778000	-0.11691000
C	1.87750500	-1.28149800	-1.59835700
C	2.35993400	-1.87746000	-2.92411400
C	3.67004100	-1.21830500	-3.37087800
C	3.49946500	0.29938100	-3.49390300
C	3.01946000	0.92250300	-2.17349100
H	4.34898600	0.79144100	3.43370500
H	0.42373100	2.26585300	4.34562200
H	-0.27291700	1.71982200	2.09864000
H	7.02645100	1.04513900	-0.48192100
H	5.45612000	-2.86399600	0.19350400
H	2.20977000	-1.73336900	1.42365800
H	4.03338300	2.76819000	0.92274200
H	0.31640400	2.62922000	-1.80151300
H	0.98308200	0.42655100	-2.46871200
H	3.39500900	-1.44384000	3.57762700
H	2.70754400	-3.06925600	3.46577100

H	4.44389800	-2.82283900	3.20330700
H	3.02815600	-3.51151300	-0.23001100
H	2.27343900	-4.14142000	1.23854600
H	4.02513000	-4.17401500	1.07374300
H	0.02604200	5.81115800	0.58604200
H	5.24460200	4.32718500	-0.49443800
H	6.48724000	3.13648800	-0.87575800
H	5.66948000	2.51535900	2.76699800
H	5.92388700	4.05333400	1.92777000
H	7.00982700	2.68538000	1.62434900
H	1.72798200	3.76297200	0.66697500
H	2.55115100	3.32313200	-0.81774900
H	2.09523600	5.77114700	-0.76309400
H	1.25154800	4.99665700	-2.09957700
H	4.84254200	2.91081700	-1.47954500
H	-0.28431500	6.57455300	-0.97007000
H	-2.12873900	4.98930700	-0.29821800
H	-1.36175300	4.49353700	-1.80700600
H	-0.73578200	3.36518000	0.96597100
H	-1.65855500	2.53149200	-0.25652800
H	2.59716900	-1.52471700	-0.81933700
H	0.91772300	-1.72861500	-1.31082100
H	2.49138200	-2.96117300	-2.81794500
H	1.58786300	-1.72437300	-3.69044600
H	4.44688600	-1.43096100	-2.62549500
H	4.01150900	-1.64357500	-4.32210100
H	4.44403600	0.76830700	-3.79500100
H	2.76994800	0.51793300	-4.28613900
H	3.80497100	0.82031200	-1.42717500
H	2.84354700	1.99134300	-2.32500100
C	7.60759100	-1.57877400	-0.88009500
H	8.25326700	-0.74492000	-1.18458700
C	7.26088600	-2.38414000	-2.14283100
H	8.16747500	-2.79076100	-2.60358500
H	6.60068200	-3.22538600	-1.90573800
H	6.75088800	-1.75992700	-2.88169900
C	8.39714000	-2.43807100	0.12216300
H	9.31998900	-2.81502700	-0.33140600
H	8.66187800	-1.86040800	1.01288600
H	7.80831500	-3.30221800	0.44786600
C	-3.90062400	-3.52067300	-2.51441900
C	-3.02534300	-2.45431400	-2.30116700
C	-2.72425200	-2.04376900	-0.99617400
C	-3.25951400	-2.75896200	0.09115300

C	-4.17689600	-3.81185300	-0.12109500
C	-4.49138400	-4.17472000	-1.43302000
H	-4.12931300	-3.83466200	-3.52976200
H	-2.59297500	-1.93620500	-3.14861400
H	-5.19569000	-4.98450600	-1.60663700
C	-4.81724600	-4.53714500	1.03896900
H	-5.60326900	-5.21251100	0.69025600
H	-4.09196500	-5.13443300	1.60214500
H	-5.26725200	-3.83934200	1.75507400
C	-2.78102400	-2.37176900	1.45299500
C	-0.66344400	-1.42145000	2.17379500
C	-1.78569600	-3.38033700	2.10813700
C	-1.94137600	-1.04590600	1.40753300
C	-0.41839100	-2.84882400	1.65150100
H	0.41293300	-3.35135900	2.15485500
H	-0.26761100	-2.89470200	0.56964000
C	-1.00484400	-1.69288500	3.66330300
H	-0.08110800	-1.75404300	4.24791600
H	-1.60585900	-0.88811700	4.09073700
C	-1.74243600	-3.06787600	3.61873900
H	-1.17933000	-3.83815400	4.15593400
H	-2.74433800	-3.02904300	4.05936800
H	0.14977000	-0.71852200	2.05396200
H	-2.00246900	-4.42229800	1.86571200
C	-2.68161500	0.16409100	1.88763600
O	-2.17282900	1.10809700	2.50580600
H	-3.63092500	-2.26492300	2.14183200
N	-4.02592200	0.20848100	1.58904300
H	-4.45579200	-0.61179400	1.18705300
C	-4.88350900	1.24715600	2.13976300
C	-4.77632200	2.62430800	1.45752500
C	-6.38349400	0.87150200	2.05078800
H	-4.59737500	1.38629200	3.18899900
C	-6.07741300	3.31017900	1.88650500
H	-3.86361100	3.14841700	1.74751900
C	-7.13541500	2.19492000	1.74249300
H	-6.72526400	0.40511200	2.97886800
H	-6.54891800	0.13812300	1.25282100
H	-6.00129500	3.62595000	2.93431600
H	-6.31503600	4.20006500	1.29637700
H	-7.99975300	2.34713900	2.39449300
H	-7.51109400	2.17696800	0.71370900
H	2.79153700	1.79509100	5.06499600
H	-4.76274800	2.49455800	0.36899300

C	-7.00370200	0.45058700	-2.87615100
H	-7.99272000	0.72202000	-2.49396300
H	-6.97553400	-0.63639200	-3.00496500
H	-6.88703700	0.90795900	-3.86408100
C	-5.90097100	0.91281300	-1.92063900
H	-6.04998600	0.45879700	-0.93492500
H	-5.95975700	1.99867800	-1.77752000
C	-4.49887700	0.51961100	-2.45262700
H	-4.33373500	0.94211100	-3.44657000
H	-4.46733900	-0.56855700	-2.54325700
C	-3.45929300	0.98449100	-1.49751800
H	-3.58460600	0.68782100	-0.46393200
H	-3.04003800	1.97107300	-1.63806000
Br	-1.40053300	0.44770300	-3.07264800

17

C	3.15883200	1.76371500	2.74772700
C	2.33920900	2.57018200	3.52539900
C	1.04018200	2.82060700	3.08910100
C	0.60941800	2.24797100	1.90139400
C	1.42254100	1.42985500	1.08289700
C	2.74514800	1.18605800	1.52830600
C	3.83009200	0.39901300	0.84751700
C	4.79363900	1.07938000	0.07122900
C	5.87239000	0.35957300	-0.45617200
C	6.04519100	-1.00106300	-0.21155500
C	5.10506400	-1.64582900	0.59725500
C	4.00690900	-0.97472200	1.13866700
C	3.05366700	-1.71326800	2.07361700
C	4.73468400	2.58879500	-0.14048600
P	0.43479200	0.88542300	-0.41096600
C	0.16486200	2.52428300	-1.30548000
C	1.31303500	-0.15048000	-1.68266300
Pd	-2.00201100	-0.40608100	-0.40439300
C	3.51034200	-1.57920100	3.53911900
C	2.87598800	-3.20109700	1.73390900
C	5.03450500	3.02307800	-1.58402300
C	5.69826500	3.29981200	0.82871800
C	1.31805600	3.53452700	-1.22791200
C	1.04765300	4.73924900	-2.14283100
C	-0.29471400	5.40778400	-1.82112500
C	-1.44243700	4.39136700	-1.86035800
C	-1.16267000	3.20522300	-0.93073400
C	1.61942400	-1.56053400	-1.16385800

C	2.04915000	-2.48685900	-2.30601300
C	3.24855700	-1.90092100	-3.05994300
C	2.92918400	-0.49780500	-3.58776800
C	2.49615800	0.44477500	-2.45456900
H	4.17419200	1.56432500	3.07318400
H	0.36325100	3.44186700	3.66720700
H	-0.41005000	2.44078500	1.59299600
H	6.60877700	0.87814800	-1.06298600
H	5.23505800	-2.69970500	0.81593700
H	2.07618900	-1.23052900	1.98803000
H	3.72320100	2.92037100	0.10331100
H	0.05177800	2.18644400	-2.34130400
H	0.47820300	-0.23884100	-2.39112300
H	3.54473500	-0.53661600	3.85979700
H	2.82246200	-2.11402600	4.20324300
H	4.50906100	-2.00993400	3.66919600
H	2.61874100	-3.35854800	0.68420500
H	2.07568100	-3.62704700	2.34520200
H	3.78410300	-3.77362500	1.94941500
H	-0.24276100	5.85196700	-0.81665900
H	4.85660000	4.09777000	-1.69381000
H	6.07947600	2.83899300	-1.85364800
H	5.45677900	3.07482000	1.87025800
H	5.64611900	4.38572700	0.69515900
H	6.73114500	2.98429000	0.64628300
H	1.43227100	3.87971400	-0.19291100
H	2.26205600	3.06508200	-1.50731800
H	1.86679600	5.46275800	-2.05348000
H	1.04089900	4.39945800	-3.18751700
H	4.40617700	2.49993600	-2.30813700
H	-0.48675500	6.23081100	-2.51891500
H	-2.38896200	4.86999900	-1.58224800
H	-1.57080400	4.00893100	-2.88097600
H	-1.12303100	3.57213500	0.10300400
H	-1.97871800	2.48291200	-1.00621100
H	2.43302500	-1.50371100	-0.44389900
H	0.74713500	-1.97507500	-0.65205700
H	2.29246200	-3.47822200	-1.90522800
H	1.20914200	-2.62584200	-2.99922600
H	4.10206500	-1.83705300	-2.37279000
H	3.54652300	-2.56059400	-3.88350600
H	3.80039400	-0.07475000	-4.10207700
H	2.12260400	-0.56279400	-4.33071800
H	3.33693400	0.60008200	-1.77734000

H	2.22321000	1.41651700	-2.87663400
C	7.25275500	-1.74477200	-0.75683000
H	7.79298200	-1.04962100	-1.41225500
C	6.85598000	-2.96854600	-1.59764500
H	7.74636600	-3.46591800	-1.99631600
H	6.30798100	-3.70170200	-0.99631000
H	6.21732000	-2.68327700	-2.43787800
C	8.20388500	-2.14721000	0.38426800
H	9.10304200	-2.63189500	-0.01057200
H	8.51113700	-1.27388200	0.96746200
H	7.71596300	-2.85022500	1.06792700
C	-1.57309700	-4.36775100	-1.82015600
C	-1.52272400	-2.97581200	-1.72167600
C	-1.91338400	-2.39622600	-0.52076700
C	-2.35146900	-3.13448600	0.58413700
C	-2.45584700	-4.53402300	0.44860200
C	-2.05881000	-5.12709100	-0.75711300
H	-1.27027000	-4.85162000	-2.74428700
H	-1.23417800	-2.36028900	-2.56403500
H	-2.14314800	-6.20560400	-0.86299100
C	-3.00415400	-5.40396800	1.55605200
H	-3.49230800	-6.28914600	1.13830000
H	-2.21382200	-5.75773300	2.22849500
H	-3.73628400	-4.87041600	2.16785500
C	-2.64741500	-2.37212400	1.84745600
C	-1.05349200	-0.66172800	2.56268800
C	-1.68589700	-2.78080200	3.00042400
C	-2.29063800	-0.86177800	1.64682200
C	-0.40081700	-2.05144500	2.57423600
H	0.40163500	-2.12617400	3.31391200
H	-0.02429000	-2.37154600	1.60091800
C	-1.55842100	-0.58308300	4.02776000
H	-0.70967600	-0.34855800	4.67913100
H	-2.31388400	0.18918600	4.18521000
C	-2.09389300	-2.02287800	4.28469300
H	-1.63158300	-2.47174900	5.16912800
H	-3.17750100	-2.03442700	4.42938100
H	-0.41350800	0.16924800	2.29476400
H	-1.60067900	-3.85854300	3.13350900
C	-3.40523300	0.10310900	1.98941200
O	-4.49293900	-0.23768800	2.45160600
H	-3.69414900	-2.47370200	2.15169000
N	-3.09821100	1.41311400	1.73296300
H	-2.19889900	1.61141000	1.31808100

C	-4.04800600	2.50400900	1.86172400
C	-3.38731800	3.81718100	2.37734900
C	-4.74546600	2.88741100	0.53614500
H	-4.79911700	2.15016100	2.57042700
C	-3.85878700	4.93953100	1.42296100
H	-3.69413000	4.01181400	3.40908700
C	-5.10738700	4.36380800	0.72892100
H	-5.59859500	2.23824300	0.32242400
H	-4.03495100	2.78375200	-0.29171300
H	-4.05209100	5.88239200	1.94216300
H	-3.08671800	5.13773100	0.67104100
H	-5.98045900	4.45463200	1.38739200
H	-5.34929400	4.87354300	-0.20821700
H	2.70849700	2.99210100	4.45472700
H	-2.29570800	3.72897500	2.39101300
C	-6.48692600	-2.45410500	-3.25600700
H	-7.54065200	-2.27448000	-3.49331300
H	-6.38771400	-3.49757500	-2.93659800
H	-5.90848200	-2.33337600	-4.17841700
C	-5.98570300	-1.49818200	-2.17033900
H	-6.59238100	-1.61658600	-1.26272900
H	-6.11863500	-0.46021600	-2.50133100
C	-4.50062300	-1.73509200	-1.83837700
H	-3.90326900	-1.56475300	-2.73672600
H	-4.36151600	-2.77841000	-1.53915000
C	-4.06218100	-0.81168000	-0.72510000
H	-4.46045200	-1.11845700	0.23786100
H	-4.31029000	0.23344000	-0.93090700
Br	-2.00269700	0.38885700	-2.92185500

TS5

C	2.82939300	2.11570400	2.40230400
C	1.99778100	3.12369100	2.87149900
C	0.82932300	3.40702500	2.16735500
C	0.51056900	2.63468200	1.05964200
C	1.31024200	1.56624700	0.59169500
C	2.53731700	1.33414500	1.26335400
C	3.67954900	0.44804600	0.84430800
C	4.69095900	1.01439600	0.03434800
C	5.82740600	0.25517900	-0.26547300
C	6.00536700	-1.03634500	0.22387400
C	5.01324500	-1.56300500	1.05452700
C	3.86338500	-0.84343400	1.38987500
C	2.86558400	-1.43879500	2.37636200

C	4.61363600	2.45169500	-0.46929400
P	0.41482700	0.69346900	-0.79726400
C	0.23712300	2.04516500	-2.09632400
C	1.35660200	-0.63959600	-1.69263100
Pd	-1.79476600	-0.52209800	-0.49861700
C	3.19659000	-1.01683400	3.82122800
C	2.77199300	-2.97161200	2.31243500
C	5.05174000	2.60920300	-1.93421600
C	5.44818200	3.37994800	0.43308100
C	1.40105700	3.04176800	-2.18249400
C	1.24319700	3.94446300	-3.41558600
C	-0.10817400	4.66998600	-3.41727900
C	-1.27159100	3.67939800	-3.27943000
C	-1.10558500	2.79439200	-2.03820000
C	1.47000500	-1.92078900	-0.85682600
C	1.94663400	-3.09237900	-1.72192100
C	3.27162500	-2.75571700	-2.41536000
C	3.14081900	-1.48224500	-3.25856400
C	2.66455300	-0.29048800	-2.41257100
H	3.77165700	1.92850700	2.90602800
H	0.17115600	4.21477800	2.47263800
H	-0.39480500	2.87243700	0.51654800
H	6.60252900	0.68534700	-0.89253000
H	5.14544600	-2.55978700	1.45976400
H	1.88318800	-1.02773700	2.13052700
H	3.57419500	2.77690600	-0.39814300
H	0.21272000	1.44674500	-3.01366400
H	0.60842800	-0.84195800	-2.46916300
H	3.14715800	0.06517400	3.95159300
H	2.48868600	-1.47187100	4.52262500
H	4.20377800	-1.34904700	4.09469300
H	2.63511400	-3.33739600	1.29244600
H	1.92629100	-3.31858300	2.91158200
H	3.67066500	-3.44336100	2.72287100
H	-0.13618700	5.37563300	-2.57455600
H	4.82225400	3.62023500	-2.28570900
H	6.12989700	2.46266600	-2.05289000
H	5.09568100	3.35392500	1.46705400
H	5.38855200	4.41509100	0.07997700
H	6.50120000	3.07866900	0.42726600
H	1.42301000	3.66099700	-1.27758300
H	2.35667700	2.51839200	-2.22662600
H	2.06712400	4.66717300	-3.45264300
H	1.32454400	3.32737800	-4.32075700

H	4.54426100	1.89722200	-2.58944900
H	-0.21752600	5.26687100	-4.33002000
H	-2.22589200	4.21653800	-3.22780700
H	-1.32002600	3.03374000	-4.16575500
H	-1.14531700	3.43465900	-1.14989800
H	-1.92775100	2.07925800	-1.97003500
H	2.18363800	-1.76166700	-0.05019700
H	0.50126100	-2.15821900	-0.40508500
H	2.05398100	-3.99107300	-1.10252200
H	1.17875100	-3.31703800	-2.47422400
H	4.04317900	-2.60096400	-1.65045000
H	3.60328200	-3.59353000	-3.03996700
H	4.09970200	-1.23450200	-3.72956600
H	2.42293500	-1.65761100	-4.07121400
H	3.43929600	-0.03337700	-1.69073900
H	2.51627500	0.57697900	-3.06300100
C	7.25513300	-1.83227900	-0.11029400
H	7.88103400	-1.19820600	-0.75130400
C	6.92202200	-3.10955700	-0.89875200
H	7.83573100	-3.65661900	-1.15380500
H	6.28390400	-3.77873900	-0.31167800
H	6.39238300	-2.87453100	-1.82621100
C	8.06469700	-2.15995900	1.15574700
H	8.99319000	-2.68028800	0.89809500
H	8.32118900	-1.24971000	1.70603300
H	7.49531100	-2.80861300	1.82983100
C	-2.44017000	-4.70488100	-1.09755300
C	-2.34709400	-3.33935300	-1.35542700
C	-2.56315500	-2.43744200	-0.30946200
C	-2.81550500	-2.87638300	1.00425600
C	-3.02288000	-4.25346300	1.22662200
C	-2.82171100	-5.14787600	0.16709100
H	-2.26329700	-5.41792600	-1.89761100
H	-2.13623900	-2.97193200	-2.35120100
H	-2.97612900	-6.20966500	0.34260600
C	-3.50119200	-4.80815100	2.55147000
H	-4.16724800	-5.65856300	2.37637400
H	-2.67676200	-5.17232100	3.17560200
H	-4.05320100	-4.06621100	3.13287300
C	-2.81635600	-1.83390700	2.09280600
C	-0.95745600	-0.28492300	2.49272100
C	-1.86424300	-2.19640400	3.26844600
C	-2.20772700	-0.46840600	1.59514800
C	-0.50834300	-1.73587300	2.72056900

H	0.29284900	-1.81673900	3.45960200
H	-0.21419600	-2.25221000	1.80409000
C	-1.41757200	0.09772300	3.92483800
H	-0.53819700	0.34570800	4.52913400
H	-2.08017100	0.96479600	3.94630300
C	-2.10551100	-1.20493200	4.42801500
H	-1.64521300	-1.56817000	5.35221300
H	-3.17244400	-1.06303900	4.62304700
H	-0.20602400	0.39324200	2.09997400
H	-1.91477600	-3.23793900	3.57413300
C	-3.20706300	0.66551500	1.70763900
O	-4.40485800	0.48975600	1.94606700
H	-3.83219900	-1.66001700	2.46368300
N	-2.69256900	1.91881200	1.51912800
H	-1.68722600	1.99651500	1.50798800
C	-3.45725800	3.12101700	1.77900900
C	-3.20248000	3.74669200	3.17120800
C	-3.16826200	4.27595800	0.81042200
H	-4.50668700	2.82833600	1.69551600
C	-3.55270900	5.25147800	3.01991500
H	-3.78034300	3.24083300	3.94900800
C	-3.82977700	5.47198400	1.50647700
H	-3.53910400	4.08496200	-0.20014300
H	-2.08350600	4.43737700	0.74019500
H	-4.41773900	5.53415800	3.62599000
H	-2.71819000	5.87501000	3.35587400
H	-4.90875000	5.44837100	1.31598800
H	-3.46122600	6.43579400	1.14457500
H	2.27234200	3.69379600	3.75323300
H	-2.14336700	3.61852400	3.42549600
C	-6.91048300	-1.73033300	-3.19181900
H	-7.82744000	-1.18733300	-3.44272100
H	-7.19810800	-2.71960500	-2.81876500
H	-6.34198600	-1.87645600	-4.11670200
C	-6.07830100	-0.97145600	-2.15483200
H	-6.67186000	-0.81190500	-1.24537400
H	-5.82475400	0.02369900	-2.54168700
C	-4.77894400	-1.71923000	-1.80613100
H	-4.17176500	-1.80759700	-2.70926000
H	-5.01522900	-2.72934800	-1.45666100
C	-4.02473500	-0.95808900	-0.74088000
H	-4.47206300	-1.01108800	0.24392800
H	-3.91045300	0.09124800	-1.03451600
Br	-1.79274400	-0.47053300	-3.16811600

18

C	2.61368200	1.52703200	2.97229200
C	1.58331000	2.14615800	3.66726100
C	0.35239200	2.31622600	3.03637000
C	0.18779100	1.84338800	1.74345000
C	1.21457400	1.19253100	1.02470100
C	2.47381600	1.04492900	1.65352400
C	3.74960100	0.49832500	1.07599600
C	4.68650400	1.40967000	0.53900800
C	5.93238300	0.93446700	0.11399500
C	6.28920400	-0.40690700	0.22522400
C	5.36283400	-1.28557100	0.79390500
C	4.10595500	-0.86260600	1.23387900
C	3.16813600	-1.85880600	1.91219900
C	4.40688700	2.90735700	0.47015600
P	0.54603100	0.62423100	-0.61367400
C	0.15132300	2.22688300	-1.52273800
C	1.71602200	-0.19277600	-1.80884400
Pd	-1.29058700	-0.81058500	-0.57719300
C	3.30155500	-1.79886700	3.44594800
C	3.36880000	-3.31032000	1.44837900
C	4.80824600	3.54323800	-0.87100200
C	5.11127800	3.63619200	1.62962600
C	1.07750800	3.39766200	-1.15777700
C	0.81754200	4.60379800	-2.07128100
C	-0.65145900	5.03936400	-2.01739100
C	-1.58291200	3.86793100	-2.35041100
C	-1.31805400	2.66037500	-1.44290800
C	2.08906500	-1.61877000	-1.40019200
C	2.76641800	-2.35958200	-2.55683300
C	3.99617800	-1.58636100	-3.04793700
C	3.61534300	-0.16019600	-3.46035000
C	2.93066400	0.59857900	-2.31212200
H	3.58168900	1.40736200	3.44715300
H	-0.48054500	2.78768300	3.54761700
H	-0.78739900	1.94045500	1.28775700
H	6.65116800	1.63237200	-0.30521200
H	5.63283800	-2.32939500	0.90479300
H	2.14538900	-1.56626600	1.66068900
H	3.33249400	3.05417400	0.59854600
H	0.33328300	1.93479500	-2.56406100
H	1.00940000	-0.28263800	-2.64413400
H	3.03901100	-0.81596200	3.83863000

H	2.63712300	-2.53407900	3.91218200
H	4.32882200	-2.02746700	3.74987600
H	3.36887700	-3.40444200	0.35978000
H	2.56483200	-3.93856800	1.83991300
H	4.31093500	-3.72401900	1.82289500
H	-0.87933900	5.40627100	-1.00627700
H	4.46472000	4.58213400	-0.90890700
H	5.89459400	3.55635900	-1.00450800
H	4.77426700	3.26093100	2.59886900
H	4.90485400	4.71114100	1.59072400
H	6.19599200	3.49591400	1.57203300
H	0.89991100	3.68745100	-0.11570900
H	2.12448400	3.09910700	-1.22302000
H	1.47586000	5.43203000	-1.78389900
H	1.07970400	4.33649600	-3.10421000
H	4.37528600	3.01079000	-1.72116600
H	-0.82754900	5.87641700	-2.70246200
H	-2.63184000	4.17400900	-2.25911300
H	-1.43561500	3.56445600	-3.39515400
H	-1.56703900	2.93039600	-0.41145700
H	-1.95052800	1.82262300	-1.74807600
H	2.77201400	-1.58096300	-0.55485900
H	1.18983200	-2.15214100	-1.07947800
H	3.05142700	-3.36852100	-2.23451100
H	2.04797400	-2.47805500	-3.37870000
H	4.73359600	-1.53973600	-2.23643400
H	4.47219300	-2.11048500	-3.88488100
H	4.50373500	0.39559600	-3.78290300
H	2.93493500	-0.20185200	-4.32143700
H	3.64670000	0.74906800	-1.50438000
H	2.62184300	1.58579000	-2.66791300
C	7.66168000	-0.88703000	-0.21492400
H	8.18300600	-0.02303300	-0.64675900
C	7.57515600	-1.96997600	-1.30217200
H	8.57647100	-2.27960100	-1.61929700
H	7.05263000	-2.85940500	-0.93425300
H	7.03502500	-1.60591600	-2.18051700
C	8.48658400	-1.37656300	0.98783600
H	9.49558100	-1.66528800	0.67508500
H	8.57210800	-0.59643000	1.75019800
H	8.01858800	-2.24970900	1.45504300
C	-3.96495100	-3.06413300	-2.69345900
C	-4.67928800	-2.29956300	-1.77858200
C	-4.21815900	-2.11436700	-0.47678200

C	-2.95208500	-2.66956000	-0.07189200
C	-2.26917500	-3.51662600	-1.00201000
C	-2.79947800	-3.68712600	-2.28951000
H	-4.33016800	-3.18879000	-3.70760200
H	-5.61892600	-1.85806500	-2.08352600
H	-2.25449700	-4.31056500	-2.99084200
C	-0.99631400	-4.30480300	-0.75411700
H	-0.95560300	-5.13708900	-1.46094200
H	-0.10502700	-3.69870400	-0.93502700
H	-0.92097600	-4.71950100	0.24621100
C	-2.51630000	-2.36162200	1.38440500
C	-0.52577300	-1.36146400	2.40260500
C	-1.60550300	-3.33178100	2.17527600
C	-1.70583700	-1.00408500	1.46886300
C	-0.18797300	-2.78250600	1.92680300
H	0.56300400	-3.26776300	2.55706000
H	0.14339200	-2.80965600	0.89208700
C	-0.98935900	-1.66662900	3.84998400
H	-0.09673600	-1.82098700	4.46723300
H	-1.58238600	-0.86727400	4.28395900
C	-1.78577200	-2.99362100	3.67986900
H	-1.37294000	-3.79518900	4.30077800
H	-2.84055900	-2.87858900	3.94563900
H	0.28385600	-0.63915600	2.36741900
H	-1.78688600	-4.38521100	1.95689900
C	-2.60622600	0.14049900	1.93977300
O	-3.06443200	0.18244400	3.08404100
H	-3.43596000	-2.25244300	1.95967900
N	-2.95759200	1.08893500	1.02367800
H	-2.64359600	0.95519900	0.06920100
C	-3.95834100	2.10671400	1.31049200
C	-3.38709800	3.43729900	1.89996400
C	-4.73151900	2.51546000	0.03705800
H	-4.63472600	1.66564600	2.04761200
C	-3.82083300	4.55515100	0.92953900
H	-3.80863900	3.60316400	2.89585700
C	-5.08280800	3.99265700	0.25541000
H	-5.60193800	1.88042800	-0.13855100
H	-4.07921300	2.41960700	-0.83858600
H	-3.98959900	5.51254200	1.43120700
H	-3.04777900	4.72019700	0.16998600
H	-5.94058300	4.07795400	0.93452700
H	-5.34614600	4.50897900	-0.67246700
H	1.74152400	2.49039100	4.68443900

H	-2.30262900	3.38602700	2.01905100
C	-8.55816300	0.44634100	0.57647500
H	-9.13016500	0.91611300	1.38279500
H	-9.20341200	-0.29988900	0.09948400
H	-8.33957900	1.21762900	-0.17103800
C	-7.26963800	-0.19140900	1.09976300
H	-7.50800100	-0.92792500	1.87805600
H	-6.65393900	0.57346100	1.59011500
C	-6.45220100	-0.87062600	-0.00391500
H	-6.24375400	-0.14404400	-0.79982500
H	-7.05916200	-1.66231100	-0.46066000
C	-5.13764000	-1.44207300	0.53144400
H	-5.37959500	-2.18044200	1.31034300
H	-4.61979500	-0.64040400	1.05295800
Br	-1.48750100	-0.57752200	-3.14456100

16'

C	2.23234100	-0.13110900	3.05275800
C	1.25506800	0.10706900	4.01145600
C	0.01797100	0.59758400	3.60111200
C	-0.20022700	0.84168200	2.25084100
C	0.79788700	0.66101700	1.26513100
C	2.04548800	0.13383700	1.68115500
C	3.22674500	-0.23261900	0.82687800
C	4.32112000	0.65097200	0.71239200
C	5.45724800	0.23982000	0.00438900
C	5.55704500	-1.03024900	-0.55920900
C	4.48272100	-1.90816400	-0.39029700
C	3.32316000	-1.54390300	0.29806800
C	2.22132600	-2.57561600	0.51706500
C	4.33522900	2.00540400	1.41035700
P	0.13449600	1.25161900	-0.37476200
C	0.13626700	3.13156100	-0.19899600
C	1.15763800	0.98757000	-1.90810700
Pd	-2.31832800	0.99612300	-0.43755800
C	2.45427200	-3.33844300	1.83607000
C	2.07377300	-3.58727100	-0.62927300
C	4.88082000	3.14353200	0.53272200
C	5.14192300	1.92288200	2.72008500
C	1.27390900	3.75685500	0.61495600
C	1.18789700	5.29032100	0.61867600
C	-0.17485200	5.77905400	1.12446900
C	-1.31969300	5.15453300	0.31642700
C	-1.22564700	3.62257500	0.32939500

C	1.37632400	-0.49523000	-2.23423900
C	1.91825700	-0.66814400	-3.65652100
C	3.22386600	0.11593400	-3.83636500
C	3.02901400	1.59712300	-3.49309800
C	2.46130100	1.78139000	-2.07692500
H	3.18861200	-0.54306200	3.35665600
H	-0.77857400	0.77124600	4.31756200
H	-1.19010300	1.15837100	1.93451800
H	6.29737300	0.92127900	-0.09330600
H	4.55097600	-2.90969900	-0.80043000
H	1.26662700	-2.05183100	0.59023800
H	3.30591600	2.25062200	1.67892600
H	0.21983700	3.47228600	-1.24114400
H	0.43227600	1.38230700	-2.63975800
H	2.43232600	-2.67427700	2.70234300
H	1.67738700	-4.09711400	1.97377500
H	3.42500900	-3.84681900	1.82099800
H	2.02859300	-3.09832900	-1.60444500
H	1.14018500	-4.13922100	-0.49849600
H	2.89627700	-4.31139400	-0.64453400
H	-0.28829200	5.50081200	2.18139500
H	4.73375000	4.10683400	1.03210100
H	5.95474500	3.03362500	0.35154800
H	4.72036600	1.18030000	3.40164500
H	5.14528400	2.89104800	3.23267600
H	6.18078800	1.64188600	2.51699200
H	1.21640600	3.38505200	1.64530800
H	2.23880600	3.44139700	0.21872500
H	1.99535000	5.70514400	1.23324400
H	1.34954400	5.66162500	-0.40293800
H	4.38395600	3.18420900	-0.43970400
H	-0.23094500	6.87250000	1.07898400
H	-2.29032000	5.47295400	0.71288800
H	-1.26961200	5.50786700	-0.72242300
H	-1.37381600	3.26621400	1.35507100
H	-2.04752800	3.21321000	-0.28897400
H	2.11929100	-0.88324400	-1.53980500
H	0.46871200	-1.07614400	-2.06766300
H	2.08201700	-1.73277600	-3.86048000
H	1.17225400	-0.31965300	-4.38530400
H	3.98086300	-0.30689300	-3.16374800
H	3.60559100	0.00883500	-4.85858300
H	3.97849300	2.13871400	-3.57959100
H	2.34042500	2.05115300	-4.21987000

H	3.19191900	1.42538300	-1.34715200
H	2.29897500	2.84696900	-1.88760100
C	6.82265400	-1.46773000	-1.27757600
H	7.49263100	-0.59888200	-1.31284800
C	6.54984700	-1.90662500	-2.72506800
H	7.48076000	-2.20203500	-3.22058200
H	5.86898800	-2.76371600	-2.75726000
H	6.09537800	-1.09892100	-3.30537200
C	7.53979900	-2.57981000	-0.49228100
H	8.48353100	-2.85185900	-0.97685600
H	7.75699900	-2.26100800	0.53159300
H	6.91919600	-3.48046300	-0.43661700
C	-6.29862700	2.00245400	0.81971900
C	-4.94337600	2.08770400	0.49353600
C	-4.29831800	1.00654300	-0.12055800
C	-5.03345200	-0.15833500	-0.41764000
C	-6.39603300	-0.25953000	-0.07546700
C	-7.01138900	0.83466700	0.54329200
H	-6.79922600	2.84048300	1.29852200
H	-4.39280900	2.99700100	0.72842500
H	-8.06233200	0.76734900	0.81406000
C	-7.18430400	-1.51696600	-0.35433400
H	-8.17727600	-1.46746900	0.10100200
H	-7.31937200	-1.68534200	-1.42876000
H	-6.67708400	-2.40579700	0.03889000
C	-4.26827800	-1.24554300	-1.10879300
C	-2.34379400	-1.00459600	-2.59569500
C	-4.57128800	-1.38754900	-2.63334100
C	-2.72924300	-0.92762100	-1.11185500
C	-3.58652900	-0.38621700	-3.26408000
H	-3.55990200	-0.45017200	-4.35721800
H	-3.76338900	0.64824900	-2.96066000
C	-2.44795000	-2.48371200	-3.06465200
H	-2.00275000	-2.58516900	-4.05990500
H	-1.91144000	-3.15678600	-2.39535800
C	-3.98739500	-2.73577200	-3.10616600
H	-4.32451700	-2.96876400	-4.12145000
H	-4.29714300	-3.56418500	-2.46048100
H	-1.38615300	-0.54495300	-2.83129800
H	-5.62581700	-1.24262400	-2.87639400
C	-1.88264900	-1.71244500	-0.15263500
O	-0.76041500	-2.14839100	-0.44471300
H	-4.45075900	-2.21421600	-0.62358100
N	-2.41942500	-1.92533700	1.08645000

H	-3.23362600	-1.37586700	1.32695700
C	-1.59757300	-2.43448500	2.17205200
C	-2.22054000	-2.19136100	3.54773500
C	-1.37725100	-3.95778100	2.15384400
H	-0.62063800	-1.93781000	2.12993300
C	-1.35331200	-3.06495800	4.46681900
H	-2.22821000	-1.13522700	3.83133600
C	-0.99153300	-4.31603400	3.61251300
H	-0.62758100	-4.24691300	1.41561800
H	-2.32039400	-4.43781400	1.86995200
H	-0.44280000	-2.51391400	4.72742400
H	-1.85584300	-3.32118700	5.40362800
H	0.07354300	-4.54836800	3.70227500
H	-1.53604600	-5.20164100	3.95280900
H	1.45322300	-0.10316100	5.05791700
H	-3.25986200	-2.54728200	3.54186100

TS4'

C	2.61822500	0.01008500	2.98782000
C	1.83249000	0.47885800	4.03248900
C	0.63698800	1.13130700	3.73407800
C	0.26687400	1.29369000	2.40602100
C	1.07997900	0.87727200	1.32620800
C	2.28350500	0.19958600	1.63081600
C	3.28528600	-0.36983300	0.66764900
C	4.47466300	0.34362200	0.40285600
C	5.45749200	-0.24376700	-0.40212500
C	5.30847700	-1.52107200	-0.93640500
C	4.13963200	-2.22525400	-0.63338500
C	3.13080300	-1.68736700	0.17060700
C	1.94024400	-2.55874000	0.56424300
C	4.74670300	1.71353200	1.01270900
P	0.26235900	1.40040600	-0.26635600
C	0.50143700	3.27088500	-0.27078000
C	1.05287500	0.91498800	-1.88541900
Pd	-1.99090700	0.80347500	-0.37252800
C	2.21314400	-3.23872300	1.92124900
C	1.57899900	-3.63881300	-0.46720200
C	5.29624100	2.72852200	-0.00323800
C	5.71053400	1.59269700	2.20753700
C	1.80450100	3.77379600	0.36516100
C	1.95669300	5.29363500	0.21193300
C	0.74622400	6.04026000	0.78480800
C	-0.55973600	5.53398500	0.15903100

C	-0.70785900	4.01548300	0.32283300
C	0.88660600	-0.58327300	-2.16458000
C	1.21759300	-0.91303900	-3.62305000
C	2.63378100	-0.44564200	-3.97817000
C	2.80360100	1.05316500	-3.70285800
C	2.46157200	1.40463200	-2.24593700
H	3.53709500	-0.52302600	3.20753700
H	-0.01316800	1.48981600	4.52600800
H	-0.69587000	1.74192500	2.18003100
H	6.37158000	0.30531500	-0.60931600
H	4.01515800	-3.23009200	-1.02149100
H	1.05898200	-1.92111800	0.67229400
H	3.80007800	2.10043000	1.39514800
H	0.53108400	3.50330200	-1.34568400
H	0.34413400	1.44250900	-2.54551500
H	2.30183300	-2.51429500	2.73298100
H	1.39874200	-3.92553400	2.16852500
H	3.14208400	-3.81810700	1.87664600
H	1.52322600	-3.24024000	-1.48251000
H	0.59545500	-4.04523600	-0.22420400
H	2.30250700	-4.46204500	-0.46216400
H	0.70814700	5.88171800	1.87171900
H	5.33504300	3.72675900	0.44523000
H	6.31336400	2.47359500	-0.31768600
H	5.30113700	0.94456200	2.98612500
H	5.90151900	2.57650600	2.65000000
H	6.67021300	1.17122700	1.88964600
H	1.80246600	3.51397700	1.43069500
H	2.66277300	3.26857500	-0.07836200
H	2.87980300	5.62551200	0.70198000
H	2.06263100	5.53918100	-0.85421700
H	4.67573900	2.78206700	-0.90115300
H	0.85314500	7.11989400	0.62808600
H	-1.42134600	6.04349400	0.60601100
H	-0.56802900	5.78287500	-0.91173200
H	-0.78964900	3.77979400	1.39154800
H	-1.63161100	3.65842900	-0.14496000
H	1.57837100	-1.12572400	-1.52258800
H	-0.11877100	-0.91831700	-1.89685600
H	1.11792300	-1.99223500	-3.78971100
H	0.48943200	-0.42377000	-4.28628100
H	3.35059400	-1.00319800	-3.36303300
H	2.86735900	-0.66933000	-5.02596900
H	3.83008500	1.36977500	-3.92370500

H	2.14676200	1.62130000	-4.37714000
H	3.19159100	0.93623000	-1.58443000
H	2.54063500	2.48753700	-2.10505600
C	6.40787200	-2.14292100	-1.78064100
H	7.21530200	-1.40283000	-1.85446800
C	5.93179700	-2.45689800	-3.20786100
H	6.74644300	-2.88424500	-3.80240400
H	5.10985000	-3.18053100	-3.19841700
H	5.57575000	-1.55476300	-3.71299200
C	6.98692500	-3.39773800	-1.10492000
H	7.82308900	-3.80022600	-1.68657000
H	7.34579800	-3.17153200	-0.09636500
H	6.22949700	-4.18422600	-1.02100900
C	-5.28100400	2.67246400	-1.43565700
C	-4.09795500	1.93197500	-1.56323900
C	-4.02553200	0.70016100	-0.88015400
C	-5.18343800	0.16379500	-0.29547200
C	-6.38087500	0.87433100	-0.20206900
C	-6.38659500	2.16881700	-0.74387300
H	-5.34505200	3.65342600	-1.89931300
H	-3.27857300	2.31627700	-2.16187200
H	-7.29118300	2.76836200	-0.67627100
C	-7.62682000	0.25289200	0.37746400
H	-8.30456700	1.01610300	0.77113500
H	-8.17805800	-0.31227600	-0.38453800
H	-7.38914600	-0.44398300	1.18651400
C	-4.85033300	-1.28917900	-0.21562600
C	-3.38099100	-1.83443400	-2.11151600
C	-5.49999600	-2.12439500	-1.35627900
C	-3.37153600	-1.13540000	-0.74262000
C	-4.81296200	-1.56813300	-2.62177500
H	-5.04696400	-2.15828100	-3.51331100
H	-5.03271100	-0.51966700	-2.82502200
C	-3.46984100	-3.36711400	-1.86290800
H	-3.36658600	-3.88634500	-2.82112600
H	-2.68174000	-3.72570800	-1.20427500
C	-4.90659100	-3.55008100	-1.28209000
H	-5.49759500	-4.24836600	-1.88272800
H	-4.89531700	-3.93097300	-0.25547500
H	-2.55656700	-1.53784300	-2.75915200
H	-6.59204100	-2.08779700	-1.34134400
C	-2.27875800	-1.60346500	0.21317800
O	-1.28828600	-2.24722600	-0.15899100
H	-4.95387100	-1.79051600	0.75150500

N	-2.56136500	-1.44868800	1.55496000
H	-3.21605200	-0.71562800	1.79205500
C	-1.57059400	-1.78809700	2.56513500
C	-1.95234800	-1.25083900	3.94635000
C	-1.43211300	-3.30127900	2.81153800
H	-0.59619400	-1.37583300	2.27418100
C	-1.01121400	-2.01719500	4.88869500
H	-1.85172000	-0.16448000	4.02339300
C	-0.83175200	-3.41902200	4.23480000
H	-0.83676300	-3.78406500	2.03606200
H	-2.43504200	-3.74174300	2.77548600
H	-0.04780800	-1.49955900	4.93100900
H	-1.39585100	-2.07157400	5.91107800
H	0.22616700	-3.69326400	4.20145300
H	-1.34102400	-4.19817700	4.80956600
H	2.14098200	0.32285900	5.06159800
H	-2.99998100	-1.51031000	4.15186100

16'H

C	2.22528000	1.12041800	3.05123200
C	1.24820200	1.66385800	3.87662900
C	-0.04076500	1.82605300	3.37533800
C	-0.30438700	1.46982900	2.05802300
C	0.68657600	0.96738100	1.18366100
C	1.98427100	0.75228300	1.71266500
C	3.16063800	0.09790000	1.04255900
C	4.21096500	0.87675600	0.51272300
C	5.33979500	0.23310600	-0.00968700
C	5.47751600	-1.15300700	0.01222000
C	4.45193300	-1.90339500	0.59434400
C	3.30192700	-1.31093800	1.12156200
C	2.26678900	-2.17611500	1.83303000
C	4.19447800	2.39906500	0.57291000
P	-0.05289800	0.80259100	-0.51969300
C	-0.11671300	2.58217400	-1.14511900
C	0.93944800	-0.05732800	-1.84033300
Pd	-2.49794800	0.51158100	-0.37369300
C	2.60778300	-2.28817000	3.33223800
C	2.11193900	-3.58580100	1.24373100
C	4.63024800	3.06985100	-0.74004700
C	5.07833500	2.89544700	1.73272000
C	1.00533400	3.51845200	-0.68720700
C	0.86660800	4.91209500	-1.31556300
C	-0.50749800	5.52773400	-1.02327100

C	-1.63919300	4.59538100	-1.47532700
C	-1.49135400	3.20720000	-0.83695500
C	1.22128000	-1.53006500	-1.51269200
C	1.74923800	-2.27206500	-2.74552500
C	3.01289400	-1.59149800	-3.28476400
C	2.75282100	-0.11407600	-3.59973900
C	2.20124700	0.63392500	-2.37623600
H	3.22134400	0.94945200	3.44529300
H	-0.83826600	2.21704200	4.00009100
H	-1.32081500	1.56169100	1.68431700
H	6.14524600	0.83053400	-0.42730100
H	4.55283300	-2.98185400	0.64918300
H	1.29125800	-1.69558800	1.74563700
H	3.17116200	2.71193100	0.78860100
H	-0.05318700	2.46302800	-2.23620600
H	0.18259500	-0.03642700	-2.64246500
H	2.62099500	-1.31154000	3.82059600
H	1.86373500	-2.91023700	3.84120600
H	3.59121000	-2.75141200	3.47175300
H	1.98806000	-3.56632200	0.15903800
H	1.21879100	-4.05124200	1.66767300
H	2.96997400	-4.22595100	1.47923000
H	-0.60000600	5.70603900	0.05706200
H	4.46632100	4.15102500	-0.68280600
H	5.69539500	2.91389000	-0.93811900
H	4.73801100	2.49754000	2.69196400
H	5.05932900	3.98916300	1.79222100
H	6.11729700	2.58059800	1.58854600
H	0.97097200	3.60360400	0.40593300
H	1.97513700	3.09067900	-0.93848300
H	1.66493800	5.56686100	-0.94722800
H	1.00412000	4.83160600	-2.40293600
H	4.07467900	2.68590300	-1.59907500
H	-0.60255500	6.50348400	-1.51281200
H	-2.61575900	5.02202100	-1.22058100
H	-1.61321000	4.49165300	-2.56850800
H	-1.62285400	3.29733000	0.24754300
H	-2.30327800	2.55800900	-1.22031100
H	1.99076600	-1.55901800	-0.74325600
H	0.34368100	-2.01812500	-1.08641700
H	1.96056900	-3.31567700	-2.48465000
H	0.97643100	-2.29280500	-3.52739800
H	3.79691700	-1.65573900	-2.52008200
H	3.38591800	-2.11193900	-4.17469800

H	3.67400800	0.37262000	-3.94146700
H	2.03133700	-0.03863000	-4.42570800
H	2.96060800	0.64639500	-1.59153500
H	1.99263500	1.67316500	-2.64892400
C	6.73933200	-1.81729100	-0.51295600
H	7.34796400	-1.03195200	-0.97970700
C	6.44345800	-2.87851500	-1.58420900
H	7.37431100	-3.32058500	-1.95496200
H	5.82914000	-3.68966200	-1.17957600
H	5.90758000	-2.44678600	-2.43384400
C	7.55856500	-2.41786800	0.64310100
H	8.49638300	-2.84700800	0.27441100
H	7.79822300	-1.65694600	1.39190400
H	6.99862400	-3.21430000	1.14486100
C	-6.48440800	1.90376300	0.41179100
C	-5.14197200	1.85423500	0.03054700
C	-4.46657700	0.62764300	-0.00731600
C	-5.15701400	-0.55321700	0.33123300
C	-6.50569600	-0.50947000	0.73552700
C	-7.15281400	0.73110100	0.76718000
H	-7.00915900	2.85548500	0.44238900
H	-4.62504200	2.77654100	-0.22854700
H	-8.19342100	0.77689500	1.07922700
C	-7.24509300	-1.76227700	1.14109400
H	-8.23696300	-1.52325500	1.53447300
H	-7.37776500	-2.45004800	0.29861700
H	-6.70127500	-2.31780300	1.91422800
C	-4.36092500	-1.81947100	0.23088800
C	-2.49384400	-2.28844000	-1.27754700
C	-4.69883100	-2.70646400	-1.00855100
C	-2.84025300	-1.50347100	-0.00442100
C	-3.78553000	-2.11817900	-2.09903500
H	-3.78795500	-2.71231600	-3.01922300
H	-4.00749800	-1.07489400	-2.33518800
C	-2.53467600	-3.80822900	-0.95432200
H	-2.11823400	-4.37380400	-1.79444500
H	-1.94178000	-4.04949300	-0.07150900
C	-4.05948800	-4.09333000	-0.78289700
H	-4.41551200	-4.81003000	-1.53010000
H	-4.30519000	-4.49989200	0.20361900
H	-1.56888900	-1.97099700	-1.75446300
H	-5.76546100	-2.73374100	-1.23933000
C	-1.92294700	-1.68463500	1.16706800
O	-0.78468400	-2.15240000	1.06471000

H	-4.48429500	-2.42357200	1.13996900
N	-2.42889200	-1.31554900	2.39260000
H	-3.21211300	-0.67647100	2.40013700
H	1.48722600	1.93307900	4.90087800
H	-1.73800700	-1.18875100	3.11889500

TS4'H

C	2.22748600	0.45116300	3.18919700
C	1.31734500	1.01405500	4.07380500
C	0.11940700	1.52257400	3.57310600
C	-0.12322800	1.46011500	2.20742100
C	0.80853900	0.93059500	1.28258700
C	2.01084800	0.39164800	1.79605500
C	3.12033000	-0.27813800	1.03653700
C	4.30195700	0.44093300	0.75518500
C	5.38074600	-0.22571400	0.16243300
C	5.33276600	-1.58383900	-0.14094600
C	4.16575700	-2.28554400	0.17612400
C	3.06252600	-1.66987200	0.77291600
C	1.85682500	-2.51184100	1.18088600
C	4.45982600	1.91130400	1.12372200
P	0.11025700	1.13405300	-0.43737500
C	0.28013900	2.98612400	-0.74463800
C	1.05409300	0.42860600	-1.88176300
Pd	-2.12726600	0.42817000	-0.47584400
C	1.94062200	-2.91485800	2.66644600
C	1.65747700	-3.78057000	0.33848400
C	5.05570700	2.75594300	-0.01489500
C	5.31326800	2.06458600	2.39603900
C	1.50088700	3.65138700	-0.09590700
C	1.61941800	5.12564800	-0.50566700
C	0.33921000	5.90278900	-0.17624800
C	-0.88950900	5.23450800	-0.80686800
C	-1.00212200	3.76112100	-0.39195000
C	0.97935300	-1.10294200	-1.91819400
C	1.47587700	-1.64983600	-3.26028100
C	2.89880400	-1.16176800	-3.55735000
C	2.96943600	0.36928600	-3.53260900
C	2.46791700	0.93645400	-2.19557300
H	3.15005400	0.02616800	3.57011600
H	-0.62514600	1.95109500	4.23733400
H	-1.07649300	1.81457100	1.82594000
H	6.28923100	0.32714700	-0.05896900
H	4.11699400	-3.34768000	-0.03517100

H	0.95402000	-1.91148400	1.04679700
H	3.46693300	2.30649000	1.34705800
H	0.39936100	3.03692700	-1.83691300
H	0.38616400	0.79999300	-2.67736900
H	1.98181700	-2.04850500	3.32886700
H	1.06229100	-3.50951700	2.93932400
H	2.83358100	-3.52360100	2.84818500
H	1.71551600	-3.57970000	-0.73396200
H	0.66369900	-4.18303700	0.54260900
H	2.39900500	-4.55013500	0.58193000
H	0.20980200	5.93393400	0.91475000
H	5.00708400	3.81986700	0.23967200
H	6.10810900	2.51140300	-0.19086200
H	4.86258300	1.54283200	3.24400100
H	5.41887500	3.12130600	2.66492300
H	6.31600600	1.65183500	2.24189600
H	1.40439200	3.58337700	0.99465900
H	2.41136100	3.11464000	-0.36249500
H	2.48410600	5.58146400	-0.00873100
H	1.81223100	5.18447200	-1.58617200
H	4.51920500	2.60473100	-0.95484400
H	0.42494600	6.94245800	-0.51275600
H	-1.80319800	5.77172800	-0.52724700
H	-0.81239800	5.29480600	-1.90180600
H	-1.17094400	3.70817500	0.69092200
H	-1.86928500	3.28653700	-0.86427000
H	1.61987200	-1.49337400	-1.12956000
H	-0.03574900	-1.44578600	-1.69930400
H	1.44223800	-2.74560800	-3.24613500
H	0.79954700	-1.32520600	-4.06424700
H	3.57532100	-1.56131600	-2.79162000
H	3.24722800	-1.54392000	-4.52428800
H	3.99679900	0.70904200	-3.71082700
H	2.35749200	0.77377500	-4.35157700
H	3.14906200	0.63017700	-1.40005900
H	2.48365900	2.03045500	-2.23496800
C	6.52904900	-2.28394400	-0.76299700
H	7.31881900	-1.53034300	-0.87938100
C	6.20623100	-2.83870600	-2.15986800
H	7.08974400	-3.31120900	-2.60245400
H	5.41327100	-3.59268900	-2.11142400
H	5.86949300	-2.04402900	-2.83151800
C	7.07197500	-3.38983600	0.15747100
H	7.97136700	-3.84455800	-0.27126400

H	7.32436500	-2.99162500	1.14480800
H	6.33121200	-4.18411400	0.29749600
C	-5.61654100	1.78055200	-1.69205200
C	-4.44027200	1.02060200	-1.74322200
C	-4.16941300	0.17522500	-0.65109800
C	-5.14661700	-0.04108100	0.33358900
C	-6.33748600	0.68641500	0.37216300
C	-6.52819400	1.63881000	-0.64149800
H	-5.82895500	2.48729800	-2.48998100
H	-3.76777000	1.10827200	-2.59062000
H	-7.43386800	2.24048200	-0.63883400
C	-7.40252600	0.41075800	1.40422300
H	-8.00257000	1.30382400	1.60253300
H	-8.08945800	-0.37499000	1.06571700
H	-6.96762700	0.07460600	2.34989000
C	-4.73891100	-1.35324300	0.92444100
C	-3.80396400	-2.67636100	-0.92530900
C	-5.62690600	-2.52557000	0.41370700
C	-3.44597500	-1.53698500	0.04601200
C	-5.32915500	-2.53254600	-1.10150700
H	-5.76463000	-3.40112300	-1.60504100
H	-5.64460900	-1.62890000	-1.62336400
C	-3.76216100	-3.99992200	-0.10892100
H	-3.91472800	-4.84143500	-0.79224100
H	-2.80842900	-4.15191500	0.39277700
C	-4.96951500	-3.84956700	0.86875100
H	-5.67083800	-4.68427800	0.77415200
H	-4.65280200	-3.80503900	1.91579900
H	-3.19171900	-2.69235800	-1.82605700
H	-6.67551200	-2.42039000	0.70164700
C	-2.11944100	-1.73530100	0.75550400
O	-1.22249700	-2.45173200	0.29694700
H	-4.58953800	-1.40864000	2.00706000
N	-2.04345500	-1.26314600	2.06411500
H	-2.58117800	-0.42947200	2.26252100
H	1.53280500	1.03837200	5.13753100
H	-1.08898200	-1.19636500	2.39583900

TS6

C	-2.51790300	2.79522600	-1.80554800
C	-1.54338300	3.76394800	-2.00387100
C	-0.36978500	3.68843200	-1.25786300
C	-0.19379000	2.62768400	-0.37851900
C	-1.16513800	1.62973900	-0.15900000

C	-2.38336600	1.74183700	-0.87628800
C	-3.62983900	0.91295600	-0.74700200
C	-4.69136500	1.40191700	0.04923100
C	-5.89920200	0.69543500	0.06921800
C	-6.09862700	-0.45525300	-0.69196100
C	-5.04947400	-0.89735100	-1.50097300
C	-3.81989900	-0.23678900	-1.54528000
C	-2.71578800	-0.74323500	-2.46669600
C	-4.57264700	2.69938200	0.84962400
P	-0.48408800	0.31583600	0.97828500
C	0.22448800	1.26408000	2.44743300
C	-1.77167400	-0.73310000	1.82101700
Pd	1.25628900	-1.13091900	0.14587800
C	-2.78128700	-0.04086800	-3.83603700
C	-2.73027200	-2.26619500	-2.66457400
C	-5.25253700	2.64262500	2.22861900
C	-5.15471600	3.88391500	0.05380900
C	-0.42866800	2.61371600	2.79741000
C	0.13405100	3.15404400	4.12065400
C	1.66131200	3.28576900	4.06354000
C	2.31619200	1.94822700	3.69668700
C	1.75858200	1.38631700	2.38474000
C	-2.29890800	-1.87613200	0.94628600
C	-3.16565500	-2.84049100	1.76350600
C	-4.30398100	-2.09573600	2.46940200
C	-3.74776500	-0.98983700	3.37184900
C	-2.88385900	0.00074400	2.57594700
H	-3.44337800	2.84652700	-2.36866100
H	0.40618000	4.44108300	-1.35998600
H	0.74645600	2.55385600	0.14552700
H	-6.71209900	1.05326700	0.69348300
H	-5.19105100	-1.78593400	-2.10533600
H	-1.76120800	-0.47635600	-2.00295700
H	-3.50756800	2.89518900	1.01095400
H	0.00691400	0.56219200	3.26269900
H	-1.12057000	-1.20915200	2.56270600
H	-2.66230100	1.04026100	-3.74137100
H	-1.99004200	-0.41149600	-4.49599600
H	-3.74476800	-0.23652800	-4.31901000
H	-2.74268300	-2.80176300	-1.71246300
H	-1.84099500	-2.57969100	-3.21676500
H	-3.59853200	-2.58802100	-3.24842700
H	1.92758800	4.03781300	3.30679600
H	-5.00169700	3.54214400	2.79967800

H	-6.34317900	2.61380600	2.13888300
H	-4.63062800	4.03634200	-0.89101100
H	-5.07970100	4.80889500	0.63551500
H	-6.21259400	3.70861600	-0.16945400
H	-0.22754700	3.34374300	2.00665800
H	-1.51760800	2.52177400	2.85466700
H	-0.32722700	4.12195800	4.34988700
H	-0.14088200	2.47214000	4.93711800
H	-4.94084100	1.77343200	2.81069600
H	2.04732200	3.65356500	5.02126800
H	3.40306800	2.06046000	3.61340400
H	2.13505600	1.22136400	4.50021200
H	2.06346300	2.03934600	1.56078500
H	2.19481900	0.40670900	2.17968900
H	-2.89798100	-1.47706500	0.13030400
H	-1.44881500	-2.41387000	0.51971200
H	-3.56849000	-3.61882400	1.10418900
H	-2.53597500	-3.34653300	2.50682900
H	-4.96002900	-1.64155700	1.71539400
H	-4.91666900	-2.79252800	3.05378400
H	-4.56429300	-0.44903500	3.86616700
H	-3.14025400	-1.44110700	4.16807200
H	-3.51638400	0.53195100	1.86822900
H	-2.45998400	0.74178600	3.25937000
C	-7.42686800	-1.19179300	-0.66002600
H	-8.05988700	-0.68542900	0.07989900
C	-7.26397500	-2.65422000	-0.21352300
H	-8.23802700	-3.15212100	-0.16513800
H	-6.63893300	-3.21500100	-0.91642800
H	-6.79568300	-2.71816100	0.77243900
C	-8.13855300	-1.10683700	-2.02129100
H	-9.12005700	-1.59070900	-1.97753600
H	-8.28094300	-0.06602200	-2.32741600
H	-7.55358100	-1.60711400	-2.80058000
C	3.71311400	-5.38113400	-0.12591400
C	4.34855100	-4.25406500	0.38308600
C	3.77307700	-2.98382000	0.27052800
C	2.53686100	-2.85327000	-0.39227000
C	1.84119500	-3.99597800	-0.84035000
C	2.45822800	-5.24700400	-0.71033800
H	4.17156600	-6.36125700	-0.03228700
H	5.29713100	-4.35261200	0.90451100
H	1.92010800	-6.12935800	-1.04815000
C	0.42541800	-3.98106700	-1.36949200

H	-0.08153100	-4.90880500	-1.09041300
H	-0.14701800	-3.15670400	-0.94462200
H	0.37837400	-3.89984700	-2.46083700
C	2.68742600	-1.24089200	-1.75741400
C	1.12190300	0.24404600	-2.74751600
C	2.13447400	-1.75388200	-3.07376100
C	2.03241400	0.02977800	-1.52685400
C	0.69837300	-1.19814500	-3.05860800
H	0.19334100	-1.29699400	-4.02383900
H	0.07940200	-1.62268100	-2.27469300
C	2.05121800	0.52232100	-3.96984700
H	1.44172400	0.76441700	-4.84654300
H	2.73909300	1.35275900	-3.80425600
C	2.78860900	-0.83808700	-4.15504000
H	2.61501900	-1.25852500	-5.14989700
H	3.87069900	-0.75504500	-4.01922300
H	0.31135600	0.96267200	-2.61509900
H	2.27096800	-2.81917600	-3.25067500
C	2.91279800	1.13250200	-1.01516000
O	3.88300700	0.93116300	-0.28063000
H	3.75103700	-1.29371800	-1.57888900
N	2.63815900	2.39016500	-1.47005200
H	1.81821400	2.54077900	-2.03610300
C	3.50197200	3.52163600	-1.18207600
C	3.54073600	4.52758100	-2.34560000
C	3.12533800	4.36751300	0.07723900
H	4.49685700	3.09872400	-1.02601800
C	4.01799500	5.82318400	-1.68169200
H	4.17319500	4.18607900	-3.17003500
C	3.22710400	5.85036400	-0.35960800
H	3.80791600	4.13373200	0.89833000
H	2.12064300	4.12507900	0.42944100
H	5.09381700	5.75758300	-1.47785500
H	3.85466100	6.71130600	-2.29883900
H	3.69002400	6.48622900	0.39992900
H	2.22533800	6.25592600	-0.54642500
H	-1.70369700	4.56526800	-2.71832100
H	2.52688600	4.67135700	-2.74681800
C	7.88276500	0.05585300	0.52049700
H	8.36135000	0.85456400	1.09731700
H	7.75518500	0.41789100	-0.50635300
H	8.57688500	-0.79222400	0.48696700
C	6.53695200	-0.34878800	1.12559400
H	5.86623700	0.51615100	1.14965200

H	6.68030600	-0.66991100	2.16662400
C	5.84727200	-1.47162700	0.34681300
H	6.49251900	-2.36039100	0.32533600
H	5.72458500	-1.15274400	-0.69631500
C	4.47502300	-1.82473200	0.93859600
H	3.84751100	-0.93598000	0.90488700
H	4.59559200	-2.08205200	1.99885700
Br	1.05659100	-2.44100200	2.33562600

19

C	-2.61733400	2.90612700	-1.33931200
C	-1.65542600	3.89871200	-1.46471900
C	-0.40599000	3.69199200	-0.88489000
C	-0.14857300	2.48865600	-0.24183500
C	-1.11186900	1.46896600	-0.08590800
C	-2.39886600	1.70226600	-0.63503000
C	-3.64869700	0.87519800	-0.50420900
C	-4.58281000	1.22597200	0.49670600
C	-5.81218700	0.55856900	0.54158900
C	-6.15719600	-0.42158700	-0.38572600
C	-5.23513300	-0.72567100	-1.39131600
C	-3.99417600	-0.09042900	-1.47870000
C	-3.05717700	-0.41133300	-2.64036900
C	-4.32295800	2.35895200	1.48491600
P	-0.32939600	0.05440200	0.85840800
C	0.06453100	0.84800700	2.52308000
C	-1.48842800	-1.32259000	1.35608500
Pd	1.72815900	-1.19564800	-0.02130100
C	-3.26146500	0.57027600	-3.80984300
C	-3.19085900	-1.85182400	-3.15681800
C	-4.69949700	2.01050500	2.93438000
C	-5.06928500	3.63281900	1.04510700
C	-0.91742000	1.93892500	2.97632600
C	-0.63095800	2.36445700	4.42309300
C	0.81929700	2.83383900	4.58670500
C	1.80420600	1.76419800	4.10031200
C	1.51520400	1.34064200	2.65388000
C	-1.92296800	-2.18532700	0.16816700
C	-2.60462900	-3.47482900	0.63859100
C	-3.79285600	-3.15779600	1.55272900
C	-3.34570800	-2.31251700	2.74996900
C	-2.65795300	-1.01432300	2.29855700
H	-3.60122300	3.06065800	-1.76917000
H	0.36450500	4.45252400	-0.93656900

H	0.84255600	2.32200200	0.15947300
H	-6.52874100	0.82035600	1.31454800
H	-5.49590500	-1.47548000	-2.12940700
H	-2.03473600	-0.27883500	-2.27606400
H	-3.25434600	2.58180900	1.46538200
H	-0.02628200	-0.01443700	3.19437400
H	-0.76347000	-1.91777000	1.92498100
H	-3.06605300	1.60176100	-3.51203000
H	-2.58557400	0.32337500	-4.63638600
H	-4.28909700	0.51141400	-4.18406200
H	-3.11293800	-2.58705900	-2.35248200
H	-2.40445100	-2.06327000	-3.88639600
H	-4.14641300	-2.00700000	-3.66772500
H	0.96619400	3.75189700	3.99964700
H	-4.37580800	2.81276200	3.60530200
H	-5.78181500	1.90226300	3.05730100
H	-4.76079900	3.95496800	0.04780800
H	-4.87205300	4.45363500	1.74295600
H	-6.15035300	3.45841900	1.02318800
H	-0.81799400	2.81168100	2.32003300
H	-1.94874300	1.59727300	2.88380100
H	-1.32930100	3.15562200	4.72174000
H	-0.81534400	1.51249500	5.09196700
H	-4.23070900	1.08185400	3.26643000
H	1.02088900	3.09428600	5.63221600
H	2.83368700	2.12655000	4.18071500
H	1.73168800	0.87804500	4.74520200
H	1.68848000	2.19741700	1.99033900
H	2.20106900	0.54969800	2.35026800
H	-2.62414900	-1.62517300	-0.44575700
H	-1.05586800	-2.42628700	-0.44817600
H	-2.93305000	-4.05863200	-0.23002900
H	-1.87673500	-4.09403000	1.17964800
H	-4.54271700	-2.59848400	0.97883200
H	-4.27321600	-4.08193200	1.89504900
H	-4.20321000	-2.06737700	3.38811500
H	-2.64817500	-2.89640400	3.36555500
H	-3.39107300	-0.38455900	1.79447600
H	-2.30274800	-0.47238000	3.17912500
C	-7.50930100	-1.11202600	-0.32425900
H	-8.04891700	-0.68932700	0.53284100
C	-7.37128400	-2.62501500	-0.08835000
H	-8.35719400	-3.09792200	-0.02777800
H	-6.82105400	-3.10350700	-0.90558800

H	-6.83347200	-2.83294400	0.84051700
C	-8.33963700	-0.82405300	-1.58672000
H	-9.33483100	-1.27379100	-1.50711300
H	-8.45958300	0.25228400	-1.74259600
H	-7.85679100	-1.23883800	-2.47797000
C	4.70751600	-5.03027700	-0.65622300
C	5.27076300	-3.80099300	-0.33808600
C	4.48990900	-2.64256300	-0.18129000
C	3.09813500	-2.75921600	-0.34273900
C	2.50661700	-3.99840000	-0.65064300
C	3.32934000	-5.12127000	-0.81435900
H	5.33519700	-5.90866700	-0.77515200
H	6.34711800	-3.71791100	-0.20964100
H	2.86847200	-6.07723000	-1.05096500
C	1.01343200	-4.19292200	-0.75309800
H	0.77426900	-5.23304100	-0.99337200
H	0.53760300	-3.94171300	0.19861300
H	0.56292000	-3.56320400	-1.52458900
C	2.57585600	-0.98979500	-2.15769300
C	0.75678600	0.30396000	-2.83456300
C	1.76986700	-1.68080400	-3.23239100
C	1.95156400	0.22579000	-1.88085000
C	0.34721200	-1.17610300	-2.93491800
H	-0.34621200	-1.36354300	-3.75795000
H	-0.07186800	-1.56504700	-2.00783900
C	1.37733500	0.50232900	-4.26012900
H	0.57611800	0.67887700	-4.98428900
H	2.06104300	1.35240500	-4.30404900
C	2.09180600	-0.85888100	-4.52534100
H	1.67834600	-1.36477800	-5.40270900
H	3.16797800	-0.74942200	-4.68302400
H	-0.02809900	1.01186200	-2.57058800
H	1.92600000	-2.75514400	-3.32006900
C	2.78908100	1.39424400	-1.46123400
O	3.79276700	1.27829000	-0.75866300
H	3.64026200	-1.13273200	-2.06299000
N	2.44301800	2.60102400	-1.98917300
H	1.54561300	2.71514900	-2.43415600
C	3.26381700	3.77730400	-1.73863900
C	2.87569300	4.94689000	-2.66004000
C	3.19738300	4.34543300	-0.28487000
H	4.29687800	3.47874800	-1.93816900
C	3.34492600	6.18579800	-1.88726000
H	3.30889600	4.85487900	-3.66005500

C	2.94621400	5.86483000	-0.43513800
H	4.13697700	4.13884000	0.23183000
H	2.41359700	3.85392400	0.29527700
H	4.43493600	6.27969900	-1.96728900
H	2.90787600	7.11608100	-2.26140300
H	3.49655400	6.45937000	0.29922700
H	1.88243700	6.09207200	-0.29286300
H	-1.88247800	4.81900500	-1.99382100
H	1.78326500	4.98053200	-2.77728200
C	5.30302500	1.53649000	2.70604600
H	6.03214800	2.32470700	2.92457800
H	5.08854900	1.00884300	3.64263100
H	4.37687300	2.01775500	2.37545500
C	5.80872800	0.57681400	1.62830100
H	6.79751100	0.18634300	1.90703200
H	5.94083700	1.13219400	0.69265500
C	4.85086800	-0.59085200	1.37331200
H	3.83887600	-0.19913600	1.25298700
H	4.82692500	-1.26948500	2.23383900
C	5.23182500	-1.35234600	0.10068100
H	6.30231200	-1.58817600	0.13837700
H	5.10374100	-0.65026000	-0.73110900
Br	1.70699900	-2.28978300	2.26072700

20

C	-2.69098800	-3.23344500	0.25079500
C	-1.77218900	-4.26503800	0.10609500
C	-0.45236000	-3.95230800	-0.20619300
C	-0.09338100	-2.62246800	-0.38060400
C	-1.02788400	-1.56688900	-0.32012800
C	-2.36028500	-1.88195500	0.03749500
C	-3.47571300	-0.91541400	0.30621200
C	-4.49773700	-0.70516500	-0.64485900
C	-5.55906700	0.14775100	-0.31807200
C	-5.65925300	0.76524000	0.92862600
C	-4.67308100	0.48766300	1.87893000
C	-3.59052200	-0.34891800	1.59868300
C	-2.61883000	-0.72843200	2.70991200
C	-4.52175000	-1.45272700	-1.97474300
P	-0.19538500	-0.00105600	-0.88148900
C	0.09993900	-0.39540100	-2.69500500
C	-1.17243300	1.58876400	-0.94303300
Pd	1.80646700	0.87261800	0.29599500
C	-3.17490000	-1.92201100	3.50932800

C	-2.27052600	0.42107600	3.66679200
C	-4.90212000	-0.58021200	-3.18200400
C	-5.48572200	-2.65188600	-1.88502100
C	-1.05967700	-1.12919900	-3.38902200
C	-0.81943100	-1.19277700	-4.90459600
C	0.52108500	-1.86158800	-5.23322500
C	1.68038800	-1.18992200	-4.48585500
C	1.41895500	-1.13816600	-2.97477600
C	-1.49907000	2.12538400	0.45853300
C	-2.05270500	3.55379800	0.39778500
C	-3.26586200	3.63585500	-0.53435000
C	-2.90567100	3.13718200	-1.93701300
C	-2.36656100	1.70007400	-1.89548900
H	-3.70990000	-3.46164700	0.54409700
H	0.29833100	-4.73043200	-0.29078300
H	0.94915900	-2.38415600	-0.56316900
H	-6.34125700	0.32646200	-1.05046400
H	-4.75670700	0.92120700	2.86980500
H	-1.69334100	-1.07932400	2.25231500
H	-3.51898800	-1.84944500	-2.15035500
H	0.20458000	0.60515200	-3.12893900
H	-0.37177500	2.22269100	-1.34954600
H	-3.36399600	-2.77883400	2.85872500
H	-2.45445800	-2.23303200	4.27232200
H	-4.11507900	-1.65370600	4.00401700
H	-1.92935100	1.31368400	3.13512600
H	-1.47269200	0.10268900	4.34527600
H	-3.12502400	0.71003100	4.28741600
H	0.47211200	-2.91963100	-4.93921500
H	-4.80477700	-1.16176700	-4.10444100
H	-5.94069200	-0.23929600	-3.12286600
H	-5.19946400	-3.33974100	-1.08625800
H	-5.49432300	-3.20998100	-2.82740700
H	-6.50636200	-2.30956300	-1.68317000
H	-1.13144900	-2.14654800	-2.98674300
H	-2.01513600	-0.64532700	-3.18421300
H	-1.64419400	-1.72913200	-5.38891300
H	-0.82619600	-0.17182800	-5.31073700
H	-4.26566500	0.30208200	-3.27079800
H	0.70029700	-1.84435400	-6.31449500
H	2.61656000	-1.72394100	-4.68262900
H	1.81856400	-0.16465400	-4.85425500
H	1.35227000	-2.16417500	-2.59459200
H	2.24502600	-0.64220400	-2.46318500

H	-2.24085900	1.47914600	0.92941200
H	-0.59599800	2.10583000	1.07756000
H	-2.32118100	3.88560300	1.40781300
H	-1.26713600	4.23224000	0.03804600
H	-4.06963000	3.00702600	-0.13089400
H	-3.64838000	4.66232900	-0.57755000
H	-3.78115500	3.17833000	-2.59593800
H	-2.14659300	3.79863100	-2.37669900
H	-3.16243800	1.03392900	-1.56335000
H	-2.07332400	1.39568400	-2.90352500
C	-6.85625800	1.63848500	1.26662200
H	-7.39117600	1.83176900	0.32787900
C	-6.45547900	2.99556500	1.86502600
H	-7.34378000	3.60664700	2.05557400
H	-5.93098800	2.87145200	2.81799100
H	-5.79729600	3.55030200	1.19108900
C	-7.81688900	0.88808000	2.20711700
H	-8.71006900	1.48750000	2.41331500
H	-8.13302800	-0.06327300	1.76887800
H	-7.32927000	0.66897800	3.16329000
C	5.76833700	3.42755700	1.53370900
C	5.86908900	2.07871300	1.20634100
C	4.72746800	1.32910800	0.88719100
C	3.48368600	1.96868900	0.90307500
C	3.35565500	3.32884000	1.22030700
C	4.51798700	4.04416300	1.53814900
H	6.65771700	3.99781900	1.78563000
H	6.84018300	1.58845600	1.19651600
H	4.43441000	5.09974500	1.78541900
C	2.02491700	4.03977500	1.18000900
H	2.12308400	5.07902900	1.50617600
H	1.62635900	4.02796700	0.16081300
H	1.27363200	3.55917400	1.81746700
H	-2.07858400	-5.29471300	0.26169600
C	5.27711100	-1.96013500	-2.94972100
H	5.12003300	-2.99821700	-3.26180100
H	6.31126100	-1.69095900	-3.19152600
H	4.62298300	-1.32338700	-3.55425700
C	4.99256300	-1.76508900	-1.45915600
H	5.66075800	-2.40734800	-0.86779400
H	3.96920400	-2.09828300	-1.23459300
C	5.14065700	-0.30870600	-1.01288000
H	4.44769300	0.31881100	-1.58235000
H	6.14974400	0.05566200	-1.24633200

C	4.86261400	-0.12153600	0.48818700
H	5.66645900	-0.59277600	1.06809200
H	3.94107500	-0.65311600	0.74461100
Br	2.30074100	2.08911100	-1.85848500
O	0.36898400	-2.36137500	2.61830300
O	2.57455000	-1.92670100	2.25170600
C	2.70636200	-3.52902700	4.10672000
C	4.57007800	-3.15164000	2.45790000
C	2.47688100	-4.32254100	1.70470400
C	3.05876600	-3.26582800	2.64171500
C	1.27719300	-1.59514300	2.35090800
C	1.03913100	-0.13434900	2.18826700
C	1.98393000	0.79935900	2.57240200
H	3.09184500	-2.72329800	4.73886200
H	3.17268700	-4.46526500	4.42775000
H	1.62841100	-3.60814400	4.24666300
H	4.82012600	-2.96064700	1.41233300
H	5.04958800	-4.08470600	2.76713800
H	4.97210400	-2.33521500	3.06370400
H	1.40078800	-4.41539300	1.84056900
H	2.94937800	-5.28823100	1.90977700
H	2.68620700	-4.05601400	0.66407800
H	-0.00956900	0.12489200	2.18306900
H	1.68544000	1.79529700	2.87200900
H	2.97359800	0.47735200	2.86423800

TS7

C	-2.40009300	3.27724700	0.68462400
C	-1.45831400	4.16591200	1.18642100
C	-0.17984300	3.69978100	1.48016500
C	0.11811000	2.36086000	1.26985500
C	-0.85029000	1.42736800	0.84491600
C	-2.13914400	1.90396700	0.51698200
C	-3.28110100	1.11679300	-0.05264400
C	-4.38865100	0.78105700	0.75698500
C	-5.48412700	0.13714900	0.16864400
C	-5.52899300	-0.15355000	-1.19423000
C	-4.44195700	0.23051100	-1.98462300
C	-3.32080800	0.86462700	-1.44542200
C	-2.19889100	1.34836400	-2.35550000
C	-4.45032300	1.15610800	2.23630100
P	-0.15547100	-0.28428300	0.94632200
C	0.19304000	-0.43545100	2.78744500
C	-1.24530000	-1.76264400	0.61696500

Pd	1.69616200	-0.83450000	-0.32176700
C	-2.46137600	2.79791200	-2.80465700
C	-1.95359700	0.46240300	-3.58526300
C	-4.97500500	0.03272600	3.14662200
C	-5.32026800	2.41305000	2.43289300
C	-0.87363900	0.20957100	3.69147200
C	-0.63428600	-0.19399100	5.15497800
C	0.77778300	0.18462700	5.62026900
C	1.84852200	-0.38429500	4.68029400
C	1.59200800	0.02868900	3.22568300
C	-1.54604500	-1.96305800	-0.87319900
C	-2.18805300	-3.33039800	-1.12996000
C	-3.44681400	-3.51625500	-0.27556700
C	-3.12089400	-3.34341800	1.21093800
C	-2.48637200	-1.97237400	1.48972200
H	-3.38297400	3.63955000	0.40454500
H	0.58866100	4.37369400	1.84340300
H	1.13517500	2.02338600	1.43237500
H	-6.33377300	-0.13662200	0.78750100
H	-4.47115000	0.03663500	-3.05126500
H	-1.27622500	1.37654200	-1.77451400
H	-3.43481000	1.40134000	2.56015800
H	0.17335200	-1.52318900	2.91913600
H	-0.50967300	-2.52956700	0.89557600
H	-2.55666800	3.46623300	-1.94679100
H	-1.62594700	3.15759800	-3.41273700
H	-3.38156500	2.86088400	-3.39674200
H	-1.81522600	-0.58878500	-3.31787100
H	-1.05121100	0.80291700	-4.10335400
H	-2.77695200	0.52013600	-4.30549700
H	0.86393300	1.28035000	5.63930100
H	-4.90401900	0.34313300	4.19412400
H	-6.02804700	-0.18949500	2.94639700
H	-4.93811300	3.26381300	1.86506000
H	-5.35146900	2.69738100	3.49020400
H	-6.34709600	2.22306700	2.10239400
H	-0.81349900	1.29955300	3.59754000
H	-1.88420300	-0.07167800	3.38649500
H	-1.38784700	0.27796600	5.79657300
H	-0.77150100	-1.27962800	5.25372300
H	-4.40969200	-0.89338000	3.02994100
H	0.94416100	-0.16108000	6.64711900
H	2.84476700	-0.04733900	4.99017600
H	1.85386900	-1.48060000	4.73881300

H	1.66212100	1.11969700	3.15523000
H	2.34947000	-0.40213900	2.57068400
H	-2.22523100	-1.18366000	-1.21743400
H	-0.61618600	-1.87346400	-1.44149400
H	-2.42945400	-3.42702400	-2.19529100
H	-1.46375900	-4.12148800	-0.89278500
H	-4.19023700	-2.76242500	-0.56484300
H	-3.89524700	-4.49994500	-0.45786400
H	-4.02717500	-3.45270800	1.81852000
H	-2.42859200	-4.13521000	1.52776700
H	-3.21775800	-1.19411300	1.27675300
H	-2.22416700	-1.90739200	2.54872600
C	-6.75555800	-0.80607700	-1.80911000
H	-7.40477900	-1.12061900	-0.98171900
C	-6.41023000	-2.05678200	-2.63261900
H	-7.32102800	-2.52015400	-3.02601400
H	-5.77115300	-1.80829100	-3.48650100
H	-5.88304200	-2.79874300	-2.02687300
C	-7.53932900	0.21065000	-2.65831300
H	-8.45579600	-0.23740300	-3.05708300
H	-7.81404200	1.08880500	-2.06624900
H	-6.93632800	0.55505900	-3.50543300
C	4.29781200	-3.82658800	-1.32565400
C	4.88913000	-2.62664800	-0.96000800
C	4.36461000	-1.39659700	-1.37775600
C	3.21058400	-1.39130700	-2.21032500
C	2.60361400	-2.62941500	-2.57463900
C	3.15642300	-3.82490700	-2.12577900
H	4.71327500	-4.76614000	-0.97555300
H	5.76503800	-2.62918800	-0.31786100
H	2.68509300	-4.76382300	-2.39996200
C	1.40454200	-2.66923700	-3.49237500
H	0.95190300	-3.66352200	-3.48606900
H	0.63394100	-1.95101500	-3.20462000
H	1.68859200	-2.43913600	-4.52733300
H	-1.71396600	5.21218600	1.32221100
C	4.88078400	1.74866800	2.56346100
H	5.51694700	2.49230900	3.05402200
H	4.77439600	0.89465900	3.24131500
H	3.88484200	2.18904200	2.43817100
C	5.45590000	1.31045000	1.21429000
H	6.47398800	0.92206600	1.35143200
H	5.54872700	2.18364000	0.55764700
C	4.59120900	0.24641600	0.53848100

H	3.55656900	0.61046300	0.47178900
H	4.55240500	-0.65125200	1.16619700
C	5.05770800	-0.14451400	-0.87642600
H	6.13658800	-0.34065600	-0.85189000
H	4.90175300	0.70310100	-1.54612200
Br	2.09871900	-2.84182500	1.21741200
O	0.65390300	2.66952200	-1.52233900
O	2.90572100	2.39574700	-1.65412400
C	2.49903600	4.53489900	-2.81377100
C	4.72315700	3.85912300	-1.87913100
C	2.84026700	4.43029100	-0.30079500
C	3.21132700	3.82923700	-1.65550700
C	1.62366200	1.94146000	-1.67913200
C	1.53811100	0.48889700	-1.95307000
C	2.66300700	-0.09850400	-2.81948900
H	2.72066400	4.02539600	-3.75692100
H	2.86681400	5.56297800	-2.88936500
H	1.42054200	4.55271900	-2.66584700
H	5.24596500	3.33176200	-1.07864400
H	5.07840600	4.89326200	-1.90218100
H	4.97915500	3.38295500	-2.83004200
H	1.75958400	4.42433900	-0.17082400
H	3.20450800	5.46068500	-0.23568100
H	3.30128400	3.85132700	0.50584300
H	0.54344700	0.28382700	-2.34373800
H	2.29269400	-0.30422200	-3.82838500
H	3.46714900	0.62683000	-2.91939400

21

C	-2.40009300	3.27724700	0.68462400
C	-1.45831400	4.16591200	1.18642100
C	-0.17984300	3.69978100	1.48016500
C	0.11811000	2.36086000	1.26985500
C	-0.85029000	1.42736800	0.84491600
C	-2.13914400	1.90396700	0.51698200
C	-3.28110100	1.11679300	-0.05264400
C	-4.38865100	0.78105700	0.75698500
C	-5.48412700	0.13714900	0.16864400
C	-5.52899300	-0.15355000	-1.19423000
C	-4.44195700	0.23051100	-1.98462300
C	-3.32080800	0.86462700	-1.44542200
C	-2.19889100	1.34836400	-2.35550000
C	-4.45032300	1.15610800	2.23630100
P	-0.15547100	-0.28428300	0.94632200

C	0.19304000	-0.43545100	2.78744500
C	-1.24530000	-1.76264400	0.61696500
Pd	1.69616200	-0.83450000	-0.32176700
C	-2.46137600	2.79791200	-2.80465700
C	-1.95359700	0.46240300	-3.58526300
C	-4.97500500	0.03272600	3.14662200
C	-5.32026800	2.41305000	2.43289300
C	-0.87363900	0.20957100	3.69147200
C	-0.63428600	-0.19399100	5.15497800
C	0.77778300	0.18462700	5.62026900
C	1.84852200	-0.38429500	4.68029400
C	1.59200800	0.02868900	3.22568300
C	-1.54604500	-1.96305800	-0.87319900
C	-2.18805300	-3.33039800	-1.12996000
C	-3.44681400	-3.51625500	-0.27556700
C	-3.12089400	-3.34341800	1.21093800
C	-2.48637200	-1.97237400	1.48972200
H	-3.38297400	3.63955000	0.40454500
H	0.58866100	4.37369400	1.84340300
H	1.13517500	2.02338600	1.43237500
H	-6.33377300	-0.13662200	0.78750100
H	-4.47115000	0.03663500	-3.05126500
H	-1.27622500	1.37654200	-1.77451400
H	-3.43481000	1.40134000	2.56015800
H	0.17335200	-1.52318900	2.91913600
H	-0.50967300	-2.52956700	0.89557600
H	-2.55666800	3.46623300	-1.94679100
H	-1.62594700	3.15759800	-3.41273700
H	-3.38156500	2.86088400	-3.39674200
H	-1.81522600	-0.58878500	-3.31787100
H	-1.05121100	0.80291700	-4.10335400
H	-2.77695200	0.52013600	-4.30549700
H	0.86393300	1.28035000	5.63930100
H	-4.90401900	0.34313300	4.19412400
H	-6.02804700	-0.18949500	2.94639700
H	-4.93811300	3.26381300	1.86506000
H	-5.35146900	2.69738100	3.49020400
H	-6.34709600	2.22306700	2.10239400
H	-0.81349900	1.29955300	3.59754000
H	-1.88420300	-0.07167800	3.38649500
H	-1.38784700	0.27796600	5.79657300
H	-0.77150100	-1.27962800	5.25372300
H	-4.40969200	-0.89338000	3.02994100
H	0.94416100	-0.16108000	6.64711900

H	2.84476700	-0.04733900	4.99017600
H	1.85386900	-1.48060000	4.73881300
H	1.66212100	1.11969700	3.15523000
H	2.34947000	-0.40213900	2.57068400
H	-2.22523100	-1.18366000	-1.21743400
H	-0.61618600	-1.87346400	-1.44149400
H	-2.42945400	-3.42702400	-2.19529100
H	-1.46375900	-4.12148800	-0.89278500
H	-4.19023700	-2.76242500	-0.56484300
H	-3.89524700	-4.49994500	-0.45786400
H	-4.02717500	-3.45270800	1.81852000
H	-2.42859200	-4.13521000	1.52776700
H	-3.21775800	-1.19411300	1.27675300
H	-2.22416700	-1.90739200	2.54872600
C	-6.75555800	-0.80607700	-1.80911000
H	-7.40477900	-1.12061900	-0.98171900
C	-6.41023000	-2.05678200	-2.63261900
H	-7.32102800	-2.52015400	-3.02601400
H	-5.77115300	-1.80829100	-3.48650100
H	-5.88304200	-2.79874300	-2.02687300
C	-7.53932900	0.21065000	-2.65831300
H	-8.45579600	-0.23740300	-3.05708300
H	-7.81404200	1.08880500	-2.06624900
H	-6.93632800	0.55505900	-3.50543300
C	4.29781200	-3.82658800	-1.32565400
C	4.88913000	-2.62664800	-0.96000800
C	4.36461000	-1.39659700	-1.37775600
C	3.21058400	-1.39130700	-2.21032500
C	2.60361400	-2.62941500	-2.57463900
C	3.15642300	-3.82490700	-2.12577900
H	4.71327500	-4.76614000	-0.97555300
H	5.76503800	-2.62918800	-0.31786100
H	2.68509300	-4.76382300	-2.39996200
C	1.40454200	-2.66923700	-3.49237500
H	0.95190300	-3.66352200	-3.48606900
H	0.63394100	-1.95101500	-3.20462000
H	1.68859200	-2.43913600	-4.52733300
H	-1.71396600	5.21218600	1.32221100
C	4.88078400	1.74866800	2.56346100
H	5.51694700	2.49230900	3.05402200
H	4.77439600	0.89465900	3.24131500
H	3.88484200	2.18904200	2.43817100
C	5.45590000	1.31045000	1.21429000
H	6.47398800	0.92206600	1.35143200

H	5.54872700	2.18364000	0.55764700
C	4.59120900	0.24641600	0.53848100
H	3.55656900	0.61046300	0.47178900
H	4.55240500	-0.65125200	1.16619700
C	5.05770800	-0.14451400	-0.87642600
H	6.13658800	-0.34065600	-0.85189000
H	4.90175300	0.70310100	-1.54612200
Br	2.09871900	-2.84182500	1.21741200
O	0.65390300	2.66952200	-1.52233900
O	2.90572100	2.39574700	-1.65412400
C	2.49903600	4.53489900	-2.81377100
C	4.72315700	3.85912300	-1.87913100
C	2.84026700	4.43029100	-0.30079500
C	3.21132700	3.82923700	-1.65550700
C	1.62366200	1.94146000	-1.67913200
C	1.53811100	0.48889700	-1.95307000
C	2.66300700	-0.09850400	-2.81948900
H	2.72066400	4.02539600	-3.75692100
H	2.86681400	5.56297800	-2.88936500
H	1.42054200	4.55271900	-2.66584700
H	5.24596500	3.33176200	-1.07864400
H	5.07840600	4.89326200	-1.90218100
H	4.97915500	3.38295500	-2.83004200
H	1.75958400	4.42433900	-0.17082400
H	3.20450800	5.46068500	-0.23568100
H	3.30128400	3.85132700	0.50584300
H	0.54344700	0.28382700	-2.34373800
H	2.29269400	-0.30422200	-3.82838500
H	3.46714900	0.62683000	-2.91939400

22

C	3.22794600	-3.34409100	-1.16792800
C	2.49656500	-4.47356700	-1.51352700
C	1.11888400	-4.47718200	-1.30610300
C	0.51364800	-3.36689300	-0.73332800
C	1.25295700	-2.24064100	-0.31158800
C	2.63843300	-2.21384300	-0.57084200
C	3.54445400	-1.03744700	-0.38531400
C	4.46663900	-0.99015600	0.68256100
C	5.35477000	0.08991200	0.75625200
C	5.37637800	1.09628300	-0.20889300
C	4.48270800	1.00495300	-1.27945300
C	3.55892500	-0.03698200	-1.38731200
C	2.60587300	-0.09648600	-2.57796400

C	4.54160700	-2.10386500	1.72572700
P	0.12881200	-0.96516000	0.40656000
C	-0.73787700	-1.87463600	1.81510900
C	0.82612100	0.48685600	1.35261300
Pd	-1.48114200	-0.02896700	-1.04413000
C	3.18840100	-0.96683300	-3.70717000
C	2.23023700	1.28303800	-3.13473500
C	4.81952700	-1.60642800	3.15500600
C	5.62024800	-3.13609500	1.34236800
C	0.07028400	-3.00829200	2.46869400
C	-0.66602400	-3.56097900	3.69696300
C	-2.07234200	-4.04663500	3.32499400
C	-2.88581200	-2.93206400	2.65541100
C	-2.15455900	-2.34722300	1.43936800
C	1.32208000	1.63894800	0.46882200
C	1.57896000	2.89959300	1.30252100
C	2.55628500	2.61085000	2.44848700
C	2.04361400	1.46923800	3.33324600
C	1.78455100	0.19879500	2.51003000
H	4.28787700	-3.30117400	-1.39283300
H	0.51168500	-5.32290900	-1.61205700
H	-0.56450600	-3.35957000	-0.63815000
H	6.05407000	0.14814900	1.58485500
H	4.49278700	1.77514500	-2.04235600
H	1.67538700	-0.57272600	-2.25688500
H	3.57377900	-2.61768900	1.72860200
H	-0.85723200	-1.08000200	2.56400000
H	-0.12238400	0.83129100	1.79288900
H	3.39344700	-1.98365500	-3.36751500
H	2.47606600	-1.02674800	-4.53576900
H	4.12313600	-0.53434300	-4.08237900
H	1.91782100	1.96883100	-2.34395900
H	1.39945400	1.17297800	-3.83692000
H	3.06248900	1.74657700	-3.67660800
H	-1.98517600	-4.89393200	2.63090800
H	4.72303200	-2.43820200	3.86001000
H	5.83875700	-1.21917500	3.25379800
H	5.41002000	-3.60451600	0.38000400
H	5.68069800	-3.92716900	2.09763100
H	6.60129300	-2.65330100	1.27722200
H	0.21797900	-3.81431100	1.74313000
H	1.07103100	-2.65968100	2.74376300
H	-0.08502800	-4.37731300	4.14113700
H	-0.74122900	-2.77585900	4.46270700

H	4.13143500	-0.81787300	3.46617800
H	-2.59628000	-4.41885700	4.21257600
H	-3.86786200	-3.30988600	2.34929400
H	-3.07284300	-2.13281000	3.38569300
H	-2.09686300	-3.11171300	0.65595000
H	-2.72209900	-1.51605900	1.00796200
H	2.24608000	1.34631700	-0.02770300
H	0.58568700	1.84732300	-0.31209600
H	1.96803300	3.69184500	0.65355700
H	0.62839800	3.27182800	1.70717100
H	3.52719700	2.31892500	2.02681200
H	2.72375500	3.51307700	3.04822400
H	2.76145700	1.25077800	4.13296200
H	1.11000600	1.77796200	3.82537200
H	2.72589000	-0.16044200	2.09635000
H	1.38930200	-0.58724800	3.16066600
C	6.35750800	2.25172500	-0.10853600
H	6.89544600	2.13963600	0.84165900
C	5.63935800	3.61131800	-0.08246800
H	6.36000000	4.42754700	0.03456000
H	5.08913300	3.78436100	-1.01324600
H	4.92323100	3.66495500	0.74260000
C	7.39398100	2.19741200	-1.24391500
H	8.12896900	3.00282100	-1.14031500
H	7.92742400	1.24216200	-1.24384500
H	6.90976400	2.30851400	-2.21995100
C	-0.91247100	5.72060400	0.21021200
C	-1.78309000	5.15731800	1.13667300
C	-2.37733000	3.91354500	0.90359600
C	-2.10320500	3.22352700	-0.30420800
C	-1.20766400	3.78694400	-1.24235500
C	-0.62861100	5.03114500	-0.96258900
H	-0.45247400	6.68480200	0.40417400
H	-2.00460700	5.68055300	2.06270400
H	0.06049800	5.45688900	-1.68622700
C	-0.81743200	3.11553200	-2.53658700
H	0.08159200	3.58226600	-2.94451500
H	-0.61171400	2.04816100	-2.41357200
H	-1.60272000	3.20591000	-3.29515000
H	2.99129600	-5.32343000	-1.97340000
C	-2.57626400	0.65004500	4.80098000
H	-3.20770200	0.18862900	5.56655200
H	-1.74092500	1.14501300	5.30893200
H	-2.15678900	-0.15495300	4.18788500

C	-3.36335800	1.64059100	3.94018800
H	-3.78654800	2.42909500	4.57625900
H	-4.21690200	1.12981300	3.47453300
C	-2.50131000	2.27378700	2.84621800
H	-2.12549000	1.47625600	2.19471000
H	-1.61307500	2.73999800	3.29243300
C	-3.24029800	3.33142300	2.00713600
H	-3.55197700	4.14513300	2.67115600
H	-4.16818800	2.90232900	1.61091500
Br	-1.16983500	-1.43762500	-3.04332300
O	-4.81682400	0.03511000	-2.85757100
O	-4.68765900	-0.02324200	-0.57567400
C	-7.08284600	-0.40610500	-1.00843900
C	-5.92528800	-1.03977100	1.12859500
C	-5.40551900	-2.31843000	-0.98617500
C	-5.79692200	-0.96374200	-0.39302300
C	-4.27485600	0.35588200	-1.81846100
C	-3.06597200	1.20773400	-1.74354400
C	-2.73388500	1.86205000	-0.46623600
H	-7.27837200	0.59991700	-0.62388700
H	-7.92538300	-1.04691600	-0.72933700
H	-7.01103900	-0.36150200	-2.09388100
H	-4.98947800	-1.37602000	1.58001800
H	-6.71627700	-1.74280200	1.40503900
H	-6.17602800	-0.05777100	1.54169100
H	-5.26808800	-2.24156000	-2.06505500
H	-6.18952900	-3.05359700	-0.77879100
H	-4.47147300	-2.67150900	-0.54035700
H	-2.82696600	1.66527600	-2.69087600
H	-1.93454500	1.13864000	0.14113600
H	-3.54522100	1.70535600	0.23861900

TS8

C	3.12876600	-3.29539300	-1.31655500
C	2.36743600	-4.38642400	-1.71577800
C	0.99043300	-4.36430400	-1.50501900
C	0.41613200	-3.26726700	-0.87825700
C	1.18505000	-2.18273900	-0.40480100
C	2.57067800	-2.17978300	-0.66348700
C	3.51332400	-1.04305100	-0.42105300
C	4.44433900	-1.08560900	0.63915300
C	5.37372800	-0.04519600	0.76019300
C	5.42504700	1.00929600	-0.15099000
C	4.51732900	1.00960800	-1.21366800

C	3.55595000	0.00836900	-1.36884200
C	2.59921600	0.03954800	-2.55703300
C	4.48252600	-2.25178300	1.62565000
P	0.09742900	-0.92491900	0.39828200
C	-0.75328900	-1.88753000	1.77720400
C	0.84140300	0.47324400	1.38742500
Pd	-1.49813900	0.05890400	-0.98783100
C	3.15463000	-0.78841800	-3.73103000
C	2.26044200	1.45413500	-3.04456300
C	4.76834200	-1.83393100	3.07846800
C	5.53116000	-3.29585400	1.19467900
C	0.06862700	-3.03992900	2.38054700
C	-0.64845000	-3.63279200	3.60135700
C	-2.05760200	-4.11448100	3.23507300
C	-2.88483800	-2.98647200	2.60571300
C	-2.16932200	-2.36091600	1.40097300
C	1.33411600	1.65158200	0.53754800
C	1.63012400	2.87341200	1.41427300
C	2.62802000	2.52617700	2.52555500
C	2.11751500	1.35701500	3.37492300
C	1.82225800	0.12402000	2.50801400
H	4.18924900	-3.26967400	-1.54129100
H	0.36055500	-5.17735800	-1.85089500
H	-0.66131100	-3.23506200	-0.78153300
H	6.08355800	-0.05676800	1.58199000
H	4.55055000	1.81777400	-1.93576900
H	1.65501000	-0.42615600	-2.26188400
H	3.49967700	-2.73552900	1.60164500
H	-0.87105500	-1.11833100	2.55266100
H	-0.09094200	0.81247900	1.86228800
H	3.33389100	-1.82595400	-3.44335300
H	2.43596700	-0.78882500	-4.55606100
H	4.09902700	-0.36300200	-4.09000900
H	1.94995800	2.10510400	-2.22382200
H	1.43683400	1.39416200	-3.76086200
H	3.10811400	1.92789700	-3.55257800
H	-1.97568100	-4.94287600	2.51785200
H	4.64611300	-2.69676300	3.74100100
H	5.79721100	-1.48034400	3.19952600
H	5.31202600	-3.70847500	0.20896200
H	5.56357400	-4.12565300	1.90905200
H	6.52689400	-2.84099700	1.15770900
H	0.20500000	-3.82092300	1.62564300
H	1.07310900	-2.70050200	2.65240300

H	-0.05765100	-4.45900900	4.01307600
H	-0.71597400	-2.87076700	4.39079100
H	4.10053900	-1.04341300	3.42614300
H	-2.56799100	-4.51269200	4.11929400
H	-3.86672700	-3.36275000	2.29700500
H	-3.07180400	-2.21045400	3.36032200
H	-2.10974900	-3.10498400	0.59847300
H	-2.74578900	-1.52238400	0.99791000
H	2.24243800	1.36568000	0.00900000
H	0.58060000	1.90077600	-0.21410900
H	2.01702900	3.68501100	0.78827000
H	0.69431600	3.24264700	1.85451000
H	3.58532600	2.23822900	2.07161500
H	2.82145600	3.40112700	3.15715700
H	2.84877600	1.09617700	4.14927000
H	1.19891300	1.65884200	3.89861700
H	2.74902900	-0.23128000	2.06004700
H	1.42886400	-0.68063800	3.13630100
C	6.45718100	2.11464200	-0.00673900
H	6.99657500	1.93474000	0.93224400
C	5.80382400	3.50342100	0.08720600
H	6.56315200	4.27870000	0.23439300
H	5.25595300	3.74494700	-0.82959300
H	5.09696500	3.55322300	0.92041900
C	7.48182100	2.06472200	-1.15318100
H	8.25303100	2.83117500	-1.02103800
H	7.97161100	1.08752900	-1.20043200
H	6.99549500	2.24042300	-2.11861400
C	-0.83491400	5.60663700	0.42113900
C	-1.72328200	5.02597600	1.31959000
C	-2.37252300	3.82597300	1.01809200
C	-2.13519800	3.19734200	-0.23308500
C	-1.22525100	3.78444700	-1.14786100
C	-0.59072500	4.98096400	-0.79605400
H	-0.33180500	6.53613800	0.66962500
H	-1.91656100	5.50144900	2.27705600
H	0.10984600	5.42225300	-1.49878100
C	-0.87898300	3.18173300	-2.48597800
H	-0.00004400	3.67671400	-2.90385900
H	-0.65910700	2.11160900	-2.42114600
H	-1.69369900	3.30130200	-3.20862700
H	2.83910200	-5.22519500	-2.21828400
C	-2.62701900	0.49363000	4.84756900
H	-3.26708700	0.01864100	5.59752300

H	-1.80415300	0.98949900	5.37456100
H	-2.19083200	-0.30062500	4.23245300
C	-3.40748300	1.48854800	3.98581800
H	-3.83868500	2.27088400	4.62431500
H	-4.25531200	0.98026800	3.50721700
C	-2.53458400	2.13258800	2.90677100
H	-2.17290500	1.34717600	2.23244000
H	-1.63915700	2.57303000	3.36474300
C	-3.25497800	3.22431500	2.09555900
H	-3.55720300	4.02349000	2.78124400
H	-4.18708500	2.82271700	1.68260000
Br	-1.05136100	-1.13336800	-3.14129100
O	-4.81948600	0.03984100	-2.88028100
O	-4.72920600	-0.03922600	-0.59813500
C	-7.10278600	-0.50107900	-1.07051200
C	-5.95256400	-1.12171400	1.07524800
C	-5.35938000	-2.35371300	-1.04747000
C	-5.80717000	-1.02151000	-0.44334400
C	-4.31400400	0.36986400	-1.82681100
C	-3.15458500	1.29044900	-1.72751900
C	-2.84325600	1.91067300	-0.48216100
H	-7.34018900	0.49161800	-0.67519900
H	-7.92576700	-1.17546400	-0.81322800
H	-7.01732500	-0.43871500	-2.15419500
H	-5.01163200	-1.43232500	1.53444100
H	-6.72285300	-1.85456200	1.33190000
H	-6.24138500	-0.15425600	1.49746400
H	-5.21311900	-2.26035300	-2.12388900
H	-6.11786200	-3.11952500	-0.85687400
H	-4.41842900	-2.67688700	-0.59386700
H	-2.85693600	1.69946900	-2.67944700
H	-1.87896800	0.94098500	0.27995900
H	-3.56584200	1.65810600	0.28292000

20'

Pd	1.75086000	-0.11359300	-0.17359900
C	5.96771100	1.82061700	-1.51747200
C	5.96269100	0.73065000	-0.65339500
C	4.75710500	0.12583200	-0.26094800
C	3.55485900	0.67890900	-0.71618200
C	3.53661900	1.75824900	-1.61229200
C	4.75876600	2.31841200	-2.00540600
H	6.90675900	2.27309100	-1.82289500

H	6.90161700	0.31985500	-0.28855300
H	4.75732000	3.15177300	-2.70421400
C	2.24397400	2.28658500	-2.18902000
H	2.42124900	3.17007700	-2.80934500
H	1.77033500	1.51968700	-2.81098300
H	1.52528300	2.56641200	-1.41222900
C	5.24757500	-4.93162000	-0.36167000
H	5.20665400	-5.84950300	0.23450400
H	6.21032600	-4.91582500	-0.88473200
H	4.46064900	-4.98831100	-1.12166900
C	5.07126500	-3.68443800	0.50691700
H	5.83906000	-3.66443700	1.29282100
H	4.10530100	-3.73997500	1.02722400
C	5.12378700	-2.38516100	-0.30078500
H	4.39401600	-2.42696600	-1.11586200
H	6.11068700	-2.27223000	-0.76792800
C	4.81389900	-1.14727100	0.55616200
H	5.56685300	-1.05351000	1.35102800
H	3.85088700	-1.31879800	1.04582200
Br	2.02482800	-1.47931600	-2.25228100
O	0.89450100	3.64260200	1.00732400
O	3.03927300	2.99617100	1.40318500
C	5.12113000	4.05375800	1.51800900
C	3.08720800	5.15325200	2.54177200
C	3.35120500	5.02981400	0.02062000
C	3.63174900	4.34982100	1.36029300
C	1.73110900	2.79019200	1.25968800
C	1.34560800	1.37106700	1.52498900
C	2.23909000	0.41156900	1.94752200
H	5.31516700	3.55491700	2.47202800
H	5.69011700	4.98768200	1.49245600
H	5.46437200	3.40553900	0.70824800
H	2.01686900	5.33352300	2.43196300
H	3.60055900	6.11816900	2.59330600
H	3.26651400	4.62018100	3.48039100
H	3.71428500	4.40682000	-0.79735800
H	3.88820500	5.98317900	-0.00762900
H	2.28722900	5.22027200	-0.11354200
H	0.28034100	1.24427200	1.67110700
H	3.29172200	0.65321000	2.00895000
H	1.89691300	-0.47833300	2.46055200
C	-2.83944600	0.36940700	3.24424300
C	-2.09117400	-0.04270300	4.33886900
C	-0.97181000	-0.84444100	4.12353500

C	-0.62059300	-1.18014000	2.82338600
C	-1.35939800	-0.76226300	1.69179700
C	-2.51583800	0.02044100	1.91682200
C	-3.53059800	0.46873400	0.90522700
C	-4.67264200	-0.33765900	0.70317900
C	-5.69682700	0.13540900	-0.12508800
C	-5.63148600	1.38420700	-0.74050900
C	-4.49921200	2.17162400	-0.51330700
C	-3.44670900	1.74488100	0.30028600
C	-2.24884800	2.66078700	0.53566400
C	-4.84003000	-1.68152000	1.40875800
P	-0.47180100	-1.24174700	0.13316800
C	-0.28266700	-3.10912500	0.24867100
C	-1.35722300	-1.06301900	-1.49152100
C	-2.40923700	3.48511700	1.82644000
C	-1.94932900	3.61336500	-0.63199500
C	-5.42483400	-2.78444000	0.51135800
C	-5.71270500	-1.52097800	2.66796100
C	-1.41173900	-3.84280500	0.99079800
C	-1.25198300	-5.36378700	0.85166300
C	0.12619100	-5.82976800	1.33905700
C	1.25374800	-5.08144700	0.61710600
C	1.10060800	-3.56118400	0.75471900
C	-1.38219300	0.38671500	-1.98617400
C	-1.80182300	0.44886300	-3.45846200
C	-3.15943700	-0.23382000	-3.66418500
C	-3.12438600	-1.68712400	-3.17646300
C	-2.69670900	-1.77240300	-1.70291200
H	-3.72600600	0.97501200	3.39929400
H	-0.37171900	-1.20023900	4.95526700
H	0.25902000	-1.79531600	2.67486000
H	-6.57521700	-0.48170500	-0.28895000
H	-4.43319900	3.14571500	-0.98416400
H	-1.36813000	2.02395100	0.66056200
H	-3.84977700	-2.01378500	1.73282500
H	-0.32674600	-3.39638200	-0.80975600
H	-0.60598600	-1.57570200	-2.10747300
H	-2.52410000	2.84891100	2.70589000
H	-1.52463800	4.11090700	1.97107900
H	-3.29139600	4.13125500	1.75695800
H	-1.91765500	3.09406900	-1.59319400
H	-0.97917600	4.08306600	-0.46090100
H	-2.69884700	4.40926300	-0.70354000
H	0.20544100	-5.64416900	2.41972400

H	-5.40959100	-3.74088400	1.04401500
H	-6.46677500	-2.58110000	0.24423000
H	-5.27438300	-0.81088900	3.37263800
H	-5.82860400	-2.48142000	3.18173800
H	-6.70998100	-1.15731900	2.39800500
H	-1.38721000	-3.57308400	2.05284800
H	-2.38984200	-3.52693100	0.61605000
H	-2.04744600	-5.87296400	1.40825900
H	-1.37712600	-5.64419900	-0.20337400
H	-4.85787200	-2.90226600	-0.41444300
H	0.23337600	-6.91131400	1.19801100
H	2.23134300	-5.39360100	1.00147700
H	1.24102400	-5.34058900	-0.45040500
H	1.22876100	-3.28621500	1.81038300
H	1.88173000	-3.04922900	0.18880400
H	-2.09695300	0.95519900	-1.39533700
H	-0.39671800	0.84231500	-1.84709700
H	-1.84631600	1.49415800	-3.78652000
H	-1.03883900	-0.04620900	-4.07391500
H	-3.92089100	0.31321700	-3.09337100
H	-3.45586900	-0.19271700	-4.71882100
H	-4.10742600	-2.15703600	-3.30021000
H	-2.41835800	-2.26006600	-3.79323900
H	-3.45988500	-1.30192500	-1.08353900
H	-2.62661200	-2.82224300	-1.40112200
C	-6.78062900	1.89075400	-1.59615200
H	-7.51017600	1.07445800	-1.67497200
C	-6.33265700	2.25595900	-3.02034200
H	-7.18652400	2.59223700	-3.61785500
H	-5.59610300	3.06613500	-3.00900300
H	-5.87746300	1.39940000	-3.52510200
C	-7.48165600	3.08074100	-0.91781000
H	-8.34391000	3.41167900	-1.50639100
H	-7.83033100	2.81299200	0.08415700
H	-6.79755800	3.93002400	-0.81692300
H	-2.38279700	0.25046600	5.34235700
TS7'			
Pd	2.13391300	0.30316100	0.03456200
C	6.70510400	1.47275200	-1.21802500
C	6.49787600	0.41495000	-0.33961800
C	5.22671800	0.16019800	0.19382900
C	4.17079200	1.01389100	-0.15709900
C	4.35570200	2.07209400	-1.06785200

C	5.63335800	2.28484600	-1.59031800
H	7.69633900	1.66187800	-1.61949800
H	7.32735400	-0.23055900	-0.06247900
H	5.78410700	3.09289900	-2.30159000
C	3.19634600	2.90227000	-1.55090800
H	3.54004700	3.81800300	-2.04188200
H	2.61321700	2.32078700	-2.27437400
H	2.52718200	3.17279300	-0.73296300
C	5.46975600	-4.90152200	0.50291600
H	5.31880500	-5.77636800	1.14401900
H	6.51548500	-4.90326700	0.17582800
H	4.84707400	-5.02638700	-0.38887400
C	5.12818800	-3.59965200	1.23177500
H	5.77462500	-3.49242600	2.11378800
H	4.09942300	-3.64523200	1.61276200
C	5.28210400	-2.36911900	0.33556600
H	4.59172600	-2.42349800	-0.51413300
H	6.29228800	-2.35846100	-0.09221600
C	5.03645900	-1.04850600	1.08393800
H	5.71949700	-0.99433800	1.94435500
H	4.01585200	-1.06052700	1.48316800
Br	2.61964900	-0.79452100	-2.20879800
O	-0.28351400	2.48220800	1.90069100
O	1.53363900	3.69487700	1.26421700
C	1.93924600	5.92881700	0.68508700
C	0.02659600	5.39433700	2.22747100
C	-0.09007200	4.74796700	-0.22819000
C	0.80906100	4.94670500	0.99082300
C	0.90850800	2.56777600	1.66469100
C	1.85871200	1.43952300	1.84480000
C	3.25206500	1.62846800	1.68807100
H	2.60217600	6.03276900	1.54865400
H	1.52276000	6.91163400	0.44662000
H	2.53073600	5.58597500	-0.16748500
H	-0.79171600	4.71058400	2.44739300
H	-0.37783200	6.39620400	2.05270600
H	0.68945500	5.44257700	3.09679900
H	0.50032700	4.44692300	-1.09760000
H	-0.59889600	5.68671200	-0.46803100
H	-0.84142300	3.98693500	-0.03175100
H	1.49227800	0.70187100	2.54786800
H	3.61022500	2.61952200	1.45054600
H	3.92351200	1.01222500	2.27025300
C	-2.79767500	-0.91137900	3.18226600

C	-1.91274000	-1.23641900	4.20235600
C	-0.56280200	-1.38628400	3.89831400
C	-0.14088900	-1.18122800	2.59120000
C	-1.01970500	-0.84557000	1.53715100
C	-2.40209500	-0.72382000	1.84309400
C	-3.54513500	-0.46215000	0.89606300
C	-4.32807300	-1.54747800	0.43343900
C	-5.39220000	-1.29589800	-0.44107800
C	-5.73800200	-0.00861700	-0.83946000
C	-5.02063800	1.05545600	-0.28872300
C	-3.95245400	0.86174300	0.59075800
C	-3.33000800	2.06685300	1.28524000
C	-4.12649300	-2.97881600	0.91832300
P	-0.03265500	-0.76826000	-0.04671000
C	0.26139200	-2.57331800	-0.44247300
C	-0.83600000	-0.07026900	-1.56966900
C	-3.96548000	2.27426600	2.67540000
C	-3.46089200	3.37942000	0.49855400
C	-4.30089800	-4.03358800	-0.18849800
C	-5.10295100	-3.29132700	2.06984100
C	-0.95590800	-3.47629000	-0.23462100
C	-0.68905500	-4.88348600	-0.78441300
C	0.54698500	-5.50438700	-0.12411000
C	1.76779000	-4.58383000	-0.24570800
C	1.47539500	-3.17399800	0.28620700
C	-0.96640300	1.45403300	-1.43895200
C	-1.38446800	2.09683400	-2.76631200
C	-2.65759000	1.45196200	-3.32370400
C	-2.46936200	-0.05937600	-3.49168800
C	-2.08715600	-0.73015000	-2.16295200
H	-3.85214000	-0.80457400	3.40992600
H	0.15801700	-1.64982900	4.66613400
H	0.91467900	-1.28959000	2.36693700
H	-5.97649800	-2.13009500	-0.81661500
H	-5.31467600	2.06779200	-0.53973400
H	-2.26932100	1.87036100	1.44277700
H	-3.11470200	-3.06482300	1.31552800
H	0.51514800	-2.52924600	-1.50794200
H	-0.00661300	-0.25515600	-2.26696200
H	-3.79841000	1.42078900	3.33296800
H	-3.52860000	3.15529800	3.15738200
H	-5.04603600	2.43325200	2.58528000
H	-3.11370600	3.28953400	-0.53428100
H	-2.87003300	4.15706300	0.98920600

H	-4.49735600	3.73325800	0.47291600
H	0.33230400	-5.67596400	0.94031600
H	-3.94180600	-5.00638600	0.16143800
H	-5.35398900	-4.15842500	-0.46011700
H	-4.95130500	-2.62552400	2.92187300
H	-4.96816400	-4.32162900	2.41700200
H	-6.13948000	-3.17815900	1.73475500
H	-1.16269500	-3.54265500	0.83985100
H	-1.84207600	-3.04661300	-0.69847200
H	-1.56803600	-5.51909900	-0.62776500
H	-0.53321300	-4.82095700	-1.87018100
H	-3.75328200	-3.77465800	-1.09767800
H	0.76387300	-6.48544000	-0.56233200
H	2.61767100	-5.01528400	0.29210300
H	2.06829600	-4.50274500	-1.29875800
H	1.26406600	-3.23201600	1.36198000
H	2.34823600	-2.53300400	0.15100200
H	-1.69563400	1.69534500	-0.66500600
H	-0.00688200	1.86687700	-1.11321100
H	-1.52765900	3.17500900	-2.62459000
H	-0.56829300	1.97945500	-3.49224300
H	-3.48780700	1.63271900	-2.63027200
H	-2.93308200	1.91170300	-4.28002300
H	-3.38579700	-0.52035900	-3.87867800
H	-1.68275400	-0.24536500	-4.23593600
H	-2.92626900	-0.65709400	-1.47343500
H	-1.90030900	-1.79379500	-2.33800100
C	-6.89020800	0.22791000	-1.79997800
H	-7.29010900	-0.75729100	-2.07255900
C	-6.42137000	0.91531300	-3.09281900
H	-7.25370300	1.02719100	-3.79576800
H	-6.02305900	1.91416600	-2.88595200
H	-5.63222500	0.33820100	-3.58310200
C	-8.02438000	1.02400200	-1.13262100
H	-8.87095300	1.14089800	-1.81743400
H	-8.37938800	0.52099400	-0.22819200
H	-7.68599300	2.02557500	-0.84678500
H	-2.27606800	-1.37436800	5.21594500

21'

Pd	2.03923000	0.57250500	-0.41144000
C	5.89026500	-0.07626500	-1.49770200
C	5.51743600	-0.86100300	-0.40492500
C	4.73271400	-0.33445200	0.61851100

C	4.32202600	1.03009400	0.55024900
C	4.70565600	1.82260200	-0.56156500
C	5.48610600	1.24633200	-1.57378800
H	6.48399600	-0.50971200	-2.29637300
H	5.83725800	-1.89534800	-0.36328200
H	5.75621500	1.84857600	-2.43493700
C	4.33470900	3.28213800	-0.67168100
H	4.60036000	3.66429500	-1.65979400
H	3.26996200	3.44735100	-0.51140100
H	4.86556700	3.88413000	0.07646900
C	4.08932200	-4.99941500	2.63938500
H	3.57868800	-5.55468100	3.43240600
H	5.15209400	-5.26289100	2.67747900
H	3.69617500	-5.35080900	1.67851000
C	3.88803900	-3.49031400	2.78934800
H	4.24913300	-3.15919400	3.77225300
H	2.81287600	-3.26629400	2.76722700
C	4.58492700	-2.68845300	1.68652100
H	4.22222000	-3.03949400	0.71498900
H	5.66186800	-2.89861000	1.70745200
C	4.33715000	-1.18293200	1.81293100
H	4.85635700	-0.80997300	2.70819200
H	3.27405700	-1.02452400	2.01546200
Br	2.39573800	0.10662200	-2.89323600
O	-0.10914600	2.40450500	1.78966700
O	1.67452900	3.64749800	1.13488600
C	2.01655300	5.91875800	0.66093500
C	0.33002100	5.26703000	2.40533500
C	-0.12491000	4.81281900	-0.05596100
C	0.93224000	4.91096200	1.04378200
C	1.07719600	2.48755900	1.50726200
C	2.01720000	1.33903100	1.53232500
C	3.51609900	1.63724200	1.70521200
H	2.81469200	5.92692700	1.40855100
H	1.58652400	6.92263900	0.60029300
H	2.45322000	5.67141800	-0.31000700
H	-0.43569600	4.54917500	2.69548800
H	-0.11388400	6.26625000	2.35656100
H	1.11198600	5.27840400	3.17101800
H	0.33792400	4.50253700	-0.99760000
H	-0.58886400	5.79234100	-0.20862400
H	-0.89740000	4.09559000	0.21154500
H	1.62256800	0.59851300	2.22170900
H	3.67972500	2.71344400	1.73598100

H	3.87258600	1.23022600	2.65598200
C	-2.27786300	-1.50331200	2.99921400
C	-1.26292700	-1.94934500	3.83565000
C	0.04767700	-1.94134300	3.36590100
C	0.29732100	-1.47711700	2.08219800
C	-0.71693200	-1.02242300	1.21141400
C	-2.05505600	-1.04169700	1.68571100
C	-3.32168500	-0.66691700	0.96053800
C	-4.11835300	-1.68406200	0.38602700
C	-5.33884800	-1.34164000	-0.20767900
C	-5.81162200	-0.03260400	-0.22846200
C	-5.04276200	0.94715900	0.40409200
C	-3.82362100	0.65669400	1.02209400
C	-3.12186600	1.73496900	1.83719600
C	-3.73356100	-3.15687800	0.44675900
P	0.05021700	-0.60964900	-0.43583100
C	0.52974600	-2.28526600	-1.12979200
C	-1.00628600	0.17066300	-1.74336100
C	-3.58015500	1.67690300	3.30833200
C	-3.34364200	3.16101800	1.31171300
C	-3.96558000	-3.89815000	-0.88098400
C	-4.49884600	-3.86792600	1.57900200
C	-0.50860100	-3.38776700	-0.89248700
C	-0.12610100	-4.66998600	-1.64549300
C	1.27275300	-5.15651900	-1.24904400
C	2.31320200	-4.04575700	-1.43503100
C	1.91679100	-2.77232900	-0.67821500
C	-1.36301300	1.61009300	-1.35646700
C	-2.02046500	2.35143700	-2.52407600
C	-3.24043900	1.58532300	-3.04712900
C	-2.84953300	0.16325400	-3.46411600
C	-2.20191800	-0.61088200	-2.30485300
H	-3.30174700	-1.51155500	3.35600600
H	0.87033300	-2.28075100	3.98755700
H	1.31992500	-1.46090900	1.72878500
H	-5.94488800	-2.12100600	-0.65988500
H	-5.41355700	1.96553500	0.43647200
H	-2.04934700	1.54178300	1.82069000
H	-2.67139200	-3.21726000	0.68580700
H	0.60073000	-2.06242700	-2.20122700
H	-0.24259300	0.22839200	-2.53102200
H	-3.34949800	0.71539700	3.76978400
H	-3.07357100	2.45566900	3.88814800
H	-4.66107300	1.84186600	3.38357500

H	-3.14737800	3.24641100	0.23983900
H	-2.67085200	3.84624400	1.83320700
H	-4.36722100	3.50764400	1.49274500
H	1.25961000	-5.46303900	-0.19310700
H	-3.49769500	-4.88728700	-0.84692900
H	-5.03193300	-4.05138700	-1.07472700
H	-4.28140200	-3.42135700	2.55211600
H	-4.22280400	-4.92716800	1.62272200
H	-5.57957200	-3.80501100	1.41320900
H	-0.56158800	-3.60112400	0.18198100
H	-1.49952500	-3.05831500	-1.19887000
H	-0.87400900	-5.44803100	-1.45188000
H	-0.14981300	-4.47138200	-2.72561800
H	-3.55076300	-3.35298900	-1.73274600
H	1.54755600	-6.04387000	-1.83081500
H	3.29920200	-4.38574500	-1.09583100
H	2.41416800	-3.80437200	-2.50108300
H	1.89359100	-2.99229900	0.39574200
H	2.66014800	-1.99076900	-0.84468600
H	-2.04254700	1.59833500	-0.50504000
H	-0.45698900	2.13141500	-1.04105600
H	-2.30727700	3.36024800	-2.20326600
H	-1.28693700	2.47325900	-3.33258800
H	-3.99694700	1.53159200	-2.25485800
H	-3.69684400	2.11674400	-3.89046200
H	-3.72832700	-0.38868300	-3.81840400
H	-2.14476100	0.21402200	-4.30517400
H	-2.94715800	-0.77922400	-1.52798800
H	-1.87358200	-1.59080600	-2.66531800
C	-7.13817700	0.30553000	-0.88659600
H	-7.57298800	-0.63878900	-1.23890200
C	-6.94463400	1.21542500	-2.11076200
H	-7.90386700	1.41982200	-2.59830700
H	-6.50512400	2.17534300	-1.81949500
H	-6.27744800	0.75340000	-2.84408300
C	-8.12558800	0.92846300	0.11407000
H	-9.09719000	1.10418400	-0.35955400
H	-8.27654700	0.27401600	0.97775200
H	-7.75807600	1.89108600	0.48481200
H	-1.49535900	-2.29592800	4.83775600
20''			
C	-3.15086300	-0.97842700	3.14950800
C	-2.39868000	-1.59584100	4.14023800

C	-1.09789600	-1.99881400	3.84390700
C	-0.59910600	-1.79142800	2.56434500
C	-1.36337400	-1.20862200	1.52612200
C	-2.66870500	-0.76556100	1.84213700
C	-3.61423300	-0.01747000	0.94829400
C	-4.65829400	-0.69495200	0.28313100
C	-5.58004200	0.04993000	-0.46180100
C	-5.51858300	1.44109800	-0.54193800
C	-4.50761300	2.09542200	0.16741000
C	-3.56168800	1.39645600	0.92021700
C	-2.56120500	2.16515400	1.77792800
C	-4.85138500	-2.20059200	0.43270200
P	-0.35188400	-1.20096200	-0.03844300
C	-0.21742500	-3.03406500	-0.41924700
C	-1.07892000	-0.48278000	-1.59350600
Pd	1.86775800	-0.08215100	0.00364300
C	-3.20544500	2.54055100	3.12626200
C	-1.98339900	3.42310000	1.11179900
C	-5.22205600	-2.91945900	-0.87416400
C	-5.92082600	-2.49080200	1.50361800
C	-1.49647100	-3.84705000	-0.16230100
C	-1.34605200	-5.27016900	-0.72060700
C	-0.11917700	-5.98008500	-0.13393500
C	1.15402500	-5.14423800	-0.31924700
C	0.98363200	-3.72904900	0.24728300
C	-1.17022300	1.04723000	-1.51862900
C	-1.49015300	1.65350500	-2.88954000
C	-2.76579900	1.03874700	-3.47579300
C	-2.64151700	-0.48510300	-3.57551700
C	-2.33185300	-1.11158800	-2.20750100
H	-4.15228200	-0.62930400	3.37704800
H	-0.47051800	-2.45935500	4.60060600
H	0.42651700	-2.07899100	2.35750500
H	-6.37988500	-0.46644900	-0.98437100
H	-4.46438900	3.17926300	0.14658000
H	-1.72852300	1.49211200	1.99302700
H	-3.90791400	-2.62137500	0.78947900
H	-0.01007000	-3.01634300	-1.49566200
H	-0.23328000	-0.71672800	-2.25617900
H	-3.54290300	1.65422800	3.66806900
H	-2.48897700	3.07414800	3.76000000
H	-4.07196900	3.19142300	2.96774500
H	-1.55077800	3.21024900	0.13215100
H	-1.19405500	3.84244300	1.74406700

H	-2.74175300	4.20226300	0.98447400
H	-0.28407500	-6.14673100	0.94001100
H	-5.23574600	-4.00169700	-0.71011200
H	-6.21904300	-2.63366200	-1.22458800
H	-5.64545300	-2.06703700	2.47218000
H	-6.05396500	-3.57031900	1.63144300
H	-6.88480800	-2.06160800	1.21003600
H	-1.68030300	-3.89412200	0.91822800
H	-2.36876100	-3.36363900	-0.60494800
H	-2.25620100	-5.84694700	-0.51730600
H	-1.24636500	-5.21442800	-1.81336300
H	-4.51236200	-2.70815300	-1.67640600
H	0.00138700	-6.96955700	-0.58979000
H	2.00583200	-5.63613600	0.16281300
H	1.39766700	-5.06855200	-1.38736000
H	0.81627900	-3.80343000	1.32868000
H	1.89036900	-3.14430000	0.08611800
H	-1.95879700	1.32360800	-0.81840200
H	-0.22665200	1.45214100	-1.13765200
H	-1.59583400	2.74092300	-2.79512000
H	-0.64706500	1.47397100	-3.57030700
H	-3.61153800	1.28253100	-2.82050600
H	-2.98399800	1.47055400	-4.45954200
H	-3.56525900	-0.91982600	-3.97560400
H	-1.83921500	-0.73970600	-4.28137800
H	-3.18225200	-0.95467200	-1.54405700
H	-2.19431300	-2.18995700	-2.32619100
C	-6.57383200	2.22116300	-1.30805000
H	-7.16221100	1.49307800	-1.88106000
C	-5.96856000	3.22121300	-2.30513800
H	-6.76083500	3.73964800	-2.85494000
H	-5.37002700	3.98247900	-1.79382200
H	-5.32169200	2.71902400	-3.02927900
C	-7.53002600	2.93023000	-0.33170900
H	-8.33172300	3.44275500	-0.87381600
H	-7.98463500	2.21698800	0.36239300
H	-6.99356100	3.67825100	0.26227900
C	6.28375300	1.66726700	-0.98479600
C	6.13732800	0.64450300	-0.05299200
C	4.87236700	0.11549500	0.24108000
C	3.75992500	0.66107000	-0.40591900
C	3.88174800	1.66512700	-1.37540300
C	5.16320300	2.16043600	-1.65078700
H	7.26751700	2.07462100	-1.19876400

H	7.00897000	0.24088300	0.45730200
H	5.27629200	2.94090400	-2.39955600
C	2.68815200	2.16729400	-2.15055300
H	2.95466400	3.02444500	-2.77688600
H	2.30237900	1.37287600	-2.79705300
H	1.87893800	2.46906400	-1.48052700
H	-2.81456400	-1.74052200	5.13231900
C	4.98331100	-4.94252000	0.55349300
H	4.76026900	-5.81382600	1.17871400
H	6.02446700	-5.02695400	0.22253300
H	4.35018300	-4.99609000	-0.33868600
C	4.75010100	-3.62996000	1.30505900
H	5.37837700	-3.59998200	2.20611600
H	3.70970700	-3.59148300	1.65689500
C	5.02514500	-2.40009000	0.43765200
H	4.39325400	-2.43211200	-0.45615300
H	6.06443500	-2.41540700	0.08416100
C	4.76034900	-1.07353700	1.16950400
H	5.46005800	-0.96737300	2.00883600
H	3.75127800	-1.11964100	1.59666100
Br	2.34252800	-1.41388300	-2.08282300
O	3.97929000	3.04372900	1.97901100
O	2.08726100	3.44674000	0.76963900
C	1.17575400	5.31840000	-0.31252900
C	3.67801900	5.10522400	-0.15283400
C	2.30310200	5.58769800	1.92517700
C	2.34753300	4.88516100	0.56677200
C	2.92113000	2.68797600	1.50084700
C	2.34870700	1.34219200	1.80352900
C	1.00184900	1.07043400	1.74994200
H	1.18289200	4.77091000	-1.25849300
H	1.25055100	6.38764200	-0.52993100
H	0.22316200	5.13162200	0.18955700
H	4.51444400	4.75372700	0.44885300
H	3.80055400	6.17525700	-0.34916500
H	3.68974800	4.57599200	-1.10632800
H	1.36030500	5.36782600	2.43617000
H	2.36799100	6.67033400	1.78024200
H	3.13317100	5.26936300	2.55649300
H	3.01446600	0.73683600	2.40605200
H	0.32583900	1.80401600	1.32733400
H	0.57271400	0.29429400	2.36771300

TS7''

C	-3.03642500	-0.66448100	3.23564900
C	-2.26173200	-1.24439800	4.23179400
C	-0.99666500	-1.72909500	3.90435500
C	-0.55536200	-1.64071000	2.59019800
C	-1.34827500	-1.10224000	1.55124100
C	-2.61221100	-0.57313600	1.89487000
C	-3.54819900	0.17292300	0.99174300
C	-4.67295300	-0.46784900	0.43105100
C	-5.57389700	0.29156600	-0.32497200
C	-5.41092600	1.66416100	-0.51441200
C	-4.31719900	2.28686500	0.09359600
C	-3.38623300	1.57145500	0.84899100
C	-2.27132300	2.31062700	1.58176500
C	-4.96390100	-1.94090900	0.70054300
P	-0.43877300	-1.25630400	-0.06511700
C	-0.37603300	-3.11434200	-0.31629800
C	-1.21825700	-0.65211200	-1.64286300
Pd	1.69394700	-0.24684200	-0.08238100
C	-2.78417200	2.82194000	2.94172600
C	-1.64846800	3.47172500	0.79301700
C	-5.45933100	-2.72008500	-0.52803700
C	-5.98890900	-2.07567300	1.84318400
C	-1.65508200	-3.85863800	0.10321500
C	-1.58925500	-5.33187900	-0.32589200
C	-0.34159800	-6.02508300	0.23541400
C	0.93511700	-5.26011100	-0.13543300
C	0.85973500	-3.79132400	0.30115400
C	-1.25173400	0.87914300	-1.72131500
C	-1.60746100	1.35379400	-3.13436400
C	-2.93068500	0.73749800	-3.60253800
C	-2.86974600	-0.79231800	-3.54601900
C	-2.52260900	-1.28539100	-2.13300000
H	-4.00490200	-0.24508300	3.48656700
H	-0.35158700	-2.16062800	4.66335600
H	0.44460100	-1.98805000	2.35485800
H	-6.43578600	-0.19651400	-0.77044100
H	-4.19138600	3.35881100	-0.01565600
H	-1.47732700	1.58862100	1.78462200
H	-4.03249600	-2.40489300	1.03662100
H	-0.25561600	-3.18258500	-1.40445200
H	-0.41130200	-0.98354700	-2.31351600
H	-3.14845100	2.00220600	3.56480500
H	-1.98342200	3.33313000	3.48685500
H	-3.60686900	3.53088300	2.79873800

H	-1.31013200	3.16275300	-0.19799700
H	-0.78058900	3.85674600	1.33706700
H	-2.34959900	4.30359000	0.66883900
H	-0.42405500	-6.07605100	1.33046800
H	-5.54839300	-3.78261900	-0.28008100
H	-6.44864900	-2.38029000	-0.85119000
H	-5.63118700	-1.60603200	2.76210400
H	-6.19033300	-3.13075400	2.05720500
H	-6.93506000	-1.59791400	1.56700100
H	-1.76060200	-3.80081000	1.19330500
H	-2.54448800	-3.38665100	-0.32023700
H	-2.49739100	-5.85351500	-0.00108700
H	-1.57127900	-5.38438000	-1.42329200
H	-4.77935200	-2.62686300	-1.37690500
H	-0.28730200	-7.05935800	-0.12350000
H	1.81000600	-5.73657500	0.31982100
H	1.08692500	-5.29741100	-1.22252100
H	0.79770300	-3.75378600	1.39566700
H	1.75922100	-3.25528000	-0.00558200
H	-1.99820200	1.25947000	-1.02401000
H	-0.27876500	1.27890900	-1.41949200
H	-1.66783600	2.44864100	-3.15052900
H	-0.80356100	1.06838300	-3.82620900
H	-3.73728500	1.08338600	-2.94340900
H	-3.17504500	1.07414300	-4.61685000
H	-3.82685300	-1.22633600	-3.85910600
H	-2.11071900	-1.15341800	-4.25324200
H	-3.33387600	-1.01838000	-1.45574600
H	-2.43852700	-2.37569200	-2.14101200
C	-6.43981500	2.46637700	-1.29333200
H	-7.10422700	1.74674100	-1.78866300
C	-5.80846700	3.34612400	-2.38354600
H	-6.58587900	3.87007900	-2.94923300
H	-5.14846000	4.10552200	-1.95115900
H	-5.21784300	2.75057000	-3.08472000
C	-7.29793100	3.31257300	-0.33518700
H	-8.07933500	3.85037800	-0.88262100
H	-7.77684500	2.68493600	0.42230900
H	-6.68124800	4.05279700	0.18613400
C	6.12959500	1.25804100	-1.36666900
C	6.02523500	0.28839400	-0.37339900
C	4.78401400	-0.02711000	0.18968900
C	3.64903700	0.67567500	-0.25245200
C	3.72771100	1.61866900	-1.29997000

C	4.98417000	1.89562100	-1.84397400
H	7.10097800	1.50493100	-1.78487200
H	6.91186900	-0.23927200	-0.03162100
H	5.06064300	2.61054200	-2.65913600
C	2.49356300	2.21562600	-1.92629700
H	2.73579200	3.11325100	-2.50357100
H	2.04985000	1.47920000	-2.60544100
H	1.74156800	2.47687800	-1.18016700
H	-2.63077000	-1.29492300	5.25136900
C	4.74542900	-5.06533800	0.63381000
H	4.49414800	-5.91200400	1.28155100
H	5.78127700	-5.19550900	0.30102300
H	4.10638100	-5.11699700	-0.25396400
C	4.56348400	-3.72767100	1.35442300
H	5.20354200	-3.69499600	2.24711800
H	3.52927800	-3.64488800	1.71535600
C	4.86894300	-2.53261100	0.44971700
H	4.21391500	-2.55463400	-0.42784400
H	5.89665400	-2.60553200	0.07131600
C	4.68222300	-1.18020600	1.16203400
H	5.42532900	-1.07699900	1.96394800
H	3.69220000	-1.18690900	1.63143800
Br	2.23361600	-1.56231200	-2.21723300
O	4.31243000	3.00297500	1.89747800
O	2.38153700	3.57883400	0.83325700
C	1.54500400	5.56462500	-0.10477500
C	4.02372600	5.13800300	-0.15390100
C	2.85777800	5.65311000	2.04386300
C	2.73888100	5.00307100	0.66481200
C	3.23336400	2.72218900	1.41542700
C	2.67821500	1.32780600	1.51059000
C	1.28675100	1.04265900	1.53894100
H	1.42027200	5.04243900	-1.05666000
H	1.70410600	6.62715300	-0.30938600
H	0.62339500	5.45820700	0.47277100
H	4.87419200	4.70600800	0.37148600
H	4.21872800	6.19950700	-0.33555600
H	3.91858800	4.63895300	-1.11929600
H	1.94342300	5.48460700	2.62099700
H	2.99408200	6.73268400	1.92772600
H	3.70667200	5.24764200	2.59415900
H	3.31161500	0.73994400	2.16130700
H	0.60344600	1.82219000	1.22010200
H	0.92145300	0.39173100	2.32652500

21"

C	-2.57374800	0.06022000	3.27589000
C	-1.68328100	-0.20261400	4.30876300
C	-0.42033300	-0.70579600	4.00031900
C	-0.09568400	-0.95627200	2.67384500
C	-1.00809500	-0.74879600	1.61510000
C	-2.26946500	-0.19421100	1.92365600
C	-3.32163200	0.24272900	0.94869700
C	-4.46903700	-0.54726500	0.72938300
C	-5.48193900	-0.04991400	-0.09974400
C	-5.40354600	1.20984600	-0.69284600
C	-4.27436400	1.99190800	-0.43008200
C	-3.23673100	1.53978700	0.38719600
C	-2.08951800	2.47627700	0.75189400
C	-4.66109000	-1.88829500	1.43133500
P	-0.25283100	-1.33005000	0.02171700
C	-0.12029300	-3.17978600	0.28739200
C	-1.18993200	-1.20379300	-1.58202800
Pd	1.73498100	-0.35274200	-0.49152400
C	-2.47169000	3.30408200	1.99443000
C	-1.64093300	3.41439200	-0.37890300
C	-5.19703500	-3.00039800	0.51518800
C	-5.59539900	-1.72443300	2.64547000
C	-1.32822700	-3.79435500	1.01688500
C	-1.24510900	-5.32789000	0.99219200
C	0.07289400	-5.82758600	1.59631100
C	1.28223000	-5.17310900	0.91637800
C	1.18934800	-3.64173100	0.94912200
C	-1.27968600	0.24206000	-2.08563500
C	-1.79870000	0.29714700	-3.52611900
C	-3.14363300	-0.42676900	-3.65192200
C	-3.02316300	-1.87921300	-3.18110400
C	-2.51423500	-1.95854800	-1.73358700
H	-3.54245700	0.49343600	3.50049200
H	0.31192400	-0.88943100	4.78032700
H	0.90308700	-1.30638600	2.43820200
H	-6.36588700	-0.65546100	-0.27780100
H	-4.20706700	2.98546600	-0.86092900
H	-1.23054300	1.85954800	1.02323300
H	-3.68523300	-2.20775600	1.80746900
H	-0.09215100	-3.54516100	-0.74659000
H	-0.43890900	-1.70961400	-2.20666400
H	-2.73389500	2.66172900	2.83759800

H	-1.63749400	3.94058000	2.30226400
H	-3.33245600	3.94555000	1.77545300
H	-1.44745700	2.87635000	-1.30923000
H	-0.71482700	3.91767900	-0.08479700
H	-2.38543900	4.19083100	-0.58457500
H	0.08881400	-5.58379900	2.66805300
H	-5.21737500	-3.95053700	1.05861800
H	-6.22024400	-2.79404100	0.18516000
H	-5.20091200	-1.00109700	3.36268100
H	-5.72406700	-2.68049600	3.16406000
H	-6.58328400	-1.37575400	2.32599500
H	-1.33311000	-3.44556200	2.05642600
H	-2.27070600	-3.46575900	0.57354600
H	-2.10029500	-5.75360900	1.53042100
H	-1.32354500	-5.67319100	-0.04784500
H	-4.57859100	-3.13253500	-0.37459200
H	0.13525000	-6.91939600	1.52197600
H	2.20987200	-5.49787200	1.40017300
H	1.34150200	-5.49914500	-0.13041400
H	1.21669100	-3.30875400	1.99367200
H	2.03831700	-3.19627200	0.42738900
H	-1.95963400	0.80265500	-1.44435200
H	-0.29150900	0.71002600	-2.01834200
H	-1.89502200	1.34299100	-3.84162700
H	-1.06391600	-0.17155800	-4.19430600
H	-3.88503100	0.08794400	-3.02759400
H	-3.50780500	-0.38828600	-4.68527400
H	-3.99135600	-2.38888600	-3.25318200
H	-2.32950400	-2.41927500	-3.83960100
H	-3.26120600	-1.52392500	-1.06967800
H	-2.38764100	-3.00791500	-1.45345500
C	-6.55118900	1.74467700	-1.53358400
H	-7.27097000	0.92544200	-1.65766700
C	-6.10270700	2.18819000	-2.93476700
H	-6.95851400	2.54948500	-3.51445100
H	-5.37275600	3.00257000	-2.88018800
H	-5.64119400	1.36359000	-3.48422200
C	-7.26954100	2.89041700	-0.79862000
H	-8.13432000	3.23944000	-1.37273400
H	-7.61709800	2.56852800	0.18764200
H	-6.59603900	3.74190900	-0.65358600
C	4.96872900	0.26659000	-2.83258800
C	5.23393200	-0.25332600	-1.57274700
C	4.54641600	0.20082300	-0.44293700

C	3.60154900	1.25569400	-0.59238100
C	3.30010500	1.75263300	-1.89269300
C	3.99311400	1.24479300	-2.99126800
H	5.49646400	-0.11922200	-3.69897000
H	5.95322400	-1.05688700	-1.47002000
H	3.75713900	1.62128700	-3.98220400
C	2.30021200	2.86041500	-2.13018900
H	2.79510400	3.83639300	-2.08728300
H	1.84973600	2.75288700	-3.12041500
H	1.49094800	2.86984200	-1.39967700
H	-1.96288300	0.00673800	5.33658500
C	5.02655200	-4.22724200	2.01261500
H	4.81377100	-4.73603100	2.95855200
H	6.06935400	-4.43524600	1.74806100
H	4.39581900	-4.67613000	1.23807800
C	4.77406700	-2.72159600	2.11063000
H	5.41624300	-2.28589900	2.88845800
H	3.73841600	-2.54409400	2.43140100
C	5.00495500	-2.00134500	0.78029400
H	4.31682300	-2.39750400	0.02433000
H	6.01875400	-2.22162500	0.42358400
C	4.79510200	-0.48089600	0.89345900
H	5.65574400	-0.02167000	1.40048300
H	3.93559600	-0.32109400	1.55004600
Br	2.25124600	-2.18914800	-2.22523300
O	4.08032800	3.94598400	0.26232600
O	2.03713700	3.99366800	1.25827100
C	0.71186900	5.70312000	2.17695500
C	2.11886400	6.18957700	0.15019900
C	3.21094100	5.81737100	2.41710400
C	2.05148500	5.45090000	1.48836300
C	3.08485900	3.38478700	0.67467700
C	2.91512100	1.86802400	0.64163100
C	1.50603700	1.28471200	0.74447700
H	-0.11934500	5.45856000	1.51153200
H	0.62958600	6.75726800	2.45658500
H	0.62487300	5.09444600	3.08120000
H	3.08193000	6.03704600	-0.33567500
H	1.97224300	7.26112800	0.31865800
H	1.32397800	5.83906300	-0.51527000
H	3.15341900	5.23316100	3.34065600
H	3.14393600	6.87750500	2.68032200
H	4.17186900	5.63324300	1.93809100
H	3.48228900	1.55069900	1.52145900

H	0.74712400	1.92755600	0.29947100
H	1.21120400	1.02820200	1.76090100
20''			
C	2.71260600	-0.23082100	3.37491400
C	1.74102700	0.00435100	4.33884100
C	0.48030700	0.43883000	3.93298200
C	0.23575300	0.64049100	2.58094700
C	1.22297100	0.45065800	1.58589400
C	2.49039600	-0.02387100	1.99836900
C	3.64298200	-0.40884700	1.11650500
C	4.69632100	0.49888600	0.87516500
C	5.79533700	0.07491500	0.11951300
C	5.89809800	-1.22449100	-0.37741600
C	4.87269200	-2.12426500	-0.07560000
C	3.75610300	-1.74884200	0.67552900
C	2.75662400	-2.81696100	1.11084200
C	4.70400000	1.88909400	1.50034700
P	0.49965300	0.91113600	-0.06964000
C	0.30651200	2.77042200	0.07574900
C	1.51623500	0.69674200	-1.61364100
Pd	-1.61421600	-0.22047100	-0.70138900
C	3.32047700	-3.58844400	2.31986900
C	2.35275500	-3.80262100	0.00338400
C	5.21807300	2.99463400	0.56525000
C	5.53472100	1.87701900	2.79825900
C	1.47353900	3.49080100	0.76776100
C	1.30875800	5.01410600	0.66097000
C	-0.03608300	5.47695300	1.23425800
C	-1.20560700	4.72238500	0.58987100
C	-1.02707700	3.20349700	0.70884100
C	1.72127000	-0.78457100	-1.95816700
C	2.29729400	-0.95627300	-3.36819500
C	3.59146400	-0.15258400	-3.53548500
C	3.35550000	1.32876800	-3.22546300
C	2.79367500	1.52005900	-1.80867000
H	3.68708300	-0.60005300	3.67654300
H	-0.31151900	0.60689100	4.65635700
H	-0.76158600	0.93819900	2.27511300
H	6.60456500	0.77223200	-0.07638800
H	4.95417400	-3.15210700	-0.41394900
H	1.85258300	-2.30851400	1.45327300
H	3.67560800	2.13382600	1.77444200
H	0.26814600	3.07204300	-0.97797200

H	0.76453900	1.08281200	-2.31754900
H	3.53606600	-2.91643500	3.15409100
H	2.60446900	-4.34177400	2.66528800
H	4.25042000	-4.09969800	2.04962400
H	1.96818700	-3.29273200	-0.88252400
H	1.57180500	-4.47498300	0.37285200
H	3.19449600	-4.42804500	-0.31018800
H	-0.04470900	5.29263400	2.31792800
H	5.07243900	3.97380700	1.03248000
H	6.28894800	2.88892800	0.36402700
H	5.13600100	1.16261300	3.52231500
H	5.53412900	2.86832700	3.26393900
H	6.57334400	1.60012300	2.58810800
H	1.49620400	3.19965800	1.82519100
H	2.43007000	3.19098500	0.33886100
H	2.13824300	5.51311400	1.17613800
H	1.37363500	5.30649800	-0.39620800
H	4.69644700	2.99646700	-0.39416300
H	-0.15564400	6.55803800	1.09897500
H	-2.15207000	5.02127600	1.05237000
H	-1.27732600	4.98666600	-0.47366000
H	-1.03736600	2.93113300	1.77131300
H	-1.85268400	2.68396100	0.22082000
H	2.41133500	-1.22786800	-1.23880600
H	0.76437400	-1.31345700	-1.88130400
H	2.47752600	-2.01983800	-3.56444700
H	1.55621800	-0.61759700	-4.10462300
H	4.34587900	-0.54404500	-2.84133600
H	3.99073600	-0.27387500	-4.54918200
H	4.28853700	1.89562100	-3.32670600
H	2.64950600	1.74637100	-3.95616100
H	3.54632700	1.20865300	-1.08394100
H	2.58813600	2.58112400	-1.64218000
C	7.13693500	-1.66541000	-1.13974600
H	7.71217300	-0.75997400	-1.37181600
C	6.80513400	-2.36198900	-2.46804900
H	7.72455600	-2.63137900	-2.99790400
H	6.23774900	-3.28397500	-2.30432800
H	6.21130900	-1.71589700	-3.11982800
C	8.01696400	-2.56527000	-0.25335100
H	8.93818700	-2.84554900	-0.77493700
H	8.28809200	-2.05740300	0.67707700
H	7.48555400	-3.48577000	0.01155400
C	-5.96214900	-1.55138600	-2.38334400

C	-5.84692700	-0.74981700	-1.25316100
C	-4.58788200	-0.35381800	-0.77506500
C	-3.45248700	-0.79870400	-1.45753300
C	-3.54180000	-1.56310700	-2.62888000
C	-4.81449700	-1.94183600	-3.07251200
H	-6.94112000	-1.86306300	-2.73537500
H	-6.73912900	-0.41534500	-0.72795600
H	-4.90057100	-2.54623800	-3.97219900
C	-2.32016000	-1.92225300	-3.43852600
H	-2.58868900	-2.52322400	-4.31182700
H	-1.81979700	-1.00977200	-3.77885700
H	-1.58296100	-2.48833200	-2.85816100
H	1.95982800	-0.16764300	5.38805400
C	-5.04824100	4.46479000	0.76854600
H	-4.99520800	5.14848900	1.62269200
H	-6.05056300	4.55021300	0.33407400
H	-4.33407900	4.81183000	0.01425400
C	-4.75029800	3.02036100	1.17648300
H	-5.47036500	2.69597300	1.94093300
H	-3.76100200	2.96736500	1.65002000
C	-4.79356500	2.05351000	-0.00907500
H	-4.06965300	2.35827300	-0.77249300
H	-5.78102300	2.10293300	-0.48652800
C	-4.50968000	0.59962000	0.39754500
H	-5.23471200	0.30485200	1.16592000
H	-3.52029900	0.53478700	0.86638400
Br	-1.87545600	1.60737500	-2.40851300
O	-3.82418600	-3.75126900	0.22216500
O	-3.44990900	-2.09575000	1.74631800
C	-4.13959500	-3.88042300	3.26278200
C	-5.87704500	-2.53706000	1.99798500
C	-4.44781200	-1.42838200	3.75576600
C	-4.50984600	-2.51379700	2.68261600
C	-3.17750100	-2.81415800	0.64506100
C	-1.87854100	-2.42888000	0.01948800
C	-0.86483100	-1.81758900	0.71888800
H	-4.16203300	-4.65018500	2.49054500
H	-4.85314600	-4.15169400	4.04669900
H	-3.13972300	-3.84690500	3.70654200
H	-6.10009500	-1.56967800	1.54627200
H	-6.64489900	-2.75314000	2.74783400
H	-5.91212300	-3.29675300	1.21912000
H	-3.45332800	-1.39579000	4.21072300
H	-5.18238800	-1.63372000	4.53959000

H	-4.66316400	-0.44799900	3.32374800
H	-1.67030300	-2.99010900	-0.88226700
H	0.16040600	-1.93563200	0.39939400
H	-1.02929800	-1.46443900	1.72879400
TS7'''			
C	2.58401600	-0.37082100	3.42308900
C	1.62578300	-0.04256600	4.37319100
C	0.43291000	0.54412900	3.95303700
C	0.24110700	0.79979700	2.60165000
C	1.22150400	0.51762100	1.62384300
C	2.41524100	-0.10872100	2.04886100
C	3.52080200	-0.61675700	1.17161700
C	4.67725000	0.15931600	0.94467500
C	5.71415200	-0.38373400	0.17799700
C	5.65651200	-1.67911600	-0.33841800
C	4.53128000	-2.45293500	-0.04475500
C	3.46646400	-1.95222500	0.70830000
C	2.32597900	-2.88402500	1.10614100
C	4.85129300	1.52607600	1.59826400
P	0.60168100	1.07568200	-0.04174900
C	0.56344900	2.94169400	0.12051000
C	1.63150600	0.81515700	-1.57092400
Pd	-1.45700700	0.08867100	-0.64882200
C	2.76941800	-3.77410600	2.28267700
C	1.78578800	-3.75376400	-0.03929500
C	5.52559700	2.57664400	0.70235000
C	5.64775000	1.37964600	2.90964500
C	1.75369600	3.53805000	0.88949000
C	1.74061400	5.07145000	0.80831500
C	0.41399600	5.64823300	1.31631400
C	-0.78032000	5.02328300	0.58454300
C	-0.76045300	3.49179500	0.67646600
C	1.72297900	-0.66421900	-1.96495800
C	2.29002900	-0.82726200	-3.37913000
C	3.64849700	-0.12939700	-3.50912000
C	3.53634500	1.35281500	-3.13714100
C	2.97613400	1.53327500	-1.71769900
H	3.49969700	-0.86319200	3.73274700
H	-0.34906900	0.78794200	4.66548900
H	-0.70824400	1.21411500	2.28097600
H	6.60113900	0.21296300	-0.01311800
H	4.48588400	-3.47754300	-0.39906800
H	1.50274600	-2.26389200	1.46750500

H	3.85633500	1.89598100	1.85825600
H	0.61421500	3.25480700	-0.92982700
H	0.92387000	1.28275400	-2.27215200
H	3.08927300	-3.17227500	3.13714700
H	1.94703100	-4.41961200	2.60875400
H	3.60841000	-4.41364100	1.98794300
H	1.45213500	-3.15115900	-0.88641600
H	0.93328400	-4.34321500	0.31390700
H	2.53802000	-4.45983900	-0.40487700
H	0.32351900	5.44192000	2.39229100
H	5.51809500	3.54939900	1.20435500
H	6.57228600	2.32565900	0.50227500
H	5.14832800	0.70627900	3.60980200
H	5.76512900	2.35227800	3.39934600
H	6.64611100	0.97690000	2.70777400
H	1.69021800	3.22695700	1.93964800
H	2.70122400	3.15474200	0.50674800
H	2.58229900	5.48013100	1.38005100
H	1.89263800	5.37502900	-0.23667600
H	5.01817500	2.68796300	-0.25802900
H	0.40489600	6.73853000	1.20396100
H	-1.71969800	5.40670000	0.99633400
H	-0.75841700	5.31364900	-0.47449100
H	-0.87097100	3.20157100	1.72831800
H	-1.59437100	3.06284000	0.11849200
H	2.37210800	-1.18664300	-1.26151200
H	0.72752600	-1.11713100	-1.90403400
H	2.38204000	-1.89346300	-3.61796000
H	1.58510100	-0.39727400	-4.10327900
H	4.36363200	-0.61171000	-2.83012900
H	4.04299000	-0.24042900	-4.52589800
H	4.51534600	1.84168100	-3.20747700
H	2.87613900	1.85918400	-3.85431500
H	3.68925400	1.12553400	-1.00091300
H	2.86402500	2.60065700	-1.50781600
C	6.83040200	-2.25311100	-1.11426700
H	7.48386500	-1.41217700	-1.38029300
C	6.40762700	-2.94601000	-2.41828100
H	7.28822100	-3.29719100	-2.96588900
H	5.77493900	-3.81806100	-2.22187700
H	5.84913000	-2.26724500	-3.06837700
C	7.64096200	-3.21119000	-0.22232200
H	8.52190000	-3.58774400	-0.75296500
H	7.97609000	-2.70994300	0.69065100

H	7.03128100	-4.07173000	0.07405700
C	-5.69968700	-1.07942200	-2.71481500
C	-5.66122600	-0.43683500	-1.48086300
C	-4.45621700	-0.29740900	-0.78252100
C	-3.28455900	-0.82893900	-1.35582700
C	-3.29704700	-1.42972800	-2.63173400
C	-4.52114000	-1.55029600	-3.29357700
H	-6.64474000	-1.19997700	-3.23613800
H	-6.57205300	-0.02760200	-1.05062700
H	-4.54684300	-2.01189600	-4.27692600
C	-2.02750400	-1.82769400	-3.34042300
H	-2.24007600	-2.45561700	-4.20978800
H	-1.51307000	-0.92122800	-3.67826300
H	-1.32424800	-2.36672300	-2.69792800
H	1.79910300	-0.26165700	5.42217700
C	-4.55389700	4.37075700	1.18601600
H	-4.39029000	4.97230100	2.08651700
H	-5.56346200	4.58633300	0.81873300
H	-3.84858100	4.70942300	0.42023200
C	-4.37949400	2.87591400	1.46213100
H	-5.10920100	2.55139800	2.21744100
H	-3.38770700	2.69454000	1.89786100
C	-4.52994800	2.02630300	0.19931500
H	-3.76293500	2.30031400	-0.53272200
H	-5.49600000	2.23973200	-0.27696300
C	-4.43551500	0.51854200	0.48879700
H	-5.27221500	0.23082700	1.13615600
H	-3.51852800	0.31657200	1.05032100
Br	-1.71329400	1.85192800	-2.48603700
O	-4.01734400	-3.70448500	-0.06747400
O	-3.85509200	-2.20797900	1.64341000
C	-4.70684300	-4.16603100	2.84129000
C	-6.28509100	-2.64423200	1.56305600
C	-5.07083900	-1.79297100	3.60310000
C	-5.00804000	-2.73258700	2.40020700
C	-3.48493400	-2.75993800	0.48060200
C	-2.22723800	-2.14687600	-0.06872000
C	-1.26314800	-1.49228900	0.74189900
H	-4.64872800	-4.83418200	1.98211900
H	-5.50039400	-4.51665900	3.50823200
H	-3.75971000	-4.20307700	3.38808000
H	-6.45364600	-1.62045000	1.22259900
H	-7.13725500	-2.94533400	2.18038400
H	-6.22921000	-3.29575800	0.69204100

H	-4.13593100	-1.83240100	4.16935300
H	-5.89091500	-2.08763700	4.26387300
H	-5.23637200	-0.76206500	3.28011800
H	-1.85179100	-2.76522200	-0.87310100
H	-0.23146200	-1.80073700	0.62594800
H	-1.54527500	-1.17788200	1.74111400

21'''

C	1.83241100	-1.39159600	2.98562900
C	0.83277500	-1.29783300	3.94449700
C	-0.21026300	-0.39453500	3.74354400
C	-0.22596800	0.37755000	2.59061400
C	0.78982700	0.31340100	1.61038800
C	1.84579400	-0.60349600	1.81643900
C	2.99557600	-0.87119400	0.89241000
C	4.17873600	-0.10317700	0.98319500
C	5.24918100	-0.41099400	0.13752600
C	5.19795900	-1.47187000	-0.76952900
C	4.04928600	-2.26387500	-0.78595500
C	2.95237100	-1.99739000	0.03908400
C	1.78921700	-2.98481800	0.05053600
C	4.33367200	0.96687300	2.05995600
P	0.34144600	1.42928700	0.18471700
C	0.29008400	3.14862800	0.92515500
C	1.48206400	1.63405600	-1.26997800
Pd	-1.60950200	0.81109600	-0.78650300
C	2.23347700	-4.30670000	0.70284800
C	1.18727000	-3.25001600	-1.33885400
C	5.24135200	2.14355200	1.67262000
C	4.85910600	0.32483400	3.35986100
C	1.39586500	3.42350900	1.95863200
C	1.41139000	4.90880900	2.35014900
C	0.04330900	5.37166700	2.86592100
C	-1.06592500	5.05938500	1.85379600
C	-1.08246000	3.57259600	1.47788800
C	1.58237500	0.36072500	-2.12004600
C	2.28876000	0.63696600	-3.45108200
C	3.66551700	1.27008600	-3.22136600
C	3.54341900	2.55564900	-2.39672200
C	2.84683300	2.29390100	-1.05222500
H	2.64066200	-2.10306600	3.11993900
H	-1.01625400	-0.29992000	4.46438000
H	-1.07526300	1.02622700	2.42232900
H	6.15558300	0.18439200	0.18798100

H	4.00673100	-3.12352700	-1.44760700
H	0.99450500	-2.57394700	0.67538500
H	3.33931400	1.36699000	2.27438400
H	0.46583900	3.76646500	0.03476800
H	0.84653900	2.33857900	-1.82830700
H	2.58317200	-4.14566800	1.72672200
H	1.40129200	-5.01756700	0.73347400
H	3.05077700	-4.76945500	0.13972200
H	0.87367200	-2.32328800	-1.82406700
H	0.30876900	-3.89579600	-1.23971100
H	1.89976800	-3.75103600	-2.00221000
H	-0.17620700	4.85478600	3.81105800
H	5.18526500	2.91920800	2.44273400
H	6.29009100	1.83719000	1.60179800
H	4.18498300	-0.45217200	3.72525500
H	4.96280900	1.08052400	4.14591900
H	5.84180000	-0.12839200	3.19075400
H	1.21346300	2.81144500	2.85039200
H	2.37632900	3.13215800	1.57486100
H	2.18659700	5.08320200	3.10566200
H	1.68891600	5.50618300	1.47069500
H	4.95684100	2.59358400	0.71917600
H	0.06706200	6.44374000	3.09279300
H	-2.04351500	5.34755000	2.25659300
H	-0.91467100	5.65325000	0.94268900
H	-1.32131300	2.99026800	2.37540600
H	-1.85274700	3.37625000	0.72999200
H	2.13802900	-0.40230700	-1.57390600
H	0.57332900	-0.02640600	-2.29757400
H	2.38654800	-0.29854300	-4.01446700
H	1.66983300	1.31211000	-4.05711100
H	4.29854800	0.55946900	-2.67500200
H	4.16000800	1.47545500	-4.17792300
H	4.53331800	2.99097300	-2.21491100
H	2.96863100	3.30040300	-2.96364800
H	3.47122100	1.63408700	-0.45093700
H	2.73547800	3.23653800	-0.50911300
C	6.39759400	-1.80015300	-1.64248900
H	7.08080000	-0.94267000	-1.58919900
C	6.02288700	-2.00851200	-3.11767100
H	6.92101000	-2.18505400	-3.71834100
H	5.36772000	-2.87669700	-3.24433500
H	5.50495200	-1.13616900	-3.52503600
C	7.14266500	-3.02783000	-1.08744600

H	8.04150300	-3.23936500	-1.67641900
H	7.44161700	-2.86982800	-0.04685400
H	6.50129600	-3.91541200	-1.11943000
C	-5.12095300	1.05060100	-2.71644500
C	-5.21563400	0.72069100	-1.37128700
C	-4.33665600	-0.20021800	-0.78893500
C	-3.34387700	-0.81567600	-1.59941500
C	-3.25145900	-0.47374800	-2.97652300
C	-4.14376900	0.45611700	-3.50975400
H	-5.79967200	1.77954200	-3.14748800
H	-5.97756500	1.18359300	-0.75090300
H	-4.05810300	0.72901700	-4.55653500
C	-2.21180600	-1.09292800	-3.88194400
H	-2.28973400	-0.67432000	-4.88759300
H	-1.19540000	-0.89650600	-3.52605900
H	-2.33446200	-2.17919400	-3.96106600
H	0.86321600	-1.92637900	4.82906000
C	-3.74569600	1.43520500	4.00816700
H	-3.71215500	1.11793100	5.05568000
H	-4.49287400	2.23170700	3.92420300
H	-2.77401200	1.87705200	3.76181600
C	-4.07838800	0.26865100	3.07529700
H	-5.04029400	-0.17309400	3.36846600
H	-3.32964800	-0.52673900	3.19721600
C	-4.13010500	0.67277300	1.60023000
H	-3.15368400	1.06316400	1.28489400
H	-4.84003100	1.49698100	1.45855600
C	-4.50600300	-0.50552400	0.68549100
H	-5.55034200	-0.78747500	0.86778500
H	-3.91235000	-1.37013900	0.98102400
Br	-1.91686200	3.02714700	-2.02986200
O	-4.10856100	-3.50538200	-0.78676100
O	-2.25889500	-3.59640900	0.54207200
C	-2.83927400	-5.97814800	0.46224100
C	-3.98489100	-4.39464800	2.08854100
C	-1.53176000	-4.90429000	2.33550400
C	-2.69007600	-4.74339700	1.35155900
C	-3.04138400	-3.06256000	-0.41633500
C	-2.36073300	-1.82608600	-0.99640700
C	-1.43055900	-1.08265900	-0.04084400
H	-3.65947900	-5.85146200	-0.24454400
H	-3.03666400	-6.85780100	1.08293000
H	-1.91396700	-6.15468600	-0.09489500
H	-3.85308200	-3.47616600	2.66918200

H	-4.23936700	-5.20265100	2.78121900
H	-4.80933300	-4.25631000	1.38928600
H	-0.60356400	-5.12719800	1.80285000
H	-1.73863300	-5.72135000	3.03261200
H	-1.38436600	-3.98198100	2.90476600
H	-1.74960800	-2.22394100	-1.81099200
H	-0.41181500	-1.45275300	-0.07180800
H	-1.77123900	-1.08323000	0.99382000

TS8'

C	3.12876600	-3.29539300	-1.31655500
C	2.36743600	-4.38642400	-1.71577800
C	0.99043300	-4.36430400	-1.50501900
C	0.41613200	-3.26726700	-0.87825700
C	1.18505000	-2.18273900	-0.40480100
C	2.57067800	-2.17978300	-0.66348700
C	3.51332400	-1.04305100	-0.42105300
C	4.44433900	-1.08560900	0.63915300
C	5.37372800	-0.04519600	0.76019300
C	5.42504700	1.00929600	-0.15099000
C	4.51732900	1.00960800	-1.21366800
C	3.55595000	0.00836900	-1.36884200
C	2.59921600	0.03954800	-2.55703300
C	4.48252600	-2.25178300	1.62565000
P	0.09742900	-0.92491900	0.39828200
C	-0.75328900	-1.88753000	1.77720400
C	0.84140300	0.47324400	1.38742500
Pd	-1.49813900	0.05890400	-0.98783100
C	3.15463000	-0.78841800	-3.73103000
C	2.26044200	1.45413500	-3.04456300
C	4.76834200	-1.83393100	3.07846800
C	5.53116000	-3.29585400	1.19467900
C	0.06862700	-3.03992900	2.38054700
C	-0.64845000	-3.63279200	3.60135700
C	-2.05760200	-4.11448100	3.23507300
C	-2.88483800	-2.98647200	2.60571300
C	-2.16932200	-2.36091600	1.40097300
C	1.33411600	1.65158200	0.53754800
C	1.63012400	2.87341200	1.41427300
C	2.62802000	2.52617700	2.52555500
C	2.11751500	1.35701500	3.37492300
C	1.82225800	0.12402000	2.50801400
H	4.18924900	-3.26967400	-1.54129100
H	0.36055500	-5.17735800	-1.85089500

H	-0.66131100	-3.23506200	-0.78153300
H	6.08355800	-0.05676800	1.58199000
H	4.55055000	1.81777400	-1.93576900
H	1.65501000	-0.42615600	-2.26188400
H	3.49967700	-2.73552900	1.60164500
H	-0.87105500	-1.11833100	2.55266100
H	-0.09094200	0.81247900	1.86228800
H	3.33389100	-1.82595400	-3.44335300
H	2.43596700	-0.78882500	-4.55606100
H	4.09902700	-0.36300200	-4.09000900
H	1.94995800	2.10510400	-2.22382200
H	1.43683400	1.39416200	-3.76086200
H	3.10811400	1.92789700	-3.55257800
H	-1.97568100	-4.94287600	2.51785200
H	4.64611300	-2.69676300	3.74100100
H	5.79721100	-1.48034400	3.19952600
H	5.31202600	-3.70847500	0.20896200
H	5.56357400	-4.12565300	1.90905200
H	6.52689400	-2.84099700	1.15770900
H	0.20500000	-3.82092300	1.62564300
H	1.07310900	-2.70050200	2.65240300
H	-0.05765100	-4.45900900	4.01307600
H	-0.71597400	-2.87076700	4.39079100
H	4.10053900	-1.04341300	3.42614300
H	-2.56799100	-4.51269200	4.11929400
H	-3.86672700	-3.36275000	2.29700500
H	-3.07180400	-2.21045400	3.36032200
H	-2.10974900	-3.10498400	0.59847300
H	-2.74578900	-1.52238400	0.99791000
H	2.24243800	1.36568000	0.00900000
H	0.58060000	1.90077600	-0.21410900
H	2.01702900	3.68501100	0.78827000
H	0.69431600	3.24264700	1.85451000
H	3.58532600	2.23822900	2.07161500
H	2.82145600	3.40112700	3.15715700
H	2.84877600	1.09617700	4.14927000
H	1.19891300	1.65884200	3.89861700
H	2.74902900	-0.23128000	2.06004700
H	1.42886400	-0.68063800	3.13630100
C	6.45718100	2.11464200	-0.00673900
H	6.99657500	1.93474000	0.93224400
C	5.80382400	3.50342100	0.08720600
H	6.56315200	4.27870000	0.23439300
H	5.25595300	3.74494700	-0.82959300

H	5.09696500	3.55322300	0.92041900
C	7.48182100	2.06472200	-1.15318100
H	8.25303100	2.83117500	-1.02103800
H	7.97161100	1.08752900	-1.20043200
H	6.99549500	2.24042300	-2.11861400
C	-0.83491400	5.60663700	0.42113900
C	-1.72328200	5.02597600	1.31959000
C	-2.37252300	3.82597300	1.01809200
C	-2.13519800	3.19734200	-0.23308500
C	-1.22525100	3.78444700	-1.14786100
C	-0.59072500	4.98096400	-0.79605400
H	-0.33180500	6.53613800	0.66962500
H	-1.91656100	5.50144900	2.27705600
H	0.10984600	5.42225300	-1.49878100
C	-0.87898300	3.18173300	-2.48597800
H	-0.00004400	3.67671400	-2.90385900
H	-0.65910700	2.11160900	-2.42114600
H	-1.69369900	3.30130200	-3.20862700
H	2.83910200	-5.22519500	-2.21828400
C	-2.62701900	0.49363000	4.84756900
H	-3.26708700	0.01864100	5.59752300
H	-1.80415300	0.98949900	5.37456100
H	-2.19083200	-0.30062500	4.23245300
C	-3.40748300	1.48854800	3.98581800
H	-3.83868500	2.27088400	4.62431500
H	-4.25531200	0.98026800	3.50721700
C	-2.53458400	2.13258800	2.90677100
H	-2.17290500	1.34717600	2.23244000
H	-1.63915700	2.57303000	3.36474300
C	-3.25497800	3.22431500	2.09555900
H	-3.55720300	4.02349000	2.78124400
H	-4.18708500	2.82271700	1.68260000
Br	-1.05136100	-1.13336800	-3.14129100
O	-4.81948600	0.03984100	-2.88028100
O	-4.72920600	-0.03922600	-0.59813500
C	-7.10278600	-0.50107900	-1.07051200
C	-5.95256400	-1.12171400	1.07524800
C	-5.35938000	-2.35371300	-1.04747000
C	-5.80717000	-1.02151000	-0.44334400
C	-4.31400400	0.36986400	-1.82681100
C	-3.15458500	1.29044900	-1.72751900
C	-2.84325600	1.91067300	-0.48216100
H	-7.34018900	0.49161800	-0.67519900
H	-7.92576700	-1.17546400	-0.81322800

H	-7.01732500	-0.43871500	-2.15419500
H	-5.01163200	-1.43232500	1.53444100
H	-6.72285300	-1.85456200	1.33190000
H	-6.24138500	-0.15425600	1.49746400
H	-5.21311900	-2.26035300	-2.12388900
H	-6.11786200	-3.11952500	-0.85687400
H	-4.41842900	-2.67688700	-0.59386700
H	-2.85693600	1.69946900	-2.67944700
H	-1.87896800	0.94098500	0.27995900
H	-3.56584200	1.65810600	0.28292000