

Electronic Supplementary Information

Reaction Mechanism, Norbornene and Ligand Effects, and Origins of *meta*-Selectivity of Pd/Norbornene-Catalyzed C–H Activation

Tao Yang,^{*a} Chuncai Kong,^a Shengchun Yang,^a Zhimao Yang,^a Sen Yang^a and Masahiro Ehara^{*bc}

^aSchool of Science, MOE Key Laboratory for Non-Equilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China. E-mail: taoyang1@xjtu.edu.cn

^bResearch Center for Computational Science, Institute for Molecular Science, Nishigonaka 38, Myodaiji, Okazaki 444-8585, Japan. E-mail: ehara@ims.ac.jp

^cElements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto 615-8520, Japan.

Content

I. Possible coordination modes of amide substrate 1a with complexes 3 and 6 -----	S2
II. Free energy of dissociation of one pyridine ligand from 5 or 8 -----	S3
III. Other possible <i>ortho</i> - and <i>meta</i> -C–H activation pathways-----	S4
IV. Formation pathway of <i>ortho</i> -functionalized product-----	S5
V. Formation pathway of <i>ortho,meta</i> -difunctionalized product-----	S6
VI. Optimized structures of selected transition states-----	S7
VII. Test calculations on the calculation methods-----	S10
VIII. Cartesian coordinates of optimized structures-----	S11

I. Possible coordination modes of amide substrate **1a** with complex **3** and **6**

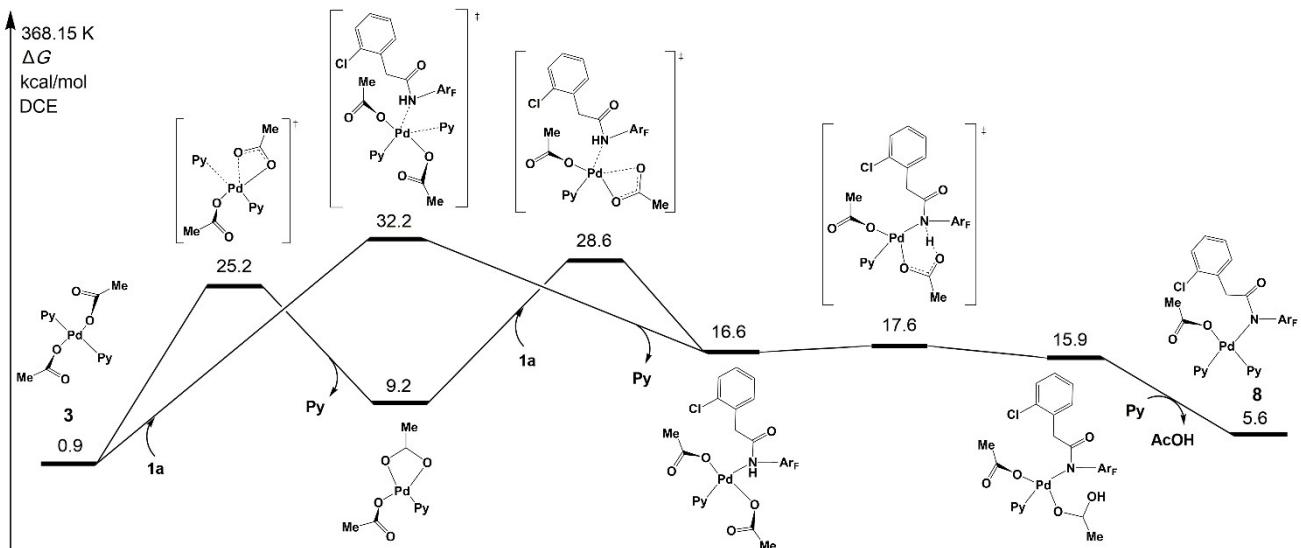


Fig. S1 Free energy profiles for substitution reactions by **1a** with N atom attacking on the Pd center.

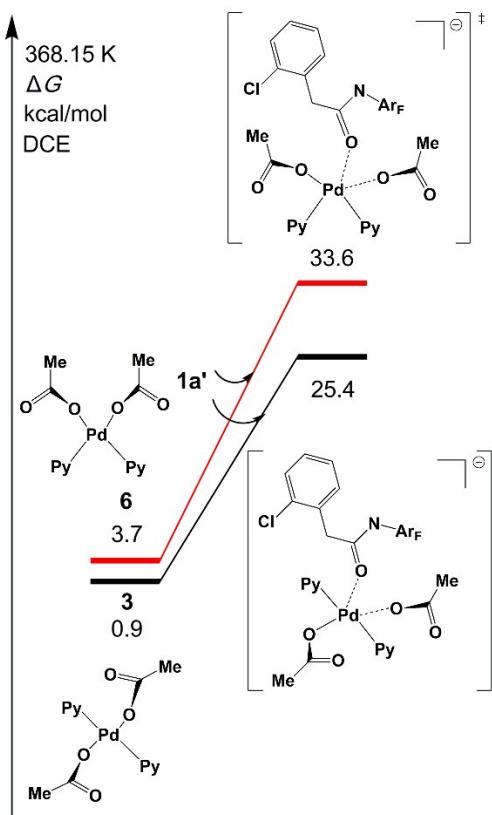


Fig. S2 Free energy profiles for substitution reactions by **1a'** with O atom attacking on the Pd center.

II. Free energy of dissociation of one pyridine ligand from **5** or **8**

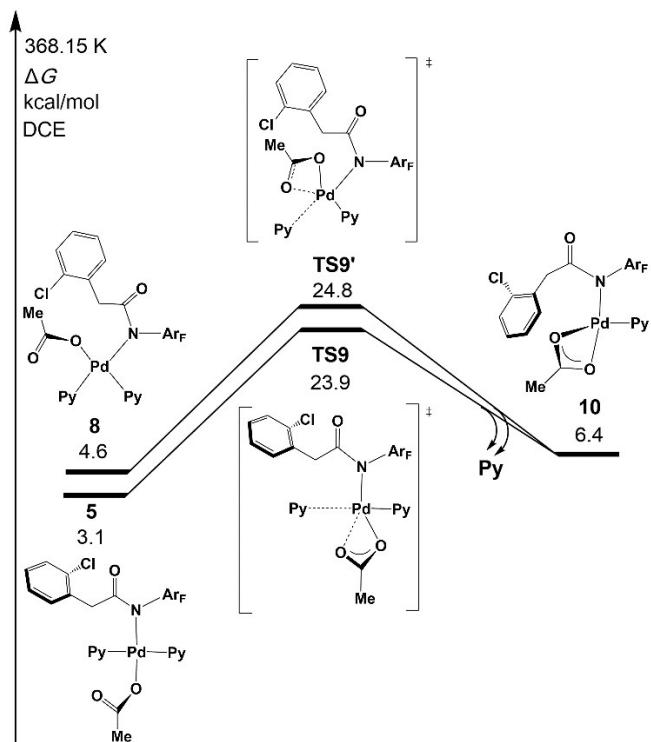


Fig. S3 Dissociation of one pyridine ligand from **5** or **8** leads to the same bidentate complex **10**.

III. Other possible *ortho*- and *meta*-C–H activation pathways

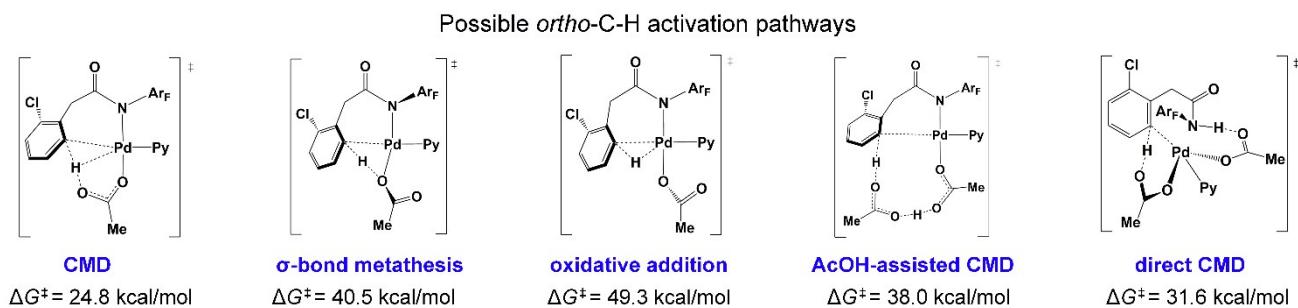


Fig. S4 Possible *ortho*-C–H activation pathways and computed activation energies at 368.15 K, where DCE was used as solvent.

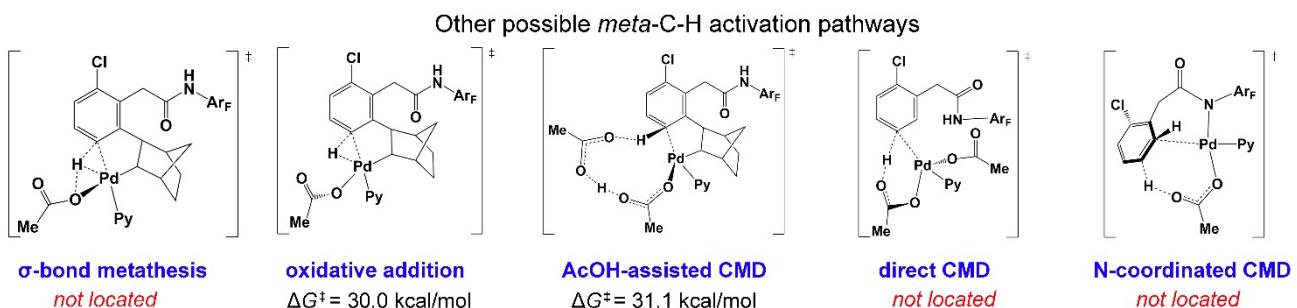


Fig. S5 Other Possible *meta*-C–H Activation Pathways and Computed Activation Energies at 368.15 K with DCE as Solvent.

IV. Formation pathway of *ortho*-functionalized product

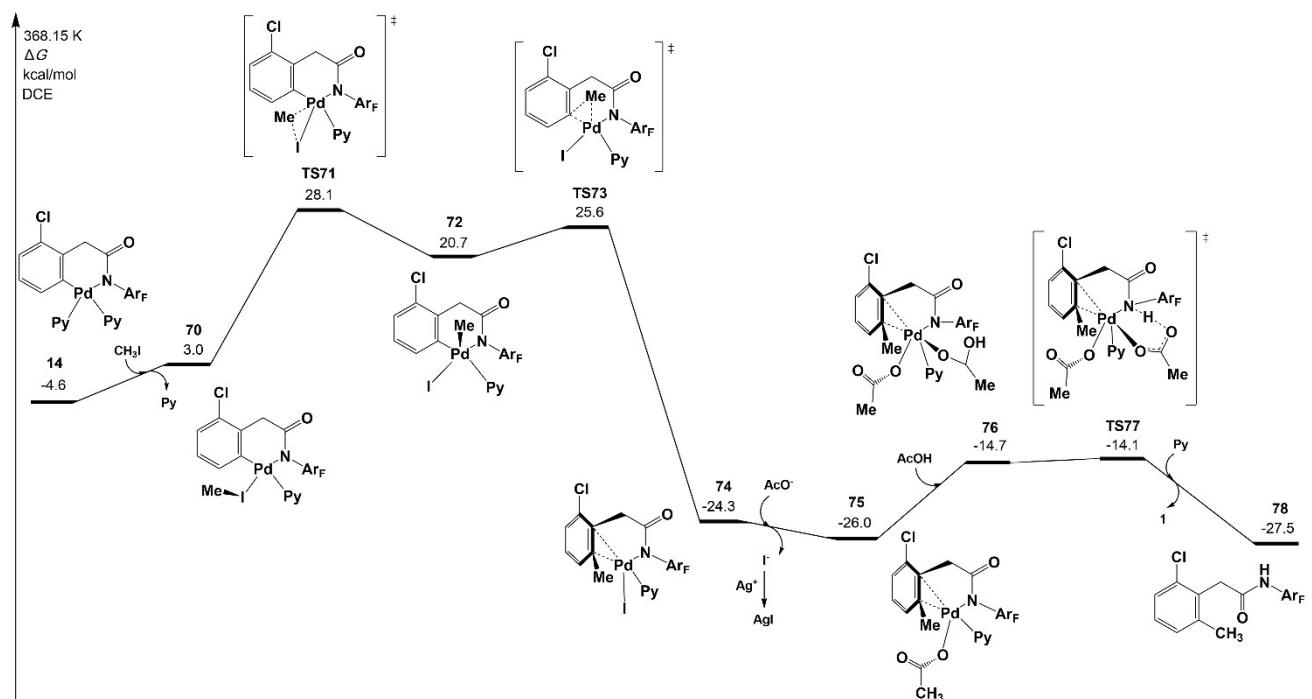


Fig. S6 Free energy profile for formation mechanism of the *ortho*-functionalized product **78** starting from intermediate **14**.

V. Formation pathway of *ortho*,*meta*-difunctionalized product

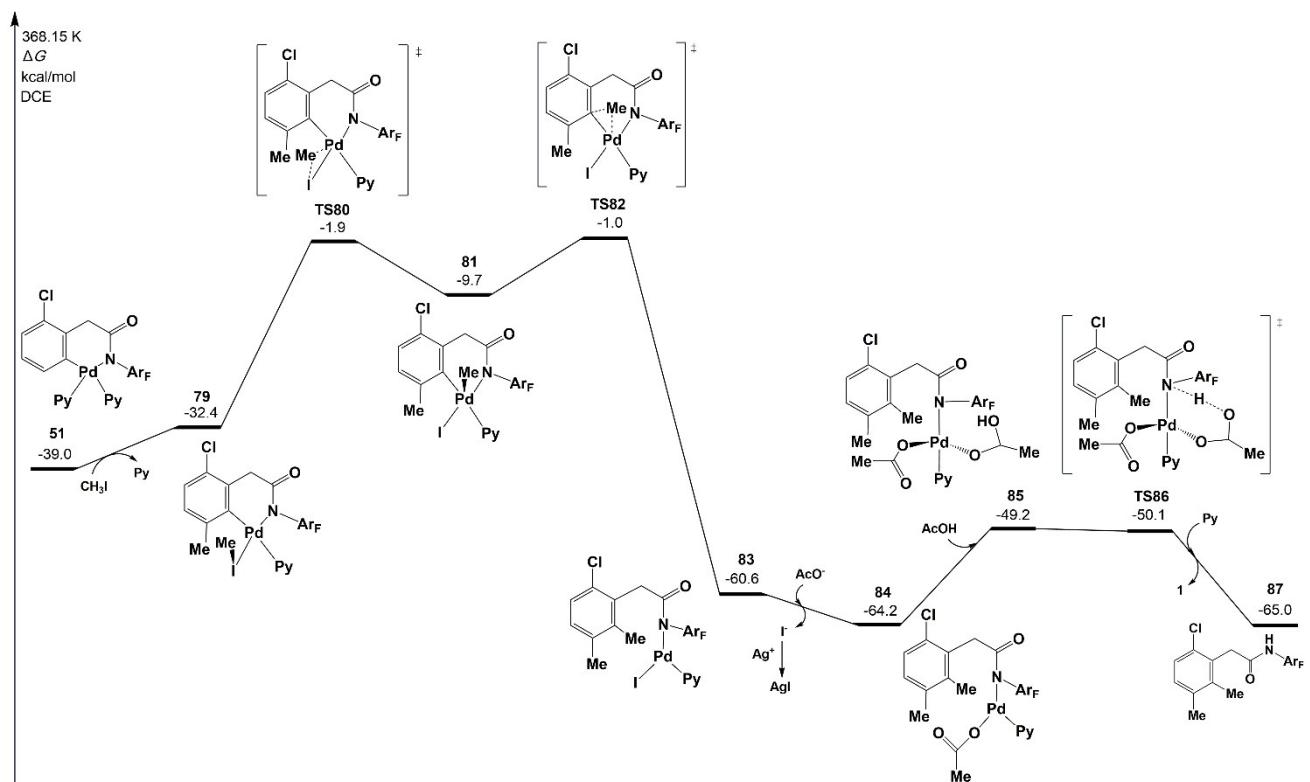


Fig. S7 Free energy profile for formation mechanism of the *ortho*,*meta*-difunctionalized product **87** starting from intermediate **51**.

VI. Optimized structures of selected transition states

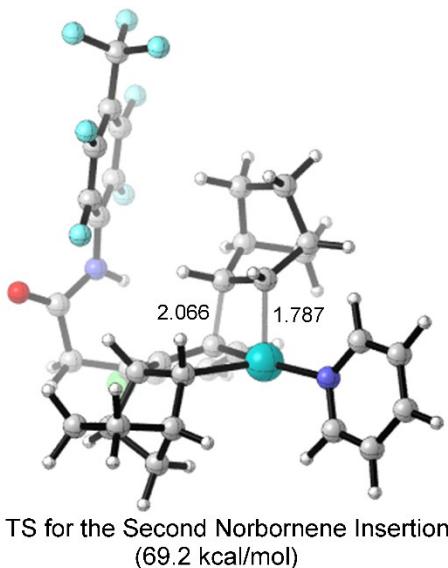


Fig. S8 Optimized structures of transition states for the second norbornene insertion into **30** with selected distances given in angstrom.

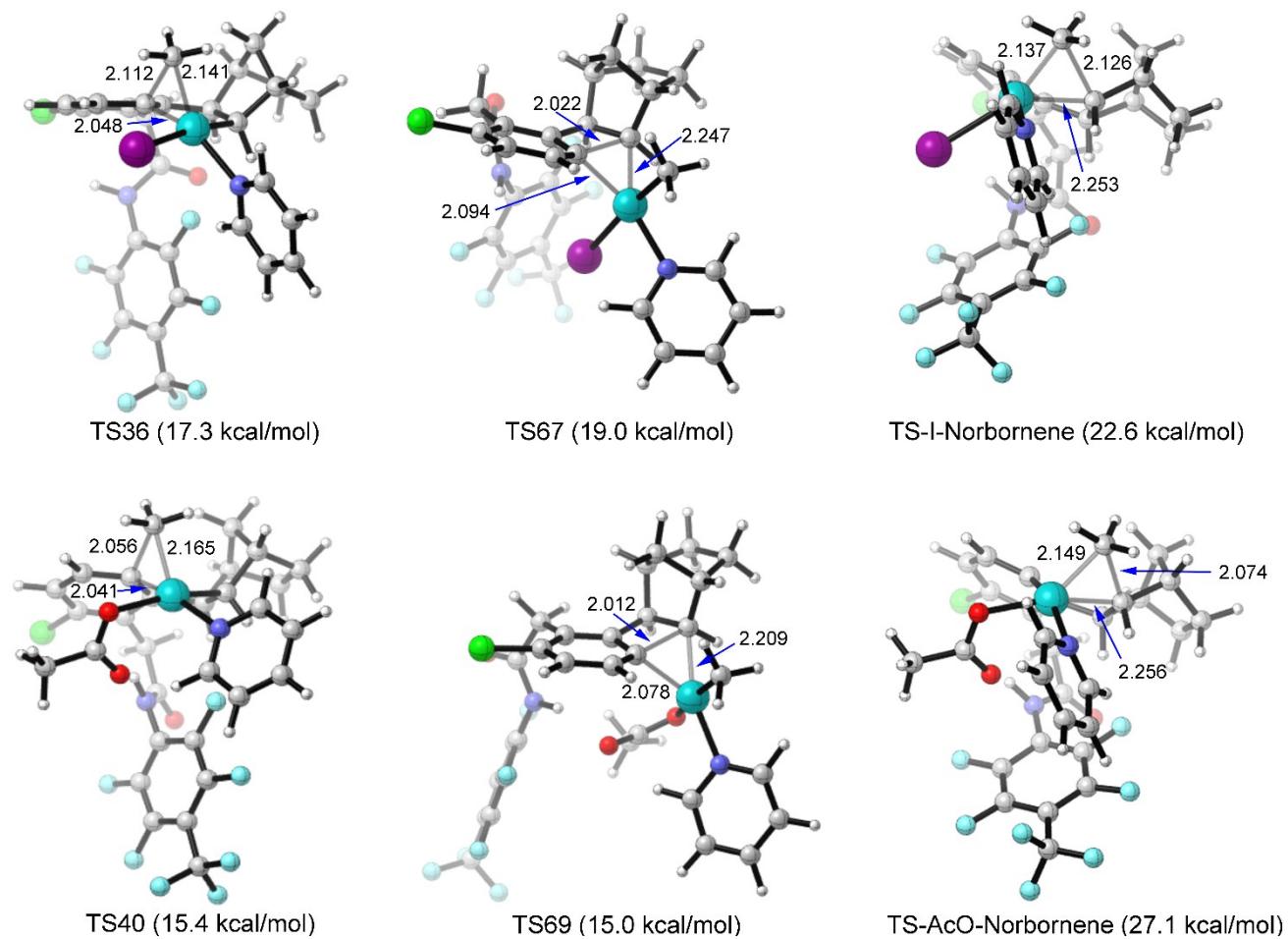


Fig. S9 Optimized structures of transition states **TS36**, **TS40**, **TS67**, **TS69**, and $\text{C}_{\text{methyl}}\text{-}\text{C}_{\text{norbornene}}$ reductive coupling transition states with selected distances given in angstrom.

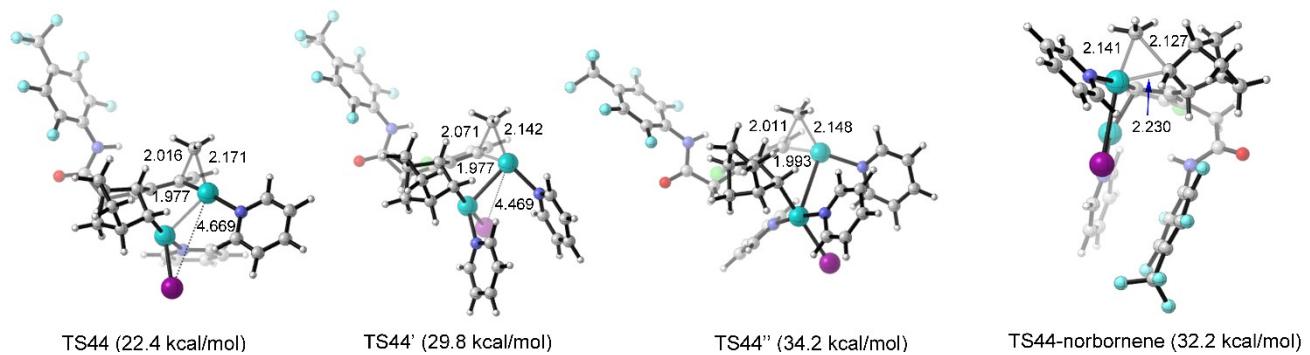


Fig. S10 Optimized structures of other possible transition states for **TS44** and C_{methyl}-C_{norbornene} reductive coupling transition states with selected distances given in angstrom.

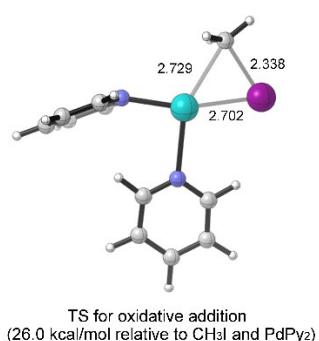


Fig. S11 Optimized structures of transition states for oxidative addition of CH₃I on PdPy₂ with selected distances given in angstrom.

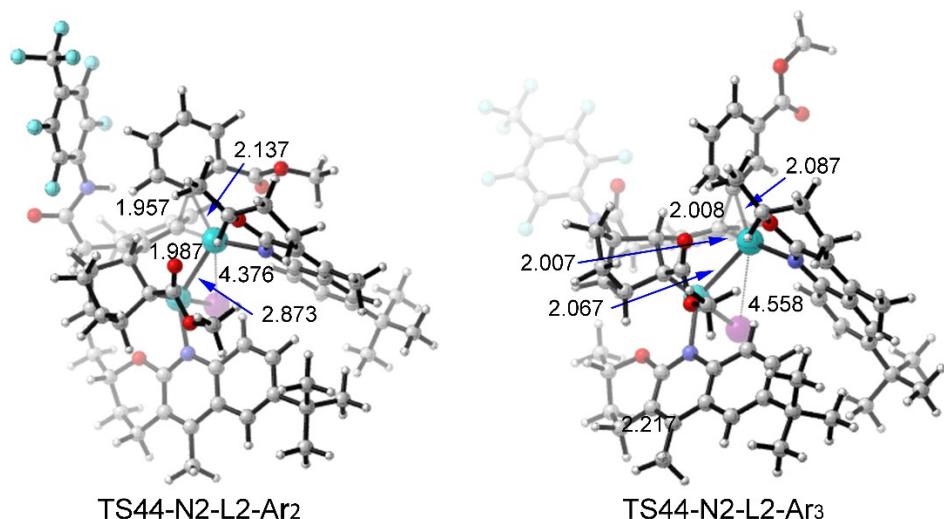


Fig. S12 Optimized structures of **TS44-N2-L2-Ar₂** and **TS44-N2-L2-Ar₃** with selected distances given in angstrom.

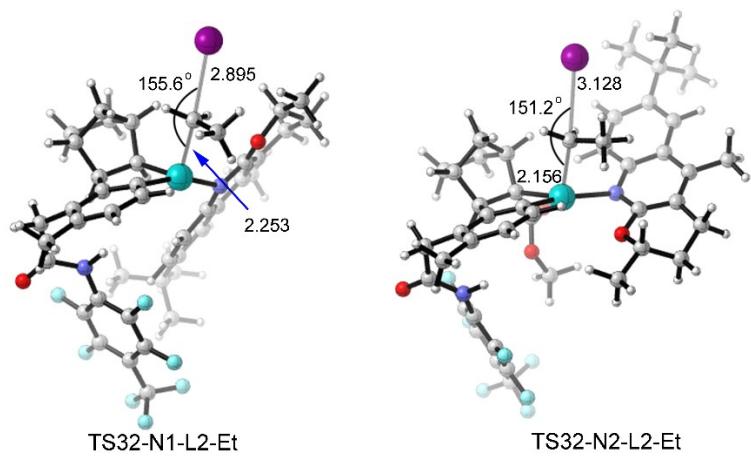
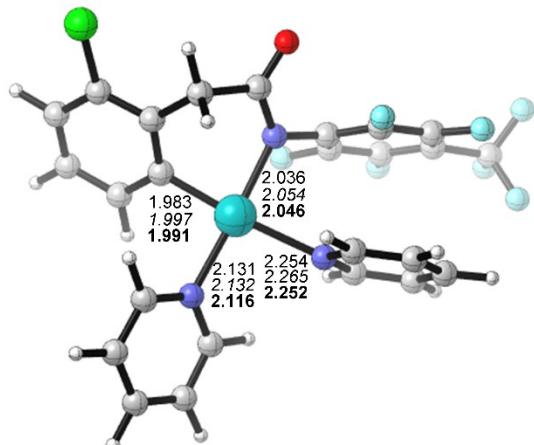


Fig. S13 Optimized structures of transition states **TS32-N1-L2-Et** and **TS32-N2-L2-Et** of amide substrate **1b** and ethyl iodide. The selected distances and angles are given in angstrom and in degree, respectively.

VII. Test calculations on the calculation methods

In this part, the reliability of ω B97XD-optimized geometries were examined, as shown in Figure S14.



14

Fig. S14 Molecular structure of intermediate **14** with selected bond distances in angstrom at the ω B97XD/Lanl2dz-6-31G(d) (regular), M06/Lanl2dz-6-31G(d) (italic), and B3LYP-D3(BJ)/Lanl2dz-6-31G(d) (bold) levels of theory.

Table S1. Relative energy between the activation energies of the selected transition states **TS40** and **TS69** at different levels of theory.

Computational Methods	$\Delta\Delta G^{\ddagger}(\text{TS40})$	$\Delta\Delta G^{\ddagger}(\text{TS69})$
M06/SDD-6-311++G(d,p)-SMD// ω B97XD/Lanl2dz-6-31G(d)	0.0	-0.4
ω B97XD/SDD-6-311++G(d,p)-SMD// ω B97XD/Lanl2dz-6-31G(d)	0.0	0.8
M06/SDD-6-311++G(d,p)-SMD// ω B97XD/SDD-6-31G(d,p)	0.0	-0.1
M06/SDD-6-311++G(d,p)-SMD//B3LYP-D3(BJ)/Lanl2dz-6-31G(d)	0.0	0.1

First of all, because the yields of meta-functionalization and benzocyclobutene products are the same (15% : 15%), the $\Delta\Delta G^{\ddagger}$ between **TS40** and **TS69** should be very close. Table S1 shows the $\Delta\Delta G^{\ddagger}$ values at different levels of theory. First, the single-point energy calculation at ω B97XD/SDD-6-311++G(d,p)-SMD gave a similar result (0.8 kcal/mol). Second, the larger basis sets (SDD-6-31G(d,p)) with ω B97XD for geometry optimizations could provide better results, however, the method is much time-consuming. Third, the B3LYP-D3(BJ) with Lanl2dz-6-31G(d) for geometry optimizations also gave very close energy for **TS40** and **TS69**. Thus, the computational methods (M06/SDD-6-311++G(d,p)-SMD// ω B97XD/Lanl2dz-6-31G(d)) used in the manuscript are reliable.

VIII. Cartesian coordinates of optimized structures

Pd₃(OAc)₆

Pd	-0.61089900	-0.08421100	1.04680300
O	-0.01282800	3.00205200	0.10885400
O	-1.16897600	1.14578800	-0.46628600
O	-1.29268500	1.21483700	2.46027400
O	0.50676000	2.49543000	2.94669700
C	-0.66159700	2.06065500	3.14915400
C	-0.88017400	2.37187200	-0.55400900
C	-1.68822100	3.18034500	-1.54022200
H	-2.07484400	2.53538200	-2.33045500
H	-2.53689200	3.62447600	-1.00948800
H	-1.08071200	3.98573800	-1.95549000
C	-1.39612100	2.64996300	4.32906700
H	-0.68706500	2.95765300	5.09889900
H	-1.93805900	3.53791300	3.98659800
H	-2.11671300	1.93298500	4.72465400
Pd	1.54092300	2.28788100	1.21647500
O	-0.32997300	-1.40335900	2.55887800
O	-0.41875400	-1.53821900	-0.36549400
O	3.20373700	2.07498200	2.37078200
O	2.63597600	2.36931100	-0.48689000
C	0.62465300	-2.22518800	2.64443800
C	0.57925900	-1.84456400	-1.07326000
O	1.69193100	-2.23161100	1.97346600
O	1.78545800	-1.53344700	-0.87226500
C	0.45936500	-3.34410100	3.64453000
H	1.41053000	-3.54172100	4.14210900
H	-0.31564300	-3.09593500	4.37015700
H	0.16307500	-4.24960600	3.10488400
C	0.28564300	-2.65563300	-2.31229900
H	-0.14179200	-1.98824100	-3.06751800
H	1.19693700	-3.10805800	-2.70381600
H	-0.45889100	-3.42096800	-2.08383000
Pd	2.52393400	-0.75185700	0.84773900
O	3.47350200	-0.16446000	2.53854100
O	3.72968500	0.39629900	-0.32620200
C	3.70735400	1.03158800	2.86803800
C	3.51922300	1.53441600	-0.82679400
C	4.67885700	1.23541600	4.00557800
H	4.11388100	1.23581300	4.94377300
H	5.40621900	0.42327800	4.03695100
H	5.17620900	2.20123700	3.90574800
C	4.41917400	1.92955600	-1.97272500
H	4.16427700	1.31856800	-2.84416200
H	4.29475500	2.98511200	-2.21417400
H	5.45840600	1.71658700	-1.71129300

AcOAg

C	0.32330700	0.96177500	-0.02050600
O	1.06336400	1.98553000	-0.01022200
O	0.76896800	-0.22359500	-0.04549600
C	-1.18208400	1.14468800	-0.00618200
H	-1.60580000	0.70863100	-0.91568100
H	-1.60486800	0.60057500	0.84305100
H	-1.44761800	2.20025000	0.05693600
Ag	2.91334400	0.59117100	-0.04592600

AcOH

C	0.33408800	1.20630400	0.07072500
O	0.94087100	2.24681400	0.14008600
O	0.95377200	0.00790200	0.04571000
H	1.90524100	0.19498000	0.09221300
C	-1.16117400	1.05501900	-0.00107900
H	-1.43843300	0.55404800	-0.93336700
H	-1.51335500	0.43048700	0.82504400
H	-1.62891500	2.03787300	0.04678200

AcO-

C	0.44212800	1.07796100	0.01214900
O	0.98390400	2.19511700	-0.14477200
O	0.96254400	-0.05346000	0.14604000
C	-1.12824900	1.07715000	0.01294300
H	-1.49365200	0.65102100	-0.93257400
H	-1.51146300	0.43655000	0.81794100
H	-1.53811100	2.08886400	0.11798500

AgI

I	0.51429100	1.85581300	1.70050300
Ag	-0.36418000	0.61350200	-0.45126300

Pyridine

C	-0.01982800	0.72626800	0.00021200
C	1.37242600	0.72046200	0.00013200
C	2.03899500	1.94070400	-0.00008000
C	1.28520800	3.10923100	-0.00019800
C	-0.10269300	3.00176600	-0.00009400
N	-0.75797800	1.83866600	0.00010400
H	3.12438300	1.98071700	-0.00015300
H	-0.57207700	-0.21132300	0.00037800
H	1.91504400	-0.21929600	0.00023300
H	1.75858400	4.08561100	-0.00037000
H	-0.72210500	3.89654200	-0.00018600

Norbornene (N1)

C	-0.18793100	1.57353300	0.02249800
C	1.32770300	1.47847200	0.02833500
C	0.78935000	3.66066800	0.02795300
C	-0.50764700	2.87093400	0.02167000
H	-0.86166000	0.73041100	-0.08692600
H	-1.49545300	3.30515400	-0.08973000
C	1.67733600	2.72253500	0.86906300
H	2.74170500	2.98428300	0.83519300
H	1.34758800	2.64065900	1.90863100
C	1.79902400	1.95165500	-1.38329000
H	2.87936400	1.80903100	-1.49204800
H	1.30746000	1.39350100	-2.18470500
C	1.42688100	3.46181900	-1.38320800
H	2.31741400	4.09013200	-1.49032500
H	0.73193700	3.72885000	-2.18381300
H	1.75253100	0.52512500	0.34834700
H	0.71930400	4.70221100	0.34761400

ICH₃

I	4.00993200	4.75907900	-1.74856400
C	2.02990100	5.14877500	-2.53796600
H	1.31300400	4.94552900	-1.74505400
H	1.99606900	6.19327900	-2.84099300
H	1.87654300	4.48636100	-3.38728500

Pd(Py)₂

Pd	0.01065300	1.25582500	-0.03908500
N	0.03941700	3.34629100	-0.01643000
C	1.15175500	4.03025800	-0.33734900
C	-1.04938500	4.05615900	0.32787100
C	1.21793600	5.41731100	-0.32516200
H	2.00997000	3.42792400	-0.61067700
C	-1.06771300	5.44429700	0.36479000
H	-1.92816000	3.47464200	0.58012400
C	0.08739400	6.14318100	0.03272900
H	2.14547800	5.91175200	-0.59278100
H	-1.97794800	5.96033500	0.65051200
H	0.10639400	7.22856700	0.05281900
N	-0.01260600	-0.83470900	-0.05851500
C	0.31936900	-1.54510600	1.03381600
C	-0.35432900	-1.51844200	-1.16472700

C	0.32265700	-2.93352500	1.06196100
H	0.58919600	-0.96364400	1.90739200
C	-0.37616800	-2.90585600	-1.22098600
H	-0.61668400	-0.91573800	-2.02610500
C	-0.03133700	-3.63224900	-0.08674100
H	0.59950600	-3.44991600	1.97473800
H	-0.65993800	-3.40016000	-2.14378500
H	-0.03863200	-4.71791100	-0.09781900

CH₃Pd(I)Py₂

Pd	0.12919700	1.34879700	0.02361700
N	0.04035700	-0.90915700	-0.18240800
C	-0.69878400	-1.63484900	0.66666000
C	0.73872100	-1.55425200	-1.12580900
C	-0.77791400	-3.01949200	0.60654400
H	-1.24336300	-1.07423700	1.42056700
C	0.71048000	-2.93675300	-1.26457400
H	1.34980800	-0.93079800	-1.76985200
C	-0.06135100	-3.68466300	-0.38330400
H	-1.38655100	-3.55928500	1.32373200
H	1.29233700	-3.41004300	-2.04765500
H	-0.10075000	-4.76675900	-0.46253300
I	2.78162300	1.37943400	-0.15633000
N	-2.01697400	1.37629400	0.19748000
C	-2.63237200	2.05478800	1.17648000
C	-2.76882800	0.66647300	-0.65725300
C	-4.01036600	2.03841800	1.34583000
H	-1.98869000	2.63036300	1.83213300
C	-4.15213000	0.60488900	-0.56372100
H	-2.23042800	0.13147200	-1.43158400
C	-4.78692700	1.30003500	0.46013000
H	-4.45792700	2.59761100	2.15978000
H	-4.71431000	0.02076700	-1.28369500
H	-5.86690100	1.26846500	0.56432800
C	0.14719600	3.35706500	0.24734600
H	0.29143500	3.56164900	1.31531100
H	0.95518500	3.82185400	-0.31782900
H	-0.81894500	3.74730500	-0.09360600

1a

C	1.11599800	-0.25848800	-0.26426900
C	1.33288600	0.26971600	1.00441300
C	1.11563200	1.62290300	1.23379100
C	0.68227200	2.48145300	0.21735400
C	0.48016100	1.92209100	-1.05061100
C	0.68814900	0.56867700	-1.29638900
H	1.27975900	-1.31400000	-0.45595000
H	1.66777300	-0.37012500	1.81430700
H	1.28233600	2.03586300	2.22521400
H	0.51639800	0.17268700	-2.29120700
C	0.48758100	3.94788800	0.50060600
H	0.29508600	4.10129900	1.56687300
H	-0.38253600	4.34523400	-0.02973200
C	1.65007300	4.88114300	0.15359200
O	1.59490300	6.06901800	0.37743000
N	2.75358100	4.27225700	-0.41443900
H	2.81386000	3.26455300	-0.36495000
C	3.93569300	4.95867900	-0.69915900
C	5.15193400	4.44630600	-0.24671800
C	3.96491200	6.12762600	-1.45462800
C	6.34671900	5.08462000	-0.51793400
C	5.16718500	6.78739500	-1.69824300
C	6.37885600	6.28119700	-1.23568100
C	7.72095800	6.93224700	-1.47995000
F	5.15135400	3.30791900	0.45404700
F	7.47544100	4.54505800	-0.06460500
F	5.10657700	7.90077500	-2.41954400
F	2.85637300	6.61916200	-1.98720500
F	8.36225200	7.13994400	-0.32098300
F	8.49927800	6.14150700	-2.23433100
F	7.61866800	8.10866000	-2.09949300

Cl -0.03584700 2.93243100 -2.38247900

1a'

C	1.50662900	-0.10318000	-0.38399700
C	1.23658700	0.50231100	0.83908100
C	0.62733600	1.75071100	0.88812800
C	0.25986400	2.43655700	-0.27664900
C	0.55461600	1.80157500	-1.48769500
C	1.16505300	0.55369100	-1.55970300
H	1.98234000	-1.07892200	-0.42945800
H	1.50095500	0.00194800	1.76643900
H	0.43519100	2.23032700	1.84113600
H	1.36433600	0.10830900	-2.52883400
C	-0.42394500	3.78692500	-0.23742200
H	-1.30646000	3.76654400	-0.88276900
H	0.26772300	4.53393000	-0.64888300
C	-0.82850400	4.24002100	1.17181300
O	0.06724800	4.51457100	1.98549300
N	-2.15663800	4.32605200	1.33249600
C	-2.64810700	4.51939600	2.57898400
C	-3.70287400	5.43864400	2.79010700
C	-2.28827700	3.77928400	3.72938100
C	-4.30062500	5.61673100	4.01783500
C	-2.88634500	3.96449100	4.96264600
C	-3.91688800	4.89022300	5.15094200
C	-4.60630600	5.15208100	6.44908600
F	-4.12819900	6.19097400	1.76523600
F	-5.27898600	6.53164200	4.13043100
F	-2.45594300	3.19883300	5.97647300
F	-1.36744400	2.80891700	3.63955900
F	-4.44033700	6.42729500	6.86458900
F	-5.94157400	4.96249300	6.35995000
F	-4.17562200	4.36631200	7.44755600
Cl	0.15751700	2.58992300	-3.01454300

1b'

C	1.49372500	-0.12281600	-0.39841800
C	1.28010600	0.48523500	0.83326100
C	0.68986000	1.74472100	0.89890900
C	0.29559200	2.41770800	-0.26011500
C	0.51669100	1.80401600	-1.50869900
C	1.11278900	0.54299800	-1.55973000
H	1.95563800	-1.10521300	-0.45945400
H	1.57325300	-0.01756200	1.75138200
H	0.53770900	2.22885500	1.85726000
H	1.27867500	0.07527400	-2.52883900
C	-0.35432900	3.78826300	-0.20557000
H	-1.23164000	3.80707300	-0.86002100
H	0.36182300	4.52719800	-0.59415400
C	-0.77543400	4.24447600	1.19682800
O	0.10632700	4.53559900	2.01873200
N	-2.10837900	4.32093800	1.34318600
C	-2.62043700	4.50999400	2.58003200
C	-3.69977900	5.40784900	2.76624300
C	-2.25806900	3.79250900	3.74546900
C	-4.31817900	5.58709000	3.98298400
C	-2.87769600	3.97997500	4.96788800
C	-3.93202100	4.88425000	5.13061600
C	-4.64328000	5.14934300	6.41522900
F	-4.12940300	6.13610000	1.72513000
F	-5.31899900	6.48072300	4.07215400
F	-2.44372500	3.23856300	5.99827400
F	-1.31487700	2.84294500	3.68063900
F	-4.50918400	6.43347900	6.81548600
F	-5.97366500	4.93233600	6.31242000
F	-4.21028500	4.38634100	7.43043100
C	0.11905800	2.49795100	-2.78825200
H	-0.96665700	2.64320500	-2.84773800
H	0.57330400	3.49347400	-2.86247000
H	0.42937700	1.91778300	-3.66395800

1			
Pd	-0.11758500	1.38881200	-0.13427500
O	-2.15204600	1.43044800	-0.05677000
O	1.91686900	1.34718800	-0.21178200
N	-0.07337800	3.43976700	-0.11958000
C	0.49071200	4.10402300	-1.13908000
C	-0.60573000	4.11415800	0.91021200
C	0.53831600	5.49054800	-1.16194800
H	0.90216000	3.48903700	-1.93385800
C	-0.58639900	5.50089600	0.95507900
H	-1.04665400	3.50753600	1.69550100
C	-0.00680200	6.20084300	-0.09768700
H	0.99715100	5.99522700	-2.00447900
H	-1.02112500	6.01352100	1.80553200
H	0.02017000	7.28617000	-0.08871200
N	-0.16177900	-0.66214200	-0.14897200
C	-0.72587600	-1.32639900	0.87052800
C	0.37058700	-1.33653500	-1.17875300
C	-0.77347000	-2.71292300	0.89340200
H	-1.13733600	-0.71141000	1.66529700
C	0.35126100	-2.72327400	-1.22361700
H	0.81151200	-0.72991300	-1.96404100
C	-0.22833900	-3.42322000	-0.17085200
H	-1.23230600	-3.21760300	1.73593100
H	0.78599400	-3.23589900	-2.07406700
H	-0.25531000	-4.50854700	-0.17982500
C	-2.67943400	1.43351200	1.12420700
C	2.44424100	1.34414900	-1.39277000
O	-2.04725600	1.41582600	2.18456600
O	1.81204400	1.36183400	-2.45311500
C	-4.19898000	1.44967400	1.10679400
H	-4.55836300	2.26952000	0.47835000
H	-4.56918200	0.51847500	0.66592600
H	-4.58833300	1.55408700	2.12069100
C	3.96378700	1.32805000	-1.37537400
H	4.33394300	2.25940100	-0.93478300
H	4.32322700	0.50840800	-0.74670100
H	4.35313100	1.22338900	-2.38925000

2			
Pd	-0.07423900	1.85707600	0.50739200
N	2.00969900	1.74877800	0.49376500
C	2.71603500	2.15456600	-0.57385600
C	2.65586300	1.29314200	1.57796600
C	4.10444400	2.10356100	-0.58774500
H	2.12366500	2.53429300	-1.40328900
C	4.03868000	1.22079700	1.63746900
H	2.03348300	0.98516700	2.41105000
C	4.77815300	1.63108700	0.53191700
H	4.63861800	2.43825000	-1.46973800
H	4.51925400	0.85093800	2.53603500
H	5.86270700	1.58520800	0.54711600
N	-0.17606500	-0.19665200	0.86433300
C	0.36814600	-1.04844500	-0.01844600
C	-0.80277400	-0.68111300	1.94877000
C	0.31014000	-2.42296400	0.14963200
H	0.85480900	-0.60040700	-0.87783600
C	-0.89267000	-2.04711000	2.18567600
H	-1.24224500	0.06885300	2.60249200
C	-0.33035400	-2.93320300	1.27504000
H	0.75660400	-3.07490900	-0.59260500
H	-1.40499700	-2.39924000	3.07381700
H	-0.39390200	-4.00504200	1.43488400
O	-0.02469100	3.84373000	0.19048300
O	-2.08043900	2.00549100	0.47881400
C	0.07795500	4.20074300	-1.05139500
C	-2.64566700	2.12493300	1.63891200
O	0.35753300	3.45293400	-1.99054100
O	-2.09220400	1.95580200	2.72731500
C	-0.18315300	5.68133800	-1.26805300
H	0.40585000	6.27923000	-0.56682900
H	0.05563300	5.95845600	-2.29610600

H	-1.23929200	5.88971500	-1.06990700
C	-4.11039800	2.51795600	1.55129200
H	-4.61267800	2.30911100	2.49748300
H	-4.17350300	3.59181900	1.34586300
H	-4.60457500	1.99474900	0.72878900

3			
Pd	0.12320700	1.31759900	0.15277500
O	-1.73403200	1.34714600	-0.65075300
O	2.11588200	1.30590500	0.59216200
N	0.04865700	3.37238500	0.24920800
C	-0.58137800	4.07354500	-0.70374500
C	0.58856100	4.00927800	1.29943800
C	-0.66957900	5.45662400	-0.65457300
H	-1.03892100	3.48874900	-1.49312900
C	0.52922900	5.39080200	1.41848900
H	1.04429100	3.37766500	2.05529900
C	-0.10175200	6.12816500	0.42323900
H	-1.18145200	5.98943700	-1.44795700
H	0.96899200	5.86963400	2.28580700
H	-0.16070100	7.21000100	0.49177800
N	0.06978300	-0.73236600	0.20010300
C	0.41659200	-1.35454600	1.33601900
C	-0.40218300	-1.44226600	-0.83266900
C	0.31468000	-2.73227500	1.46684800
H	0.76447900	-0.71446600	2.14085200
C	-0.52423300	-2.82214300	-0.77549800
H	-0.70186000	-0.87120100	-1.70358000
C	-0.15875700	-3.47947500	0.39467000
H	0.59636400	-3.20090500	2.40268900
H	-0.90734000	-3.36298300	-1.63330100
H	-0.25095800	-4.55827000	0.47260600
C	-2.70290200	1.00461100	0.16066000
C	2.48469300	1.28523200	1.83152700
O	-2.55779500	0.63056100	1.31395200
O	1.72146800	1.31275900	2.80007900
C	-4.07510700	1.12925900	-0.48445400
H	-4.28252300	2.18273800	-0.69979400
H	-4.10079100	0.59015600	-1.43616700
H	-4.84012200	0.73944800	0.18854200
C	3.99326400	1.22773000	2.01225900
H	4.38990400	0.32704000	1.53378400
H	4.45944400	2.08705600	1.52054500
H	4.24538400	1.22513000	3.07385100

TS4			
Pd	0.14252900	0.34452700	1.14883700
O	2.03657200	0.45792500	2.08227600
N	-0.13456200	2.30461800	1.57573900
C	0.89786600	3.14583800	1.41451000
C	-1.33095900	2.77074400	1.95987800
C	0.76897600	4.50708500	1.62299300
H	1.83672700	2.68744300	1.12696000
C	-1.52684600	4.13081900	2.17844000
H	-2.14508800	2.04442600	2.07400900
C	-0.47135500	5.01227800	2.00464600
H	1.62520800	5.15552300	1.47348300
H	-2.51503100	4.47211300	2.46510300
H	-0.60849400	6.07839400	2.16025800
N	0.49653600	-1.62630000	0.69336500
C	1.63558900	-2.23496200	1.05036700
C	-0.44728900	-2.30706300	0.02797900
C	1.86927300	-3.57158100	0.76596200
H	2.34928700	-1.60431900	1.56898800
C	-0.27418500	-3.64631500	-0.29570100
H	-1.34411200	-1.75224500	-0.21023100
C	0.89615600	-4.29223700	0.08097300
H	2.80330400	-4.02858200	1.07338000
H	-1.05768100	-4.16302000	-0.83836000
H	1.05214600	-5.34014500	-0.15864500
C	2.03579000	0.64567100	3.37091000

O	1.05458900	0.76311500	4.08943800
C	3.45016600	0.71310200	3.94831000
H	3.96988900	-0.23519200	3.77281600
H	4.02493600	1.49622100	3.44334000
H	3.40987900	0.91417200	5.02058100
N	-0.63486000	0.74415000	-1.10116900
C	-1.87731800	1.34964300	-1.14004400
C	-2.05856000	2.73697500	-1.02926300
C	-3.05149800	0.59436600	-1.18043200
C	-3.30924000	3.30055800	-0.88321500
C	-4.30969600	1.15501300	-1.03160600
C	-4.47211600	2.52938800	-0.87446300
C	-5.78864400	3.21388000	-0.66622800
F	-5.35918400	0.32697100	-1.06053600
F	-2.98445400	-0.73341900	-1.36145700
F	-0.99554600	3.54760200	-0.99438800
F	-3.39685000	4.62927500	-0.72030100
F	-5.82145200	3.88462000	0.49916400
F	-6.82831900	2.37074100	-0.66435400
F	-6.02905100	4.12420800	-1.63541600
C	0.23086100	1.10865100	-2.07142100
O	-0.02538400	1.79205300	-3.06493400
C	1.66635800	0.58787800	-1.84900700
H	2.18796000	1.36078600	-1.26845100
H	1.64782200	-0.30397900	-1.22494000
C	2.41708000	0.35087900	-3.13004800
C	2.72515000	1.43705200	-3.96083100
C	2.83378800	-0.90805200	-3.56835200
C	3.41695900	1.27774700	-5.15331100
H	2.37765600	2.41762200	-3.65612700
C	3.53066600	-1.09046100	-4.76145700
C	3.82544500	0.00854900	-5.55689900
H	3.63323700	2.14444600	-5.77141500
H	3.83251400	-2.09018700	-5.05580500
H	4.36568400	-0.12997200	-6.48917000
O	-2.04261000	-0.49495100	1.46146700
C	-3.22446200	-0.19787100	1.82625300
C	-4.21934400	-1.36201800	1.73987800
H	-4.43377900	-1.55490100	0.68344700
H	-3.78016800	-2.27103500	2.16273500
H	-5.15244600	-1.11682300	2.25272300
O	-3.64580600	0.91422900	2.18830200
Cl	2.48544900	-2.35034300	-2.62147400

5

Pd	0.63082000	0.51007700	0.88410400
O	1.48158800	0.19798500	2.70471700
N	0.11445900	2.45355000	1.38046100
C	0.71527100	3.50713900	0.81145500
C	-0.99548800	2.63907500	2.11692400
C	0.21169500	4.79315900	0.93419500
H	1.60133500	3.29586500	0.22524600
C	-1.56792400	3.89370900	2.26282500
H	-1.39911100	1.74626800	2.58407300
C	-0.96195900	4.98747900	1.65375800
H	0.71821100	5.61630100	0.44420900
H	-2.48631200	3.99971700	2.82785800
H	-1.40128600	5.97617900	1.73654300
N	1.03154200	-1.47328000	0.43891700
C	2.05545000	-2.09239500	1.04746500
C	0.24652000	-2.16649700	-0.40071300
C	2.33105700	-3.43373900	0.83164600
H	2.63064900	-1.48373100	1.73485200
C	0.45751000	-3.51293100	-0.65482400
H	-0.56000100	-1.61147100	-0.86060300
C	1.51721100	-4.15990900	-0.03085200
H	3.17233100	-3.89353200	1.33748900
H	-0.20303900	-4.03547400	-1.33664200
H	1.70737500	-5.21236500	-0.21523000
C	0.63176200	-0.05304200	3.65891900
O	-0.58996900	-0.04479100	3.53316800
C	1.29828800	-0.38473600	4.98237900

H	1.81794800	-1.34497600	4.89600200
H	2.04705500	0.37214100	5.23163200
H	0.54965200	-0.45035000	5.77292600
N	-0.18102900	0.86008000	-0.98348500
C	-1.43713500	1.46434900	-0.92312000
C	-1.64286800	2.79634500	-1.30550300
C	-2.51176400	0.82818700	-0.30327700
C	-2.82542800	3.45295100	-1.02752600
C	-3.70105600	1.48552800	-0.01471600
C	-3.88399400	2.81818100	-0.37431400
C	-5.09795300	3.63134100	-0.01049100
F	-4.64325400	0.79778400	0.62506100
F	-2.38458300	-0.44383000	0.09097300
F	-0.64515700	3.49231300	-1.85180100
F	-2.92293800	4.74517900	-1.34518200
F	-4.78538900	4.54564700	0.93126000
F	-6.09488100	2.88869600	0.47430200
F	-5.57236200	4.30230800	-1.06817600
C	0.45364100	0.87955200	-2.19914000
O	-0.12319600	1.12073700	-3.24860500
C	1.96335700	0.62270900	-2.13974200
H	2.41078700	1.55515400	-1.76680800
H	2.18861100	-0.13491400	-1.38940000
C	2.57897900	0.27649800	-3.46881000
C	2.51188000	1.19508900	-4.52319400
C	3.24261400	-0.92603200	-3.71952500
C	3.07718600	0.92847800	-5.76212400
H	1.98520000	2.12832100	-4.35720200
C	3.81643600	-1.21354600	-4.95567700
C	3.73161100	-0.28104400	-5.98069000
H	3.00452200	1.66344200	-6.55753800
H	4.32300900	-2.16090200	-5.10380200
H	4.17880700	-0.50039800	-6.94527000
Cl	3.39665200	-2.15006600	-2.46425100

6

Pd	-0.17075300	1.69429500	0.55556000
N	1.90333600	1.68601700	0.42476000
C	2.51392100	1.86973500	-0.75338900
C	2.63714200	1.61001400	1.54296100
C	3.89378200	1.95675700	-0.86292200
H	1.86468300	1.96089100	-1.61725800
C	4.02231600	1.68323300	1.51385000
H	2.08644000	1.51279800	2.46947500
C	4.66230400	1.85874100	0.29248800
H	4.34874300	2.10763800	-1.83517100
H	4.57954800	1.62004300	2.44129100
H	5.74432700	1.92922700	0.24140700
N	-0.19987800	-0.37555800	0.87077800
C	0.40522600	-1.21418700	0.01639300
C	-0.82006800	-0.87456600	1.95266000
C	0.41422700	-2.58691100	0.20542800
H	0.89246200	-0.75880500	-0.83872500
C	-0.84644900	-2.23986300	2.21022700
H	-1.30286600	-0.13773300	2.59160300
C	-0.22310400	-3.11127100	1.32626300
H	0.91175600	-3.22643600	-0.51491900
H	-1.35562400	-2.60214300	3.09606800
H	-0.23391100	-4.18221900	1.50371500
O	-0.15226200	3.66612300	0.18987600
O	-2.18016600	1.78742700	0.54251700
C	0.42190400	4.39987100	1.10106800
C	-2.77058400	1.86660000	1.69405400
O	1.01661300	3.98424400	2.08958800
O	-2.23914000	1.67470500	2.78804800
C	0.26644000	5.88786600	0.82771300
H	-0.77241200	6.17656600	1.01792600
H	0.92420900	6.46088600	1.48328100
H	0.48202600	6.11217800	-0.22054700
C	-4.23928100	2.24088300	1.58366600
H	-4.75145500	2.03348300	2.52475200
H	-4.31444400	3.31116800	1.36451100

H	-4.71542300	1.70246100	0.76005700
---	-------------	------------	------------

TS7

Pd	0.73454700	1.51593800	0.17577600
N	1.70807100	0.34692300	-1.22351900
C	2.08916900	0.90262300	-2.38401200
C	1.93079300	-0.95845500	-1.00617200
C	2.68019300	0.15471100	-3.39196800
H	1.87790300	1.96250900	-2.48071100
C	2.50953000	-1.76694400	-1.97633900
H	1.66287000	-1.30468800	-0.00913500
C	2.88406200	-1.20601600	-3.19147300
H	2.96427000	0.64106400	-4.31850300
H	2.66452800	-2.81982000	-1.76758200
H	3.33441300	-1.81739600	-3.96827600
N	-1.45967700	0.66416600	-0.30881800
C	-2.50209300	1.49420600	-0.22972100
C	-1.68910600	-0.64036500	-0.46847300
C	-3.81634300	1.05079800	-0.32743100
H	-2.25961700	2.54256000	-0.09773700
C	-2.96755400	-1.17137100	-0.57938800
H	-0.81084600	-1.27741400	-0.51410200
C	-4.05355300	-0.30485700	-0.51431500
H	-4.62926400	1.76690100	-0.28199100
H	-3.10096300	-2.23759600	-0.72781500
H	-5.06730000	-0.68071500	-0.61682600
O	2.26148300	1.29308400	1.53594100
O	-0.16258200	2.83200400	1.36431900
C	2.20162400	0.21868900	2.25470100
C	-0.39163200	2.69337400	2.63825000
O	1.64704000	-0.84214800	1.95687100
O	-0.20927200	1.69909800	3.32296600
C	2.89876700	0.37553100	3.59683700
H	3.83279100	0.93470300	3.49262500
H	2.22212700	0.95301700	4.23491700
H	3.08321500	-0.60074000	4.05103100
C	-0.94500300	3.99081100	3.22505500
H	-1.74044900	4.38997900	2.58843100
H	-1.31945900	3.81819200	4.23638200
H	-0.15139300	4.74497300	3.25507000
N	0.04485500	3.18329600	-1.65276600
C	0.24918000	4.37907900	-1.00028800
C	-0.77199900	5.13821500	-0.41199000
C	1.55209200	4.81202800	-0.73083900
C	-0.50072400	6.20934800	0.41190500
C	1.83139600	5.88587900	0.09596300
C	0.80463200	6.62911800	0.68026900
C	1.02698200	7.76000000	1.63618800
C	-0.77208700	3.19311500	-2.72162800
O	-1.27485300	4.18750300	-3.26380400
C	-0.97623600	1.80647600	-3.34170600
H	-0.45523100	1.80506400	-4.31003600
H	-0.48673900	1.05553900	-2.72070600
C	-2.40830300	1.38013300	-3.57182300
C	-2.71623800	0.04588200	-3.85920600
C	-3.48712700	2.27016900	-3.50337000
C	-4.02033600	-0.40350100	-4.03923100
C	-4.79676200	1.84167300	-3.68529100
H	-3.26133300	3.31250300	-3.30611600
C	-5.06998100	0.50252900	-3.94692700
H	-4.20214400	-1.45288800	-4.24609000
H	-5.60737000	2.56206500	-3.61973200
H	-6.09166600	0.16006000	-4.08614300
F	2.58479200	4.12565000	-1.24347300
F	3.11624300	6.18994700	0.30963300
F	-2.05040300	4.76087600	-0.54443700
F	-1.53031500	6.83542400	1.00039100
F	0.24136100	8.81667000	1.35112100
F	0.74221900	7.40542600	2.90683600
F	2.29011900	8.20940200	1.63391900
Cl	-1.42566000	-1.14309400	-4.01640500

8

Pd	0.95651700	2.16960700	0.63190600
N	2.21772500	1.15454900	-0.63399000
C	2.89010100	1.79289800	-1.60354000
C	2.31763000	-0.17843400	-0.51794300
C	3.69930400	1.10908300	-2.49791900
H	2.74338800	2.86431100	-1.65781800
C	3.10716600	-0.92534300	-1.37915800
H	1.71893500	-0.63443200	0.26348900
C	3.80995100	-0.27301500	-2.38556300
H	4.22282600	1.65798400	-3.27215200
H	3.15145700	-2.00185700	-1.26259500
H	4.42925800	-0.83457000	-3.07761000
N	-0.31600600	3.17694900	1.90300700
C	0.08246100	4.31241300	2.49529900
C	-1.59069400	2.78055700	2.01399200
C	-0.80006600	5.12946100	3.18281800
H	1.13048200	4.56592500	2.38455300
C	-2.53035400	3.54105000	2.69559700
H	-1.83962900	1.84046800	1.53668500
C	-2.13410500	4.74170800	3.27320500
H	-0.44862200	6.06018000	3.61149500
H	-3.55659800	3.19769000	2.75190600
H	-2.85392000	5.36875500	3.78912700
O	1.81910300	1.28839300	2.25313100
C	1.14718200	0.25182600	2.65107200
O	0.17932200	-0.22351700	2.05301300
C	1.66714700	-0.35189000	3.94299700
H	1.54011100	0.36716700	4.75844600
H	1.12616500	-1.27013900	4.17583700
H	2.73795500	-0.55735200	3.85562000
N	0.09637800	3.16934700	-0.95500800
C	-0.10545000	4.52548300	-0.71378700
C	-1.38107400	5.05807400	-0.49530700
C	0.96790800	5.38804800	-0.48748300
C	-1.56757700	6.35149500	-0.03767900
C	0.78860500	6.68003200	-0.02037600
C	-0.48536600	7.20089400	0.20175300
C	-0.65168200	8.56571000	0.81688400
C	-0.55401700	2.64013200	-2.04075300
O	-1.06603700	3.33654800	-2.90672000
C	-0.53797500	1.11765800	-2.13387400
H	0.38426300	0.84420500	-2.65927800
H	-0.45067900	0.67578200	-1.13383900
C	-1.71478600	0.49254200	-2.84196700
C	-1.61288500	-0.78468500	-3.40266700
C	-2.96642300	1.11363000	-2.91029800
C	-2.68640500	-1.41920400	-4.01846700
C	-4.05215000	0.49389000	-3.51727500
H	-3.07573700	2.10984300	-2.49869700
C	-3.91441500	-0.77248400	-4.07686900
H	-2.55418100	-2.40819600	-4.44335700
H	-5.00795500	1.00704900	-3.55746600
H	-4.75755000	-1.25960900	-4.55687900
F	2.22228100	4.93983900	-0.63950500
F	1.87466200	7.40868600	0.23763700
F	-2.45300900	4.27399700	-0.61285600
F	-2.81507800	6.73899800	0.22416400
F	-1.86422800	9.08083100	0.59821800
F	-0.47916900	8.50474300	2.15525200
F	0.24439700	9.43837000	0.34380900
Cl	-0.08869100	-1.66296400	-3.33454400

TS9

Pd	-0.58267200	1.47925200	1.07021400
O	-0.10927800	0.76202600	2.93823500
N	0.27376100	3.35179000	1.31434000
C	-0.26427300	4.46796300	0.79969300
C	1.40219400	3.43085300	2.03509600
C	0.32747700	5.70961800	0.97586100
H	-1.18206300	4.33634400	0.24124700

C	2.05111700	4.63753000	2.24737500
H	1.77361200	2.49802500	2.44330200
C	1.50781200	5.79739200	1.70576300
H	-0.13786400	6.58773400	0.54323800
H	2.96751900	4.65746900	2.82592500
H	1.99485600	6.75587900	1.85369600
N	0.67397300	-0.71602600	0.25708700
C	1.66637200	-1.18844900	1.01555700
C	0.22720800	-1.47638900	-0.74385000
C	2.25975500	-2.42756900	0.80388400
H	1.98758900	-0.54206200	1.82805400
C	0.75315500	-2.73185700	-1.03103200
H	-0.57574400	-1.05433400	-1.33868300
C	1.79089000	-3.21541100	-0.24282000
H	3.06690400	-2.76301600	1.44680400
H	0.35687100	-3.30715500	-1.86052400
H	2.22866400	-4.18963200	-0.43957200
C	-0.98213500	-0.18476900	2.88960300
O	-1.74644200	-0.26571200	1.89920200
C	-1.01172200	-1.19520300	3.99826600
H	-0.24619100	-1.95266700	3.79587800
H	-0.78099300	-0.72090800	4.95465900
H	-1.98624400	-1.68464400	4.03602200
N	-1.34566000	1.95265500	-0.74175400
C	-2.70049300	1.61752100	-0.82722100
C	-3.64364500	2.22420000	-0.00045800
C	-3.17234900	0.61332600	-1.67886700
C	-4.98161500	1.85281800	0.00248700
C	-4.50659600	0.25377400	-1.69693100
C	-5.44239600	0.85746200	-0.85471300
C	-6.87577900	0.39363900	-0.92840800
F	-4.89474700	-0.71044100	-2.53135200
F	-2.32686700	-0.03824000	-2.47867500
F	-3.25801000	3.19805000	0.83490300
F	-5.79382900	2.49302600	0.84043700
F	-7.67017700	1.02692000	-0.06145400
F	-6.96685200	-0.92021300	-0.67065100
F	-7.37920000	0.59432300	-2.15632300
C	-0.73285700	2.35775700	-1.89519300
O	-1.34999800	2.59240600	-2.92913900
C	0.78372200	2.49818900	-1.86261700
H	1.03291200	3.33681300	-2.52182200
H	1.14319700	2.73598300	-0.86437800
C	1.47209300	1.24738500	-2.36994000
C	0.95036300	0.55311000	-3.46708500
C	2.64498100	0.74504800	-1.79995400
C	1.55764100	-0.59578400	-3.95694300
H	0.04217800	0.93152400	-3.92542200
C	3.26502400	-0.40652300	-2.27421300
C	2.71551400	-1.08134800	-3.35725900
H	1.12286500	-1.11153700	-4.80754700
H	4.16481500	-0.76918900	-1.78990000
H	3.19447000	-1.98250600	-3.72742800
Cl	3.40316500	1.55880400	-0.43639100

10

Pd	-1.47417300	1.94294000	0.04399300
N	0.31500100	1.02542000	0.46603000
C	1.51699300	1.56326900	0.21050600
C	0.23525300	-0.18545300	1.03940600
C	2.69116300	0.89171700	0.51466800
H	1.50467200	2.54683000	-0.24127200
C	1.36768500	-0.91045600	1.37463200
H	-0.76574900	-0.56148800	1.22232300
C	2.61788700	-0.36519500	1.10512000
H	3.64377600	1.35851000	0.29268600
H	1.26030400	-1.88703100	1.83188300
H	3.52269600	-0.91104200	1.35267000
O	-2.82121300	0.84315600	1.22706100
C	-3.77713300	1.56572400	0.78962200
O	-3.49787900	2.52173700	0.00137000
C	-5.18880400	1.30480700	1.21319000

H	-5.36890000	1.80003600	2.17316400
H	-5.88404400	1.70841200	0.47519500
H	-5.34504400	0.23247900	1.34751500
N	-0.61243900	3.23588500	-1.24026700
C	-0.93542300	4.55844000	-0.91716600
C	-1.96236900	5.25999600	-1.55007500
C	-0.28013800	5.20980700	0.12938500
C	-2.30145900	6.55439000	-1.17803200
C	-0.62459100	6.49229100	0.51504100
C	-1.64264600	7.19488600	-0.12990100
C	-1.95508600	8.59323700	0.34408100
C	-0.27440700	2.97632000	-2.54913200
O	-0.02395500	3.85857100	-3.35453200
C	-0.13518300	1.50504000	-2.93815100
H	0.12748500	1.49929100	-4.00013200
H	0.71867100	1.08424500	-2.39801700
C	-1.36225200	0.65579600	-2.69966700
C	-1.29026300	-0.69500800	-2.34127700
C	-2.64184400	1.20502200	-2.84647700
C	-2.42793300	-1.45594300	-2.09071000
C	-3.78895200	0.45921300	-2.60791300
H	-2.73262400	2.25422500	-3.10859500
C	-3.68306200	-0.87224000	-2.21820400
H	-2.32386600	-2.49734300	-1.80624300
H	-4.76221100	0.92720800	-2.71301800
H	-4.57247100	-1.46261400	-2.02078800
F	0.70063400	4.57981200	0.78643400
F	0.04208900	7.05862400	1.52095500
F	-2.65903600	4.68600700	-2.52743100
F	-3.29076700	7.14269900	-1.84464100
F	-2.98090900	9.14549800	-0.30706900
F	-2.26187600	8.59336300	1.65108000
F	-0.89401000	9.39908600	0.18434600
Cl	0.26773900	-1.49409900	-2.19253800

11			
Pd	0.73452500	1.13361000	-0.81921000
O	1.48617300	1.69085300	1.92835300
N	-0.57001900	2.64491500	-0.27500300
C	-0.58430400	3.79218000	-0.96645000
C	-1.46559600	2.44023300	0.70201000
C	-1.54918400	4.76274600	-0.74290800
H	0.18337500	3.90709200	-1.72115500
C	-2.46187000	3.36371200	0.97750800
H	-1.37325200	1.50843600	1.24622800
C	-2.51596900	4.53613200	0.23076700
H	-1.54746200	5.66754500	-1.33929900
H	-3.19186500	3.15162900	1.74949400
H	-3.30302900	5.26203300	0.40620600
C	2.21575800	2.36094000	1.20499500
O	2.17778500	2.35053500	-0.09903100
C	3.27119100	3.29794900	1.76306900
H	3.34232300	3.18004500	2.84526300
H	4.23954500	3.09216200	1.29708700
H	3.00972000	4.33396800	1.52465200
N	-0.74885600	0.01274800	-1.63978800
C	-2.05758800	0.49771300	-1.65780300
C	-2.40595600	1.59343400	-2.44383700
C	-3.03140300	0.01293300	-0.78178200
C	-3.62999500	2.23324300	-2.30936200
C	-4.26569500	0.62906300	-0.66566000
C	-4.59390600	1.75467100	-1.42423100
C	-5.88430700	2.48272200	-1.14895400
F	-5.12171800	0.16199800	0.24294100
F	-2.73968900	-0.99615200	0.03388800
F	-1.50601300	2.11792100	-3.27866400
F	-3.83236100	3.33327200	-3.03386200
F	-6.21174200	3.33777600	-2.12128300
F	-5.78130900	3.19765300	-0.00790100
F	-6.90888200	1.63807800	-0.99630600
C	-0.55894500	-1.27943200	-2.03296800
O	-1.42769100	-2.00564300	-2.48352500

C	0.86498600	-1.78868400	-1.83952100
H	0.81899800	-2.52570400	-1.03104700
H	1.13851100	-2.33772400	-2.74504500
C	1.93416000	-0.76740400	-1.50947200
C	2.57256700	0.01192000	-2.51416100
C	2.57118600	-0.80399800	-0.24264400
C	3.77675100	0.66499600	-2.27892200
C	3.78079300	-0.16512400	-0.00929900
H	2.10988100	-1.39317500	0.54388200
C	4.38221400	0.56223700	-1.03061700
H	4.23598600	1.23917200	-3.07521200
H	4.23943400	-0.22455600	0.97140000
H	5.32839300	1.06491800	-0.85838000
Cl	1.90590700	0.05274800	-4.12266200

TS12

Pd	0.72118300	1.42561100	-0.20906800
O	3.29565000	0.88778300	1.22368200
N	-0.87855800	2.58254100	0.57729500
C	-0.89967500	3.88943800	0.27870500
C	-1.94370400	2.03111400	1.17527100
C	-2.01184200	4.68195000	0.52150200
H	-0.00306600	4.28895600	-0.18091300
C	-3.09079000	2.75801100	1.45609400
H	-1.87528800	0.96995100	1.38773500
C	-3.13440200	4.10258300	1.10383800
H	-1.99750100	5.72836700	0.23950900
H	-3.94094600	2.26481200	1.91299300
H	-4.03200800	4.68665900	1.27724100
C	2.97451500	2.09143200	1.42548400
O	2.01204700	2.67566900	0.83756300
C	3.77064300	2.88619700	2.42858300
H	3.51208600	2.53785800	3.43365000
H	4.83726200	2.70459800	2.27978700
H	3.54587800	3.94997500	2.34826700
N	-0.59491000	0.15450600	-1.12677600
C	-1.83630300	0.66557800	-1.49607400
C	-1.92705100	1.83869600	-2.24837700
C	-3.04286400	0.14884100	-1.00799500
C	-3.12937200	2.49985700	-2.44890300
C	-4.24946900	0.78384400	-1.24343100
C	-4.32669400	1.97388900	-1.96805800
C	-5.64486500	2.69494000	-2.06775800
F	-5.34652400	0.27479200	-0.68104500
F	-3.03541700	-0.88906600	-0.17404400
F	-0.81203600	2.41682300	-2.70857000
F	-3.09057600	3.65844600	-3.10624400
F	-5.63968000	3.65213000	-2.99938100
F	-5.94811300	3.28511500	-0.89188700
F	-6.64625800	1.85747800	-2.35934300
C	-0.37749200	-1.18595900	-1.33986800
O	-1.18038200	-1.93325100	-1.86838100
C	1.00689400	-1.67505800	-0.89833600
H	1.11965100	-1.51182100	0.17992900
H	1.06242500	-2.74222000	-1.10708300
C	2.04390700	-0.87851400	-1.63487900
C	2.65296400	-1.31490100	-2.81165300
C	2.32019200	0.43094200	-1.18490800
C	3.49409200	-0.48004000	-3.54451000
C	3.15727200	1.27004200	-1.94107900
H	2.66471500	0.54055200	0.08560400
C	3.74177500	0.81998300	-3.11574800
H	3.94678700	-0.85578600	-4.45606300
H	3.36500600	2.27290900	-1.57795800
H	4.39230400	1.46462600	-3.69783800
Cl	2.36492700	-2.92286600	-3.43561100

TS12 (σ -bond metathesis)

Pd	0.66849700	1.60908700	-0.36877300
O	2.24933400	1.13759100	2.23364400
N	-0.79203800	2.72671800	0.69541600

C	-0.65092800	4.05667100	0.79050100
C	-1.83821200	2.13685700	1.29092200
C	-1.55963900	4.85052900	1.47361800
H	0.22051000	4.48072900	0.30186600
C	-2.79112700	2.86174000	1.99213900
H	-1.90632800	1.06068500	1.18209400
C	-2.65253800	4.24201500	2.08332200
H	-1.41006700	5.92312900	1.52045200
H	-3.62498100	2.34421700	2.45211400
H	-3.38408000	4.83567300	2.62206500
C	2.68066400	2.14117000	1.71452300
O	2.51169200	2.43556600	0.40886900
C	3.46690400	3.20842800	2.43590600
H	4.44848700	3.32550800	1.96742500
H	2.94864700	4.16834700	2.34803500
H	3.58207400	2.94094100	3.48646500
N	-0.71388200	0.34292800	-1.10130400
C	-1.90985800	0.81946600	-1.62623900
C	-1.91410300	1.81671000	-2.60328800
C	-3.16086400	0.40533300	-1.15256000
C	-3.08937500	2.37102600	-3.09254600
C	-4.33390200	0.93992400	-1.65426100
C	-4.33005600	1.93205800	-2.63558200
C	-5.65333700	2.48115200	-3.10591800
F	-5.49226700	0.51563400	-1.14898300
F	-3.23875800	-0.46244400	-0.14370700
F	-0.75477800	2.28339000	-3.07618300
F	-2.97806300	3.32500100	-4.01477800
F	-5.52175200	3.38837300	-4.07704200
F	-6.30930100	3.07215600	-2.09170100
F	-6.44187600	1.50264600	-3.57180100
C	-0.48080800	-1.01337300	-1.09410200
O	-1.27204900	-1.84301100	-1.50190000
C	0.90869100	-1.40930700	-0.56329600
H	1.03823800	-1.02676700	0.45655900
H	0.95037200	-2.49704300	-0.54361300
C	1.95995400	-0.80719500	-1.45865000
C	2.62135500	-1.52423900	-2.45501000
C	2.17990000	0.58759600	-1.40228500
C	3.45990100	-0.89387100	-3.37623400
C	2.98337300	1.22310600	-2.35792200
H	2.53984300	1.34730500	-0.29819200
C	3.63700500	0.48207600	-3.33624900
H	3.95806100	-1.49268000	-4.13128200
H	3.12634800	2.29844900	-2.29979700
H	4.27941000	0.96742500	-4.06372400
Cl	2.41014300	-3.25263300	-2.61662500

TS12 (oxidative addition)

Pd	0.57896900	1.22921800	-0.29694500
O	1.00985700	3.59302500	-0.91544600
N	-1.17970100	2.21744600	0.73455700
C	-1.72027600	3.36879000	0.30559300
C	-1.83157300	1.50651200	1.66405700
C	-2.94643300	3.82764600	0.76373100
H	-1.14190000	3.91021600	-0.43467400
C	-3.05914400	1.89982200	2.17909500
H	-1.35941300	0.58292500	1.98022600
C	-3.63551800	3.07372300	1.70784500
H	-3.36236800	4.74407100	0.36236700
H	-3.55771400	1.27994900	2.91525200
H	-4.60833200	3.39445300	2.06605400
C	1.68443800	3.55693900	0.12916700
O	1.82689200	2.45640500	0.79379000
C	2.34297900	4.78371500	0.70322200
H	1.69117200	5.19941100	1.47945600
H	3.29746700	4.52968100	1.16933100
H	2.48174000	5.53355100	-0.07727300
N	-0.69422900	0.17860500	-1.44628400
C	-1.84864800	0.88819900	-1.79571800
C	-1.78677100	1.95134300	-2.69146100
C	-3.07781600	0.62956200	-1.18446200

C	-2.88979200	2.76654500	-2.93102500
C	-4.17342600	1.43600900	-1.42027400
C	-4.10404900	2.52291600	-2.29576400
C	-5.31706900	3.41019800	-2.42363600
F	-5.30395300	1.19067900	-0.75719100
F	-3.17632500	-0.35602500	-0.29687100
F	-0.64111200	2.23413300	-3.30176500
F	-2.72971300	3.78681300	-3.76852400
F	-5.17815700	4.35077700	-3.35857200
F	-5.55811000	4.04022600	-1.25491300
F	-6.41029000	2.69902100	-2.72178400
C	-0.63172200	-1.13501900	-1.81985200
O	-1.51884900	-1.68473800	-2.45013000
C	0.61683100	-1.89037400	-1.39297100
H	0.51108900	-2.13772400	-0.32713500
H	0.60236800	-2.83201200	-1.93733000
C	1.91223400	-1.14883100	-1.59988800
C	2.98957600	-1.70752000	-2.29895900
C	2.11706200	0.12694100	-1.05223700
C	4.20606600	-1.04603100	-2.43784100
C	3.33697900	0.78775800	-1.14302500
H	1.06211200	-0.03442700	0.42320900
C	4.37919500	0.19863600	-1.85166700
H	5.01066800	-1.51832300	-2.99016200
H	3.47935100	1.74651800	-0.66409500
H	5.33044800	0.71281800	-1.94388500
Cl	2.86234600	-3.29436200	-3.02991800

TS12 (AcOH-assisted CMD)

Pd	0.90196200	1.85579700	-0.73221700
O	2.27388600	3.19781600	2.09609400
N	-0.80325800	2.48708100	0.39502500
C	-1.67645800	3.38095800	-0.09327300
C	-1.08007000	1.85578500	1.54601000
C	-2.88600200	3.64598100	0.52834500
H	-1.39740500	3.86363400	-1.02384800
C	-2.26847900	2.07570500	2.23004300
H	-0.32990200	1.15476100	1.89724500
C	-3.19391900	2.96917000	1.70530100
H	-3.58167000	4.34674000	0.08238600
H	-2.46503300	1.53151000	3.14639300
H	-4.14636200	3.13317200	2.19843200
C	2.26193700	3.95831700	1.05568000
O	1.89313000	3.61842800	-0.08146800
C	2.76244200	5.35456100	1.29143300
H	2.30755800	5.76422500	2.19653200
H	3.84436500	5.31745300	1.45397200
H	2.54337000	5.98697900	0.43147200
N	-0.15980500	0.33741200	-1.53523800
C	-1.53727200	0.56694900	-1.63700400
C	-2.04684100	1.43350400	-2.60052300
C	-2.44323600	0.03709800	-0.71747600
C	-3.38634000	1.80262900	-2.61762700
C	-3.77634200	0.40598600	-0.72592800
C	-4.28234500	1.28819800	-1.68337900
C	-5.71338800	1.74936300	-1.57978600
F	-4.56918100	-0.06394400	0.23771200
F	-2.00359600	-0.75902100	0.25301400
F	-1.22356600	1.99921400	-3.48326500
F	-3.76957700	2.69190300	-3.53314900
F	-5.84217000	2.65915300	-0.58878800
F	-6.54024400	0.73813400	-1.29567800
F	-6.15326100	2.32347700	-2.70150400
C	0.25924400	-0.91212100	-1.90248800
O	-0.50748200	-1.79941000	-2.23970800
C	1.76826900	-1.13271100	-1.88624700
H	2.09637900	-1.22276600	-0.84494600
H	1.95228300	-2.08504400	-2.38047200
C	2.52000700	0.00028800	-2.52025800
C	3.15213900	-0.10340600	-3.75872500
C	2.59496000	1.23553300	-1.82846200
C	3.84012700	0.97288500	-4.31556400

C	3.29339800	2.31274900	-2.40335500
H	2.91263800	0.95924900	-0.56182500
C	3.91497200	2.18374400	-3.63688400
H	4.31688800	0.85160700	-5.28261400
H	3.34618600	3.25434100	-1.86719600
H	4.45389400	3.01641700	-4.07748900
H	2.05415100	2.19697100	1.90873200
O	1.84080900	0.74069800	1.93803200
C	2.75303400	0.01795200	1.45958800
C	2.98092500	-1.34255300	2.07790600
H	2.25236100	-2.04152300	1.64976600
H	3.98356000	-1.70885700	1.85256900
H	2.81282300	-1.30381700	3.15590500
O	3.48344000	0.33133300	0.46551300
Cl	3.10505200	-1.58939000	-4.68368900

TS12 (direct CMD)

Pd	0.62651700	2.21557200	-1.00458900
N	-1.25890800	2.62869400	-0.07322100
C	-2.29366200	3.03916900	-0.82312700
C	-1.47378900	2.31603000	1.21329900
C	-3.58224500	3.12986900	-0.31931500
H	-2.05742800	3.29507000	-1.84765700
C	-2.73166500	2.39917800	1.79274600
H	-0.60985300	1.96316200	1.76213000
C	-3.80937600	2.80002400	1.01201100
H	-4.39279800	3.43213500	-0.97156400
H	-2.86019600	2.12304900	2.83267800
H	-4.81155300	2.83728500	1.42640900
N	-0.50103200	-0.31510800	-2.25062000
C	-1.82772000	-0.33173900	-1.83498700
C	-2.84987200	-0.08726900	-2.75758300
C	-2.19820600	-0.46311700	-0.49465600
C	-4.16499800	0.05082400	-2.34972000
C	-3.52571300	-0.37080600	-0.09763700
C	-4.53654700	-0.09132700	-1.01289800
C	-5.97338500	0.15566200	-0.63551100
F	-3.77628600	-0.48969900	1.20551700
F	-1.27887800	-0.59216400	0.45665900
F	-2.55793400	0.03651000	-4.04795800
F	-5.09011100	0.32653900	-3.26847600
F	-6.80628800	-0.63270000	-1.32371500
F	-6.31826400	1.43229000	-0.90753500
F	-6.20971100	-0.04148500	0.66446100
C	0.44637900	-1.18458100	-1.76125800
O	0.16960800	-2.17389300	-1.11560100
C	1.91024900	-0.82818000	-2.02306700
H	2.34853600	-0.74617700	-1.02358500
H	2.35947500	-1.71688500	-2.47195700
C	2.28096200	0.40831600	-2.80631900
C	2.66988900	0.32540600	-4.14457600
C	2.33967400	1.68088100	-2.17597300
C	3.14971900	1.43027800	-4.84219300
C	2.85437300	2.77929400	-2.88393500
C	3.26588600	2.65908700	-4.20408400
H	3.44031400	1.31521500	-5.88091900
H	3.66481900	3.51320400	-4.74245700
H	-0.26543600	0.39257800	-2.96711700
O	0.04594600	3.38534100	-2.55452100
C	-0.15716400	2.92964100	-3.75212800
C	-0.30199500	4.01623900	-4.79896800
H	-0.65908800	4.95000900	-4.36053500
H	0.68654900	4.19688700	-5.23578200
H	-0.96974900	3.67981000	-5.59417800
O	-0.22159800	1.74488100	-4.07842200
O	1.20302100	1.28148200	0.74121500
C	2.42074900	1.06042300	1.00549500
C	2.73596100	0.51112600	2.37078500
H	3.81060800	0.38598800	2.49968900
H	2.34148200	1.18768200	3.13380000
H	2.23086400	-0.45221000	2.48713100
O	3.36696200	1.25356700	0.18995700

H	2.84217000	1.56626300	-0.92141900
Cl	2.55654500	-1.18678300	-5.02174800
H	2.91432700	3.74356400	-2.38871200

13			
Pd	0.64790800	1.36592700	-0.36168500
O	3.41833600	0.89774300	1.33746400
N	-0.91439000	2.65596700	0.54170900
C	-0.88754200	3.95847600	0.22772400
C	-2.02896700	2.15226000	1.08879800
C	-1.98067100	4.79398200	0.40965900
H	0.03786600	4.32520800	-0.20401400
C	-3.16599800	2.91705100	1.30781200
H	-2.01074600	1.09003600	1.31072800
C	-3.14826000	4.25932800	0.94448300
H	-1.91900800	5.83540300	0.11511100
H	-4.05524100	2.45578400	1.72201100
H	-4.03393800	4.87360000	1.06677300
C	3.03078400	2.15292900	1.34791700
O	2.08645800	2.58497200	0.68585600
C	3.85667400	3.03377700	2.23247100
H	4.00202400	2.55538100	3.20405800
H	4.84339700	3.16680500	1.77737500
H	3.37318400	4.00281000	2.35004300
N	-0.72709500	0.18178900	-1.27157500
C	-1.93553200	0.76901600	-1.62799900
C	-1.97134000	1.96894900	-2.34241900
C	-3.16627200	0.29628600	-1.15331900
C	-3.14138000	2.69200000	-2.51848800
C	-4.34093600	0.99559400	-1.36409000
C	-4.36256100	2.20974600	-2.05210900
C	-5.63683000	3.00795000	-2.11409900
F	-5.45930200	0.52331500	-0.81033500
F	-3.20772200	-0.76844600	-0.35489400
F	-0.83193600	2.50847200	-2.78962400
F	-3.04897200	3.86930100	-3.13711400
F	-5.59848500	3.96873100	-3.04169200
F	-5.87505600	3.61061800	-0.92797500
F	-6.69575900	2.23591200	-2.38155100
C	-0.57903200	-1.16205300	-1.50109800
O	-1.40158300	-1.84656800	-2.08706800
C	0.71269600	-1.77036000	-0.95783600
H	0.69199200	-1.69739000	0.13748500
H	0.70179900	-2.82570600	-1.22468400
C	1.93515900	-1.06557000	-1.49039000
C	2.96093700	-1.72269600	-2.17855800
C	2.04347400	0.32727000	-1.33156200
C	4.04375400	-1.03723800	-2.72386900
C	3.12047400	1.02147300	-1.88839900
H	2.92001800	0.41553200	0.63858100
C	4.11724100	0.34133200	-2.58457200
H	4.81340300	-1.58681600	-3.25433500
H	3.18738600	2.10063500	-1.77766400
H	4.95206100	0.88354500	-3.01850800
Cl	2.93371800	-3.46408000	-2.38865000

14			
Pd	0.26674700	1.85461700	-0.56851400
N	1.27139000	3.64640700	-0.00043800
C	0.57799100	4.70980600	0.43377000
C	2.61163500	3.72703600	-0.03059000
C	1.18801100	5.88585600	0.84346900
H	-0.49989100	4.60013300	0.45531400
C	3.29819000	4.86405800	0.37204700
H	3.13086500	2.85327800	-0.40486100
C	2.57624800	5.96657000	0.81357000
H	0.57913300	6.71814600	1.17805500
H	4.38141000	4.87616100	0.33021700
H	3.08476000	6.87212700	1.12869800
N	-0.55812600	0.06035100	-1.06525300
C	-1.93721300	-0.06149300	-0.95444400

C	-2.78737700	0.67829400	-1.77820500
C	-2.54571400	-0.80412300	0.06436700
C	-4.16187800	0.71054800	-1.58435100
C	-3.91428900	-0.77675300	0.25703700
C	-4.75900200	-0.02780100	-0.56501100
C	-6.22375900	0.04354500	-0.22997500
F	-4.42176100	-1.43850800	1.29994300
F	-1.79449300	-1.46309400	0.94366100
F	-2.27096600	1.44659000	-2.73992000
F	-4.87937700	1.49459500	-2.39036600
F	-6.95011100	0.61492000	-1.19339200
F	-6.41796000	0.77024200	0.89528000
F	-6.73975300	-1.16997800	-0.00347600
C	0.16841300	-1.07825500	-1.26559800
O	-0.32135700	-2.18990200	-1.40251100
C	1.68303700	-0.86966800	-1.30954900
H	2.02488600	-0.65631100	-0.28767100
H	2.12048700	-1.82002700	-1.61050200
C	2.09742000	0.25795200	-2.22565300
C	3.01490500	0.09049300	-3.26823300
C	1.52952800	1.53323100	-2.06309500
C	3.33938400	1.12067100	-4.14811000
C	1.83401800	2.56559200	-2.94910800
C	2.73537400	2.35941800	-3.99197300
H	4.05156700	0.94058600	-4.94573300
H	1.36972500	3.54074100	-2.83027200
H	2.96799100	3.16396200	-4.68382000
N	-1.28165300	2.08564200	1.05366200
C	-2.48927900	2.59938700	0.77479000
C	-1.14418200	1.35820300	2.16917800
C	-3.60066600	2.38910300	1.57693500
H	-2.56387700	3.16533000	-0.14957300
C	-2.20165300	1.10193100	3.03270300
H	-0.15783300	0.94402300	2.34854000
C	-3.45617400	1.61446700	2.72406100
H	-4.56435400	2.79053300	1.28699400
H	-2.04343700	0.48549200	3.91001900
H	-4.31334700	1.40070700	3.35392100
Cl	3.81986900	-1.45119500	-3.52514000

15

Pd	0.35626000	1.75738700	-0.46693200
N	1.28245500	3.61545700	-0.10560000
C	0.53254600	4.62234200	0.37050600
C	2.59646100	3.82018500	-0.29118200
C	1.06495200	5.86918000	0.66407300
H	-0.51723200	4.40315000	0.52594700
C	3.20385700	5.03543800	-0.01073600
H	3.15645700	2.98275800	-0.68893200
C	2.42539500	6.08195100	0.47069200
H	0.41600900	6.65351700	1.03679400
H	4.26910600	5.15148300	-0.17420600
H	2.87162400	7.04641600	0.69121000
N	-0.49978800	-0.10870800	-0.71001100
C	-1.89493500	-0.19583300	-0.86562600
C	-2.62949300	0.73899800	-1.59371800
C	-2.62580800	-1.21332300	-0.24076300
C	-4.01496300	0.67736600	-1.69257300
C	-4.00233100	-1.28834300	-0.35237600
C	-4.73127400	-0.34583800	-1.07876800
C	-6.23205900	-0.48611200	-1.13299800
F	-4.63967600	-2.27669000	0.27418800
F	-1.99692000	-2.11117000	0.51306900
F	-2.01119700	1.74466700	-2.22099100
F	-4.61745500	1.62971300	-2.40207700
F	-6.81288800	0.45382700	-1.88333700
F	-6.76202500	-0.39984600	0.09883500
F	-6.58451000	-1.67763000	-1.63550100
C	0.22573500	-1.16162800	-1.25512200
O	-0.27482700	-2.16706800	-1.71901400
C	1.73415200	-0.93170200	-1.25426600
H	2.06821800	-0.64657300	-0.24903500

H	2.20920500	-1.87313000	-1.52470200
C	2.05812800	0.17000000	-2.23875200
C	2.88047400	-0.01563600	-3.35420200
C	1.45402400	1.42839800	-2.07670500
C	3.08053100	0.98605400	-4.30093200
C	1.63113200	2.43019200	-3.02915300
C	2.44110600	2.20692000	-4.14113500
H	3.72114900	0.79665200	-5.15498000
H	1.13953900	3.39116500	-2.90970300
H	2.57393400	2.98653500	-4.88564500
O	-0.87388700	2.10510000	1.39745500
C	-1.01054300	1.23003300	2.25444100
C	-1.58423400	1.51321000	3.61075100
H	-1.72439900	2.58530000	3.74438300
H	-2.54499400	0.99834200	3.70735300
H	-0.91980900	1.11530500	4.38238900
O	-0.68465000	-0.02566700	2.07331300
H	-0.44244100	-0.17588800	1.11226600
Cl	3.70967500	-1.54018100	-3.61806700

TS16

Pd	0.33699900	1.82501200	-0.40080300
N	1.25267800	3.67889900	-0.10438300
C	0.51248700	4.64790700	0.45943000
C	2.54471700	3.92367000	-0.37591000
C	1.03339500	5.90051800	0.74844300
H	-0.51154100	4.38604100	0.69681000
C	3.13866000	5.14686100	-0.10269800
H	3.09836200	3.11311100	-0.83278500
C	2.36976200	6.15736200	0.46359400
H	0.39396500	6.65422900	1.19357100
H	4.18732000	5.29508600	-0.33357000
H	2.80598000	7.12695200	0.68165100
N	-0.53798900	-0.11458400	-0.50160900
C	-1.93741900	-0.20511900	-0.75677800
C	-2.61057700	0.67952400	-1.58997000
C	-2.68867500	-1.20812700	-0.14319300
C	-3.98584600	0.59351400	-1.78560300
C	-4.05499400	-1.30109100	-0.34230800
C	-4.73380700	-0.40141600	-1.16449900
C	-6.22747900	-0.56500200	-1.32234500
F	-4.72460300	-2.27370700	0.27143000
F	-2.08967200	-2.09086500	0.64656900
F	-1.95469000	1.65283500	-2.22304900
F	-4.54298000	1.49726600	-2.58685800
F	-6.76414400	0.34938800	-2.13322100
F	-6.84102100	-0.46029400	-0.13376100
F	-6.52221200	-1.77264300	-1.82226600
C	0.22672500	-1.11556900	-1.17142100
O	-0.27963500	-2.02845800	-1.77493400
C	1.72175400	-0.86508200	-1.11304600
H	2.01094600	-0.51572400	-0.11498600
H	2.23006500	-1.80423000	-1.32553500
C	2.02168500	0.19789100	-2.15389800
C	2.81355600	-0.04063500	-3.28142100
C	1.40706400	1.45711000	-2.03000500
C	2.98775800	0.92040500	-4.27374700
C	1.56232500	2.41476000	-3.03129100
C	2.34805300	2.14589700	-4.15013900
H	3.60802100	0.69629900	-5.13434900
H	1.07094000	3.37935500	-2.94166800
H	2.46270100	2.89378500	-4.92943600
O	-0.78554700	2.15371600	1.44456100
C	-0.84139500	1.19706700	2.26312200
C	-1.33608200	1.46571900	3.66338400
H	-0.62681500	1.05383100	4.38634000
H	-1.47049100	2.53468200	3.83165300
H	-2.28887900	0.94770400	3.81019200
O	-0.52343400	-0.00341600	1.99030300
H	-0.42492200	-0.15832600	0.72152300
Cl	3.63365100	-1.57627600	-3.50020500

17

Pd	0.29245200	1.81249800	-0.39459000
N	1.23164600	3.63949600	-0.05685300
C	0.50145300	4.60304100	0.53025000
C	2.53012200	3.86996400	-0.31112600
C	1.04092400	5.83901700	0.85495100
H	-0.52359500	4.34180100	0.76410000
C	3.14059300	5.07568800	-0.00049300
H	3.07483800	3.06268000	-0.78374100
C	2.38278300	6.08302200	0.58606500
H	0.41046200	6.58960100	1.31783400
H	4.19361500	5.21262800	-0.21804200
H	2.83225000	7.03942600	0.83358700
N	-0.62246500	-0.14981200	-0.49463400
C	-2.02678300	-0.16239800	-0.74594800
C	-2.56576700	0.51363300	-1.83221900
C	-2.89408600	-0.86764900	0.08240900
C	-3.93529400	0.52810600	-2.06829300
C	-4.26055800	-0.84785200	-0.14720600
C	-4.80908200	-0.15247600	-1.22385700
C	-6.31021300	-0.18500400	-1.40288400
F	-5.05226800	-1.52450800	0.67996300
F	-2.41596100	-1.57388900	1.09942500
F	-1.76947000	1.17887100	-2.66439500
F	-4.36454200	1.21468400	-3.12160400
F	-6.71831500	0.51704700	-2.46147900
F	-6.92287800	0.31895600	-0.32175600
F	-6.74028700	-1.44399200	-1.56023200
C	0.13063500	-1.11151400	-1.26807200
O	-0.41264300	-1.89777200	-1.99521000
C	1.62633300	-0.92638600	-1.14042300
H	1.89200100	-0.62384500	-0.12106300
H	2.10791600	-1.87544500	-1.37157100
C	1.99267700	0.15827200	-2.14002800
C	2.80684100	-0.08484300	-3.25109300
C	1.41268100	1.43308300	-2.00006600
C	3.03906400	0.88943800	-4.21735100
C	1.62740700	2.40178600	-2.98108300
C	2.43355800	2.13146000	-4.08427200
H	3.67587400	0.66351100	-5.06525000
H	1.16358500	3.37967800	-2.88679200
H	2.59109200	2.89035900	-4.84526400
O	-0.89926400	2.19714500	1.34782800
C	-0.83738800	1.31824600	2.27837400
C	-1.38526500	1.75422500	3.62318400
H	-0.75447700	2.55315600	4.02684800
H	-2.39141800	2.16475600	3.49838800
H	-1.40441700	0.91730900	4.32209200
O	-0.36796300	0.16937200	2.14560800
H	-0.43972100	-0.23814900	0.55520900
Cl	3.58111600	-1.64277100	-3.48061700

18

Pd	0.32164900	2.47632200	-1.55313800
N	-1.60506800	3.08642500	-0.67857000
C	-2.17756900	2.33647100	0.27340100
C	-2.32345500	4.05769200	-1.26055500
C	-3.49490000	2.52048500	0.67149900
H	-1.55907100	1.54965900	0.69472000
C	-3.64346200	4.30966000	-0.91125000
H	-1.82162100	4.60488000	-2.05230300
C	-4.24402900	3.52269800	0.06520100
H	-3.92410700	1.86725000	1.42230000
H	-4.18854600	5.10017600	-1.41491800
H	-5.28170400	3.67955500	0.34105700
N	-0.28196000	-0.94252100	-1.63226200
C	-1.66781500	-0.77618500	-1.68892300
C	-2.52850700	-0.86423800	-0.59241300
C	-2.24658600	-0.52391800	-2.93461800
C	-3.86801000	-0.53193000	-0.73529500
C	-3.58843000	-0.21626400	-3.07201000

C	-4.42522100	-0.17262200	-1.95792700
C	-5.88454000	0.20297700	-2.00673700
F	-4.03799700	0.04911000	-4.29658500
F	-1.47988000	-0.58852600	-4.02186600
F	-2.11860500	-1.26787500	0.60478000
F	-4.63405400	-0.57047500	0.35685300
F	-6.16076900	1.14832300	-1.09105400
F	-6.66641500	-0.85154000	-1.73416000
F	-6.25134000	0.68427300	-3.19605400
C	0.52238100	-0.35952300	-0.66449400
O	0.09853000	0.06302100	0.39500400
C	1.99859300	-0.34454400	-1.01888600
H	2.49956500	0.11906300	-0.16345300
H	2.34294200	-1.38176800	-1.06289600
C	2.35323800	0.38544700	-2.30357100
C	3.26887300	-0.16007000	-3.21775800
C	1.83944500	1.66476300	-2.58938100
C	3.68396700	0.51972500	-4.35603700
C	2.26071200	2.35777900	-3.72380100
C	3.17705800	1.78955100	-4.60153800
H	4.39371100	0.05676800	-5.03218200
H	1.83722000	3.33466000	-3.93599500
H	3.49294200	2.33243600	-5.48768500
O	-0.56817800	4.04150900	-3.87103800
C	-0.96350300	2.88298000	-4.04019400
C	-1.67336000	2.47260700	-5.31697900
H	-2.55213700	1.86382400	-5.09425700
H	-1.95789200	3.35465600	-5.89272600
H	-0.99419700	1.85500000	-5.91423600
O	-0.80999800	1.91550500	-3.19446000
H	0.15058200	-1.01641600	-2.54607800
C	1.09046000	3.24754700	0.40010600
C	0.82142600	4.73647300	0.55748400
C	2.20373000	3.13857200	-0.40635800
H	0.76671100	2.49188000	1.10947700
C	1.97994600	5.23608800	1.47464900
C	1.29099000	5.29170500	-0.80205000
H	-0.18018500	5.00756300	0.89238900
C	2.63518900	4.54613100	-0.76982200
H	2.89994300	2.30970700	-0.40059400
C	3.23422900	5.09938700	0.56018400
H	2.05953900	4.65209800	2.39621100
H	1.80659200	6.27900000	1.75724300
H	0.66207300	5.01723500	-1.65469300
H	1.41798200	6.37919100	-0.78323900
H	3.28068800	4.63219100	-1.64414700
H	3.99491200	4.43395500	0.97934000
H	3.70623700	6.07023400	0.38165900
Cl	3.96088900	-1.75996300	-2.95930100

TS19

Pd	0.28965200	2.96118400	-1.57234100
N	-1.49130000	4.00204700	-1.00858100
C	-2.05764900	4.79366100	-1.93287700
C	-2.11121000	3.82363800	0.16541800
C	-3.26406900	5.44138200	-1.70233800
H	-1.51780200	4.87810600	-2.87278800
C	-3.32131200	4.42996100	0.46709000
H	-1.61850900	3.16611000	0.87332000
C	-3.90871400	5.25662200	-0.48503000
H	-3.68643300	6.07326900	-2.47544100
H	-3.79095500	4.24914700	1.42729700
H	-4.85711400	5.74412900	-0.28219600
N	-0.93039600	-0.30926700	-1.95184600
C	-2.24087100	-0.78322800	-2.07617200
C	-2.50772400	-2.13212600	-2.31224200
C	-3.32391100	0.08593000	-1.98313400
C	-3.81221400	-2.57962400	-2.44126200
C	-4.63123700	-0.36009000	-2.13827800
C	-4.89929000	-1.70703500	-2.36764200
C	-6.28555400	-2.27972500	-2.54103500
F	-5.60242500	0.54550800	-2.03529200

F	-3.12044000	1.37631400	-1.72104300
F	-1.51160700	-2.99752400	-2.43706200
F	-4.02034400	-3.87547800	-2.66700400
F	-6.54353000	-3.19789100	-1.59834600
F	-6.40492300	-2.88411500	-3.73267200
F	-7.24108600	-1.34923000	-2.46724800
C	-0.13064200	-0.75277900	-0.92803000
O	-0.49196000	-1.58634000	-0.12122500
C	1.24106700	-0.08381000	-0.79922800
H	1.10742300	0.70831200	-0.05346300
H	1.88842800	-0.84256200	-0.35140300
C	1.85762000	0.48600600	-2.05111700
C	2.39033700	-0.36150900	-3.02991100
C	1.90771200	1.87060800	-2.29902000
C	2.96523900	0.12003800	-4.20000600
C	2.49524400	2.36476900	-3.46490500
C	3.01531900	1.49250000	-4.41295000
H	3.36234700	-0.57643800	-4.92998800
H	2.50227700	3.43099800	-3.65879900
H	3.45270300	1.88248400	-5.32678600
O	-0.15038600	3.98784200	-4.35871300
C	-0.56393300	2.82387100	-4.33920000
C	-0.89949900	2.08167500	-5.61941700
H	-1.85978400	1.56723100	-5.52207600
H	-0.92096600	2.76624000	-6.46871100
H	-0.13225900	1.31772300	-5.78885100
O	-0.72886100	2.13017900	-3.26077800
H	-0.69556600	0.51329000	-2.52056100
C	1.35694000	3.67344800	0.04306500
C	1.66861600	5.16395600	-0.03740700
C	2.43944900	3.00721800	-0.61540200
H	0.92858900	3.26109900	0.95784200
C	2.85656800	5.38617700	0.93505900
C	2.38397600	5.25683300	-1.39831200
H	0.81524300	5.82625500	0.11626500
C	3.36762000	4.11338300	-1.09032500
H	2.87013900	2.10025100	-0.20464600
C	4.02107700	4.64032700	0.22146500
H	2.65199100	4.99095500	1.93476200
H	3.07116000	6.45447300	1.03901200
H	1.72642100	5.06775500	-2.25337300
H	2.89335700	6.21509600	-1.54068900
H	4.08022500	3.82921700	-1.86405900
H	4.44492000	3.83264200	0.82618000
H	4.83815100	5.32241600	-0.03104900
Cl	2.32495500	-2.09598200	-2.80373000

20

Pd	-0.01838200	2.57818100	-2.53847900
N	-1.83448900	3.61454100	-2.49846300
C	-2.29081000	4.07319700	-3.67567600
C	-2.58255200	3.77050500	-1.39750900
C	-3.51905900	4.71305000	-3.77969300
H	-1.64112700	3.90318300	-4.53243700
C	-3.82016700	4.39341600	-1.42644700
H	-2.16890000	3.37778800	-0.47572400
C	-4.29891200	4.87434000	-2.64099500
H	-3.85086000	5.07115900	-4.74768500
H	-4.39372500	4.49039300	-0.51162400
H	-5.26590000	5.36408000	-2.69784800
N	-0.90362000	-0.51160100	-2.07144600
C	-2.17072000	-1.096667600	-2.18330400
C	-2.35964600	-2.46733300	-1.99802900
C	-3.28310100	-0.33263400	-2.52031800
C	-3.61827100	-3.03069300	-2.12694500
C	-4.54137400	-0.90273800	-2.67479600
C	-4.73318400	-2.26700300	-2.47624000
C	-6.06407900	-2.96621600	-2.61903700
F	-5.54321200	-0.08765200	-2.99775100
F	-3.16036100	0.98211700	-2.69099200
F	-1.32857800	-3.25287900	-1.71771400
F	-3.74918300	-4.34203800	-1.93798600

F	-6.42395800	-3.54399500	-1.46375900
F	-5.99520200	-3.93221000	-3.54687400
F	-7.04706000	-2.13618500	-2.97698400
C	-0.18728800	-0.62911600	-0.90721400
O	-0.63794200	-1.16273800	0.08749500
C	1.23538200	-0.05322200	-0.86077000
H	1.22197100	0.65750300	-0.03328900
H	1.86084400	-0.89114000	-0.53385200
C	1.81966900	0.56998800	-2.10414700
C	2.10211500	-0.22973500	-3.22105300
C	2.16622000	1.95482200	-2.17746000
C	2.60819700	0.29087000	-4.40436000
C	2.67025800	2.46266300	-3.39188300
C	2.87206900	1.64892200	-4.49601800
H	2.78804300	-0.37042700	-5.24480500
H	2.92901500	3.51118100	-3.46253500
H	3.23943400	2.07256500	-5.42361800
O	-0.12048700	2.92572600	-5.67618500
C	-0.36287800	1.74663400	-5.40097900
C	-0.49293300	0.69540100	-6.49264500
H	-1.47970300	0.22466500	-6.43757600
H	-0.35042800	1.14040400	-7.47871300
H	0.24871200	-0.09432100	-6.33097200
O	-0.53432500	1.29631600	-4.20525800
H	-0.59587900	0.04125800	-2.87860900
C	0.63749300	3.33973800	-0.79576500
C	0.73736100	4.85692900	-0.66138400
C	2.09883600	2.86160600	-0.92474300
H	0.06020500	2.85194100	0.00143300
C	1.40341600	5.15688500	0.70372600
C	1.88058700	5.18204600	-1.63456600
H	-0.20349200	5.38680700	-0.82631000
C	2.87408300	4.19849100	-0.97968700
H	2.44608600	2.27918900	-0.06481800
C	2.88692900	4.74405500	0.46525800
H	0.93625600	4.59603400	1.51995600
H	1.31981700	6.22115900	0.94751300
H	1.62300600	4.96863000	-2.67550100
H	2.22282300	6.22005300	-1.56203400
H	3.86801800	4.12400500	-1.42870100
H	3.24409700	4.00243600	1.18685900
H	3.55218700	5.61075500	0.53129000
Cl	1.83493700	-1.95703800	-3.15811400

21			
Pd	1.42385900	3.03844700	-2.75561500
N	-0.21381000	4.36382300	-2.65120300
C	-0.35949100	5.25107100	-3.64845100
C	-1.16488400	4.27121600	-1.70796200
C	-1.48144000	6.06410900	-3.74202500
H	0.45796800	5.28629300	-4.36425100
C	-2.31296200	5.04882900	-1.74052800
H	-1.01016700	3.52786100	-0.93292100
C	-2.47949400	5.95720000	-2.78071300
H	-1.56429800	6.76312700	-4.56648700
H	-3.06831500	4.92547400	-0.97278100
H	-3.37680500	6.56338900	-2.84342000
N	-0.87079700	0.64152600	-2.57169100
C	-2.11714200	1.26195400	-2.69986400
C	-3.13904100	1.08383500	-1.76740000
C	-2.38462800	2.08392500	-3.79723500
C	-4.32669100	1.80201800	-1.86390200
C	-3.57802600	2.77416900	-3.90370400
C	-4.57496600	2.65687400	-2.93515400
C	-5.81802700	3.50327300	-3.05739300
F	-3.74066200	3.59522100	-4.93864100
F	-1.45732300	2.23726000	-4.73476700
F	-3.01659200	0.21540200	-0.77248100
F	-5.22256100	1.61569600	-0.89920400
F	-6.77984900	3.13358200	-2.21090500
F	-6.32499800	3.44521200	-4.29439700
F	-5.53559700	4.79649100	-2.80181800

C	-0.15449300	0.70415500	-1.38599900
O	-0.61723800	1.19861400	-0.37660000
C	1.22402800	0.04216400	-1.39136000
H	1.60445800	0.19037900	-0.38087800
H	1.07255200	-1.03295400	-1.52918500
C	2.23059100	0.54456700	-2.41270300
C	2.39107700	-0.11199800	-3.64267600
C	3.12839300	1.62145600	-2.11835500
C	3.34972200	0.25739200	-4.57349900
C	4.09000500	1.98247400	-3.08157100
C	4.20438100	1.31141000	-4.28793300
H	3.41335600	-0.27287500	-5.51669100
H	4.76493800	2.80203800	-2.87064500
H	4.94638200	1.62233400	-5.01499200
O	2.38555100	4.49646600	-5.05203300
C	1.91254800	3.45164300	-5.53257600
C	2.08822600	3.13874800	-7.01216900
H	2.63984500	3.93440700	-7.51610200
H	2.62433900	2.18988000	-7.12263500
H	1.10881800	3.00975300	-7.48379400
O	1.26071300	2.57397800	-4.86579900
H	-0.34810900	0.51487500	-3.43142200
C	1.84269000	3.25714000	-0.79313200
C	2.38187600	4.63925300	-0.43160600
C	3.08085300	2.33350100	-0.75013100
H	1.00004400	2.92137800	-0.18375500
C	2.78361200	4.59730000	1.06179100
C	3.75788600	4.63686500	-1.11861400
H	1.71231400	5.46191700	-0.69288300
C	4.22016000	3.32976000	-0.43980600
H	3.02995100	1.57439600	0.03899200
C	4.06655200	3.71400000	1.04867900
H	1.98935700	4.17769000	1.68751500
H	2.99774700	5.60510900	1.43336300
H	3.68778600	4.60418500	-2.21014800
H	4.37998200	5.49190200	-0.83214300
H	5.22040500	2.96509100	-0.68955000
H	3.98545900	2.83579600	1.69756700
H	4.94116100	4.28348200	1.37871600
Cl	1.34143400	-1.45107400	-4.08030900

22

Pd	0.11687800	0.81989400	0.32511900
N	-0.56344500	3.33816800	0.01379500
C	-0.58037800	3.64566800	-1.28882700
C	-1.38493700	4.01550600	0.82302900
C	-1.41373200	4.61723900	-1.83011400
H	0.08461100	3.06350000	-1.92248300
C	-2.26121800	4.99631800	0.37509400
H	-1.34501400	3.74831700	1.87594500
C	-2.28042600	5.29849900	-0.98281200
H	-1.39727300	4.81169400	-2.89706300
H	-2.92274600	5.49709000	1.07313600
H	-2.96963300	6.03839300	-1.37445800
N	-1.14237800	0.22123000	-1.23436200
C	-2.24650400	0.97646700	-1.58452100
C	-2.49706500	1.39862700	-2.89540800
C	-3.12293800	1.45950600	-0.60841000
C	-3.56324500	2.23008100	-3.20819900
C	-4.16449800	2.31380300	-0.90842000
C	-4.42339600	2.71014100	-2.22064200
C	-5.55646600	3.66744800	-2.47273700
F	-4.92821600	2.76594900	0.08870100
F	-2.92185500	1.11840400	0.67722100
F	-1.65338900	1.06829400	-3.86954600
F	-3.69640100	2.59860600	-4.48142700
F	-5.75624000	3.90877600	-3.76991000
F	-5.32106600	4.85738000	-1.87912500
F	-6.70795000	3.20385700	-1.96648500
C	-0.90329500	-0.93067300	-1.93610700
O	-1.69658800	-1.46253600	-2.69483000
C	0.47044800	-1.55877100	-1.66721800

H	0.46921700	-1.98021900	-0.65329800
H	0.58858800	-2.37946200	-2.37251800
C	1.57591100	-0.54299000	-1.79310100
C	2.62572500	-0.63948300	-2.71314800
C	1.55351500	0.61120300	-1.00202400
C	3.58339600	0.36301800	-2.85694800
C	2.47904600	1.63645000	-1.13450900
C	3.50182600	1.50500200	-2.07440300
H	4.37565900	0.24408800	-3.58735800
H	2.40311100	2.53582000	-0.53123700
H	4.23703600	2.29534400	-2.19143700
C	1.47152500	-0.13693600	1.82807400
C	1.41178600	1.22933200	2.06476700
C	0.74073600	-0.81973800	2.98748300
H	2.19591900	-0.65017100	1.20581300
C	0.63531000	1.39724500	3.37641700
H	2.09955600	1.97683700	1.68662300
C	1.14466400	0.14508700	4.13084800
C	-0.78085500	-0.53308500	2.91037300
H	0.98920200	-1.87441700	3.11242700
C	-0.85219500	1.00439700	3.16181700
H	0.77628600	2.36363100	3.86272900
H	0.61626700	-0.04905700	5.07192800
H	2.22281100	0.16719500	4.31511400
H	-1.29928000	-1.08296000	3.70164100
H	-1.22489100	-0.84262200	1.95964800
H	-1.43292000	1.23049100	4.06134100
H	-1.32933600	1.55197400	2.34304400
Cl	2.78153900	-2.04641900	-3.74501700

TS23

Pd	0.28546600	1.56133800	-0.40779500
N	-1.15765800	3.08535400	0.04922700
C	-0.96291000	4.30254200	-0.48087000
C	-2.37403100	2.77834300	0.52269800
C	-1.97853600	5.24046800	-0.58669900
H	0.03624100	4.50757800	-0.84964600
C	-3.44111500	3.66339100	0.46310600
H	-2.49493200	1.77484500	0.91619600
C	-3.24669000	4.91073500	-0.11817300
H	-1.77948600	6.20016300	-1.04937900
H	-4.41356300	3.35586000	0.83042200
H	-4.07173600	5.60759400	-0.21668600
N	-1.21820800	0.39766300	-1.45451900
C	-2.33316100	1.01427000	-1.97120200
C	-2.16731600	2.10172000	-2.84316000
C	-3.65015400	0.78321800	-1.53977400
C	-3.21476300	2.91496800	-3.23382900
C	-4.70533900	1.57410600	-1.96216400
C	-4.52445000	2.65347100	-2.82769400
C	-5.66661900	3.57411600	-3.15052900
F	-5.91009600	1.33092600	-1.43930400
F	-3.89575500	-0.10555100	-0.57554800
F	-0.93098100	2.43552700	-3.23816400
F	-2.92911400	3.96981200	-4.00068800
F	-5.46039500	4.27191700	-4.27261200
F	-5.85563500	4.47460500	-2.15710500
F	-6.81989800	2.91310300	-3.29990900
C	-1.22231000	-0.95175600	-1.24438900
O	-2.06204800	-1.74641000	-1.63465100
C	0.03103100	-1.45515300	-0.47840100
H	0.05815800	-0.98749700	0.51450900
H	-0.07080200	-2.53277200	-0.35961500
C	1.24136500	-1.06680900	-1.27978800
C	1.74088600	-1.88819000	-2.29431300
C	1.74266500	0.25200200	-1.19349400
C	2.65615900	-1.42881200	-3.23738900
C	2.61236200	0.72852400	-2.17742500
C	3.06238000	-0.10382800	-3.19593000
H	3.01553000	-2.10198200	-4.00762100
H	2.96430800	1.75152700	-2.15023700
H	3.74380300	0.27875200	-3.94927200

C	1.49872900	1.95011400	1.20088600
C	2.35987000	3.19543000	1.33443300
C	2.32635300	0.92906100	0.59323900
H	0.85199200	1.68945500	2.04095500
C	3.26505100	3.07899800	0.10162700
C	3.36598800	2.87291200	2.47033600
H	1.81098500	4.13032700	1.46205900
C	3.67251900	1.62025500	0.39038200
H	2.32917300	-0.07455500	1.01075000
H	4.11893900	3.76322800	0.12894800
H	2.72028300	3.22238800	-0.83542300
H	3.95487400	3.76030400	2.72450500
H	2.86450100	2.53619300	3.38257200
C	4.25171400	1.76796800	1.82664700
H	4.34653800	1.13179400	-0.31261200
H	5.29843400	2.08004500	1.76412900
H	4.22562600	0.82348300	2.37845400
Cl	1.19271500	-3.54274300	-2.45272500

24

Pd	-0.86565500	1.97697400	-1.49101100
N	-0.26315700	3.94950900	-1.98312200
C	0.60336500	4.13657600	-2.99217000
C	-0.84142000	5.02389700	-1.42546300
C	0.93444900	5.39954500	-3.46186900
H	1.04710600	3.24036300	-3.41196400
C	-0.56510700	6.31890300	-1.83864300
H	-1.54522800	4.82504500	-0.62507800
C	0.34394800	6.51232200	-2.87328300
H	1.64568700	5.49909600	-4.27394200
H	-1.05748700	7.15463100	-1.35464600
H	0.58367700	7.51327600	-3.21768400
N	-1.71951500	0.13980800	-1.29897500
C	-3.10944500	0.23107100	-1.27166600
C	-3.77695600	1.10196800	-2.13861100
C	-3.91166500	-0.46839600	-0.36674200
C	-5.14690300	1.26037000	-2.12291900
C	-5.29530000	-0.33556100	-0.36214800
C	-5.94535400	0.53039800	-1.24076800
C	-7.43518500	0.75339200	-1.27086000
F	-5.97178500	-1.04434100	0.53864200
F	-3.35422300	-1.25451200	0.54880800
F	-3.04937300	1.83948500	-3.00973200
F	-5.70566600	2.12304100	-2.97382400
F	-7.92739300	0.54961200	-2.50267100
F	-7.73567900	2.01974400	-0.93061300
F	-8.09821700	-0.05144900	-0.43763100
C	-1.19812400	-1.11745300	-1.45293400
O	-1.87543200	-2.12031000	-1.61389900
C	0.32652800	-1.25373700	-1.33631700
H	0.54883900	-1.20347700	-0.26728000
H	0.53888900	-2.27684900	-1.65229000
C	1.21068000	-0.29634700	-2.10040900
C	1.41601300	-0.47797800	-3.47274200
C	1.89537700	0.76996200	-1.47172600
C	2.28438800	0.31683100	-4.21561300
C	2.78451500	1.54874700	-2.21199100
C	2.98518900	1.32452400	-3.57098700
H	2.41350700	0.12904700	-5.27565400
H	3.32433900	2.35604300	-1.72917000
H	3.68545300	1.93961600	-4.12875500
C	0.19629700	1.70722200	0.22350100
C	0.50426200	2.98891600	1.00750200
C	1.60992800	1.07208300	-0.00954900
H	-0.46930300	1.03905100	0.77391200
C	1.85896100	3.43664700	0.43559000
C	0.91390500	2.54579400	2.43424200
H	-0.30041600	3.72689500	1.00720600
C	2.54367000	2.08485400	0.69638200
H	1.66649400	0.12557300	0.53847500
H	2.31109400	4.25753500	1.00325000
H	1.81894200	3.71468200	-0.61863200

H	0.95375800	3.41192200	3.10346800
H	0.20210300	1.83338300	2.86243800
C	2.32776300	1.93342000	2.21600000
H	3.59229700	1.99668000	0.40247700
H	3.08966500	2.49677200	2.76434400
H	2.39532000	0.89066000	2.54197000
Cl	0.56392600	-1.74661900	-4.32252900

25

Pd	0.56609800	2.58238800	-2.13794200
N	2.05733000	4.06919100	-2.13469800
C	3.20562300	3.86625800	-2.79635900
C	1.80645900	5.28720500	-1.63574600
C	4.15810100	4.86294100	-2.95149900
H	3.35377800	2.86933100	-3.19533300
C	2.70555000	6.33789200	-1.75150300
H	0.85359700	5.40937900	-1.13332300
C	3.90832400	6.12105200	-2.41414300
H	5.07787700	4.64830800	-3.48388300
H	2.45964900	7.30421700	-1.32615800
H	4.63630600	6.91981400	-2.51485500
N	-1.08190600	1.26315600	-2.28418800
C	-2.34393600	1.89851400	-2.29607400
C	-2.65430000	3.08809400	-1.64086500
C	-3.37252900	1.33591900	-3.06423100
C	-3.89476000	3.70529000	-1.77345600
C	-4.61072500	1.93454400	-3.18700800
C	-4.90188300	3.14154100	-2.54799300
C	-6.26832100	3.74801700	-2.74399200
F	-5.53592700	1.34624300	-3.94415000
F	-3.14572100	0.19091100	-3.70756700
F	-1.76167800	3.69837100	-0.84979200
F	-4.07203700	4.85078700	-1.11642500
F	-6.42117200	4.90348500	-2.09116600
F	-7.22882200	2.91435500	-2.31838700
F	-6.49856600	3.98995300	-4.04499800
C	-1.09628300	0.06328100	-1.58893800
O	-2.02041600	-0.29660400	-0.88071300
C	0.06214500	-0.91180100	-1.81497500
H	0.15143100	-1.47630600	-0.88215300
H	-0.33288700	-1.62079800	-2.54824500
C	1.42558100	-0.43921100	-2.25532400
C	1.95335700	-0.78034600	-3.50536600
C	2.25664400	0.28620500	-1.36676700
C	3.25249800	-0.45128900	-3.88615700
C	3.56924800	0.57591500	-1.73588000
C	4.06673400	0.21389300	-2.98443200
H	3.61787600	-0.74458500	-4.86395900
H	4.21937700	1.10178700	-1.04606700
H	5.09366800	0.44683800	-3.25116200
C	0.75317100	2.02226500	-0.18493900
C	1.36617200	3.02166200	0.80717300
C	1.68009000	0.75885200	-0.04104800
H	-0.27481800	1.79473900	0.10359800
C	2.87021200	2.72079700	0.73291200
C	1.03224500	2.51262400	2.23004600
H	1.06396600	4.05883100	0.65062300
C	2.69870100	1.21963300	1.02830500
H	1.09148900	-0.06674700	0.37348000
H	3.44943500	3.23813200	1.50639200
H	3.31052600	2.93730400	-0.24165500
H	1.27363400	3.27830600	2.97555000
H	-0.02877000	2.26962600	2.34014000
C	1.95819000	1.27066300	2.38048500
H	3.61058200	0.61699100	1.05879600
H	2.67371000	1.40789500	3.19798400
H	1.40417400	0.34845000	2.58199800
Cl	1.00820200	-1.68605700	-4.67435700
O	0.44966200	3.09001200	-4.36275700
C	0.01527500	2.32772700	-5.22701700
C	0.19841300	2.59241800	-6.69426200
H	0.76398700	3.51186600	-6.84265500

H	0.71962100	1.74639400	-7.15158400
H	-0.78046900	2.67253300	-7.17575900
O	-0.63941100	1.22514500	-4.97356000
H	-0.75037700	1.11035600	-3.97580600

TS26

Pd	-0.50159600	2.04335300	-0.83919300
N	-0.38780800	3.86283800	0.18590400
C	0.49124200	4.78164200	-0.24044400
C	-1.29035400	4.21184900	1.11241100
C	0.52570000	6.06771100	0.27852800
H	1.17981800	4.45953700	-1.01189500
C	-1.32637400	5.47953100	1.67488600
H	-2.00025700	3.44550800	1.39998800
C	-0.39495000	6.42373700	1.25766000
H	1.26262900	6.77349000	-0.08770800
H	-2.07518200	5.71394100	2.42276800
H	-0.39198400	7.42199500	1.68374200
N	-0.80679700	0.26187900	-2.04566200
C	-2.14319800	-0.23091600	-2.10491400
C	-2.52322700	-0.93738700	-3.24954400
C	-3.11427300	-0.05207800	-1.12744100
C	-3.80935100	-1.41447300	-3.41718200
C	-4.41352900	-0.52589800	-1.29432000
C	-4.78709900	-1.21687300	-2.44113800
C	-6.17158000	-1.76644300	-2.69179400
F	-5.27153900	-0.29044800	-0.30485600
F	-2.84653600	0.58430500	0.01535000
F	-1.61700200	-1.17066300	-4.19538200
F	-4.10760200	-2.07497300	-4.53319800
F	-6.12826800	-3.09365000	-2.87475900
F	-6.70100900	-1.22516500	-3.79910900
F	-7.01399800	-1.52610600	-1.68465400
C	0.13774100	-0.75474100	-1.78619700
O	-0.17209600	-1.81721900	-1.29277200
C	1.56361000	-0.48210100	-2.24128700
H	2.16778200	-1.27668100	-1.79272200
H	1.55075500	-0.67149900	-3.31923600
C	2.20494600	0.86230300	-1.97654900
C	2.75902700	1.61479800	-3.01925100
C	2.35511200	1.34662300	-0.65400700
C	3.43959500	2.80918400	-2.79624300
C	3.07647500	2.52067300	-0.43781900
C	3.60927600	3.25112500	-1.49484500
H	3.85112800	3.35752300	-3.63596100
H	4.16214200	4.16583700	-1.30135200
C	0.17382200	0.85816300	0.67822300
C	0.05856600	1.32667300	2.13578000
C	1.71739800	0.58679500	0.50496700
H	-0.40216800	-0.06039600	0.54513400
C	1.36654900	2.09368400	2.36918500
C	0.27793300	0.08503500	3.03185500
H	-0.86844100	1.85374200	2.36940200
C	2.26280800	0.92580600	1.91268800
H	1.87136200	-0.48213100	0.31854800
H	1.52748700	2.35936000	3.42027800
H	1.45183000	2.99505400	1.75925100
H	0.02539300	0.31451000	4.07312900
H	-0.34264500	-0.76047000	2.72018400
C	1.80110000	-0.19113600	2.87178000
H	3.34260600	1.09517900	1.93825600
H	2.32086700	-0.10552000	3.83162800
H	2.01116700	-1.18825400	2.47239100
H	-0.60909500	0.91452100	-3.05930800
Cl	2.67454700	1.07471000	-4.68402000
O	-0.96307700	3.31004500	-2.59527700
C	-0.74790700	2.89221600	-3.75993200
C	-0.71001900	3.88519100	-4.89876700
H	-0.91035400	4.89620900	-4.54208500
H	0.27598100	3.84174800	-5.37177300
H	-1.44593000	3.60109800	-5.65619300
O	-0.54630700	1.67529200	-4.07393600

H	3.22393200	2.88257600	0.57273100
---	------------	------------	------------

27

Pd	0.60093600	2.55428400	-0.17353200
N	-1.44114200	2.96104300	0.37440000
C	-2.16095200	3.66565800	-0.51637300
C	-2.07238200	2.45362800	1.44282000
C	-3.52820200	3.85896100	-0.37980600
H	-1.59723800	4.07903200	-1.34299600
C	-3.43023200	2.62789700	1.66471400
H	-1.47227000	1.86961900	2.12648600
C	-4.17901500	3.33102800	0.72869400
H	-4.06920100	4.40539700	-1.14359900
H	-3.88947400	2.18410700	2.53988500
H	-5.25054200	3.45008600	0.85000700
N	-0.59743400	0.20485100	-1.99787900
C	-1.97911500	0.30435500	-1.84805500
C	-2.74299700	0.78724800	-2.91830400
C	-2.65940200	0.03131300	-0.66170900
C	-4.09515400	1.04203600	-2.77759200
C	-4.02748500	0.24350700	-0.54100700
C	-4.77109100	0.78013800	-1.58611800
C	-6.22122100	1.17289000	-1.48127000
F	-4.57518900	-0.02453400	0.64375200
F	-2.01438800	-0.36770800	0.43373400
F	-2.16692100	1.01666300	-4.09058700
F	-4.75930700	1.54586400	-3.81695300
F	-6.96650300	0.56807300	-2.41272300
F	-6.35772800	2.50285100	-1.66266200
F	-6.75153300	0.88730200	-0.28824300
C	0.13677000	-0.86666600	-1.55471300
O	-0.35360300	-1.84810100	-1.03179100
C	1.64153900	-0.79899200	-1.83177700
H	2.09921200	-1.48790300	-1.11830800
H	1.78312700	-1.24931900	-2.81790300
C	2.30800000	0.55390200	-1.79112600
C	2.74506100	1.17852700	-2.95419700
C	2.54209200	1.22487400	-0.54813300
C	3.37277200	2.43013300	-2.95070100
C	3.15841900	2.48758700	-0.56067100
C	3.56510500	3.08774600	-1.75884800
H	3.68409300	2.87011400	-3.89113300
H	4.03469500	4.06480300	-1.74023900
C	0.82944200	1.12025500	1.23338900
C	1.06430800	1.54720600	2.68585800
C	2.19280100	0.55331800	0.78900600
H	-0.00412900	0.42819800	1.09500000
C	2.48506400	2.12135800	2.64201100
C	1.28978200	0.24729400	3.50095000
H	0.30703400	2.21106900	3.10973000
C	3.10310400	0.85909000	2.00337600
H	2.14753500	-0.52715100	0.63501100
H	2.89661600	2.31498700	3.63857100
H	2.54838400	3.04309400	2.06069300
H	1.23413500	0.45036700	4.57549700
H	0.53893700	-0.51472000	3.26965600
C	2.72758300	-0.18527600	3.07789800
H	4.17000300	0.89674300	1.76775600
H	3.42185900	-0.12374900	3.92197700
H	2.76686500	-1.20929500	2.69415300
H	-0.16734600	1.00027300	-2.50952700
Cl	2.52207400	0.43558500	-4.51905000
O	0.53334600	4.05395200	-1.74753400
C	0.37867900	3.66813900	-2.95551700
C	0.58030200	4.73004300	-4.02516000
H	0.52526200	5.73632200	-3.60566500
H	1.57235000	4.58934500	-4.46993600
H	-0.15591600	4.60410600	-4.82286200
O	0.09799500	2.51292100	-3.32389600
H	3.42163200	2.96881500	0.37140300

TS28

Pd	1.43860200	3.82922000	-3.95069500
N	0.11145900	5.48273400	-4.02978600
C	0.52363500	6.62891800	-4.59210700
C	-1.15084000	5.39764500	-3.58658900
C	-0.30419700	7.73695800	-4.70523200
H	1.53887500	6.62992400	-4.97215200
C	-2.04299500	6.45667100	-3.67161200
H	-1.44940800	4.44529300	-3.16765300
C	-1.61016300	7.65238100	-4.23363600
H	0.07502000	8.64486600	-5.16048100
H	-3.05452600	6.33217000	-3.30194600
H	-2.28171900	8.50178400	-4.30983900
N	-0.62621700	-0.22613700	-1.62119800
C	-1.87549500	0.36312700	-1.41735600
C	-2.79813400	-0.11463000	-0.49131800
C	-2.23040000	1.49038500	-2.16095700
C	-4.00363400	0.55264000	-0.27687300
C	-3.43090800	2.13893000	-1.95893600
C	-4.34134100	1.69403400	-0.99986200
C	-5.62957400	2.46342900	-0.82718700
F	-3.69711500	3.22691900	-2.68754500
F	-1.37757500	1.95422400	-3.08269400
F	-2.56805200	-1.22869500	0.18508900
F	-4.82384100	0.03685600	0.63028600
F	-6.38681100	1.99175500	0.16211200
F	-6.35725400	2.42509000	-1.95356700
F	-5.37322100	3.75448000	-0.56186500
C	0.28556300	-0.35229200	-0.57659400
O	-0.03786600	-0.25043600	0.58562300
C	1.72496500	-0.61237800	-1.01670100
H	2.34951000	-0.19067700	-0.22501700
H	1.88149400	-1.69439000	-0.99845100
C	2.08458800	-0.03228700	-2.36623000
C	2.30116900	-0.83873100	-3.49045200
C	2.13668900	1.36702500	-2.53980100
C	2.54518700	-0.30273200	-4.75053400
C	2.41291900	1.93467200	-3.80086100
C	2.59294100	1.07441600	-4.89344400
H	2.69348800	-0.96283100	-5.59783400
H	3.23310000	2.98586500	-4.11686800
H	2.78775300	1.49937900	-5.87356800
O	4.19153700	3.64303100	-4.82454200
C	3.62342200	4.24504300	-5.79361000
C	4.53435900	4.81497300	-6.85851700
H	5.00412000	3.98958900	-7.40299800
H	3.97340800	5.43747600	-7.55678400
H	5.33569100	5.39217900	-6.38961900
O	2.37729700	4.37229300	-5.92289000
H	-0.22296700	-0.08119000	-2.53870400
C	1.12701000	3.61056300	-1.96363000
C	1.90077800	4.69802300	-1.19968800
C	1.75463900	2.29667300	-1.42082000
H	0.04842300	3.65263100	-1.77613500
C	1.51365300	4.59855200	0.29855100
C	3.32928400	4.12309100	-1.18421800
H	1.78603300	5.70407400	-1.61157300
C	2.91350800	2.80127300	-0.51489600
H	1.02145200	1.80313200	-0.77808000
C	2.26425700	3.32046900	0.78148200
H	0.42933500	4.52422900	0.43461200
H	1.85104500	5.48712700	0.84275300
H	3.77280000	4.00968800	-2.17671400
H	4.01563300	4.70341700	-0.55703600
H	3.70629900	2.06402100	-0.36122100
H	1.59783700	2.58036300	1.23697900
H	3.03280500	3.57192300	1.51971600
Cl	2.23868100	-2.58799700	-3.36720000

TS28 (oxidative addition)

Pd	1.51400100	3.89159100	-4.09444300
N	0.86143800	6.00763700	-4.20439800

C	1.75387000	7.00265800	-4.11557000
C	-0.43061300	6.31274300	-4.38622300
C	1.39358600	8.33994600	-4.19794100
H	2.78762700	6.70454000	-3.97348000
C	-0.87567200	7.62644900	-4.47161900
H	-1.09979200	5.46487900	-4.48987700
C	0.05071200	8.65805900	-4.37600900
H	2.15339300	9.10991400	-4.12534300
H	-1.93135100	7.82615600	-4.61700000
H	-0.26626600	9.69414900	-4.44398900
N	-0.52472400	-0.24432900	-1.65449100
C	-1.86131600	0.11117900	-1.43874800
C	-2.72231500	-0.68039400	-0.68700100
C	-2.36001600	1.29702900	-1.97703300
C	-4.03913800	-0.28650200	-0.46355600
C	-3.67416700	1.67558900	-1.77497200
C	-4.53961000	0.89457800	-1.00681800
C	-5.95597000	1.38585400	-0.81566100
F	-4.10031000	2.81836300	-2.30769700
F	-1.54644000	2.07577000	-2.69231800
F	-2.30890400	-1.83583300	-0.18738800
F	-4.79714200	-1.09483700	0.26878400
F	-6.69350100	0.56290800	-0.06906000
F	-6.57193500	1.52214000	-1.99916400
F	-5.96150500	2.58778900	-0.21988800
C	0.36180300	-0.34137000	-0.59344500
O	-0.00271500	-0.33901900	0.56217700
C	1.83182800	-0.46954800	-0.98567200
H	2.38762800	-0.00331200	-0.16882500
H	2.07340200	-1.53550800	-0.95591900
C	2.19856900	0.13063000	-2.32184500
C	2.63481900	-0.64436700	-3.40315500
C	2.04910700	1.51629500	-2.53633900
C	2.90616500	-0.09404700	-4.65440400
C	2.27277800	2.05567700	-3.80639200
C	2.71763900	1.26425400	-4.86208900
H	3.24241500	-0.73764700	-5.45978200
H	2.98011100	3.56635600	-3.68195300
H	2.87342100	1.70639000	-5.84027500
O	-0.49885900	3.45375300	-5.35074700
C	0.23204000	3.49437700	-6.37455800
C	-0.36215400	3.20233000	-7.73568600
H	-1.44001700	3.37513600	-7.72874300
H	0.12039100	3.81053600	-8.50423100
H	-0.18195300	2.14912400	-7.97838000
O	1.47798300	3.74756800	-6.30845700
H	-0.13602600	-0.00164200	-2.55713800
C	1.20899000	3.85506900	-2.07948000
C	2.01033100	4.83529100	-1.22008600
C	1.56551200	2.46698800	-1.47313200
H	0.13097000	4.05271300	-2.07182000
C	1.36174800	4.83723900	0.18906000
C	3.30828300	4.05849100	-0.95139000
H	2.11477800	5.83322500	-1.65004800
C	2.59358100	2.83014900	-0.36481200
H	0.66685400	2.05025900	-1.00564900
C	1.80251800	3.46829800	0.79093200
H	0.27376000	4.94622500	0.13589000
H	1.74521800	5.67386000	0.78225600
H	3.89186700	3.84486900	-1.85213600
H	3.95962600	4.54993000	-0.22062500
H	3.24169300	2.00350000	-0.06536200
H	0.95998800	2.84426800	1.10573600
H	2.44820300	3.61252700	1.66304500
Cl	2.85336400	-2.37667500	-3.23411900

TS28 (AcOH-assisted CMD)

Pd	1.47538700	3.44986300	-4.06504700
N	0.43884200	5.32469300	-4.01928600
C	1.11693500	6.45907500	-4.25090200
C	-0.87542000	5.39109600	-3.76362200
C	0.49679700	7.70162300	-4.23643500

H	2.17906500	6.34234400	-4.44754400
C	-1.56558700	6.59436000	-3.73150700
H	-1.37528400	4.44847800	-3.57700300
C	-0.86683400	7.77268900	-3.97257300
H	1.08172100	8.59422700	-4.42810800
H	-2.62887300	6.59575000	-3.51915400
H	-1.37661300	8.73089800	-3.95281200
N	-0.79831800	-0.17487500	-1.63180500
C	-2.01871300	0.48273300	-1.47210600
C	-3.00951500	0.03788600	-0.60194900
C	-2.27733200	1.63954800	-2.20926500
C	-4.19436600	0.75543800	-0.44389700
C	-3.45982100	2.33561800	-2.06849900
C	-4.44257400	1.91737000	-1.17062100
C	-5.70726300	2.73697100	-1.06791100
F	-3.64065200	3.44020000	-2.79809100
F	-1.35083900	2.07786100	-3.07101500
F	-2.86369300	-1.09302900	0.07007000
F	-5.08541100	0.26727700	0.41034400
F	-6.35404200	2.75362600	-2.24330300
F	-5.41900500	4.00960700	-0.75326400
F	-6.55181000	2.27509900	-0.14654200
C	0.05974200	-0.37728300	-0.55527900
O	-0.29547900	-0.24028100	0.59386000
C	1.48225800	-0.78070500	-0.94025600
H	2.11978800	-0.37504400	-0.15140400
H	1.54074100	-1.86958900	-0.86019000
C	1.91959700	-0.30808400	-2.30732900
C	2.07285000	-1.18644100	-3.38662100
C	2.09046800	1.07076900	-2.55429100
C	2.36115400	-0.74038100	-4.67349500
C	2.36635400	1.54847900	-3.85330700
C	2.48816000	0.62057700	-4.89628600
H	2.46891900	-1.45774300	-5.47943200
H	3.30750600	2.53151900	-4.16379800
H	2.70089500	0.97944200	-5.89883100
O	2.62364600	4.59687000	-7.19949300
C	1.57055200	3.82849000	-7.24782800
C	1.01141400	3.66192700	-8.63474300
H	0.06129700	3.12993300	-8.59345900
H	0.88146000	4.64049100	-9.10435700
H	1.72340100	3.09708600	-9.24475500
O	1.06128800	3.26763100	-6.27846200
H	-0.35690900	-0.06531000	-2.53639200
C	1.60924900	3.50146100	-2.05848400
C	2.74050800	4.35110100	-1.45110900
C	1.85575200	2.08803400	-1.46285100
H	0.62533800	3.88535300	-1.76331300
C	2.36551900	4.59570100	0.02999300
C	3.89021700	3.33927000	-1.28727300
H	2.97052100	5.26403000	-2.00703600
C	3.04823500	2.32451000	-0.50150300
H	0.97710500	1.79267900	-0.87971600
C	2.54036100	3.18494900	0.67393000
H	1.34985300	4.98978700	0.14112200
H	3.05043700	5.32192400	0.48202900
H	4.28483200	2.94282700	-2.22300900
H	4.72034100	3.73957000	-0.69314800
H	3.56532700	1.41003000	-0.19811200
H	1.61048400	2.79181200	1.09869000
H	3.28249300	3.20843600	1.47816200
Cl	1.87523300	-2.91672300	-3.17089600
H	3.02391200	4.66840700	-6.26787700
O	3.86862700	5.03863700	-4.99376200
C	4.69943700	4.21652800	-4.54090900
C	6.01145800	4.73687500	-3.99394200
H	6.27381700	5.68974900	-4.45651500
H	5.89021500	4.89314400	-2.91542800
H	6.80574800	4.00159700	-4.13730900
O	4.51889300	2.95573500	-4.46260200

Pd	2.00568000	3.87012800	-3.85234900
N	1.08719800	5.86037300	-3.91572500
C	1.77303500	6.97082100	-4.21438400
C	-0.22755500	5.96649700	-3.67489900
C	1.18062800	8.22450700	-4.27841000
H	2.83223500	6.83643300	-4.40696800
C	-0.89989900	7.18046400	-3.72118100
H	-0.74760100	5.04317500	-3.44184400
C	-0.18308600	8.33207800	-4.02650200
H	1.78070000	9.09465000	-4.52070000
H	-1.96505800	7.21292900	-3.52118300
H	-0.67847000	9.29694300	-4.06915700
N	-0.52346100	-0.11856800	-1.79127300
C	-1.74282900	0.54658700	-1.64784000
C	-2.78456900	0.04948000	-0.86492300
C	-1.94631000	1.76440000	-2.29468000
C	-3.95217000	0.78394500	-0.71189600
C	-3.11899000	2.48839000	-2.15297300
C	-4.14784300	2.01298800	-1.34320400
C	-5.45921700	2.72982500	-1.12794500
F	-3.20066100	3.65181800	-2.80080900
F	-0.97654800	2.25480800	-3.07463900
F	-2.69347900	-1.13685700	-0.28510300
F	-4.91887200	0.27538500	0.04718800
F	-5.67483800	2.94669500	0.17661300
F	-6.48364000	1.99906900	-1.58990700
F	-5.50075600	3.91544900	-1.74398800
C	0.27728300	-0.37374000	-0.67903500
O	-0.15363500	-0.33631400	0.45199200
C	1.73691800	-0.69330000	-0.99939500
H	2.30127100	-0.33706800	-0.13382900
H	1.83589100	-1.78244100	-1.01282800
C	2.23635900	-0.08255000	-2.28835400
C	2.60495100	-0.85651100	-3.39496400
C	2.22916200	1.31861800	-2.44605500
C	2.92536100	-0.27914000	-4.61724300
C	2.50226000	1.93120400	-3.68572500
C	2.85012900	1.10257400	-4.75882600
H	3.19971800	-0.91275600	-5.45421100
H	4.25015700	3.38612400	-4.42108200
H	3.03931600	1.52832600	-5.74118000
O	4.83039100	3.65070200	-5.17851700
C	4.05152400	4.13159900	-6.13330900
C	4.79440600	4.46325600	-7.39410800
H	4.16314600	5.06344900	-8.04884000
H	5.72385800	4.98875700	-7.16254100
H	5.05939000	3.53028500	-7.90222000
O	2.84067700	4.27150000	-6.00736600
H	-0.02072000	0.08017000	-2.64833800
C	1.59465800	3.68115800	-1.88343400
C	2.51804400	4.55816300	-1.02019600
C	1.84841200	2.24721900	-1.32944400
H	0.54272100	3.97263700	-1.77413600
C	1.95641300	4.57151500	0.42340100
C	3.75252200	3.65646700	-0.85870600
H	2.69538300	5.55843900	-1.42467500
C	2.96051900	2.48003900	-0.26662700
H	0.95020700	1.88656400	-0.81568500
C	2.29586600	3.14536700	0.95234000
H	0.88151500	4.78161800	0.43895500
H	2.44961600	5.34432900	1.02344200
H	4.24110500	3.42036400	-1.80852800
H	4.49616500	4.05522000	-0.15902300
H	3.54121600	1.58483500	-0.02794500
H	1.41420500	2.59135600	1.29106800
H	2.99733000	3.19430500	1.79200500
Cl	2.64887200	-2.61267100	-3.29670300

30

Pd	1.66078900	3.58005100	0.09969900
N	0.69576700	4.77741200	1.70363500
C	1.41003500	5.62487600	2.45660800

C	-0.59707800	4.59865500	2.00575100
C	0.86925300	6.31531700	3.53319300
H	2.45252000	5.74282800	2.17888100
C	-1.22131200	5.25241600	3.06017800
H	-1.13665000	3.89561300	1.38057600
C	-0.47360300	6.12567100	3.84197600
H	1.49459000	6.98140500	4.11728300
H	-2.27117500	5.07068600	3.26122700
H	-0.92803900	6.64617700	4.67919600
N	-0.01770300	-0.83467500	-2.72476000
C	-1.39930000	-0.93594100	-2.86307200
C	-1.98747800	-0.80903800	-4.12225500
C	-2.24564300	-1.12078600	-1.77127900
C	-3.35851900	-0.88631400	-4.28474800
C	-3.62210700	-1.23027300	-1.94064400
C	-4.20631500	-1.11458300	-3.19976200
C	-5.69112500	-1.20048300	-3.45946900
F	-4.35301400	-1.41044700	-0.84469900
F	-1.76168800	-1.15264600	-0.53484900
F	-1.20793800	-0.60034500	-5.18425500
F	-3.86438200	-0.75497900	-5.50930200
F	-5.96272600	-2.16371100	-4.35165400
F	-6.15110400	-0.04517000	-3.96588700
F	-6.39520400	-1.46418700	-2.35688500
C	0.74150700	-1.74523900	-2.00956400
O	0.25818600	-2.72933100	-1.49234300
C	2.23071400	-1.42384900	-1.95092800
H	2.56908100	-1.81419200	-0.98910000
H	2.71427400	-2.03497300	-2.71872500
C	2.57963000	0.03627500	-2.11655500
C	3.22851400	0.52369100	-3.25629700
C	2.18307000	0.97306500	-1.13924300
C	3.47432700	1.87930600	-3.43461800
C	2.40399900	2.35618000	-1.29696800
C	3.05471200	2.78040300	-2.46202300
H	3.97303100	2.22117100	-4.33576500
H	3.22564600	3.83836900	-2.64239200
C	0.90995300	1.83885700	0.84201900
C	1.36452500	1.58616500	2.29252800
C	1.42784900	0.56991300	0.09279100
H	-0.18518200	1.91330400	0.76958600
C	2.76005500	0.98145900	2.07360400
C	0.58216200	0.37233000	2.85444000
H	1.31869100	2.46386400	2.94311400
C	2.24941600	-0.16729700	1.19158400
H	0.58075300	-0.06701100	-0.18900200
H	3.23281900	0.62216700	2.99556700
H	3.44213600	1.66081200	1.55300900
H	0.70537200	0.29775700	3.94110500
H	-0.49131600	0.45433800	2.65129200
C	1.23507400	-0.84333700	2.13092100
H	3.01952000	-0.84093800	0.80738300
H	1.74831700	-1.49618400	2.84556800
H	0.51375900	-1.45639800	1.58107700
H	0.46397200	-0.11399300	-3.24555300
N	2.57918100	5.49840200	-0.64961300
C	1.82462100	6.56737900	-0.93313500
C	3.90852000	5.60723600	-0.77759700
C	2.36045700	7.77681200	-1.35675500
H	0.75424900	6.43507100	-0.81042200
C	4.53017700	6.77966200	-1.18868500
H	4.47618600	4.70953900	-0.55316600
C	3.74113300	7.88590600	-1.48646100
H	1.70401500	8.61016800	-1.58205400
H	5.61025400	6.81621600	-1.27844900
H	4.19406600	8.81536200	-1.81718800
Cl	3.74375000	-0.56462000	-4.54527200

31

Pd	4.21730200	3.13451800	-3.63777400
N	3.53067000	4.86555700	-4.81146500
C	4.14863900	6.05324200	-4.87019200

C	2.34826400	4.73087600	-5.43315900
C	3.61700000	7.14349400	-5.54611700
H	5.09748800	6.12233100	-4.34788500
C	1.74552000	5.76904500	-6.12970500
H	1.87514300	3.75779700	-5.35405100
C	2.39090700	6.99946700	-6.18716500
H	4.15467000	8.08495800	-5.56055400
H	0.78699100	5.60782300	-6.61002600
H	1.94470200	7.83376600	-6.71920500
N	1.02368200	-0.65991500	-2.34170300
C	-0.01989400	-0.14490000	-3.11359500
C	-1.34551300	-0.53723400	-2.95105600
C	0.25228500	0.81925600	-4.08737000
C	-2.36224600	0.05370900	-3.70018300
C	-0.75356400	1.39006600	-4.83920100
C	-2.08867300	1.02884200	-4.65643900
C	-3.13519900	1.71240600	-5.50309800
F	-0.42475700	2.32268600	-5.73875800
F	1.51711000	1.20421100	-4.28799200
F	-1.66822900	-1.50122300	-2.10331200
F	-3.60024000	-0.37175900	-3.47694200
F	-4.37321300	1.30003700	-5.23330600
F	-2.90747400	1.49131000	-6.80712500
F	-3.09949900	3.04141900	-5.31327200
C	1.02521000	-0.49485200	-0.95569500
O	0.02080800	-0.22747000	-0.33478900
C	2.39148900	-0.67001000	-0.29697000
H	2.33959100	-0.09083000	0.62873300
H	2.48106400	-1.72066600	-0.00589300
C	3.55612700	-0.24902300	-1.16588900
C	4.56574300	-1.13636700	-1.55684200
C	3.60028400	1.05549800	-1.69897900
C	5.56990700	-0.76197500	-2.44299800
C	4.55716700	1.43651700	-2.65815400
C	5.54875000	0.51239600	-3.00085000
H	6.34026100	-1.47710000	-2.71177700
H	6.31526400	0.77175100	-3.72864300
H	1.93847300	-0.61719800	-2.77588800
C	2.76600600	3.35733000	-2.25250900
C	3.04624800	4.51816900	-1.28925600
C	2.61732900	2.12424900	-1.31363300
H	1.87091100	3.52666200	-2.86301200
C	1.73452400	4.79350100	-0.51022900
C	3.90781100	3.83915400	-0.21267900
H	3.46369000	5.40989500	-1.76357500
C	2.87263600	2.74388700	0.09015000
H	1.58551300	1.75801100	-1.35619000
C	1.63533300	3.58065000	0.46219600
H	0.87049700	4.87146000	-1.17906800
H	1.80896800	5.73889300	0.03815000
H	4.85252200	3.45038000	-0.60321000
H	4.10522200	4.48198500	0.65253600
H	3.16295600	2.01188700	0.84764100
H	0.70624900	3.01295600	0.34715200
H	1.69399500	3.90813200	1.50548100
Cl	4.60278400	-2.78836800	-0.94995800

32

Pd	2.57936700	4.17553300	-3.76052800
N	2.39887600	6.37514600	-4.02914300
C	3.25506900	6.97311400	-4.87487600
C	1.49984000	7.13715100	-3.38343000
C	3.24230000	8.34413100	-5.09973200
H	4.00125600	6.35494500	-5.37569300
C	1.41998300	8.50880900	-3.55506200
H	0.82931500	6.62252900	-2.70191600
C	2.31039600	9.12640000	-4.43187800
H	3.96925000	8.76514300	-5.78506000
H	0.67706100	9.07832900	-3.00810900
H	2.27535500	10.20033300	-4.58560500
N	-0.73218600	0.09641300	-1.71878400
C	-2.08536200	0.41131600	-1.56792300

C	-3.06376200	-0.45011700	-2.06313100
C	-2.50774700	1.58687600	-0.95463200
C	-4.40898200	-0.15362700	-1.93466300
C	-3.86041300	1.87169100	-0.79958700
C	-4.83664700	1.00630700	-1.28672600
C	-6.32461800	1.25338600	-1.17318700
F	-4.17108600	3.01497900	-0.19936700
F	-1.62178300	2.48977900	-0.53536400
F	-2.68679400	-1.57248100	-2.67682100
F	-5.29863900	-1.00815000	-2.42829200
F	-6.92438000	0.23302100	-0.54681200
F	-6.87594600	1.36215500	-2.39037300
F	-6.60964300	2.36742300	-0.49785100
C	0.14491300	0.05667100	-0.64628000
O	-0.19114300	0.35316000	0.47944600
C	1.55194900	-0.39435800	-1.01219500
H	2.17602300	-0.16253400	-0.14729400
H	1.53352500	-1.48499600	-1.09876500
C	2.10403600	0.22404300	-2.27767600
C	2.52393900	-0.55000100	-3.36537200
C	2.19862600	1.62459000	-2.40790200
C	3.03181400	0.01623800	-4.53243500
C	2.67265400	2.20080900	-3.59223100
C	3.11064500	1.39729300	-4.64425500
H	3.36114200	-0.62587800	-5.34173300
H	3.51823800	1.83531500	-5.55188700
H	-0.45312400	-0.35579200	-2.57911200
C	1.81155700	4.03598200	-1.88351900
C	2.60683800	4.79870700	-0.83587400
C	1.73719200	2.58632500	-1.35009900
H	0.82877000	4.46724600	-2.12817700
C	1.68420900	4.88173500	0.41427900
C	3.63206200	3.74259900	-0.39136200
H	2.99157400	5.76556600	-1.16613900
C	2.57677600	2.68337000	-0.04303500
H	0.69343600	2.37513100	-1.09709100
C	1.71435500	3.43378300	0.98673400
H	0.67204800	5.21480200	0.16061100
H	2.09552700	5.60572000	1.12432800
H	4.31783100	3.43598500	-1.18392200
H	4.21449300	4.05858400	0.47965600
H	2.96684800	1.72918500	0.31172000
H	0.72171900	2.98812500	1.09154800
H	2.19309900	3.41302000	1.97019100
Cl	2.42329000	-2.30180100	-3.31355600
C	4.61988500	4.14099000	-3.72227900
I	6.50398900	5.47717500	-6.22802500
H	4.88678700	5.04186600	-3.16937400
H	5.08064400	3.23555700	-3.33524200
H	4.74925000	4.25229800	-4.81394500

33

Pd	1.68572700	3.49515500	0.09771400
N	0.59896500	4.63894100	1.73075600
C	1.20377600	5.66259300	2.34649000
C	-0.67733400	4.37968500	2.03786200
C	0.56841000	6.44525900	3.29984900
H	2.22678700	5.86422800	2.04924600
C	-1.39208300	5.11515300	2.97273500
H	-1.14676200	3.55693800	1.50816700
C	-0.75576400	6.16794000	3.61989300
H	1.10394800	7.26323000	3.76813700
H	-2.42717500	4.86656200	3.17759700
H	-1.28507700	6.76684500	4.35411300
N	0.05145500	-0.72911600	-2.72895200
C	-1.34123900	-0.75117100	-2.82074200
C	-1.95800400	-0.75921600	-4.07175000
C	-2.16174300	-0.72409800	-1.69626800
C	-3.33626300	-0.75641100	-4.19155000
C	-3.54708700	-0.75088500	-1.81629500
C	-4.16132900	-0.76983600	-3.06591600
C	-5.65851700	-0.77482100	-3.27587100

F	-4.25068100	-0.72159700	-0.68920900
F	-1.63855000	-0.62678900	-0.47550100
F	-1.19902800	-0.75801000	-5.16775900
F	-3.86932600	-0.75785700	-5.40924500
F	-6.02252100	-1.80377200	-4.05308400
F	-6.05257600	0.35165500	-3.88663100
F	-6.33773000	-0.87401100	-2.13178700
C	0.77272100	-1.61941100	-1.95197100
O	0.24127000	-2.48203000	-1.28682000
C	2.28348900	-1.42552000	-2.02100500
H	2.68938300	-1.94032600	-1.14910600
H	2.64040000	-1.97371300	-2.89792500
C	2.71688200	0.02152400	-2.09139900
C	3.43154600	0.53219000	-3.17810100
C	2.33524500	0.92882900	-1.07729000
C	3.75129200	1.88340700	-3.28508000
C	2.57551700	2.29992400	-1.22849500
C	3.30988900	2.77156400	-2.31595900
H	4.31552900	2.23682200	-4.14102200
H	3.50930000	3.83105600	-2.42894400
C	1.22172500	1.72590800	1.02203500
C	1.74861700	1.37519300	2.40976600
C	1.58200000	0.49737400	0.15107800
H	0.13785300	1.91774800	1.02465600
C	3.02984900	0.59053400	2.07961900
C	0.83701600	0.24504900	2.95663200
H	1.83975600	2.22566300	3.08972200
C	2.32286200	-0.41854000	1.16556700
H	0.65127700	0.00975700	-0.15537400
H	3.47894800	0.11902200	2.96029500
H	3.79307100	1.17494600	1.56395200
H	1.03308600	0.08682500	4.02227000
H	-0.22564600	0.48840600	2.85293300
C	1.25422400	-0.99666700	2.11165200
H	2.97117700	-1.16949000	0.71311000
H	1.68742900	-1.77493900	2.74755600
H	0.42139900	-1.44493200	1.56235100
H	0.55466400	-0.14265000	-3.38123000
Cl	3.95775600	-0.51637800	-4.48654400
I	1.38086900	5.78567000	-1.47419900
C	3.52349400	3.67059100	0.95522500
H	3.36873500	3.55664200	2.02825800
H	4.24493800	2.95602700	0.56916600
H	3.78963600	4.68854600	0.66561200

34

Pd	1.71048800	3.69820500	0.18064300
N	0.68630600	4.80969700	1.79850500
C	1.33154800	5.31117400	2.86046600
C	-0.64789000	4.92399900	1.75627000
C	0.67770200	5.94157900	3.91009800
H	2.41016400	5.19236800	2.85899000
C	-1.38208100	5.54304900	2.75971700
H	-1.13227400	4.49592000	0.88488000
C	-0.70725400	6.06168100	3.85886600
H	1.24751200	6.32665100	4.74832800
H	-2.46080600	5.61132600	2.67437200
H	-1.24988100	6.54869500	4.66301800
N	-0.00854400	-0.69906200	-2.75004300
C	-1.39073600	-0.84780600	-2.84400300
C	-2.01629700	-0.79287300	-4.09004500
C	-2.19874200	-1.01489700	-1.72115700
C	-3.38810900	-0.92053300	-4.20949500
C	-3.57524100	-1.17479900	-1.84566900
C	-4.19669700	-1.13105500	-3.09134200
C	-5.68519500	-1.27381500	-3.30378300
F	-4.26908600	-1.33280400	-0.72286600
F	-1.67775300	-0.98224900	-0.49919500
F	-1.27262300	-0.60476700	-5.18115600
F	-3.93200700	-0.85667500	-5.42241600
F	-5.94900800	-2.27186600	-4.15882700
F	-6.19742400	-0.14981100	-3.82923000

F	-6.34687400	-1.52741200	-2.17312000
C	0.79784000	-1.57204500	-2.03971100
O	0.35521100	-2.54434200	-1.46677000
C	2.28142000	-1.22347200	-2.06157500
H	2.68774100	-1.63898700	-1.13752800
H	2.72866800	-1.79505900	-2.88031200
C	2.59087300	0.24905600	-2.19799500
C	3.18632600	0.78328200	-3.34596500
C	2.21650600	1.14847000	-1.17850400
C	3.39802000	2.14860200	-3.49172600
C	2.41699900	2.53837300	-1.29343200
C	3.00558900	3.01157500	-2.47391500
H	3.84946500	2.52914900	-4.40210600
H	3.14466000	4.07868800	-2.63090800
C	0.97564900	1.92773600	0.85818100
C	1.45189800	1.63637100	2.28992600
C	1.50004900	0.69675200	0.05836900
H	-0.11552900	2.02849300	0.79239200
C	2.85535000	1.06395800	2.03581400
C	0.68971300	0.38599700	2.80380900
H	1.38872700	2.48479100	2.97522900
C	2.35499500	-0.06138400	1.11751200
H	0.65191900	0.06092600	-0.22089200
H	3.34188400	0.67930500	2.93978800
H	3.52136300	1.77377900	1.53484500
H	0.80963900	0.28088200	3.88778000
H	-0.38400500	0.45462900	2.59868700
C	1.36859400	-0.79195000	2.04412900
H	3.13246200	-0.70212100	0.69510600
H	1.90596900	-1.44840100	2.73709800
H	0.66054600	-1.40944600	1.48273700
H	0.43508400	0.00128600	-3.32894200
Cl	3.66971700	-0.25401100	-4.68674500
I	3.36989600	6.17839900	-0.39204400
C	5.15108100	4.94789300	-0.35359300
H	5.37130800	4.73391700	0.69002100
H	4.90714300	4.03878000	-0.90119100
H	5.95154400	5.51266000	-0.82737400

TS35

Pd	1.87174000	3.48292200	0.10944400
N	0.70063500	4.60828600	1.66833400
C	1.25107100	5.21141900	2.72833100
C	-0.62937500	4.66655000	1.52654500
C	0.50458900	5.88650900	3.68388400
H	2.33188900	5.14792400	2.80753700
C	-1.45391900	5.32506200	2.42931300
H	-1.03824100	4.16691200	0.65428400
C	-0.87648900	5.94576500	3.53104300
H	1.00077100	6.35518500	4.52630000
H	-2.52547300	5.34581000	2.26545800
H	-1.49138500	6.46819600	4.25702600
N	-0.05540000	-0.79400700	-2.67666800
C	-1.44385900	-0.79787100	-2.79459900
C	-2.03915100	-0.68526900	-4.05131000
C	-2.28386600	-0.87002000	-1.68554000
C	-3.41463900	-0.66872700	-4.19397700
C	-3.66706700	-0.88516400	-1.83292100
C	-4.25982200	-0.78615000	-3.08940600
C	-5.75172600	-0.77267900	-3.32644100
F	-4.39191600	-0.96021200	-0.72112700
F	-1.78245600	-0.88280200	-0.45460800
F	-1.26130600	-0.58174800	-5.12972700
F	-3.92727000	-0.55452400	-5.41643300
F	-6.10203600	-1.73108400	-4.19532100
F	-6.13702900	0.40238700	-3.84774000
F	-6.45374600	-0.96715000	-2.20849900
C	0.64401800	-1.74403900	-1.95173800
O	0.09452100	-2.65880900	-1.37750600
C	2.15686600	-1.55544200	-1.95736400
H	2.50740400	-2.00689400	-1.02736600
H	2.55054000	-2.17545100	-2.76821500

C	2.61642500	-0.12342600	-2.09927800
C	3.30213600	0.33423300	-3.22857700
C	2.28959500	0.82370500	-1.10596800
C	3.65777000	1.66969500	-3.37851900
C	2.59460400	2.18875600	-1.25729000
C	3.29636100	2.58740300	-2.39953100
H	4.19379100	1.98730900	-4.26662800
H	3.55012000	3.63192000	-2.55537000
C	1.18123700	1.73880200	0.93649400
C	1.78816700	1.50387700	2.32863300
C	1.56186000	0.45027700	0.14968400
H	0.09437300	1.88615200	0.98370200
C	3.09934500	0.78084400	1.97991200
C	0.98644900	0.37226600	3.01755500
H	1.87379900	2.40341200	2.94532000
C	2.40575200	-0.34026800	1.19195400
H	0.65710200	-0.12131700	-0.08626500
H	3.63861600	0.40901300	2.85832100
H	3.78066600	1.37524300	1.36227400
H	1.24977100	0.30319800	4.07897100
H	-0.09273100	0.54755300	2.95812000
C	1.43077600	-0.90318500	2.24123100
H	3.07477100	-1.08670100	0.75869200
H	1.94361600	-1.60775700	2.90426700
H	0.59486200	-1.43513400	1.77626200
H	0.46814000	-0.15413100	-3.25872200
Cl	3.73443200	-0.76406600	-4.53493600
I	2.74010900	5.93718400	-0.82553600
C	4.10176700	4.28398000	0.62528500
H	3.78711900	3.64812600	1.45261300
H	4.66062500	3.75532500	-0.13995100
H	4.58895100	5.18425800	0.98023000

TS36

Pd	1.82617600	3.28922100	0.30681400
N	0.00210800	3.95691800	1.32996600
C	0.03403700	4.97850300	2.19702100
C	-1.18338400	3.42088800	1.00877400
C	-1.11363800	5.48302100	2.79043100
H	1.00825900	5.40999300	2.39554800
C	-2.37898700	3.88073000	1.54194400
H	-1.17117600	2.60292100	0.29838200
C	-2.34387300	4.92782700	2.45503600
H	-1.03672500	6.30544700	3.49237100
H	-3.31096600	3.41968800	1.23638000
H	-3.25992900	5.31076800	2.89353300
N	0.02089800	-1.06389300	-2.90826200
C	-1.31697400	-0.66169100	-2.87322800
C	-2.21062000	-1.03343000	-3.87451000
C	-1.79176900	0.16490700	-1.85759100
C	-3.52760100	-0.60157600	-3.84802600
C	-3.11481600	0.58017000	-1.81809300
C	-4.01021700	0.20562700	-2.81729300
C	-5.46391400	0.62210100	-2.85541700
F	-3.47198300	1.37152300	-0.80709000
F	-0.95995000	0.60159500	-0.91111700
F	-1.78982500	-1.80370600	-4.87408400
F	-4.34091900	-0.98605900	-4.82630400
F	-6.26227400	-0.45330500	-2.83584600
F	-5.72870700	1.30340000	-3.97746400
F	-5.80201500	1.39599300	-1.82160900
C	0.64558400	-1.61905900	-1.80693200
O	0.01563800	-2.04741500	-0.86193600
C	2.17067300	-1.56355700	-1.85324600
H	2.52433900	-2.01302300	-0.92517100
H	2.53964200	-2.17447600	-2.68166600
C	2.62755000	-0.12450600	-1.99971600
C	2.99811900	0.40750900	-3.23725000
C	2.53765100	0.75402300	-0.90066500
C	3.24950600	1.76169200	-3.41982500
C	2.76553400	2.12687900	-1.09315900
C	3.12396000	2.62695100	-2.34426400

H	3.51961700	2.13852400	-4.39990400
H	3.27911300	3.69061700	-2.48470600
C	1.58578600	1.49785100	1.29637700
C	2.31542100	1.28124100	2.62813900
C	2.01697700	0.29253600	0.43439100
H	0.50247300	1.50411800	1.44257600
C	3.63863000	0.61864000	2.20692400
C	1.61294200	0.08057100	3.31636900
H	2.38753200	2.16914100	3.26196300
C	2.96658900	-0.48940200	1.38336400
H	1.13762700	-0.32735700	0.24888800
H	4.19478000	0.21817900	3.06186900
H	4.30639400	1.25592000	1.63302800
H	1.95712400	-0.01616000	4.35169200
H	0.52508900	0.19940000	3.34199400
C	2.06687300	-1.14074400	2.45561700
H	3.64182800	-1.18455300	0.87749300
H	2.64282700	-1.85044200	3.05799000
H	1.22843400	-1.68521700	2.01081000
H	0.56186000	-0.85566800	-3.73757400
Cl	3.08695200	-0.62159000	-4.66507000
C	3.96581400	3.23672700	0.24462000
H	3.95184300	3.53283500	1.30027900
H	4.62951500	2.38967500	0.11106300
H	4.24961400	4.06712700	-0.39638000
I	1.81632200	5.84444000	-0.91668900

37

N	-1.52905600	2.70916100	0.05749400
C	-1.61736400	3.39036900	1.20860000
C	-2.65420700	2.48559500	-0.63883300
C	-2.82744700	3.83183400	1.72328100
H	-0.68540500	3.58460500	1.72541000
C	-3.90616000	2.86614200	-0.17939000
H	-2.53018000	2.01055100	-1.60228200
C	-3.99777000	3.54814500	1.02761400
H	-2.84213800	4.38265100	2.65694800
H	-4.78262700	2.62349200	-0.76904000
H	-4.96142900	3.86453300	1.41366200
N	-0.36997100	-0.42013300	-2.49084500
C	-1.76269900	-0.43502000	-2.55960300
C	-2.38057900	-0.15148300	-3.77635700
C	-2.58233500	-0.61419300	-1.44333500
C	-3.75935700	-0.02095400	-3.88325900
C	-3.95872800	-0.51470300	-1.55979900
C	-4.57850400	-0.21307700	-2.77177100
C	-6.07712900	-0.03840300	-2.78981200
F	-4.69007700	-0.63755100	-0.45314500
F	-2.06776200	-0.76559900	-0.22728400
F	-1.62923900	0.02508300	-4.85733600
F	-4.25703200	0.27888700	-5.07592500
F	-6.56893100	0.08814000	-4.02140600
F	-6.42994200	1.06646600	-2.09997200
F	-6.69103700	-1.07709700	-2.21088200
C	0.37534800	-1.34431300	-1.79565000
O	-0.11535900	-2.31205900	-1.25324300
C	1.88394800	-1.10346500	-1.77217700
H	2.22141000	-1.55228300	-0.83857600
H	2.29350000	-1.73514800	-2.56583500
C	2.39969400	0.31005900	-1.94930200
C	2.77448600	0.72239300	-3.23006100
C	2.57919700	1.21691500	-0.84354200
C	3.33897900	1.96597900	-3.46548500
C	3.14449300	2.49873900	-1.09885100
C	3.52008800	2.82640800	-2.40499900
H	3.60696200	2.25959000	-4.47339600
H	3.93818100	3.80891400	-2.59687100
C	0.72062800	0.75773600	0.77230600
C	0.57452200	1.17018900	2.22852500
C	2.24100800	0.63549600	0.55858300
H	0.13636100	-0.12659600	0.50401500
C	1.72276600	2.17963600	2.38367400

C	1.07819900	-0.01786700	3.08841300
H	-0.42583600	1.50139100	2.50998700
C	2.80559300	1.19739700	1.88962800
H	2.54793300	-0.41193100	0.52136700
H	1.88978100	2.49558300	3.41915600
H	1.59690500	3.06586400	1.75767000
H	0.78223600	0.11201800	4.13440900
H	0.66142800	-0.96936700	2.74419700
C	2.62205900	0.06054500	2.92037600
H	3.83447500	1.55612100	1.84397000
H	3.10686000	0.33407300	3.86303100
H	3.06623300	-0.88245000	2.58669200
H	0.08707800	0.31494400	-3.02397500
Cl	2.52705500	-0.30864900	-4.62604800
C	3.36692500	3.59708500	-0.08006400
H	2.43629000	4.14512600	0.09828900
H	3.74466800	3.24423200	0.87585500
H	4.08866400	4.31684200	-0.47439200
I	-0.14132700	3.35952000	-3.17858100
Pd	0.32429100	2.05962900	-0.73922200

38

Pd	0.47385300	2.28875900	-0.61317700
N	-1.63360100	2.56306000	-0.29018200
C	-2.28119300	2.43223300	0.87479100
C	-2.35684800	2.83679900	-1.39183400
C	-3.65630600	2.57226000	0.99255500
H	-1.67424000	2.19067100	1.73496000
C	-3.73524300	2.99429800	-1.35557700
H	-1.80942100	2.87360200	-2.32543900
C	-4.40197100	2.86019400	-0.14431000
H	-4.12595400	2.44033700	1.96037700
H	-4.27215000	3.19127400	-2.27625300
H	-5.48154900	2.95482000	-0.09343100
N	-0.58985800	-0.16673200	-2.31689000
C	-1.98021200	-0.23964000	-2.23040000
C	-2.74355200	-0.00962800	-3.37884600
C	-2.67093300	-0.43573400	-1.03439200
C	-4.12447000	0.06753700	-3.31834000
C	-4.05809700	-0.39433800	-0.98530300
C	-4.81584000	-0.13665600	-2.12407500
C	-6.30952500	0.06106700	-2.09891100
F	-4.62598500	-0.54021000	0.21052900
F	-2.02678900	-0.57679300	0.12138900
F	-2.13910500	0.16230900	-4.54721100
F	-4.79147700	0.34547300	-4.43740000
F	-6.90763200	-0.56827700	-3.11578600
F	-6.60905700	1.37331300	-2.21003200
F	-6.87072900	-0.37642800	-0.96956000
C	0.23061900	-1.09257000	-1.72676000
O	-0.18717200	-2.07720400	-1.14794600
C	1.73493100	-0.87906700	-1.89417500
H	2.18791900	-1.42946000	-1.06952800
H	2.00083700	-1.43632800	-2.79667100
C	2.29843800	0.52228900	-2.00614400
C	2.61792900	1.00850200	-3.27370000
C	2.61301600	1.32612500	-0.84512100
C	3.24763400	2.23360800	-3.45101700
C	3.26737200	2.57547700	-1.03973300
C	3.56162500	2.98930700	-2.34572700
H	3.47613100	2.58552200	-4.45058700
H	4.04491300	3.95031300	-2.48974400
C	0.79200200	0.90439700	0.82747900
C	0.78162300	1.31013600	2.30262500
C	2.29126400	0.66137400	0.52622900
H	0.13761200	0.05940000	0.60735600
C	2.04439400	2.17000900	2.42117800
C	1.17655700	0.05157800	3.11485900
H	-0.13567000	1.77612900	2.66479000
C	2.97652100	1.08703200	1.84616500
H	2.49483900	-0.40262500	0.39637800
H	2.29326300	2.43008500	3.45597300

H	1.97595400	3.08694400	1.83406700
H	0.97164900	0.20072700	4.18020000
H	0.62098900	-0.83359000	2.79089800
C	2.70435200	-0.06339500	2.84371200
H	4.03958500	1.31672400	1.75995500
H	3.27897700	0.09848900	3.76131100
H	2.99493100	-1.03947200	2.44309900
H	-0.23654200	0.64185600	-2.85700400
Cl	2.24626300	0.10554200	-4.72454100
C	3.70446100	3.55760400	0.02879000
H	2.89012300	4.24578300	0.27774300
H	4.05253500	3.09399300	0.94656800
H	4.52484400	4.16610100	-0.36090500
O	0.51810800	3.75407300	-2.21585200
C	0.28212200	3.34483800	-3.39681700
C	0.60865700	4.30982200	-4.52541600
H	1.34898700	5.04765100	-4.20962400
H	0.96414000	3.75425700	-5.39699200
H	-0.30473700	4.83847300	-4.82030800
O	-0.22616000	2.24066100	-3.69379400

39

Pd	2.33019800	3.95759900	-3.61875500
N	1.22537500	5.90781800	-3.81998300
C	1.71429000	6.98071600	-4.45070800
C	-0.03172500	5.95158600	-3.35609100
C	0.97756700	8.14349200	-4.63024300
H	2.72877800	6.89411700	-4.82670400
C	-0.83579800	7.07546800	-3.48876500
H	-0.39763500	5.04722300	-2.88224700
C	-0.32186900	8.19382100	-4.13587200
H	1.41855000	8.98749000	-5.14860900
H	-1.84522200	7.05933200	-3.09301000
H	-0.92415000	9.08860400	-4.25787200
N	-0.26575600	0.67281800	-2.12139000
C	-1.59429300	1.08371000	-2.26862200
C	-2.58422700	0.23787400	-2.76240000
C	-1.94138500	2.40346900	-1.99881300
C	-3.86434300	0.71889900	-2.99498300
C	-3.20776000	2.89698500	-2.27297400
C	-4.19931800	2.05556500	-2.77268400
C	-5.60740000	2.50031300	-3.09082500
F	-3.42764800	4.18914100	-2.02635800
F	-1.04012800	3.23351700	-1.46648300
F	-2.30000000	-1.02264500	-3.05444100
F	-4.78003000	-0.11841300	-3.47651000
F	-6.49950700	1.81672600	-2.36208000
F	-5.89192500	2.28439700	-4.38355500
F	-5.80121700	3.80034900	-2.85030600
C	0.13249600	-0.25029900	-1.18122000
O	-0.65653700	-0.85894100	-0.48876200
C	1.65153000	-0.42766100	-1.00399900
H	1.88647300	0.03504100	-0.03955500
H	1.81914800	-1.49848900	-0.88140000
C	2.48677300	0.16049400	-2.11081900
C	2.95834100	-0.60165300	-3.18602200
C	2.63923500	1.55510800	-2.19686400
C	3.52360100	-0.01928600	-4.31645000
C	3.06082400	2.13894000	-3.39246600
C	3.53517900	1.36697100	-4.44239400
H	3.88508200	-0.65163100	-5.12018300
H	3.85450100	1.82591300	-5.37222600
O	0.34607200	2.93898100	-3.84506800
C	0.44956900	2.86668000	-5.12044400
C	-0.62266600	2.10167300	-5.85829800
H	-1.60897500	2.36779100	-5.46756000
H	-0.57286600	2.29197300	-6.93119000
H	-0.47356600	1.03113400	-5.67777800
O	1.41660400	3.38216500	-5.72736100
H	0.39799400	1.24934100	-2.63293800
C	2.36230700	3.97770000	-1.57892200
C	3.49595900	4.59260400	-0.75942400

C	2.28459100	2.50415700	-1.07978400
H	1.41856600	4.51516100	-1.44373900
C	2.92088900	4.80360600	0.66348000
C	4.43766400	3.40057800	-0.52246000
H	3.93523000	5.49550800	-1.18484700
C	3.34025200	2.49525800	0.05918100
H	1.28428900	2.30059000	-0.68548900
C	2.79958500	3.35331400	1.21821400
H	1.96354200	5.33458200	0.64960700
H	3.61701400	5.40054900	1.26206200
H	4.88432600	2.99876400	-1.43550300
H	5.23178300	3.62273700	0.19807000
H	3.65606100	1.49005700	0.34962500
H	1.77020400	3.08744400	1.48019400
H	3.41132500	3.22024300	2.11576000
Cl	2.81153800	-2.34939900	-3.16702600
C	4.18821300	4.73598400	-3.79609300
H	4.36369800	4.71034300	-4.87805400
H	4.96121600	4.17148200	-3.27689200
H	4.16416400	5.76548500	-3.42829700

TS40

Pd	2.20058800	3.80143300	-3.68559200
N	0.89131300	5.54872400	-3.74279100
C	1.29165000	6.75478300	-3.31683900
C	-0.36319900	5.40293500	-4.19148600
C	0.46004700	7.86401800	-3.32954400
H	2.31041600	6.81759500	-2.94799100
C	-1.26093200	6.46204900	-4.22829800
H	-0.63678600	4.39863200	-4.49700300
C	-0.84374400	7.71357000	-3.79360800
H	0.82975200	8.82014900	-2.97625900
H	-2.27204200	6.29325100	-4.57946400
H	-1.52515400	8.55846000	-3.80864900
N	-0.37114600	0.78156200	-2.00754400
C	-1.66860100	1.29654300	-2.12321200
C	-2.78536700	0.47559900	-2.24901000
C	-1.86454700	2.67166400	-2.15117400
C	-4.04554300	1.02902800	-2.42079000
C	-3.11849100	3.22675500	-2.35732700
C	-4.23785700	2.40905000	-2.49632700
C	-5.63997100	2.92564300	-2.71561700
F	-3.20363900	4.55768400	-2.39680700
F	-0.82662400	3.48913900	-1.96616900
F	-2.65133700	-0.84235900	-2.23176100
F	-5.08794900	0.20972300	-2.54143100
F	-6.16948700	2.40221200	-3.83081900
F	-5.68450700	4.25599400	-2.84016000
F	-6.43912100	2.58858800	-1.69413100
C	0.04222500	0.13894500	-0.86446200
O	-0.71417000	-0.11733600	0.05038600
C	1.53457200	-0.21955800	-0.77574700
H	1.89737500	0.25223000	0.14136500
H	1.58121300	-1.29657200	-0.60426800
C	2.34327700	0.18965300	-1.97711500
C	2.60980300	-0.70356200	-3.01571100
C	2.66739000	1.55235800	-2.16452600
C	3.12192000	-0.27890600	-4.23977200
C	3.09389000	1.98457800	-3.42775600
C	3.32576900	1.07044100	-4.45703000
H	3.30500600	-1.00145700	-5.02733800
H	3.62356500	1.41741300	-5.43990100
O	0.08240900	2.26150900	-4.52379700
C	0.69812900	2.43418700	-5.60226800
C	0.30392500	1.61712300	-6.81793400
H	-0.77013600	1.41822400	-6.81297100
H	0.59951100	2.11386200	-7.74414400
H	0.82264300	0.65272300	-6.76060100
O	1.67770600	3.23915500	-5.74291300
H	0.26781700	1.08586800	-2.73892300
C	2.36864700	4.01176600	-1.66962600
C	3.53669000	4.70668500	-0.94943500

C	2.37372000	2.57852100	-1.08552200
H	1.42480600	4.52064300	-1.45970800
C	3.01905600	5.03199200	0.47212400
C	4.50833400	3.55553800	-0.62641600
H	3.95984100	5.57200700	-1.46877000
C	3.43810700	2.67431500	0.03385100
H	1.38856600	2.36866100	-0.65997900
C	2.88761600	3.62025000	1.12363000
H	2.07149900	5.57970400	0.45391900
H	3.74717700	5.64837400	1.01090300
H	4.97175900	3.08818900	-1.49471600
H	5.29736100	3.85788200	0.07061100
H	3.78059500	1.70575900	0.40836200
H	1.85405900	3.37714100	1.39079500
H	3.48711800	3.54893300	2.03624800
Cl	2.24948100	-2.40893500	-2.85010300
C	4.33878300	3.54685300	-3.91461800
H	4.37661100	3.51282400	-5.00344800
H	5.09994500	2.89963200	-3.49118000
H	4.49916900	4.55875100	-3.53330100

41			
N	6.88092500	2.88498700	0.94568600
C	8.00166200	2.18610000	0.72167500
C	6.90293400	4.20729200	0.73850300
C	9.18177200	2.77455300	0.28773100
H	7.93351200	1.11533500	0.88968600
C	8.03707700	4.87641000	0.29608400
H	5.97813300	4.73459900	0.94914600
C	9.19919200	4.14824500	0.06807900
H	10.06314900	2.16424600	0.12499700
H	8.00229500	5.94908700	0.14126100
H	10.10368100	4.64156000	-0.27404700
N	0.75788600	0.19606400	-1.21937800
C	-0.14486100	1.22169600	-0.95882300
C	-0.67640200	1.95382600	-2.02186900
C	-0.46571000	1.63971400	0.33157100
C	-1.50380700	3.03978500	-1.80521800
C	-1.33254900	2.70550000	0.54653100
C	-1.85997100	3.43640500	-0.51488000
C	-2.83594300	4.57661100	-0.36386700
F	-1.60206700	3.01758000	1.81216600
F	0.08672300	1.06432000	1.39266200
F	-0.351166000	1.61185000	-3.26911500
F	-1.98100300	3.69858600	-2.85900900
F	-4.01918900	4.26581800	-0.90907300
F	-2.38913400	5.67954900	-0.99029200
F	-3.05588200	4.90716000	0.91250800
C	0.77495600	-1.03090800	-0.57619400
O	-0.12299700	-1.39585200	0.15007400
C	2.02649700	-1.85961900	-0.86940300
H	2.08602000	-2.59525300	-0.06469200
H	1.85667500	-2.41262700	-1.79808700
C	3.27810100	-1.01371000	-0.95977300
C	3.94923600	-0.78057800	-2.16405500
C	3.72315300	-0.31332300	0.17819300
C	5.01637800	0.10792300	-2.25087700
C	4.75999500	0.63320500	0.10189100
C	5.40459900	0.82231800	-1.12316100
H	5.51327600	0.25780000	-3.20361700
H	6.19650300	1.55827100	-1.22318600
C	3.55077000	0.64766200	2.47762500
C	4.14165200	-0.12079900	3.67395000
C	3.07671600	-0.47676000	1.51741500
H	2.72728500	1.29752500	2.78527800
C	4.78868800	-1.33638200	2.98795800
C	2.96039400	-0.78736800	4.42183400
H	4.78077400	0.47911000	4.32621300
C	3.49813800	-1.76972000	2.27536000
H	1.98758600	-0.45502200	1.42701500
H	5.15283000	-2.08992000	3.69553900
H	5.59726900	-1.07022200	2.29899500

H	3.29603800	-1.18199700	5.38714900
H	2.15404200	-0.07471300	4.62145400
C	2.53072200	-1.93669800	3.46208700
H	3.58048700	-2.65270000	1.63540100
H	2.66736900	-2.91535800	3.93438600
H	1.48436500	-1.86363400	3.14819300
H	1.45441200	0.37108500	-1.93134700
N	1.55645400	4.90396700	1.17726700
C	0.78098400	4.94231100	2.27249000
C	1.31901200	5.77493600	0.18452400
C	-0.26828800	5.83991400	2.40283500
H	1.02272000	4.23204200	3.05447600
C	0.29539200	6.70700800	0.24601700
H	1.97247600	5.70771100	-0.67735000
C	-0.51913200	6.73686900	1.37260400
H	-0.88094400	5.81719100	3.29619600
H	0.13649300	7.38597100	-0.58351200
H	-1.34166200	7.44074100	1.43938200
Cl	3.44313000	-1.58173300	-3.64990200
Pd	5.04160700	1.79789500	1.70161300
Pd	3.09502000	3.48738400	1.15664300
I	4.45092900	3.88424600	3.64245700
C	2.63712400	3.02919800	-0.74679000
H	3.43641900	3.45911800	-1.36236600
H	2.65207400	1.94257100	-0.82910900
H	1.66289600	3.43355600	-1.03691200

TS42

N	8.00419900	1.43946300	1.03611500
C	8.36986800	0.43580200	0.22560400
C	8.93500400	2.32891500	1.40518900
C	9.66689400	0.27987500	-0.24331200
H	7.58350000	-0.25556100	-0.06158700
C	10.25554200	2.25124400	0.97867200
H	8.59177000	3.12302800	2.06140200
C	10.63006000	1.20762200	0.14043200
H	9.90949200	-0.55068600	-0.89704000
H	10.97021000	2.99893000	1.30432700
H	11.65397100	1.11760400	-0.20938400
N	1.08405500	-0.00558000	-1.04421500
C	-0.11015900	0.69872500	-0.91927800
C	-0.62863800	1.35059600	-2.04033600
C	-0.78044800	0.86802800	0.28997300
C	-1.77295500	2.12115200	-1.96054500
C	-1.94872800	1.62115800	0.36303800
C	-2.47018800	2.25924600	-0.75901500
C	-3.71072100	3.12079500	-0.74452800
F	-2.51567200	1.73623800	1.55946300
F	-0.28946500	0.36899300	1.41917900
F	0.01655600	1.24399800	-3.20301700
F	-2.21178300	2.72789600	-3.05990200
F	-4.58303100	2.71606500	-1.67719800
F	-3.39924200	4.39910300	-1.01285300
F	-4.33976700	3.09790900	0.43191900
C	1.34164700	-1.25172400	-0.49966600
O	0.51475400	-1.88379200	0.11980900
C	2.73855200	-1.77409100	-0.81976900
H	2.95204400	-2.59147600	-0.13108100
H	2.66008800	-2.23677000	-1.80843700
C	3.81360500	-0.70714100	-0.84791800
C	4.63700100	-0.57913600	-1.97183200
C	3.93140100	0.27812200	0.16933800
C	5.52595600	0.48307000	-2.13957700
C	4.70573400	1.45020100	-0.05452300
C	5.53033100	1.49386000	-1.20100500
H	6.16092800	0.52240200	-3.01822400
H	6.17438600	2.35499500	-1.35313700
C	4.04555500	1.02372000	2.55550200
C	4.40630200	0.01471300	3.65117700
C	3.20330200	0.22480400	1.51465200
H	3.54762000	1.90993100	2.94895300
C	4.47920600	-1.31148300	2.87358400

C	3.11934100	-0.18836500	4.48363100
H	5.27470600	0.29480800	4.25638900
C	3.09014600	-1.14650600	2.24297000
H	2.20676300	0.66627600	1.39549100
H	4.55084200	-2.18770400	3.52699400
H	5.28967800	-1.35096600	2.13627200
H	3.33669100	-0.79018500	5.37298700
H	2.69725600	0.76207600	4.82304900
C	2.19946300	-0.94773500	3.48940100
H	2.73722400	-1.97525400	1.63910100
H	1.89907100	-1.92034400	3.89060100
H	1.28457300	-0.40092400	3.24859800
H	1.78972700	0.41099100	-1.63700400
N	3.12024500	5.22065100	1.12576300
C	3.82988600	6.35627200	1.16794800
C	1.81006400	5.27561300	1.40166100
C	3.25729800	7.58269200	1.47638700
H	4.88983800	6.26151700	0.96203900
C	1.16179300	6.45731300	1.73111900
H	1.27359800	4.33430600	1.35039500
C	1.89870000	7.63610200	1.76576200
H	3.87466200	8.47384800	1.49335300
H	0.10039600	6.44540600	1.95252600
H	1.42215200	8.57898600	2.01492500
Cl	4.60447300	-1.77103600	-3.26421900
Pd	5.86448600	1.45910700	1.80228400
Pd	4.04082100	3.32391200	0.64219500
I	5.89312800	3.95172300	3.07814900
C	2.65439400	3.09502900	-0.83645900
H	2.38207900	4.09234700	-1.19665300
H	3.00992800	2.49425900	-1.67817300
H	1.77885100	2.61512000	-0.38158700

43

N	7.47344400	-1.33041800	0.40049800
C	7.15622500	-2.30065600	-0.46339100
C	8.64782000	-0.70471200	0.25742500
C	7.98538600	-2.67456500	-1.51237400
H	6.19650900	-2.78353500	-0.30895800
C	9.53794400	-1.01350000	-0.76224600
H	8.86757100	0.06183900	0.99333200
C	9.19873900	-2.01409200	-1.66736300
H	7.67643400	-3.46166800	-2.19076600
H	10.47789900	-0.47833000	-0.83872000
H	9.87245300	-2.27845100	-2.47656600
N	1.34418900	-0.00534400	-1.14948100
C	0.12698000	0.62222000	-1.41940500
C	-0.05562100	1.30513600	-2.62130100
C	-0.91682700	0.63069600	-0.49878000
C	-1.24242000	1.95888600	-2.89734200
C	-2.12116200	1.26456800	-0.78979900
C	-2.30374200	1.94587900	-1.99099400
C	-3.56974600	2.68047500	-2.36722400
F	-3.06855100	1.21904700	0.13990000
F	-0.76999700	0.06207100	0.69165400
F	0.94050500	1.33285600	-3.50866000
F	-1.36444100	2.59767300	-4.05813900
F	-4.09576200	2.17255500	-3.49066300
F	-3.31122500	3.97702700	-2.59486400
F	-4.50475600	2.61675300	-1.41817100
C	1.42981500	-1.33437800	-0.77710100
O	0.45395000	-2.03869800	-0.63781300
C	2.84460600	-1.84908300	-0.52737100
H	2.80546400	-2.39343700	0.41379000
H	3.03215500	-2.60039700	-1.29764900
C	3.92777900	-0.79974900	-0.53063900
C	4.67225900	-0.60257300	-1.69122800
C	4.17256200	0.07918700	0.58155900
C	5.64241200	0.39729800	-1.81308100
C	5.15333200	1.11875200	0.46410700
C	5.87254600	1.23440600	-0.74888100
H	6.19793400	0.49442400	-2.73956300

H	6.62850900	2.00729800	-0.84344600
C	4.40840100	-0.03855000	3.03704600
C	3.83515300	-1.13626300	3.93805100
C	3.35250300	0.15520300	1.90698800
H	4.63697700	0.86507700	3.61988500
C	3.10138400	-2.02714400	2.92520800
C	2.65215400	-0.50094000	4.70033000
H	4.57278300	-1.62372300	4.57399400
C	2.27792900	-0.87587500	2.31919000
H	2.91315900	1.15889600	1.91845100
H	2.47695800	-2.79364500	3.39579700
H	3.79227500	-2.51453700	2.22678100
H	2.29234000	-1.18356200	5.47775900
H	2.93381100	0.43621000	5.19151100
C	1.59078300	-0.30542300	3.58213000
H	1.54026000	-1.13249800	1.56463200
H	0.67873500	-0.87177300	3.79385100
H	1.29807400	0.74069300	3.44658300
H	2.18609900	0.45690900	-1.46492800
N	6.14677300	3.41350200	3.82708700
C	6.77880400	2.72665800	4.79323000
C	5.85480800	4.70230100	4.05025700
C	7.13434800	3.30013700	6.00685700
H	7.00207600	1.68365800	4.58227000
C	6.17532300	5.35061600	5.23441100
H	5.34995500	5.22307200	3.24397700
C	6.82751700	4.63631500	6.23441000
H	7.64309300	2.69754200	6.75076100
H	5.91499200	6.39519100	5.36431500
H	7.09006500	5.11371000	7.17331800
Cl	4.43453800	-1.61401300	-3.11152800
Pd	5.97943300	-0.61869400	1.88776700
Pd	5.58656000	2.30956200	2.02553200
I	7.57874300	-1.17147600	3.96206200
C	5.41561700	3.96876600	0.87957600
H	6.32677100	4.55605300	1.04257400
H	5.28830900	3.76521500	-0.18492900
H	4.53660300	4.51404700	1.24433300

TS44

N	6.46703900	-2.20923100	-0.76704000
C	6.02861200	-3.15768500	-1.60058300
C	7.57980800	-1.54005000	-1.08917100
C	6.66729600	-3.46272000	-2.79561600
H	5.12843300	-3.68217500	-1.29529400
C	8.28371000	-1.77953300	-2.26137600
H	7.90292200	-0.78816200	-0.37581700
C	7.81473500	-2.75529200	-3.13494200
H	6.26446100	-4.23394800	-3.44227500
H	9.18097000	-1.21076100	-2.47923100
H	8.33789600	-2.96429700	-4.06297400
N	0.42173200	-0.60627900	-1.44812500
C	-0.84332200	-0.05795400	-1.66141700
C	-1.11381400	0.64914300	-2.83254100
C	-1.85445600	-0.15042800	-0.70911100
C	-2.35192200	1.22573500	-3.04920600
C	-3.10937200	0.40417300	-0.94102700
C	-3.37965100	1.10848900	-2.11201100
C	-4.70722800	1.75907600	-2.42492800
F	-4.01914800	0.26110900	0.01566200
F	-1.62926000	-0.74038000	0.45854400
F	-0.15078300	0.77658800	-3.74832800
F	-2.55576300	1.89026900	-4.18382600
F	-5.23298800	1.24547200	-3.54597400
F	-4.55050900	3.07687200	-2.62183100
F	-5.60241400	1.60154500	-1.44906800
C	0.60794400	-1.93586600	-1.10464800
O	-0.31291500	-2.70557200	-0.94894000
C	2.05695400	-2.35681000	-0.88032700
H	2.08506700	-2.77942900	0.11864900
H	2.23723800	-3.19131600	-1.56156900
C	3.10111500	-1.28439300	-1.06940400

C	3.62776700	-1.11036600	-2.35137400
C	3.54058900	-0.40418900	-0.02218900
C	4.56080200	-0.12089500	-2.66044100
C	4.47589700	0.63849700	-0.35170200
C	4.96132400	0.74743000	-1.67404800
H	4.95002800	-0.04184000	-3.66952400
H	5.65704500	1.54337300	-1.91806100
C	4.05565900	-0.77975400	2.41659400
C	3.33876100	-1.69757300	3.40243400
C	2.95726400	-0.31361300	1.42607400
H	4.60025900	0.03243600	2.90915100
C	2.34770500	-2.42528700	2.48871100
C	2.39424500	-0.79728400	4.23387400
H	4.00578000	-2.32397400	3.99342900
C	1.73459300	-1.13027900	1.91267800
H	2.74196400	0.75244400	1.56337000
H	1.61184000	-3.02964300	3.02905400
H	2.87080800	-3.06788500	1.77321200
H	1.99909400	-1.34747800	5.09416600
H	2.90760900	0.08925300	4.62041400
C	1.26871000	-0.44724900	3.21916100
H	0.91519400	-1.22809900	1.20377900
H	0.30886500	-0.87100200	3.53069000
H	1.12278800	0.63037100	3.09159900
H	1.21473600	-0.09681600	-1.81329700
N	7.38957700	1.84861600	2.37932900
C	7.84496700	0.95465100	3.27138500
C	8.00141400	3.04147900	2.30941700
C	8.91870100	1.21722600	4.11352000
H	7.33839900	-0.00582100	3.29690300
C	9.07894800	3.38438700	3.11315600
H	7.60203800	3.73873000	1.58022700
C	9.54847100	2.45313400	4.03485500
H	9.24542700	0.45469000	4.81145700
H	9.53673700	4.36243000	3.01365100
H	10.38964400	2.68921400	4.67938000
Cl	3.11987200	-2.13527100	-3.68656200
Pd	5.28229100	-1.56693400	1.01667400
Pd	5.75748200	1.30256800	0.99971000
I	6.82342200	-2.89402600	2.74708200
C	4.09422100	2.50837300	0.29819300
H	3.04886000	2.28470300	0.07894500
H	4.11748800	3.01636100	1.27151900
H	4.48522900	3.16455500	-0.48123100

TS44'

N	6.27514300	-2.54095300	1.75646000
C	6.71027200	-3.73374800	1.32321400
C	6.68847500	-2.10201800	2.95361300
C	7.56391800	-4.52825300	2.07751700
H	6.37591400	-4.03323300	0.33677500
C	7.55044900	-2.82939800	3.76017700
H	6.31457700	-1.13280400	3.26396600
C	7.99629800	-4.06948600	3.31592400
H	7.88522100	-5.48592900	1.68392800
H	7.86310300	-2.42008300	4.71419200
H	8.66804900	-4.66737600	3.92396100
N	-0.06026400	-0.28276100	-1.61297000
C	-1.39501500	0.10657200	-1.73246500
C	-1.80979900	0.86506900	-2.82677400
C	-2.34236900	-0.20927800	-0.76302900
C	-3.12468400	1.27336600	-2.95579800
C	-3.67077400	0.17856900	-0.90745800
C	-4.08610400	0.93179400	-2.00320300
C	-5.50577600	1.39953400	-2.22427600
F	-4.51160300	-0.17322500	0.05927000
F	-1.98792700	-0.86002500	0.33933300
F	-0.91482700	1.20425200	-3.75627000
F	-3.46768100	1.99231800	-4.02149200
F	-6.00032100	0.88925900	-3.36107300
F	-5.55132700	2.73600300	-2.33092700
F	-6.32622500	1.04701500	-1.23305400

C	0.30420300	-1.61122000	-1.45228300
O	-0.51057400	-2.49802200	-1.32410800
C	1.80338200	-1.87798900	-1.40317000
H	1.95913800	-2.50650800	-0.53424800
H	2.03530300	-2.50960300	-2.26441900
C	2.70840200	-0.67178700	-1.39316300
C	3.08751700	-0.13533700	-2.62182200
C	3.18026900	-0.04024400	-0.19039300
C	3.91874300	0.97862900	-2.73522700
C	4.04646900	1.09719400	-0.31878800
C	4.38381400	1.58702100	-1.59612500
H	4.19882800	1.34288000	-3.71704600
H	5.02575700	2.45647200	-1.68164700
C	3.81180400	-0.87161900	2.07608400
C	3.22222000	-2.03247800	2.87027200
C	2.64365000	-0.29593000	1.25698500
H	4.34136900	-0.13781600	2.69315800
C	2.23263300	-2.62900200	1.86367800
C	2.26622800	-1.40786600	3.91435700
H	3.95793500	-2.72045800	3.29242900
C	1.50708200	-1.29257300	1.59849800
H	2.35126700	0.69517900	1.62147100
H	1.56639900	-3.38307200	2.29517300
H	2.74927600	-3.06902500	1.00564400
H	1.95632300	-2.15636400	4.65130600
H	2.73788400	-0.58370100	4.46027800
C	1.06712600	-0.94020000	3.03940300
H	0.66086800	-1.30772100	0.91535400
H	0.15625800	-1.49248800	3.29002200
H	0.84466500	0.12520100	3.15514700
H	0.63800800	0.35261900	-1.97532200
N	7.43977900	1.12320400	1.91416000
C	7.77051400	1.36212100	3.19256400
C	8.25899700	0.35285000	1.17784900
C	8.91227100	0.83962200	3.78482400
H	7.08813500	1.99387100	3.75171100
C	9.41909400	-0.21103900	1.69492300
H	7.95737300	0.16164200	0.15189900
C	9.75196600	0.03328700	3.02126600
H	9.13256100	1.06383000	4.82290900
H	10.03427100	-0.83582000	1.05742000
H	10.65040500	-0.39517700	3.45482400
Cl	2.51379400	-0.83075600	-4.12649700
Pd	5.01760200	-1.32568700	0.51077400
Pd	5.44875600	1.50463700	1.01501900
I	6.53955600	-1.79470600	-1.79547100
C	3.70746700	2.74503600	0.88849000
H	2.66460800	2.55367800	0.63204700
H	3.75442400	2.93028900	1.97002400
H	4.05030200	3.61869000	0.33000300

TS44”

N	4.28164800	1.54457500	-0.75955500
C	4.38471800	2.19981200	-1.92469900
C	4.96322000	0.39865000	-0.60355300
C	5.15319700	1.72500400	-2.97589100
H	3.81634400	3.11838600	-2.01007900
C	5.74665000	-0.14459500	-1.60891200
H	4.88061900	-0.07859900	0.36570400
C	5.84270300	0.52903700	-2.82140500
H	5.19020100	2.28494200	-3.90226600
H	6.26839200	-1.07790200	-1.43481900
H	6.44336300	0.12916700	-3.63121000
N	0.15902000	-1.56737200	-3.30175600
C	-0.78982700	-2.49865700	-3.71932600
C	-1.36818200	-2.39179800	-4.98040600
C	-1.22195800	-3.53193400	-2.88714600
C	-2.33104600	-3.28984200	-5.42110100
C	-2.15964400	-4.44593500	-3.34020300
C	-2.73578700	-4.34627200	-4.60760700
C	-3.76383300	-5.37916300	-5.00592700
F	-2.53713000	-5.42182800	-2.51831400

F	-0.77070800	-3.62894700	-1.64298900
F	-0.99156100	-1.39222500	-5.78102300
F	-2.82753500	-3.10655400	-6.64024600
F	-4.23609900	-5.18833600	-6.23960200
F	-4.80909600	-5.35583500	-4.16536300
F	-3.23848400	-6.61132700	-4.95912000
C	1.39961600	-1.93996600	-2.80969300
O	1.72418200	-3.09762200	-2.66310500
C	2.31050500	-0.78583800	-2.41684100
H	2.49960400	-0.90416100	-1.35492300
H	3.26519600	-0.97977300	-2.90992900
C	1.84141600	0.61207700	-2.73465600
C	2.05331100	1.07914700	-4.04630000
C	1.26277400	1.48133100	-1.78420400
C	1.74833500	2.36891300	-4.43888100
C	0.98305000	2.82360000	-2.17539900
C	1.21239700	3.23329200	-3.49663900
H	1.92201100	2.68719400	-5.46051500
H	0.95180100	4.24307800	-3.79609400
C	1.60600400	1.65419700	0.88682600
C	1.51625900	0.48414500	1.88890800
C	0.82875900	1.09840700	-0.36722900
H	1.03592100	2.51195800	1.25445500
C	1.72585900	-0.73168500	0.97807300
C	0.04189300	0.30457500	2.31968100
H	2.20336900	0.56925400	2.73414900
C	0.55348700	-0.37907800	0.04603300
H	-0.14505600	1.59570900	-0.30736500
H	1.58905600	-1.69312200	1.48296400
H	2.70927900	-0.72267600	0.50325700
H	-0.03279200	-0.35022200	3.19398500
H	-0.42028200	1.26066500	2.58558100
C	-0.60477900	-0.34989900	1.06600400
H	0.34000100	-1.06574400	-0.76972600
H	-0.93461600	-1.37107600	1.28034500
H	-1.47234000	0.20154600	0.69101700
H	0.05036000	-0.61434900	-3.62018100
N	1.96176000	6.06816700	0.22890400
C	3.26484400	6.13229600	0.54544500
C	1.13161400	6.96499200	0.78828500
C	3.77788800	7.05750000	1.44577400
H	3.91901600	5.39394200	0.09470800
C	1.56227900	7.92681500	1.69035200
H	0.08809900	6.88862100	0.50132200
C	2.91152500	7.96965100	2.03327200
H	4.83609700	7.02781200	1.67862000
H	0.84871500	8.62525900	2.11301400
H	3.27712500	8.70240900	2.74532500
Cl	2.74072400	0.01507000	-5.26754700
Pd	3.50762700	2.46228400	0.92673600
Pd	1.22051500	4.35089000	-0.91727600
I	6.07807700	3.60199100	1.23886300
C	-0.72268300	3.67231600	-1.53151000
H	-1.09731500	4.03380900	-0.56290200
H	-1.02913100	4.34891100	-2.33066000
H	-1.17527300	2.69706800	-1.70553300
N	2.92427800	3.30700400	2.76739400
C	3.65231300	3.00330700	3.85489700
C	1.91810200	4.18248700	2.89681600
C	3.39957100	3.56306600	5.09790300
H	4.46818700	2.30704500	3.70450300
C	1.61691400	4.80327400	4.10020300
H	1.34965000	4.39139100	1.99814100
C	2.36981800	4.48841000	5.22449500
H	4.01582700	3.28077100	5.94319300
H	0.80589000	5.52073500	4.14022500
H	2.16035500	4.95498000	6.18142200

TS44-norbornene

N	7.11486500	-0.58016300	0.54936200
C	8.27732300	-0.85260600	-0.05906200
C	7.15344500	-0.09521500	1.79713900

C	9.51120400	-0.65160500	0.54293400
H	8.20713000	-1.24542900	-1.06904200
C	8.34318200	0.12805300	2.47891700
H	6.19489600	0.14086100	2.24615800
C	9.54529900	-0.15153900	1.84087400
H	10.42181000	-0.88140800	0.00084900
H	8.31594100	0.52565100	3.48723700
H	10.49255800	0.01893700	2.34283200
N	0.33533400	0.23456400	0.09770800
C	0.45783900	1.31807800	0.96978100
C	0.03811600	2.57243000	0.52659800
C	1.07015900	1.24554100	2.21452100
C	0.26256600	3.70932000	1.27613200
C	1.26126000	2.38619300	2.98784000
C	0.87329000	3.64042700	2.52843300
C	1.09718200	4.92974700	3.28004000
F	1.87011900	2.22680900	4.15728600
F	1.55414500	0.09386700	2.67131300
F	-0.56622700	2.67261200	-0.65901700
F	-0.12974100	4.88575800	0.78602800
F	1.84755400	5.77352600	2.55650700
F	1.70725800	4.74926800	4.45224400
F	-0.07164000	5.54513300	3.52436900
C	-0.14000300	-1.01879900	0.41684800
O	-0.58441600	-1.30673100	1.50801800
C	-0.09468600	-1.98875900	-0.76538900
H	-0.30025300	-2.98612400	-0.37920000
H	-0.94189800	-1.73570600	-1.40982500
C	1.19369700	-1.86907000	-1.55598300
C	1.15165900	-1.56085000	-2.94023500
C	2.44192400	-1.83943600	-0.92038000
C	2.25490200	-1.13509000	-3.64689000
C	3.54200600	-1.22894100	-1.58186500
C	3.46205100	-0.89469200	-2.96130000
H	2.18931100	-0.97722000	-4.71828900
H	4.35516400	-0.65041400	-3.53083400
C	4.23570800	-2.50809900	0.82400100
C	4.22468300	-3.92186600	1.44023100
C	2.71139400	-2.23531600	0.51845300
H	4.64131700	-1.80915700	1.56166000
C	3.06608200	-4.61240800	0.70677300
C	3.62971800	-3.75975700	2.86126000
H	5.18590900	-4.43612600	1.44337700
C	2.04197900	-3.52802400	1.05691100
H	2.42264600	-1.38124300	1.14202300
H	2.81643800	-5.58767300	1.13767800
H	3.21384700	-4.73308800	-0.37059300
H	3.77917800	-4.68533500	3.42711100
H	4.11297800	-2.95340300	3.42261800
C	2.12179300	-3.49512400	2.59288000
H	1.03606300	-3.70714400	0.69269400
H	1.49977500	-4.28695200	3.02124800
H	1.76536100	-2.54500600	2.99751000
H	0.68772800	0.39253100	-0.83884800
N	2.12460000	2.55196200	-2.31068400
C	2.15017800	3.78984200	-1.79707500
C	1.22569600	2.28609200	-3.26774900
C	1.28655000	4.79469800	-2.21396100
H	2.88701500	3.96233300	-1.01757100
C	0.32638700	3.23012200	-3.74576700
H	1.23188500	1.27184700	-3.65633000
C	0.35543700	4.51106800	-3.20611600
H	1.34304900	5.77407400	-1.75265000
H	-0.38523000	2.95511800	-4.51650100
H	-0.33868700	5.27216600	-3.54891700
Cl	-0.35693900	-1.70929800	-3.83686400
Pd	5.18468000	-1.01328100	-0.53134100
Pd	3.50817100	0.90016800	-1.50599300
I	4.46997700	2.14340300	0.68971100
C	5.61523300	-3.10503100	-0.68090800
H	4.93185600	-3.89245300	-0.98109400
H	6.10808800	-2.74794500	-1.60509700
H	6.37314500	-3.45682500	0.01571900

45

N	6.07863600	-2.19544300	-0.34977900
C	5.87544500	-3.49588500	-0.60661700
C	6.74645000	-1.46961000	-1.25561700
C	6.31496500	-4.10979000	-1.77205100
H	5.35177500	-4.05493200	0.16244800
C	7.23246500	-2.00516600	-2.44109200
H	6.88108200	-0.41952600	-1.00895600
C	7.00836800	-3.35046800	-2.70821300
H	6.11785900	-5.16383500	-1.93244500
H	7.76730600	-1.37027500	-3.13869300
H	7.36824300	-3.80030900	-3.62839400
N	0.65546100	-0.34841500	-1.38100800
C	-0.62415500	-0.12110700	-1.88714900
C	-0.82321500	0.82062100	-2.89576000
C	-1.73962200	-0.78410500	-1.38417200
C	-2.08674400	1.07259800	-3.39735500
C	-3.00670700	-0.55223600	-1.91084700
C	-3.20442700	0.38215500	-2.92528400
C	-4.54954500	0.70214000	-3.53510000
F	-4.01581300	-1.23382100	-1.38072800
F	-1.61641000	-1.62558300	-0.36554200
F	0.22870200	1.49154500	-3.37163900
F	-2.22144600	1.98262600	-4.35903100
F	-4.52962900	0.49564100	-4.85951100
F	-4.86299800	1.99134900	-3.33434300
F	-5.53632900	-0.03667600	-3.02647300
C	1.21373400	-1.61741200	-1.32751300
O	0.60757900	-2.61218500	-1.65465900
C	2.62231900	-1.67941300	-0.74980500
H	2.51867800	-2.19203000	0.20217400
H	3.19417700	-2.35274900	-1.39240000
C	3.34328900	-0.36354300	-0.58694000
C	3.92657800	0.21313300	-1.74217100
C	3.42483200	0.33688200	0.63769000
C	4.59620500	1.41538600	-1.72134700
C	4.08489800	1.64107700	0.67463600
C	4.67774100	2.13991500	-0.51972500
H	5.02227400	1.81965600	-2.63268000
H	4.98804600	3.18074200	-0.57061900
C	3.76677000	-0.64806200	2.92232900
C	2.96103400	-1.67238900	3.71928600
C	2.72032900	-0.03367300	1.96377500
H	4.32469400	0.07134400	3.52968000
C	2.13227700	-2.33567400	2.61106300
C	1.86664800	-0.89847500	4.50204900
H	3.56720900	-2.33501100	4.33377100
C	1.51619500	-1.01234000	2.10742200
H	2.36796800	0.92310000	2.35597100
H	1.36846600	-3.02344700	2.98826100
H	2.76364500	-2.88325000	1.90515400
H	1.44038600	-1.53049200	5.28736700
H	2.27068300	-0.00370200	4.98778000
C	0.81264600	-0.56042100	3.40651200
H	0.83732800	-1.05957700	1.25471400
H	-0.10706900	-1.13611000	3.55173000
H	0.53493700	0.49885700	3.38730000
H	1.28793300	0.43990000	-1.35692200
N	8.28438800	0.80049400	1.20676800
C	8.69759700	-0.40942400	1.61474200
C	9.20557200	1.76853000	1.06612700
C	10.02833300	-0.69249600	1.89659200
H	7.93280200	-1.17005400	1.72947900
C	10.55408400	1.56807100	1.32145700
H	8.83518800	2.73285400	0.73464900
C	10.97621200	0.31118900	1.74639400
H	10.29644200	-1.68823500	2.23167800
H	11.25538700	2.38475000	1.18957000
H	12.02441400	0.12214800	1.95642300
Cl	3.80733700	-0.61366800	-3.28572700
Pd	5.02945500	-1.35040300	1.49703500

Pd	6.17304900	1.21939800	0.84349700
I	6.22283800	-3.10527900	3.14151600
C	3.79742000	2.64100700	1.78286300
H	2.73606400	2.92506000	1.79128200
H	4.05050500	2.25943100	2.77542700
H	4.37890900	3.55250400	1.62214200

TS46

Pd	-0.42095500	1.96072200	-0.78481100
N	-0.37003300	3.78220800	0.23505200
C	0.47458200	4.73337700	-0.18906500
C	-1.28928400	4.09521400	1.15803400
C	0.45680400	6.02034800	0.32837800
H	1.18171400	4.43479000	-0.95429500
C	-1.37838900	5.36180900	1.71668600
H	-1.96283900	3.29838500	1.45042100
C	-0.48312200	6.34138900	1.30142900
H	1.16973400	6.75263800	-0.03318400
H	-2.13798500	5.56763300	2.46211800
H	-0.52195600	7.33962200	1.72575200
N	-0.69758600	0.18685100	-2.02077900
C	-2.06520700	-0.19977100	-2.15348900
C	-2.49261400	-0.73459500	-3.37022400
C	-3.01694500	-0.08267500	-1.14804400
C	-3.81480000	-1.08279800	-3.58202800
C	-4.34874400	-0.42587700	-1.35787100
C	-4.77618500	-0.92613100	-2.58341400
C	-6.20068100	-1.32529500	-2.88763800
F	-5.18482500	-0.25995900	-0.33552200
F	-2.68783000	0.37303100	0.06324800
F	-1.60885200	-0.93504400	-4.34197100
F	-4.16093500	-1.58374000	-4.76568100
F	-6.28591400	-2.64265900	-3.12249200
F	-6.64612600	-0.69228100	-3.98295400
F	-7.04096200	-1.03815300	-1.89056600
C	0.13586700	-0.90429100	-1.70353500
O	-0.30749800	-1.97532600	-1.34886300
C	1.63908800	-0.71896600	-1.86318500
H	2.08816600	-1.35578500	-1.09775600
H	1.86504100	-1.21033800	-2.81398700
C	2.25059200	0.66346200	-1.86275700
C	2.66015900	1.22181400	-3.07821600
C	2.47724300	1.37998400	-0.64999200
C	3.26323800	2.46848100	-3.14070300
C	3.16936700	2.60893000	-0.70740900
C	3.51933600	3.13266100	-1.95765400
H	3.55451900	2.88912100	-4.09619200
H	4.03191400	4.09030800	-1.99943500
C	0.33947100	0.80065500	0.71348300
C	0.08776000	1.18536400	2.17643300
C	1.91174900	0.72068300	0.61784900
H	-0.12139300	-0.17166000	0.52646800
C	1.24528900	2.13593400	2.49905900
C	0.46094100	-0.04190200	3.04274200
H	-0.92187400	1.55288700	2.37413200
C	2.33725700	1.14905000	2.04965300
H	2.18870200	-0.33438100	0.53403800
H	1.31907000	2.38043500	3.56503900
H	1.20272500	3.06285400	1.92962000
H	0.10820600	0.09133100	4.07134700
H	0.01499900	-0.96426900	2.65859700
C	2.01627200	-0.04721800	2.97572500
H	3.37085700	1.47905000	2.14480800
H	2.45310600	0.12052800	3.96588300
H	2.42456300	-0.98887800	2.59510500
H	-0.43393100	0.86695300	-3.01135900
Cl	2.47534600	0.36856900	-4.59671300
C	3.62770600	3.42491500	0.48261000
H	2.83952400	3.63225000	1.20449100
H	4.44341700	2.92707900	1.01675600
H	4.01663000	4.38824900	0.13880900
O	-1.04203600	3.21273800	-2.49154800

C	-0.78029900	2.84447500	-3.66371000
C	-0.89901900	3.84933100	-4.78653000
H	-1.59124100	3.47093200	-5.54401000
H	-1.24504200	4.81292700	-4.41068900
H	0.07755700	3.96361600	-5.26716300
O	-0.41380600	1.67297900	-3.99598500

47

Pd	-0.37302300	1.82841100	-0.80625700
N	-0.37785400	3.69004100	0.17421200
C	0.47929400	4.64896900	-0.20431200
C	-1.35264900	3.99852800	1.04007700
C	0.41538900	5.94014200	0.29936600
H	1.23855400	4.35134400	-0.91920600
C	-1.48874000	5.26742600	1.58448700
H	-2.03191900	3.19461400	1.29988800
C	-0.58335600	6.25561800	1.21437600
H	1.13989800	6.67864000	-0.02468200
H	-2.29044000	5.46822400	2.28599900
H	-0.65821600	7.25568100	1.62956300
N	-0.62706800	0.06412000	-1.92940400
C	-1.98101700	-0.28445700	-2.12693800
C	-2.41155800	-0.76679400	-3.36907800
C	-2.96468600	-0.14906600	-1.14933900
C	-3.73822200	-1.06448800	-3.61659900
C	-4.30390700	-0.42862400	-1.39779800
C	-4.72138400	-0.89327200	-2.64041500
C	-6.14921700	-1.23072600	-2.98748000
F	-5.15878800	-0.24435700	-0.39209100
F	-2.64989200	0.26502100	0.08540800
F	-1.52500000	-0.93528000	-4.34736700
F	-4.07669100	-1.51540600	-4.82438200
F	-6.27727700	-2.53312300	-3.28170300
F	-6.55574200	-0.53752500	-4.06359800
F	-7.00090600	-0.95807600	-1.99468900
C	0.20800500	-1.03677700	-1.90521100
O	-0.18522000	-2.18743300	-1.99969100
C	1.71689800	-0.81312400	-1.75698900
H	1.98991600	-1.34198200	-0.84202300
H	2.15283600	-1.40650200	-2.56376600
C	2.30686700	0.57645800	-1.78836900
C	2.67034900	1.12015100	-3.02384200
C	2.55104900	1.32988700	-0.60356100
C	3.26067500	2.37009100	-3.13308500
C	3.22444800	2.56479500	-0.70305200
C	3.54449400	3.06335800	-1.97179600
H	3.51979600	2.77156400	-4.10622500
H	4.04847800	4.02360700	-2.04714500
C	0.42279900	0.71843000	0.71214900
C	0.10072100	1.14895500	2.14932900
C	1.99659200	0.70378700	0.68009600
H	0.00726300	-0.27409900	0.52606300
C	1.20892500	2.15841600	2.47826400
C	0.49134000	-0.02946600	3.07433100
H	-0.92923700	1.48105500	2.29765900
C	2.35394200	1.20214700	2.10738600
H	2.32754500	-0.33822000	0.65265800
H	1.22909200	2.44334400	3.53667500
H	1.16122700	3.06286000	1.87413700
H	0.09293200	0.12483800	4.08307000
H	0.09757400	-0.98266700	2.70851600
C	2.04710000	0.02812800	3.06580700
H	3.36911200	1.57755400	2.22656700
H	2.43769300	0.25003600	4.06454100
H	2.50756000	-0.90912000	2.73742100
H	-0.35928800	1.09498700	-3.40555500
Cl	2.40575600	0.23345600	-4.51341300
C	3.68065900	3.41090700	0.46639700
H	2.88925700	3.62981300	1.18324400
H	4.49753000	2.92830800	1.01265700
H	4.06565900	4.36800400	0.10086000
O	-1.17256900	3.10763800	-2.52167900

C	-0.95649600	2.87411600	-3.71004600
C	-1.22195000	3.88304800	-4.79019500
H	-1.61611800	4.80136900	-4.35604000
H	-0.29214200	4.08732800	-5.32920400
H	-1.93422300	3.47084100	-5.51063500
O	-0.47514300	1.74378800	-4.16036500

48

Pd	-0.41600900	1.52451500	-0.77671700
N	-0.45435000	3.52256800	-0.04897700
C	0.41407500	4.42432500	-0.53502100
C	-1.38508300	3.93402600	0.82651200
C	0.39885100	5.75598100	-0.14461300
H	1.14889100	4.04843200	-1.23876300
C	-1.46916300	5.24768000	1.26311200
H	-2.06883600	3.17388700	1.18753100
C	-0.55622400	6.17655800	0.77397600
H	1.12876500	6.44349400	-0.55675800
H	-2.23593300	5.52949000	1.97559500
H	-0.59148700	7.21068200	1.10170100
N	-0.62390100	-0.25600400	-1.71477800
C	-1.95514200	-0.56917500	-2.00635300
C	-2.42223300	-0.66388800	-3.32177400
C	-2.89797700	-0.75219700	-0.99450800
C	-3.75182900	-0.93417000	-3.59384700
C	-4.23673200	-1.00107600	-1.26357700
C	-4.69066700	-1.11459700	-2.57571300
C	-6.12840600	-1.36704100	-2.95062400
F	-5.05846600	-1.13236100	-0.22157100
F	-2.51897800	-0.66613500	0.28780000
F	-1.58775800	-0.46081800	-4.33547800
F	-4.13998500	-0.99622200	-4.86804700
F	-6.22816000	-2.36346800	-3.84154800
F	-6.67602700	-0.27487200	-3.51258800
F	-6.88607600	-1.69603500	-1.89962100
C	0.30187600	-1.18686300	-2.08839100
O	0.02479200	-2.24839400	-2.62699300
C	1.76313600	-0.91241200	-1.70381900
H	1.89561700	-1.36335800	-0.71826000
H	2.34795100	-1.52683600	-2.39155500
C	2.29754500	0.50295600	-1.73647800
C	2.59343100	1.05573900	-2.98630400
C	2.56482600	1.26797900	-0.56462300
C	3.18513400	2.30234300	-3.11889900
C	3.22871400	2.50663100	-0.68944100
C	3.51929600	2.99397700	-1.97021800
H	3.40021400	2.70556500	-4.10204000
H	4.02468600	3.95150700	-2.06563200
C	0.47684500	0.56329400	0.78672000
C	0.10366100	1.10666500	2.16626700
C	2.04403800	0.65178900	0.74135900
H	0.10192500	-0.44879700	0.64089900
C	1.16765000	2.18372300	2.42048800
C	0.52655800	0.02053800	3.18575800
H	-0.94310500	1.40100500	2.26475700
C	2.35303500	1.24596300	2.14302200
H	2.43827200	-0.36931200	0.75732700
H	1.15849200	2.56173000	3.44893000
H	1.09788300	3.02662600	1.73350500
H	0.11636100	0.24987000	4.17494500
H	0.16231700	-0.97156600	2.90293400
C	2.07812000	0.12804200	3.17479700
H	3.34993900	1.66626300	2.25359600
H	2.45853100	0.42630300	4.15714900
H	2.56878800	-0.81342500	2.90855900
Cl	2.21480100	0.18335100	-4.45330200
C	3.70071800	3.37952600	0.45517800
H	2.91044800	3.64833100	1.15776500
H	4.50282400	2.89886900	1.02395200
H	4.11188500	4.31225700	0.05766100

TS49

Pd	0.09858400	1.12692100	0.14663800
N	-1.91847400	1.76027400	0.48631200
C	-2.35896400	2.86050400	-0.14569100
C	-2.81899100	0.92155200	1.01573300
C	-3.70725500	3.14498300	-0.29413900
H	-1.59682700	3.50756800	-0.56659200
C	-4.18651200	1.13599000	0.91546300
H	-2.42204300	0.03862000	1.50347500
C	-4.64041500	2.25903300	0.23453700
H	-4.01675100	4.02339700	-0.84758300
H	-4.87559200	0.41178100	1.33392300
H	-5.70197400	2.43431700	0.09775400
N	-0.50333800	0.11742600	-1.67976800
C	-1.61771000	0.57090400	-2.34966900
C	-1.53707400	1.75449500	-3.09495800
C	-2.90692800	0.04106900	-2.18412500
C	-2.65372500	2.38059700	-3.62481900
C	-4.02118900	0.66260200	-2.71639700
C	-3.92928200	1.83890100	-3.46348900
C	-5.18254200	2.54063500	-3.90328200
F	-5.22073800	0.14669700	-2.43294300
F	-3.10052600	-1.00702500	-1.38161800
F	-0.35038700	2.35469200	-3.23622000
F	-2.46788400	3.53534600	-4.26833900
F	-4.95763700	3.46463300	-4.84151100
F	-5.76748500	3.17620700	-2.85831300
F	-6.08997300	1.68716700	-4.39203100
C	-0.23617100	-1.22052900	-1.65617000
O	-0.76423200	-2.08004400	-2.34384200
C	0.89170700	-1.61559000	-0.65688700
H	0.50721900	-1.49162400	0.36477500
H	1.10273300	-2.67173500	-0.81691000
C	2.08790500	-0.73803900	-0.89872700
C	3.08180100	-1.11571400	-1.79872400
C	2.09918000	0.58786300	-0.38481900
C	4.03193200	-0.20771100	-2.25185100
C	2.95243100	1.55039500	-0.96396000
C	3.92338500	1.11738700	-1.87088600
H	4.80074900	-0.52831200	-2.94585900
H	4.60076500	1.84875600	-2.30381600
C	0.67122400	0.99523000	2.10791600
C	0.92230500	2.14458500	3.06943600
C	1.96375500	0.63702200	1.53336100
H	0.02564600	0.19057500	2.47198100
C	2.04755600	2.90151200	2.36034500
C	1.69491600	1.51708300	4.26033100
H	0.03737300	2.71920600	3.34854900
C	2.92617400	1.65188900	2.14954200
H	2.27021400	-0.40334400	1.60197800
H	2.53612600	3.64414600	2.99970800
H	1.70807100	3.38460100	1.44701700
H	1.80152100	2.24519700	5.07107200
H	1.18661600	0.63858800	4.66935900
C	3.07304700	1.17276500	3.62323600
H	3.87567500	1.77212300	1.62753300
H	3.88429000	1.72647600	4.10531400
H	3.32050800	0.10897900	3.69038800
Cl	3.15463600	-2.74261200	-2.44184800
C	2.83872500	3.04380300	-0.76002400
H	1.80801900	3.34203400	-0.55943100
H	3.47702200	3.41861900	0.04648400
H	3.14412300	3.55105000	-1.67975000

50

Pd	1.34157500	1.52067200	-0.75500900
N	-0.40778000	0.49379300	-1.21142300
C	-1.18790000	0.89757500	-2.28039800
C	-0.60897600	1.13162700	-3.53152000
C	-2.53985500	1.25169500	-2.15521200
C	-1.30226700	1.71451700	-4.58004200
C	-3.24465900	1.79526100	-3.21396400

C	-2.65047900	2.04204600	-4.45246000
C	-3.43410200	2.76988800	-5.50956800
F	-4.50619700	2.17613300	-2.99979600
F	-3.13576700	1.21421200	-0.96474500
F	0.69373100	0.87234400	-3.71277500
F	-0.62564700	1.96161800	-5.70238700
F	-2.83395000	2.75387800	-6.70308900
F	-3.60021600	4.06748000	-5.16814200
F	-4.65601100	2.24782500	-5.66758600
C	-0.86483500	-0.52676600	-0.41639800
O	-1.89378100	-1.15145900	-0.61444100
C	0.06396900	-0.86738300	0.75322500
H	0.14749500	0.00291900	1.41707300
H	-0.40100000	-1.67989800	1.30862500
C	1.42137800	-1.24825300	0.21509400
C	1.97694500	-2.52214000	0.36404100
C	2.11586800	-0.32178000	-0.57315000
C	3.15594600	-2.88137400	-0.27928500
C	3.27616000	-0.66767500	-1.27084700
C	3.78202500	-1.96078800	-1.10490000
H	3.56177700	-3.87821800	-0.14854900
H	4.68527100	-2.25198500	-1.63556200
C	3.08384500	1.94824700	0.74027800
C	2.65290900	2.57847800	2.04984300
C	3.05282200	2.93582200	-0.21742900
H	3.68288000	1.04736100	0.70317900
C	1.67236100	3.66229600	1.57674200
C	3.87910400	3.46244100	2.44287100
H	2.31418400	1.88926200	2.82337300
C	2.61797800	4.20914100	0.49320300
H	3.64932500	2.94287100	-1.12485000
H	1.45273500	4.40088400	2.35418900
H	0.73488200	3.25893200	1.18669500
H	3.73810600	3.86524800	3.45028900
H	4.81474800	2.89603100	2.44071600
C	3.85034100	4.59120800	1.37094200
H	2.24160900	5.01198400	-0.14081700
H	3.69236900	5.57174000	1.83029400
H	4.77307300	4.64452000	0.78599200
N	0.35886500	3.41329700	-1.50638900
C	0.88441000	3.97764200	-2.60310300
C	-0.89975400	3.72485400	-1.17347200
C	0.17049900	4.84307500	-3.41836100
H	1.90691500	3.70068600	-2.83930800
C	-1.68486600	4.58558200	-1.92888500
H	-1.30019200	3.22193400	-0.29882000
C	-1.14693000	5.14175100	-3.08345000
H	0.63300400	5.25163200	-4.30956300
H	-2.71082100	4.77618900	-1.63498300
H	-1.74894800	5.78243900	-3.71863000
C	4.00230200	0.29697500	-2.17962800
H	4.64285800	-0.24370900	-2.88280000
H	3.30214700	0.90267100	-2.76304400
H	4.64959000	0.97649700	-1.61033000
Cl	1.20243900	-3.73601600	1.36692700

51

Pd	1.25888500	1.45728800	-0.93362600
N	-0.41117700	0.42972900	-1.46517900
C	-1.13066300	0.87581400	-2.56278600
C	-0.56265000	0.86379400	-3.83883700
C	-2.37942200	1.49882300	-2.44315600
C	-1.17922100	1.46061700	-4.92953400
C	-2.99963000	2.08524500	-3.53067000
C	-2.42307000	2.07596200	-4.80245000
C	-3.08895800	2.84193100	-5.91263300
F	-4.14821500	2.73509300	-3.32809000
F	-2.93868900	1.64472500	-1.24415600
F	0.65131000	0.33444200	-4.01520400
F	-0.52441400	1.44526900	-6.09167600
F	-2.56968700	2.57342300	-7.11314600
F	-2.95488700	4.17432800	-5.71358600

F	-4.40095200	2.58833600	-5.97639000
C	-0.99179500	-0.48083900	-0.62748300
O	-2.07966500	-1.00120300	-0.82360700
C	-0.16177600	-0.82025600	0.61439800
H	-0.17630900	0.05084000	1.28381900
H	-0.67826100	-1.63343200	1.12196200
C	1.26593900	-1.18862600	0.27870600
C	1.84646700	-2.39344800	0.68534800
C	2.03699300	-0.32671800	-0.51992300
C	3.12390200	-2.76306400	0.27839700
C	3.30107500	-0.70192700	-0.99118300
C	3.83005100	-1.92682600	-0.57145500
H	3.54348700	-3.70750900	0.60665200
H	4.81133200	-2.23518700	-0.92509100
N	0.22926000	3.38043300	-1.52133800
C	0.26418600	3.78813500	-2.79896500
C	-0.73795500	3.85848400	-0.72847400
C	-0.66837700	4.66306200	-3.33613800
H	1.05248400	3.36158900	-3.41304700
C	-1.70935800	4.74222500	-1.18064000
H	-0.74320100	3.48881800	0.29143200
C	-1.68333300	5.14012100	-2.51222200
H	-0.62227200	4.92984500	-4.38528900
H	-2.48591300	5.08077800	-0.50457400
H	-2.44878700	5.79876600	-2.90906100
C	4.10797900	0.15620200	-1.93913800
H	4.75897400	-0.46636500	-2.56116600
H	3.45678300	0.73172600	-2.60336100
H	4.74909100	0.86618700	-1.40117200
Cl	0.98710000	-3.51149800	1.73488600
C	3.54929800	1.98336500	0.98718000
C	3.42395200	3.58928000	-0.66384100
C	4.64676100	2.60531800	1.56514200
H	3.14166000	1.06305200	1.38878700
C	4.52099800	4.26621900	-0.15174400
H	2.90085100	3.94794900	-1.54285300
C	5.14694900	3.76498700	0.98480300
H	5.09830000	2.17572700	2.45206100
H	4.87342800	5.16707800	-0.64119700
H	6.00901000	4.26920900	1.40969300
N	2.94674200	2.46400200	-0.11204300

TS52

Pd	0.17753000	1.92754300	-0.48963900
N	-1.92227800	2.44003000	-0.11815400
C	-2.63534800	2.04770000	0.94718700
C	-2.57562700	3.04740600	-1.12460700
C	-4.00582500	2.23640300	1.05099000
H	-2.09046500	1.53875300	1.72964200
C	-3.94780700	3.25405100	-1.10810200
H	-1.95180300	3.36379100	-1.95216500
C	-4.68136700	2.83922300	-0.00325100
H	-4.52917900	1.88244300	1.93135600
H	-4.42831400	3.71927600	-1.96101100
H	-5.75836100	2.96773000	0.02651900
N	-0.71208300	-0.18252300	-2.34111000
C	-2.09980800	-0.17578700	-2.26886500
C	-2.80889700	0.21090700	-3.41660300
C	-2.86297800	-0.42681400	-1.12535600
C	-4.18088300	0.37148600	-3.40718800
C	-4.24890100	-0.30728300	-1.13597000
C	-4.94024400	0.10910300	-2.26694200
C	-6.41879600	0.39053100	-2.29982200
F	-4.87611600	-0.54387000	0.01550200
F	-2.30776900	-0.69563200	0.05544500
F	-2.14394600	0.45266200	-4.54208700
F	-4.77999000	0.78632900	-4.52227700
F	-7.01537700	-0.23239800	-3.32276700
F	-6.64084100	1.71259600	-2.45561900
F	-7.04380900	0.01798300	-1.17981000
C	0.11646400	-1.03802800	-1.65798800
O	-0.27519200	-1.94010500	-0.94063800

C	1.60128600	-0.90035500	-1.97556800
H	2.10411400	-1.56416600	-1.26173800
H	1.70951200	-1.39563700	-2.94452100
C	2.33400900	0.42768400	-2.04229100
C	3.35598900	0.55830900	-2.99473600
C	2.13851500	1.50202200	-1.14093200
C	4.15793900	1.68484200	-3.07119000
C	2.93889400	2.66218000	-1.21456000
C	3.93859800	2.72351800	-2.18406400
H	4.93541600	1.74687300	-3.82376800
H	4.54872700	3.61974100	-2.25816400
C	0.39370200	0.70419200	1.18370900
C	0.43694900	1.35522400	2.56516300
C	1.75509300	0.66926500	0.74354000
H	-0.24857000	-0.15823500	1.01442000
C	1.56657000	2.37897500	2.40328000
C	1.11844900	0.30116800	3.48097500
H	-0.50571800	1.73951500	2.95744000
C	2.56520200	1.36234500	1.82337500
H	2.15543200	-0.24592700	0.32794500
H	1.90491800	2.79601000	3.35733100
H	1.30514400	3.19172500	1.72519200
H	1.05939100	0.61309400	4.52861100
H	0.64572700	-0.68159700	3.39811000
C	2.58802600	0.30742900	2.97042300
H	3.55127200	1.71642600	1.52255000
H	3.28215400	0.63482200	3.75003900
H	2.92396800	-0.67431700	2.62342100
H	-0.28522200	0.53723300	-2.97026600
Cl	3.70577200	-0.71456100	-4.15394900
C	2.74334300	3.89387200	-0.36048800
H	1.68694000	4.15431800	-0.26968500
H	3.16408800	3.77138400	0.64199300
H	3.24884000	4.74694400	-0.82186200
O	0.13058800	3.28897300	-2.15646200
C	0.40670300	2.96460700	-3.36821100
C	0.89228500	4.10996400	-4.23955100
H	1.96264500	4.24959900	-4.04935300
H	0.75351700	3.87613400	-5.29646400
H	0.38260700	5.04103600	-3.98014100
O	0.33108600	1.82627700	-3.85667300

53

Pd	0.40841400	1.70898000	-0.03699600
N	-1.81851500	2.18348500	0.50036400
C	-2.46962100	2.12736400	1.66906100
C	-2.54101400	2.49745000	-0.58929400
C	-3.83475600	2.34414600	1.79818800
H	-1.87434400	1.89813500	2.54247300
C	-3.90830100	2.73736900	-0.55179700
H	-2.00400200	2.53358500	-1.52729500
C	-4.57580800	2.64726800	0.66244300
H	-4.29994300	2.26674100	2.77441600
H	-4.43664700	2.96477700	-1.47058100
H	-5.64831100	2.80099700	0.71862700
N	-0.78696100	-0.16847700	-2.14896600
C	-2.17122300	-0.27267700	-2.01241200
C	-2.99118800	0.10487900	-3.07938000
C	-2.80443000	-0.62900900	-0.82038600
C	-4.36852300	0.15777600	-2.94576100
C	-4.18733900	-0.60843500	-0.70165400
C	-5.00170700	-0.21353400	-1.75917700
C	-6.49185600	-0.03232700	-1.62338700
F	-4.69632700	-0.90684000	0.49196900
F	-2.10745200	-0.89423200	0.28135500
F	-2.44202200	0.45385200	-4.23700800
F	-5.08509600	0.58234600	-3.98491700
F	-7.14437500	-0.46220000	-2.70788600
F	-6.79181800	1.27562300	-1.46981600
F	-6.99528000	-0.67909100	-0.56974200
C	0.05907200	-1.13999500	-1.69038400
O	-0.34176900	-2.18918900	-1.21458800

C	1.55994200	-0.91317300	-1.80737700
H	1.96307600	-1.34891000	-0.88570800
H	1.87565000	-1.60025400	-2.59600300
C	2.22196500	0.43486100	-2.01876900
C	3.18960700	0.57999000	-3.02906000
C	2.08085600	1.51334600	-1.12905100
C	4.02003700	1.68757300	-3.10678600
C	2.95226400	2.61094300	-1.13630200
C	3.91774600	2.67662000	-2.14017900
H	4.75630900	1.75641000	-3.89926800
H	4.59741600	3.52450800	-2.17246000
C	0.58818300	-0.03068500	1.37596300
C	0.01911600	0.17378700	2.76800200
C	1.83487600	0.56895900	1.38393000
H	0.30075900	-0.88222200	0.76811100
C	0.60341000	1.54641800	3.15880400
C	0.88232800	-0.76343400	3.66887900
H	-1.05285300	0.01142100	2.87012500
C	2.03790100	1.17505200	2.75877300
H	2.67875200	0.26645100	0.77694600
H	0.50310100	1.76047500	4.22777400
H	0.21405800	2.39056500	2.58125600
H	0.45865600	-0.80353000	4.67692800
H	0.91095300	-1.78469000	3.27970400
C	2.27537900	-0.07317500	3.66398400
H	2.80148400	1.94902300	2.83844500
H	2.56714800	0.24864400	4.66825100
H	3.07003700	-0.71876900	3.27929800
H	-0.44048400	0.69212100	-2.61624500
Cl	3.42327600	-0.65885600	-4.25490700
C	2.86415300	3.71971400	-0.11632300
H	1.99277300	4.34896700	-0.31802800
H	2.75138400	3.31750600	0.89586800
H	3.76530300	4.34064000	-0.13740900
O	0.13579700	3.37604600	-1.30355100
C	0.06467000	3.29848400	-2.58494700
C	0.43400200	4.57428400	-3.31525900
H	1.52716000	4.60981000	-3.39179200
H	0.01280600	4.57625800	-4.32180900
H	0.10735800	5.45448800	-2.75668300
O	-0.26072300	2.29246400	-3.23265100

54

N	-1.12548100	2.96114200	0.16380800
C	-0.99904100	3.21503800	1.47183900
C	-2.34659200	3.04465000	-0.38364200
C	-2.07675900	3.53922100	2.28393200
H	0.00508000	3.14753500	1.87841900
C	-3.48134500	3.34376800	0.35818400
H	-2.38485000	2.86436100	-1.45204900
C	-3.34648200	3.59080000	1.71871900
H	-1.91862100	3.73343200	3.33894400
H	-4.45092500	3.35415300	-0.12628300
H	-4.21518700	3.81927700	2.32809000
N	-0.55086900	-0.57065400	-2.06748200
C	-1.91559700	-0.50426900	-1.80487100
C	-2.80752000	-0.69861600	-2.86467500
C	-2.47588600	-0.15193400	-0.57218000
C	-4.17584900	-0.50896500	-2.72392800
C	-3.84487500	-0.00368600	-0.42695100
C	-4.72759700	-0.16073300	-1.49238600
C	-6.18948100	0.12229600	-1.26381300
F	-4.30889700	0.36511000	0.76843600
F	-1.72496200	0.13708200	0.49071700
F	-2.34047000	-1.06833200	-4.05098700
F	-4.93278700	-0.68695300	-3.80238000
F	-6.94819800	-0.18277200	-2.31704300
F	-6.38003300	1.43151800	-0.99837400
F	-6.65947100	-0.56356300	-0.21347100
C	0.37852800	-1.05447800	-1.18714300
O	0.08038800	-1.64837400	-0.16370000
C	1.84062500	-0.89924600	-1.57840300

H	2.37523200	-0.81366300	-0.62619600
H	2.12382300	-1.87825100	-1.97453600
C	2.31991100	0.18960500	-2.51933400
C	3.24991800	-0.13057200	-3.52168700
C	1.97740900	1.54758800	-2.36986900
C	3.84403200	0.83418200	-4.32107000
C	2.59724100	2.54316700	-3.14291100
C	3.52625900	2.16640500	-4.11240700
H	4.55636100	0.54183100	-5.08405000
H	4.00468200	2.92812700	-4.72319400
H	-0.26203800	-0.06495900	-2.92513100
C	2.28619600	4.01233300	-2.95966900
H	2.43612000	4.33188000	-1.92056700
H	2.93008900	4.62982800	-3.59412400
H	1.24234300	4.22651500	-3.20601400
O	-0.62389700	2.79249500	-2.71295600
C	-0.80508900	2.23361000	-3.86479400
C	-1.61225800	3.08666900	-4.83039800
H	-2.67899700	2.92585900	-4.63492200
H	-1.40078700	4.14906300	-4.69046400
H	-1.40583700	2.78455700	-5.85845900
O	-0.43576900	1.10838900	-4.20692700
Cl	3.74921200	-1.79502400	-3.81812700
C	1.33797600	0.79595000	1.41512200
C	3.03424500	2.10733000	0.54440600
C	2.14874400	0.37362500	2.45907900
H	0.32789000	0.42512500	1.30049900
C	3.89867800	1.73770300	1.56290900
H	3.34843900	2.76851700	-0.25408900
C	3.45060500	0.85245500	2.53834100
H	1.75746200	-0.33347600	3.18114300
H	4.90761200	2.13386700	1.57723800
H	4.10967300	0.53512600	3.34017000
N	1.77250400	1.65054600	0.47341500

TS55

Pd	0.70884200	1.74717800	-1.19558100
N	-0.93710300	2.03638800	0.26091300
C	-1.99091400	2.77433700	-0.12486100
C	-1.00714500	1.36762500	1.41988400
C	-3.15698400	2.84404600	0.62547900
H	-1.87338000	3.28497300	-1.07662600
C	-2.13440900	1.38787000	2.22841500
H	-0.13267700	0.78230600	1.68560600
C	-3.23606100	2.13072400	1.81634600
H	-3.99595100	3.42592800	0.26262800
H	-2.15305500	0.80992300	3.14527900
H	-4.14820700	2.14144700	2.40393400
N	-0.58152700	0.32028200	-2.62459000
C	-1.90039200	0.19867000	-2.15560700
C	-2.99155800	0.82859100	-2.75479700
C	-2.16110100	-0.48534700	-0.96369100
C	-4.24881600	0.80596100	-2.16578400
C	-3.41638300	-0.52406900	-0.38504200
C	-4.50003800	0.12153500	-0.97979900
C	-5.86043300	0.20775200	-0.34102500
F	-3.53648700	-1.15430600	0.78369300
F	-1.14983300	-1.04962400	-0.29730900
F	-2.85862800	1.48754200	-3.90079600
F	-5.22917100	1.47679700	-2.77044300
F	-6.84035900	0.06121700	-1.23893900
F	-6.03803000	1.41247500	0.24540000
F	-6.04272200	-0.71785600	0.60516700
C	0.09334500	-0.90735100	-2.78177100
O	-0.47580400	-1.97635700	-2.80492100
C	1.61469600	-0.85635500	-2.79949100
H	1.88735000	-1.06284400	-1.75374600
H	1.94037100	-1.72240200	-3.37443400
C	2.31558100	0.40334300	-3.24611500
C	3.21814900	0.39382400	-4.31826400
C	2.12420800	1.61758200	-2.57144800
C	3.91376500	1.53253300	-4.69834600

C	2.82550200	2.78065700	-2.92215900
C	3.71591000	2.71141800	-3.99542000
H	4.60222100	1.49213800	-5.53484100
H	4.26184700	3.60359600	-4.29276500
H	-0.42919700	1.09647600	-3.52156500
C	2.64246900	4.09552700	-2.19916700
H	3.06937000	4.05675400	-1.19006700
H	3.14743100	4.90403500	-2.73745200
H	1.58203400	4.34932800	-2.10965200
O	-0.45057200	3.35115000	-2.67581600
C	-0.30669400	3.15314800	-3.91053500
C	-0.11280500	4.34617700	-4.82222500
H	-0.53849200	5.24743800	-4.37666400
H	0.96576200	4.49629000	-4.95244600
H	-0.54751900	4.15750300	-5.80593000
O	-0.25869900	2.00867500	-4.45533600
N	2.22130900	1.98464900	0.29711200
C	3.35521600	1.26671000	0.27613600
C	2.05159300	2.88922900	1.27509500
C	4.34955700	1.42050200	1.23215300
H	3.46139700	0.56521200	-0.54264000
C	3.00028800	3.10478100	2.26359900
H	1.12419100	3.44989700	1.244817500
C	4.17240100	2.35642000	2.24428500
H	5.24632800	0.81429800	1.17226200
H	2.81779600	3.85214600	3.02749300
H	4.93454000	2.50172900	3.00322800
Cl	3.52778800	-1.07020500	-5.23976900

56

Pd	1.60415600	1.45841200	-1.61607000
N	0.13820300	0.34675000	-2.44179100
C	-0.24762200	0.60992300	-3.75109000
C	0.69577700	0.67925600	-4.78223100
C	-1.56727600	0.91372300	-4.09939800
C	0.34119200	1.03361400	-6.07084700
C	-1.92996700	1.24928700	-5.39700000
C	-0.98110700	1.31569100	-6.41507400
C	-1.28699000	1.69767300	-7.84033000
F	-3.21013600	1.54573300	-5.61535200
F	-2.50790400	0.97395500	-3.15577300
F	1.98294500	0.42225900	-4.52794600
F	1.29609400	1.09378400	-7.00039300
F	-0.87174100	0.75041800	-8.69366200
F	-0.65445000	2.83705300	-8.17416800
F	-2.59074900	1.88869700	-8.05756300
C	-0.48701600	-0.66897100	-1.76419400
O	-1.37644400	-1.36038800	-2.23097700
C	0.04193600	-0.89510400	-0.34403700
H	-0.14962900	0.00512300	0.25400200
H	-0.53127600	-1.71607400	0.08338600
C	1.52298500	-1.19588400	-0.37396300
C	2.07347500	-2.38034300	0.12647400
C	2.38181800	-0.28283100	-1.01381000
C	3.42132800	-2.67773800	-0.03962800
C	3.73261000	-0.59356300	-1.24300500
C	4.23404700	-1.79581200	-0.73692400
H	3.82146700	-3.60347900	0.35881200
H	5.27848800	-2.05044500	-0.89757800
N	0.73284700	3.33881400	-2.36993100
C	1.53175500	4.29840100	-2.85503600
C	-0.59415600	3.50607400	-2.44900500
C	1.03793800	5.45061700	-3.45039500
H	2.59798300	4.12507800	-2.75333700
C	-1.17104700	4.62845800	-3.02714300
H	-1.19977300	2.69905600	-2.05120700
C	-0.34016000	5.61711100	-3.54245500
H	1.72469600	6.19476000	-3.83794700
H	-2.25072800	4.71253300	-3.07701200
H	-0.75949200	6.50279000	-4.00918100
C	4.63248200	0.31543500	-2.04684100
H	5.60666600	-0.15208200	-2.21838400

H	4.18188400	0.53306300	-3.02012200
H	4.80349900	1.27565400	-1.54907300
O	3.00559400	2.71643400	-0.54435900
C	3.40562300	2.55036700	0.60915500
O	3.25919200	1.43575300	1.28463200
H	2.86057700	0.74570000	0.70092100
C	4.12747200	3.62456900	1.36289300
H	3.66104600	3.76489300	2.34155800
H	5.16227200	3.31164400	1.53268600
H	4.10941700	4.55460700	0.79614200
Cl	1.08743900	-3.54948200	0.98464900

TS57

Pd	1.95454600	1.44735800	-1.38618300
N	0.43108600	0.36156500	-2.17391800
C	-0.01562000	0.66232600	-3.45734600
C	0.89050900	0.75355000	-4.52009400
C	-1.34666900	0.97324200	-3.74833300
C	0.48841800	1.13009800	-5.78787100
C	-1.75758700	1.32831400	-5.02721700
C	-0.84690700	1.41320200	-6.07775200
C	-1.20545500	1.81639200	-7.48528700
F	-3.04489500	1.62506500	-5.19379700
F	-2.25167300	1.02028100	-2.77031100
F	2.18640100	0.50028800	-4.31130800
F	1.40786200	1.21079700	-6.75064300
F	-0.81606500	0.88446700	-8.36690800
F	-0.59023300	2.96398700	-7.82236500
F	-2.51684400	2.00376100	-7.65230400
C	-0.17581000	-0.67009200	-1.49847600
O	-1.12537700	-1.30658200	-1.91563300
C	0.52474400	-1.01861800	-0.17806300
H	0.54181900	-0.14289600	0.48117700
H	-0.03704400	-1.81963100	0.30002600
C	1.92944700	-1.41864300	-0.53512900
C	2.28866200	-2.74613200	-0.75779900
C	2.87259900	-0.39594400	-0.80543400
C	3.54247800	-3.06781200	-1.26800800
C	4.14210700	-0.72582800	-1.33979600
C	4.45452700	-2.06481300	-1.56410300
H	3.79464700	-4.10885000	-1.44068700
H	5.42554800	-2.33400700	-1.96991400
N	1.05394600	3.23372700	-2.10034400
C	1.83162700	4.17281400	-2.65728600
C	-0.27045200	3.43133300	-2.04135300
C	1.30702700	5.33570400	-3.20163300
H	2.89723500	3.97531400	-2.65139500
C	-0.86933700	4.57154200	-2.55627200
H	-0.85215800	2.63712900	-1.58843200
C	-0.06832200	5.53790300	-3.15433800
H	1.97083000	6.06288000	-3.65507200
H	-1.94524500	4.68563400	-2.49170500
H	-0.50866300	6.43516400	-3.57725500
C	5.19299900	0.32401800	-1.59268900
H	6.00387800	-0.07496900	-2.20819700
H	4.78168300	1.20581300	-2.08845700
H	5.62806000	0.65297500	-0.64058400
O	3.36000200	2.69211500	-0.47995100
C	3.78595100	2.33588300	0.65977800
O	3.55924500	1.20777800	1.17778000
H	3.06011000	0.42937900	0.20220200
C	4.65700500	3.30681700	1.41585900
H	5.70459300	3.09005600	1.17995500
H	4.43891000	4.33334900	1.11826600
H	4.51817500	3.17673200	2.49018700
Cl	1.17612300	-4.05865900	-0.44353700

58

Pd	1.96595100	0.65063300	-2.65396100
N	0.18540700	-0.22727100	-2.42828400
C	-0.94761700	0.40984900	-2.94274000

C	-1.12023100	0.55395000	-4.31774700
C	-1.89215500	1.00347600	-2.10905700
C	-2.17602400	1.28291500	-4.83419900
C	-2.96478500	1.71934100	-2.62379500
C	-3.12964400	1.86978400	-4.00065700
C	-4.21093700	2.71798500	-4.62000300
F	-3.80711400	2.27737500	-1.75636200
F	-1.75122100	0.92448900	-0.79008300
F	-0.22883700	0.02537100	-5.15297900
F	-2.26230000	1.42865000	-6.15727400
F	-4.78785100	2.09626500	-5.65750500
F	-3.69350700	3.87149100	-5.08373600
F	-5.18048400	3.03385000	-3.75798800
C	-0.00913300	-1.36091400	-1.69823200
O	-1.08314100	-1.91002400	-1.52954700
C	1.25434700	-1.91369900	-1.04570900
H	1.17138900	-1.68681200	0.02238100
H	1.21475900	-3.00221100	-1.14014500
C	2.58344000	-1.40146500	-1.55327900
C	3.20800300	-1.93636500	-2.70806500
C	3.38592300	-0.58449600	-0.72346600
C	4.56076300	-1.73354100	-2.95377400
C	4.74804300	-0.37155500	-0.95263700
C	5.32247600	-0.97505500	-2.06934800
H	5.01605400	-2.18457000	-3.82872200
H	6.38133400	-0.83514000	-2.26987700
N	3.74933900	1.66997100	-3.04581200
C	4.46133000	1.38288400	-4.14358000
C	4.15891400	2.65394500	-2.23157200
C	5.63671400	2.04993700	-4.45473100
H	4.06719500	0.59771900	-4.77910700
C	5.32735000	3.36284200	-2.47487800
H	3.50216700	2.87655900	-1.39817400
C	6.08335700	3.05223500	-3.59980100
H	6.18122100	1.78841000	-5.35491100
H	5.62672000	4.14860200	-1.79073500
H	7.00092100	3.59094000	-3.81461900
C	5.57172000	0.46628800	-0.00916100
H	6.27314200	1.10208300	-0.55838800
H	4.93819800	1.11250700	0.60520000
H	6.15751600	-0.16723700	0.66679400
O	1.05599400	2.22681400	-3.54421300
C	0.81071700	3.19353900	-2.70144100
O	1.21441400	3.23398700	-1.54339200
H	2.92576600	-0.17056400	0.17066100
C	-0.05131400	4.28523000	-3.30611500
H	-1.00762100	3.86378000	-3.63131700
H	-0.22524000	5.07202900	-2.57122600
H	0.43588800	4.70146700	-4.19278500
Cl	2.30616900	-2.96474300	-3.78052600

59

Pd	1.90929200	1.44030400	-2.83271700
N	0.18069800	0.73674200	-1.93239600
C	-0.94890000	1.08421900	-2.69944800
C	-1.54639400	0.21170800	-3.61241700
C	-1.44177300	2.38425300	-2.66834200
C	-2.59165500	0.62469200	-4.41567000
C	-2.48676300	2.80806300	-3.47881100
C	-3.09182300	1.92678200	-4.36898300
C	-4.23130300	2.29162600	-5.28653400
F	-2.87360700	4.07751800	-3.36568400
F	-0.87028800	3.28342000	-1.85357400
F	-1.07781600	-1.02016300	-3.77242800
F	-3.10123000	-0.24838400	-5.28582900
F	-5.29541200	1.50643100	-5.06140200
F	-3.88074400	2.12893500	-6.57204100
F	-4.62901600	3.55813900	-5.13733700
C	0.07478500	-0.47636200	-1.23278300
O	-0.99177000	-1.02755000	-1.05962200
C	1.33075900	-0.98560900	-0.51377400
H	1.53408800	-0.28260800	0.30360500

H	1.01880400	-1.92750600	-0.05543600
C	2.59983300	-1.18227800	-1.30683500
C	2.71330100	-2.14629400	-2.31356300
C	3.73942600	-0.42825400	-1.01330800
C	3.90197800	-2.32810600	-3.00736200
C	4.93980400	-0.57050000	-1.70718200
C	5.00568300	-1.53975200	-2.70708300
H	3.94801800	-3.06857200	-3.79688800
H	5.92860800	-1.68107800	-3.26388700
N	3.66126200	2.15692300	-3.70295200
C	4.41990700	1.34840200	-4.46061900
C	4.08975700	3.39756000	-3.42443400
C	5.64951000	1.76425300	-4.95592300
H	4.00099300	0.36579900	-4.66068700
C	5.30030000	3.88125000	-3.89390200
H	3.44064100	4.00004100	-2.80073800
C	6.09873400	3.04728700	-4.67173800
H	6.23507900	1.08061100	-5.55987400
H	5.60455100	4.89316400	-3.65166200
H	7.05331300	3.39710200	-5.05242200
C	6.10447100	0.33842200	-1.40835300
H	5.94129800	1.33129700	-1.84743600
H	6.24121200	0.47591100	-0.33062200
H	7.03741100	-0.05766700	-1.82067200
O	1.08510600	0.97586800	-4.59692800
C	1.44431200	-0.04542000	-5.32629000
O	2.40593100	-0.77399300	-5.11759500
H	3.68161700	0.31142100	-0.22032400
C	0.51495100	-0.25285300	-6.50855500
H	0.28115600	0.70067900	-6.98863200
H	0.97343900	-0.93801700	-7.22303200
H	-0.42288800	-0.68672700	-6.15027500
O	2.59278700	2.43648700	-1.04594900
C	1.95115500	2.69201200	-0.01594300
C	2.54815300	3.52655900	1.07670700
H	2.41037900	3.02896600	2.03997400
H	3.60634000	3.70035800	0.88354000
H	2.01791000	4.48305100	1.12242500
O	0.74369200	2.27694000	0.21119200
H	0.40786600	1.75756400	-0.59927200
Cl	1.34555200	-3.14594700	-2.71984900

TS60

Pd	1.97379100	1.43377400	-2.83224400
N	0.19703900	0.77201600	-1.88691500
C	-0.91311200	1.15723200	-2.68048300
C	-1.45055000	0.32826400	-3.66722800
C	-1.42844500	2.44545700	-2.59372000
C	-2.46889900	0.76925900	-4.49061500
C	-2.44843300	2.89350200	-3.42426300
C	-3.00141400	2.05411100	-4.38542500
C	-4.09740100	2.46270300	-5.33826200
F	-2.85975400	4.14886600	-3.26150400
F	-0.90745400	3.30743600	-1.71449600
F	-0.95957900	-0.88752700	-3.87479300
F	-2.91791600	-0.06115100	-5.43233100
F	-4.60919500	3.66232600	-5.05095200
F	-5.10532000	1.57921800	-5.31202300
F	-3.63893100	2.50990700	-6.59887900
C	0.07017500	-0.52152900	-1.27937200
O	-0.99382900	-1.08594400	-1.22488100
C	1.29693600	-1.05102800	-0.53829700
H	1.50408200	-0.34165900	0.27155800
H	0.95996400	-1.98417200	-0.07981500
C	2.56841000	-1.27574500	-1.32281200
C	2.67949600	-2.25862000	-2.31126200
C	3.70683600	-0.51644800	-1.04336500
C	3.86857000	-2.45599800	-2.99970600
C	4.90749900	-0.67442500	-1.73367000
C	4.97285700	-1.66284500	-2.71402100
H	3.91326500	-3.20793200	-3.77841300
H	5.89394900	-1.81180100	-3.27181700

N	3.73660600	2.10694300	-3.68178000
C	4.48326600	1.28471700	-4.43637300
C	4.19117700	3.33428500	-3.38541600
C	5.72733800	1.67510900	-4.91516800
H	4.04570300	0.31190100	-4.64452900
C	5.41833200	3.79067300	-3.83827800
H	3.55238200	3.94318100	-2.75813500
C	6.20435800	2.94437200	-4.61486300
H	6.30281000	0.98203000	-5.51814700
H	5.74567000	4.79185700	-3.58207000
H	7.17170100	3.27343900	-4.98156100
C	6.07818200	0.22567400	-1.43044800
H	6.86013100	0.13067100	-2.18997200
H	5.76101400	1.27472700	-1.40089500
H	6.52556400	-0.01062800	-0.45789900
O	1.16528200	0.98116800	-4.60749000
C	1.51801500	-0.03894300	-5.34120800
O	2.44042000	-0.80774500	-5.10084400
H	3.64501400	0.24894500	-0.27594400
C	0.64409200	-0.18342800	-6.57382600
H	-0.34548600	-0.53915500	-6.27393700
H	0.51483400	0.78351300	-7.06708900
H	1.08969100	-0.90436000	-7.26068000
O	2.65938300	2.39089900	-1.07986800
C	1.95698000	2.59525100	-0.05367900
C	2.52777400	3.45077600	1.04480500
H	3.59101900	3.62932400	0.88268200
H	1.99400500	4.40642700	1.05808400
H	2.36242400	2.96922300	2.01154500
O	0.78893000	2.12924600	0.12238500
H	0.42275700	1.53422900	-0.85056300
Cl	1.30737500	-3.25752100	-2.70925600

61

Pd	1.96041600	1.39496900	-2.96993700
N	0.15112800	0.57643300	-2.06457600
C	-0.96517900	1.24886000	-2.64803300
C	-1.53242200	0.86041900	-3.86085700
C	-1.47599600	2.38983000	-2.03792200
C	-2.55783700	1.60058100	-4.42448700
C	-2.50090500	3.13317300	-2.60737300
C	-3.06788800	2.74595200	-3.81725900
C	-4.18356600	3.49103200	-4.51135100
F	-2.90993700	4.21100700	-1.94528400
F	-0.96274500	2.79958000	-0.87548200
F	-1.09265400	-0.19828300	-4.52618600
F	-3.05383800	1.19284700	-5.58799800
F	-5.24187600	2.68919000	-4.69929900
F	-3.78808100	3.92550100	-5.71500300
F	-4.60179800	4.55168800	-3.81621000
C	0.00473700	-0.86205300	-1.87909100
O	-0.99837800	-1.42832400	-2.21057700
C	1.14444100	-1.53036200	-1.12304900
H	1.20719300	-1.03867500	-0.14568700
H	0.82030100	-2.56246800	-0.97228600
C	2.50648200	-1.47916100	-1.77576300
C	2.82983100	-2.23936900	-2.90398700
C	3.49308500	-0.64174100	-1.25332700
C	4.09043900	-2.16417500	-3.48106100
C	4.75541500	-0.51710800	-1.83415700
C	5.04368000	-1.30103600	-2.94953800
H	4.31627900	-2.76948900	-4.35230600
H	6.02119200	-1.23278900	-3.42030700
N	3.67692500	2.17923100	-3.80910600
C	4.37712400	1.44695300	-4.68774600
C	4.11546900	3.39600600	-3.45596000
C	5.56202600	1.91072600	-5.23928100
H	3.95089800	0.48164700	-4.93339400
C	5.28566100	3.92675300	-3.97773700
H	3.51168900	3.91961600	-2.72518500
C	6.02531200	3.17146700	-4.88103500
H	6.10405100	1.28639700	-5.94044300

H	5.60452600	4.91709900	-3.67330300
H	6.94653300	3.56174100	-5.30204300
C	5.73700600	0.48880500	-1.29172100
H	5.33949200	1.50436200	-1.41197400
H	5.92173800	0.33350400	-0.22334300
H	6.69697100	0.43631300	-1.81373400
O	1.78614900	0.19574700	-4.56415600
C	1.18376100	0.76541800	-5.58023600
O	0.74597800	1.90756200	-5.57120200
H	3.24535400	-0.04542200	-0.37926900
C	1.11024500	-0.13742000	-6.79445400
H	0.84818100	-1.15518500	-6.49661700
H	0.37894500	0.25370000	-7.50307000
H	2.09265900	-0.17157300	-7.27867600
O	2.29298300	2.67931300	-1.39219900
C	1.98857300	2.42886000	-0.16804700
C	2.46351400	3.46443500	0.82844800
H	2.55778500	3.01446200	1.81807300
H	3.41116800	3.90679500	0.51382600
H	1.71460200	4.26191500	0.88170500
O	1.33375100	1.44720100	0.21957300
H	0.42215200	0.96940700	-1.12441300
Cl	1.64393900	-3.29888600	-3.62151700

62

N	0.97837100	-1.00825700	-1.21211700
C	0.01617800	-2.00414000	-1.39054100
C	-0.00275600	-3.11279000	-0.54368500
C	-0.92160100	-1.95639100	-2.41899400
C	-0.93344200	-4.12232500	-0.70525900
C	-1.87881500	-2.95737200	-2.55963000
C	-1.90305300	-4.05856900	-1.70729600
C	-2.89414300	-5.19433300	-1.81408700
F	-2.74148700	-2.83068000	-3.56165400
F	-0.90151600	-0.97252100	-3.30768000
F	0.90468700	-3.19646200	0.43235100
F	-0.90145600	-5.15833300	0.12904300
F	-3.54162700	-5.36673800	-0.65304800
F	-2.26372400	-6.34426000	-2.09720400
F	-3.81171800	-4.99242800	-2.76066000
C	0.66271100	0.33822300	-1.14052000
O	-0.46990300	0.75333900	-1.24195400
C	1.87539100	1.24680800	-0.96145700
H	1.47974400	2.24674500	-0.77580700
H	2.45055600	0.93945700	-0.08258300
C	2.73905300	1.24922600	-2.20255700
C	3.88696000	0.47010700	-2.34699900
C	2.35705700	2.03884300	-3.29168100
C	4.63714400	0.48822800	-3.51809600
C	3.07867800	2.07377500	-4.48191800
C	4.23146400	1.28910700	-4.57614200
H	5.53063000	-0.12155800	-3.59515600
H	4.81976400	1.30130800	-5.48980000
H	1.89992000	-1.30250200	-0.91476800
C	2.62069000	2.91532200	-5.64571200
H	2.12377700	2.29504500	-6.40077400
H	1.90950600	3.68300800	-5.32819200
H	3.46560600	3.41289000	-6.13241500
H	1.45396000	2.63730700	-3.19564600
Cl	4.42781000	-0.58164200	-1.04316000

TS63

Pd	1.96139100	3.63107100	0.15680700
N	0.33989100	5.20523200	0.63671100
C	0.54509500	6.51936300	0.48330000
C	-0.92273700	4.75825500	0.58369300
C	-0.48361600	7.42596200	0.25270300
H	1.57978500	6.84437700	0.53291900
C	-2.01314500	5.58687400	0.34246200
H	-1.05154100	3.68964100	0.71968000
C	-1.78817300	6.94886800	0.17078100

H	-0.25999700	8.48004400	0.12881900
H	-3.00815600	5.16334600	0.27455200
H	-2.61410100	7.62563600	-0.02517600
N	0.66043500	0.49509400	-2.65985600
C	-0.48479100	1.28538900	-2.70084500
C	-0.87267300	1.86479200	-3.90943700
C	-1.23243700	1.61343300	-1.56992300
C	-1.92571900	2.75915700	-3.97853100
C	-2.32397000	2.46713300	-1.65419200
C	-2.68382600	3.07770100	-2.85256900
C	-3.74538000	4.14298500	-2.95360000
F	-2.98247400	2.71542000	-0.52041400
F	-0.89645700	1.16466500	-0.36697900
F	-0.18118500	1.59049300	-5.01506500
F	-2.19235000	3.32932600	-5.15243100
F	-4.50821100	3.98104700	-4.03839800
F	-3.17543200	5.36281200	-3.04180800
F	-4.55657500	4.16568300	-1.89102500
C	0.79500500	-0.66978100	-1.91912900
O	-0.15678300	-1.25514800	-1.45282500
C	2.24796300	-1.12130900	-1.75548600
H	2.24548500	-1.86751300	-0.95684800
H	2.57597300	-1.61918000	-2.67349300
C	3.12093700	0.06365700	-1.42045700
C	4.20982500	0.52252300	-2.17498000
C	2.76144800	0.86134400	-0.34085400
C	4.91859400	1.67243400	-1.81631300
C	3.28585200	2.14513200	-0.10260400
C	4.46944600	2.49899600	-0.78365600
H	5.79920200	1.94630200	-2.38916700
H	5.00979400	3.41271400	-0.55635700
C	2.43219300	1.97219700	1.56259100
C	3.45756500	1.59932500	2.65072000
C	2.02517200	0.59606400	0.93664000
H	1.58965300	2.50411400	2.03418100
C	4.10356300	0.30332400	2.12705600
C	2.62959200	1.03246200	3.82538500
H	4.13716300	2.40872800	2.92448400
C	2.76145700	-0.40324600	1.86124200
H	0.95379900	0.39250400	0.87381800
H	4.69271300	-0.20438400	2.89861900
H	4.72802700	0.43215100	1.24083100
H	3.27006700	0.85967000	4.69757600
H	1.82804200	1.71139300	4.13515300
C	2.09112500	-0.31545400	3.25076400
H	2.82260600	-1.41755700	1.45742600
H	2.38883100	-1.16142200	3.87861500
H	0.99880800	-0.33238200	3.17438000
H	1.49823800	0.91004700	-3.04738300
N	1.39994400	4.25790800	-2.21771700
C	0.36775100	4.98481900	-2.65560600
C	2.19458000	3.69487000	-3.13790300
C	0.09453500	5.19206300	-4.00444400
H	-0.27824100	5.41493000	-1.89682800
C	1.99460500	3.83366600	-4.50647600
H	3.02785900	3.11733100	-2.74854800
C	0.92354500	4.60263300	-4.95092400
H	-0.76822600	5.78043000	-4.29542600
H	2.66757800	3.34506200	-5.20296400
H	0.73164300	4.72890400	-6.01161800
Cl	4.75087500	-0.37023200	-3.59354900

64

N	-0.52335600	0.01661800	-0.38762900
C	-1.57791800	-0.00630900	-1.30531300
C	-2.72588700	0.76886000	-1.14041700
C	-1.516111500	-0.84886200	-2.41189300
C	-3.74087700	0.71893600	-2.08374400
C	-2.54760800	-0.92106400	-3.33795600
C	-3.68253500	-0.12599400	-3.19236800
C	-4.85052400	-0.12869100	-4.15124300
F	-2.39525900	-1.75627700	-4.36027700

F	-0.43421600	-1.61358500	-2.58016300
F	-2.87926400	1.53592000	-0.07069200
F	-4.81261700	1.48334900	-1.89324400
F	-5.01365900	1.08200100	-4.70290500
F	-5.98752800	-0.43621000	-3.51085900
F	-4.69773600	-1.00797700	-5.14360200
C	0.12648000	1.19011400	-0.03754100
O	-0.25183400	2.28422700	-0.39219500
C	1.38769800	0.96714200	0.79026900
H	1.59106700	1.90842300	1.30460000
H	1.23321700	0.18402000	1.53753600
C	2.53755200	0.63606600	-0.13055100
C	3.00098900	-0.65672300	-0.42129900
C	3.19780600	1.63269000	-0.83329300
C	4.04793300	-0.91840100	-1.30855200
C	4.23558700	1.39753900	-1.72393500
C	4.69881000	0.11941000	-1.98305500
H	4.34434300	-1.94868100	-1.47303600
H	5.50859300	-0.09793500	-2.67252700
H	-0.01298600	-0.85006900	-0.26612400
C	4.42601500	2.87107200	-2.03579500
C	5.60680200	3.60249300	-1.37287000
C	3.23301600	3.13648700	-1.01722400
H	4.26744700	3.16277400	-3.07793000
C	5.32878900	5.11309100	-1.53548100
C	5.33431100	3.41050700	0.13125000
H	6.58948600	3.28381300	-1.72961800
C	3.90427700	3.98014500	0.08101900
H	2.31599500	3.58328200	-1.40916600
C	4.15952100	5.37245000	-0.53603600
H	5.06755600	5.37273900	-2.56661100
H	6.21515700	5.69606600	-1.26536300
H	5.39007800	2.37038600	0.46442600
H	6.00118300	4.01407100	0.75582300
H	3.35943400	4.00314900	1.02818100
H	3.26625000	5.77276300	-1.02577600
H	4.45572200	6.08619200	0.23907500
Cl	2.23379400	-2.04589800	0.34779700

TS65

Pd	4.72168900	2.50238600	-4.00147600
N	5.05761400	2.59794400	-6.16414600
C	6.18340800	3.08977000	-6.70286100
C	4.10233200	2.15040900	-6.99485700
C	6.39816000	3.15354400	-8.07312700
H	6.92957800	3.44279600	-5.99969700
C	4.23517500	2.17870800	-8.37691600
H	3.20643000	1.76138800	-6.52560500
C	5.40472600	2.68953300	-8.92852100
H	7.32692800	3.56248000	-8.45538900
H	3.43030800	1.80712100	-9.00139500
H	5.53958800	2.72759700	-10.00505100
N	1.15407500	-0.66347400	-2.29823100
C	0.26999500	-0.19292800	-3.26982300
C	-1.11519300	-0.32153300	-3.16412500
C	0.77624000	0.41230000	-4.41871600
C	-1.93865100	0.19675800	-4.15394600
C	-0.04715400	0.90418400	-5.41823000
C	-1.43206800	0.81506800	-5.29750000
C	-2.41030100	1.33041800	-6.32660900
F	0.53985800	1.46959400	-6.47353500
F	2.10360600	0.51703100	-4.55727500
F	-1.66535800	-0.96680600	-2.14736600
F	-3.25358400	0.06346000	-4.00849700
F	-3.23826500	2.23319100	-5.78450700
F	-3.16290200	0.33112000	-6.80844700
F	-1.80176400	1.91220700	-7.36389200
C	1.07409700	-0.24562000	-0.96901600
O	0.10573500	0.32514100	-0.52159700
C	2.31715000	-0.58057700	-0.15926600
H	2.18426100	-0.12167500	0.82465200
H	2.35102200	-1.66487300	-0.00891400

C	3.58865400	-0.10084500	-0.82354400
C	4.81053100	-0.78173000	-0.74901400
C	3.61088100	1.10273600	-1.52804200
C	5.98604000	-0.25461100	-1.28143700
C	4.74820500	1.60222300	-2.17853400
C	5.97635300	0.95291800	-1.97931500
H	6.91395700	-0.80226100	-1.15333600
H	6.90766100	1.35368700	-2.36482800
H	2.09192500	-0.84645000	-2.63411200
C	3.75032900	3.22926100	-2.19911100
C	4.19586800	4.15822900	-1.05436800
C	2.69661700	2.29244800	-1.53510700
H	3.33859000	3.84009800	-3.02490200
C	3.05651000	5.19256800	-0.90800500
C	3.96601200	3.32572600	0.22080700
H	5.18755400	4.59359300	-1.18821400
C	2.51905700	2.94135700	-0.14383300
H	1.74940800	2.19447900	-2.07618000
C	1.87683200	4.32973000	-0.36181300
H	2.81901200	5.68882500	-1.85464700
H	3.34077900	5.96994700	-0.19050800
H	4.64372200	2.47667000	0.33552900
H	4.01805800	3.93839400	1.12717300
H	1.97891200	2.31316000	0.56771500
H	1.03553600	4.27900700	-1.06096800
H	1.49253600	4.73084500	0.58100300
Cl	4.91592200	-2.31926000	0.09469900

66

Pd	4.60964200	1.10965100	-3.87717100
N	3.40769000	1.71309000	-5.59361500
C	2.31055500	2.45099600	-5.34472800
C	3.71263100	1.45149800	-6.87331300
C	1.50361100	2.95928800	-6.35314400
H	2.06959900	2.62095100	-4.30067900
C	2.95356800	1.91444100	-7.94079500
H	4.59801600	0.84683700	-7.03640200
C	1.83096400	2.69086400	-7.67792600
H	0.62756600	3.54299000	-6.09236800
H	3.23882900	1.66140600	-8.95547700
H	1.21313700	3.06279800	-8.48798000
N	0.66132100	-0.08577300	-2.58281500
C	0.43867200	-0.10611100	-3.96376500
C	-0.66220400	0.51399200	-4.55146700
C	1.33120000	-0.77358600	-4.79868700
C	-0.82305500	0.49739400	-5.92930700
C	1.16229600	-0.79763900	-6.17438900
C	0.08883900	-0.13902400	-6.77129000
C	-0.15166400	-0.15753800	-8.26135300
F	2.07088500	-1.44847800	-6.89558800
F	2.37942700	-1.39647400	-4.26147900
F	-1.58627900	1.10377300	-3.80573100
F	-1.89577500	1.10197500	-6.43597300
F	-0.60496600	1.02774000	-8.69807700
F	-1.06778400	-1.07994300	-8.58818700
F	0.96025800	-0.42989900	-8.95272600
C	0.83932600	1.10800800	-1.89772000
O	0.55276300	2.18703000	-2.37426000
C	1.53659900	0.93915000	-0.55076700
H	1.37029400	1.85591800	0.01785300
H	1.13687000	0.08947100	0.00853100
C	2.99904000	0.77541600	-0.89146000
C	3.65550700	-0.46538000	-1.08461700
C	3.74034800	1.86748300	-1.28879700
C	4.92240100	-0.58652400	-1.63169400
C	5.03287100	1.80154800	-1.85020900
C	5.67192000	0.55483100	-2.05102900
H	5.36088500	-1.57358200	-1.72910100
H	6.72774800	0.44599600	-2.28244900
H	1.14414000	-0.89506400	-2.20862300
C	5.25014100	3.30754600	-1.72368000
C	6.06626400	3.81524100	-0.52168600

C	3.75617800	3.37993500	-1.18285500
H	5.48352500	3.83855000	-2.64864100
C	5.81605700	5.33731700	-0.44250300
C	5.25927800	3.32260200	0.69360000
H	7.12210300	3.53399400	-0.54730800
C	3.93203800	3.95471800	0.23375600
H	3.02012700	3.91688100	-1.78599600
C	4.34388700	5.43252200	0.06534500
H	5.95967000	5.82777400	-1.41084400
H	6.50836600	5.80228200	0.26689600
H	5.22061400	2.23430600	0.79604600
H	5.62306600	3.74924700	1.63450500
H	3.07203900	3.79911700	0.89058100
H	3.69019600	5.96220600	-0.63522500
H	4.29017100	5.95727300	1.02459500
Cl	2.81889200	-1.95919100	-0.64586600

TS67

Pd	0.51453800	4.02891400	-0.96553300
N	-0.57176900	5.84683700	-1.36399700
C	-1.04797200	6.61808700	-0.37638100
C	-0.81005100	6.20740900	-2.63444100
C	-1.77874900	7.77204300	-0.61670800
H	-0.83259400	6.29262100	0.63469800
C	-1.51875100	7.35565800	-2.95781800
H	-0.43826600	5.53663200	-3.39956700
C	-2.01628800	8.15167900	-1.93317800
H	-2.15179900	8.35463200	0.21790700
H	-1.68292800	7.60393000	-4.00000100
H	-2.58202600	9.05082600	-2.15572100
N	0.01859500	-0.87898900	-2.75276700
C	-1.34632100	-1.18402100	-2.73497100
C	-2.05920000	-1.15636300	-3.93319600
C	-2.05429700	-1.45218900	-1.56792300
C	-3.42109700	-1.39292000	-3.96061900
C	-3.41964500	-1.71587300	-1.59895400
C	-4.12979600	-1.68815300	-2.79571600
C	-5.61334300	-1.94581000	-2.91124400
F	-4.01418900	-1.96358100	-0.43555100
F	-1.45195700	-1.41483800	-0.38129300
F	-1.41615700	-0.88139500	-5.06640200
F	-4.05279900	-1.35302300	-5.13124900
F	-5.85075600	-2.99294600	-3.71617900
F	-6.23956000	-0.88473000	-3.43957200
F	-6.18641700	-2.20663000	-1.73425700
C	0.98065100	-1.61227600	-2.09966500
O	0.73751800	-2.63614700	-1.49487000
C	2.40412000	-1.08657500	-2.25585200
H	2.99332500	-1.57554300	-1.47388600
H	2.77918600	-1.47772800	-3.20758000
C	2.58955500	0.41056500	-2.20632100
C	3.55346700	1.08235200	-2.97180700
C	1.84610800	1.20912100	-1.33710300
C	3.80244400	2.44398800	-2.82893100
C	2.01141400	2.59285700	-1.25297900
C	3.04893000	3.21663100	-1.94734900
H	4.58617100	2.90468100	-3.42022400
H	3.26324200	4.27479000	-1.85428200
C	0.89745200	2.29147600	0.40696600
C	1.77351400	2.24171000	1.65991000
C	0.96879300	0.86257500	-0.18192900
H	-0.11918900	2.63134500	0.63921300
C	2.78497300	1.11832700	1.37169100
C	0.87044800	1.53687200	2.70631900
H	2.17137900	3.19870200	1.99505700
C	1.71398000	0.09930700	0.94106800
H	0.00035500	0.42786000	-0.42736300
H	3.31998400	0.80825600	2.27489500
H	3.51599000	1.36109400	0.59705100
H	1.35415100	1.57673600	3.68759400
H	-0.11081100	2.01204100	2.80597600
C	0.78759700	0.07483500	2.17405700

H	2.06322700	-0.88766300	0.63228700
H	1.15408400	-0.63948600	2.91698400
H	-0.23065700	-0.22204300	1.90721500
H	0.27567500	-0.02462200	-3.23376000
Cl	4.54892100	0.20284600	-4.11394400
C	1.74770400	5.16880100	0.20316700
H	1.24850300	5.31877000	1.16706500
H	2.70935200	4.67603200	0.36224200
H	1.89376900	6.12965300	-0.29874600
I	-1.32216800	2.63265300	-2.59932000

68

Pd	1.05348200	4.46989700	-1.82803400
N	-0.27831700	5.97740000	-2.41705600
C	-1.60279000	5.78821000	-2.32524900
C	0.18099100	7.11355600	-2.95884600
C	-2.51481100	6.73612500	-2.76360100
H	-1.92433800	4.84273500	-1.90633600
C	-0.66812400	8.10377000	-3.43063900
H	1.25791400	7.21706000	-3.01805300
C	-2.04140800	7.91459700	-3.32929200
H	-3.57645800	6.54009200	-2.66795800
H	-0.25032000	9.00184700	-3.87087800
H	-2.73200200	8.67023500	-3.68956100
N	-0.21323300	-0.33379700	-2.73936300
C	-1.53430600	-0.73715200	-2.54367000
C	-2.43741000	-0.66223300	-3.60720500
C	-2.02130100	-1.18911200	-1.31906000
C	-3.76165400	-1.02819800	-3.44875900
C	-3.34708800	-1.58360000	-1.16968400
C	-4.24460600	-1.50969700	-2.23108600
C	-5.70095300	-1.89842000	-2.14350800
F	-3.72096800	-2.00029700	0.03653400
F	-1.24111900	-1.21431700	-0.24108700
F	-2.01435100	-0.23461400	-4.79330600
F	-4.57758700	-0.93430700	-4.49605500
F	-5.99914500	-2.83420000	-3.05576900
F	-6.48853000	-0.83868600	-2.38474100
F	-6.03502000	-2.38370600	-0.94574600
C	0.87512900	-1.09372500	-2.37167800
O	0.77771400	-2.16369200	-1.80589500
C	2.21200200	-0.50195300	-2.79567000
H	2.98428000	-1.19705700	-2.45279000
H	2.24561700	-0.50225700	-3.89156500
C	2.49137800	0.89006300	-2.29009700
C	3.45709700	1.73322100	-2.89672700
C	1.87682300	1.44440000	-1.19135800
C	3.79262800	2.98448500	-2.41295200
C	2.18248000	2.71721300	-0.66844500
C	3.17726100	3.51376700	-1.25470500
H	4.55973500	3.55690800	-2.92143300
H	3.59407200	4.40069100	-0.79133500
C	1.41054600	2.45230900	0.62358200
C	2.22153800	2.02796000	1.86155500
C	1.00306500	1.06233700	-0.01446800
H	0.60857000	3.15326500	0.86352400
C	2.90256400	0.72188800	1.41083000
C	1.18974300	1.48588500	2.87613600
H	2.87849600	2.80718300	2.25694600
C	1.59674600	0.03596800	0.96427600
H	-0.05277800	0.90175300	-0.23255000
H	3.38669600	0.20020200	2.24282400
H	3.63748200	0.85105900	0.61014900
H	1.65933100	1.34189400	3.85435300
H	0.35027600	2.17531200	3.01494000
C	0.75444300	0.12290600	2.25427500
H	1.68460900	-0.96871900	0.54640000
H	0.99524400	-0.70951000	2.92245400
H	-0.31766200	0.07300300	2.04346000
H	-0.06658800	0.51422700	-3.29025900
Cl	4.30541700	1.17100200	-4.31533100
C	1.41412100	5.68066700	-0.22337900

H	0.45042300	6.01622600	0.17143000
H	1.96491700	5.15336400	0.56059800
H	1.99193800	6.54579200	-0.56903900
I	0.15766700	3.05971200	-4.10372400

TS69

Pd	0.91040100	3.71104600	0.13991300
N	-0.24003000	5.43376700	-0.41063200
C	-0.19029700	6.62203600	0.20571700
C	-1.09631400	5.26012600	-1.43155000
C	-1.00037800	7.68507100	-0.16410700
H	0.52661900	6.71392800	1.01412800
C	-1.93213500	6.28056500	-1.86518600
H	-1.09321200	4.27741200	-1.89730100
C	-1.88911400	7.51118900	-1.22017800
H	-0.93000500	8.62688000	0.36823300
H	-2.60502300	6.10006700	-2.69573400
H	-2.53688300	8.32312100	-1.53556200
N	-0.65259500	-0.71263300	-2.54072400
C	-1.81281600	-0.78787700	-3.31208800
C	-1.93721500	0.01631400	-4.44507100
C	-2.89683300	-1.58418300	-2.95589400
C	-3.10042100	0.01038900	-5.19400400
C	-4.05463300	-1.61013900	-3.72594800
C	-4.17736000	-0.81326800	-4.86211000
C	-5.40749300	-0.77037100	-5.73588900
F	-5.04440800	-2.39650600	-3.31111700
F	-2.86290200	-2.29673000	-1.83477100
F	-0.92614400	0.79527800	-4.81394200
F	-3.17385700	0.80064100	-6.26466600
F	-5.09178000	-1.00973100	-7.01711800
F	-5.98357500	0.44218000	-5.68677200
F	-6.32918700	-1.66683000	-5.37718000
C	0.08419000	-1.81868900	-2.19422900
O	-0.22172200	-2.95051500	-2.50545900
C	1.31636200	-1.53208000	-1.32636500
H	1.01710500	-1.73219400	-0.29166000
H	2.05709300	-2.28746100	-1.60008600
C	1.86004900	-0.13563200	-1.44236300
C	2.49720300	0.33005700	-2.60004200
C	1.69378000	0.79826000	-0.42374100
C	2.98211200	1.62865400	-2.71237400
C	2.06527300	2.13454700	-0.56701800
C	2.78052200	2.55264600	-1.68830100
H	3.49268000	1.92831000	-3.62105100
H	3.14148600	3.56638700	-1.81091300
C	1.73923900	2.11186800	1.41862000
C	3.07656900	2.01304400	2.15567800
C	1.38582200	0.65045100	1.02961100
H	0.98259000	2.59968700	2.04770500
C	3.72978700	0.74164500	1.58706500
C	2.68765200	1.51179600	3.56956200
H	3.67149900	2.92690700	2.15578300
C	2.48165500	-0.13709400	1.79496600
H	0.36828300	0.34426900	1.28548400
H	4.57771000	0.40923800	2.19445000
H	4.05527200	0.82543000	0.54844400
H	3.56483000	1.53527900	4.22434300
H	1.91341500	2.12867300	4.03696400
C	2.22051100	0.04771800	3.30529300
H	2.57052200	-1.17896400	1.47831500
H	2.80783700	-0.66652900	3.88983900
H	1.16677700	-0.10821000	3.55774200
H	-0.34230000	0.24149800	-2.34293600
Cl	2.72370800	-0.75328700	-3.95218600
C	2.54520600	4.89292200	0.38270600
H	2.45560700	5.35517500	1.37426100
H	3.47726500	4.32428300	0.33703900
H	2.54526000	5.66710600	-0.39133500
O	-0.92478700	2.57373100	0.24778200
C	-1.38988300	1.97147700	-0.77707000
C	-2.60521300	1.09117300	-0.52296600

H	-2.28281300	0.04539500	-0.45956700
H	-3.10239700	1.35934700	0.41074700
H	-3.30374200	1.16621800	-1.36080200
O	-0.91212800	2.04400100	-1.92707100

TS-I-norbornene

Pd	1.40702800	2.85671000	-0.37986900
N	-0.27044300	3.86460000	0.66603200
C	-0.23139200	5.16426600	0.98083600
C	-1.43676600	3.21439400	0.77628300
C	-1.35061700	5.86152300	1.41438100
H	0.72875800	5.65626600	0.86272000
C	-2.60560000	3.83359800	1.19206000
H	-1.42764900	2.16389200	0.50928400
C	-2.56200300	5.18561000	1.51491400
H	-1.26977900	6.91652700	1.65073200
H	-3.52625600	3.26407500	1.23405900
H	-3.45957000	5.70593900	1.83369900
N	0.19075900	-0.77002000	-2.51430900
C	-1.12600700	-0.31661500	-2.41379200
C	-1.80578400	0.04403700	-3.57414200
C	-1.76903800	-0.07102200	-1.20042800
C	-3.05633800	0.64928500	-3.54024700
C	-3.02073600	0.51290800	-1.16851200
C	-3.69241000	0.89431700	-2.32668600
C	-5.03108300	1.57501600	-2.18219200
F	-3.55946100	0.76452000	0.03028000
F	-1.16657900	-0.29985500	-0.02963900
F	-1.21576700	-0.14740400	-4.75137600
F	-3.61119600	0.97539300	-4.70041600
F	-5.89541500	0.78883300	-1.52230000
F	-5.58206000	1.88770200	-3.35401800
F	-4.90821200	2.71068900	-1.47372900
C	0.73969600	-1.80198700	-1.78087600
O	0.06908300	-2.54970600	-1.09959100
C	2.26624600	-1.91900000	-1.89558500
H	2.57829300	-2.51464600	-1.03607500
H	2.49072800	-2.51385900	-2.78615500
C	2.93345300	-0.56201800	-1.98737700
C	3.66978700	-0.15769400	-3.10478300
C	2.60506100	0.43427900	-1.04176500
C	4.00264100	1.17767300	-3.32805800
C	2.74195000	1.77925200	-1.37502700
C	3.47886500	2.15682400	-2.49341700
H	4.58516000	1.44702700	-4.20226100
H	3.59433600	3.20303400	-2.75550400
C	1.72315200	1.31477700	1.23235900
C	2.42835600	0.87671400	2.53052900
C	1.96911700	0.09238600	0.28176200
H	0.66691300	1.49438900	1.43831800
C	3.64670600	0.09864500	2.01492700
C	1.55696900	-0.26529600	3.12019600
H	2.61481300	1.67134000	3.25284600
C	2.81769400	-0.86797600	1.16448800
H	0.98835700	-0.35402200	0.10787700
H	4.19827400	-0.40521900	2.81540500
H	4.34766000	0.69423200	1.42257000
H	1.85545500	-0.45218500	4.15658000
H	0.49247000	-0.00906500	3.13177500
C	1.87346100	-1.48484400	2.20702900
H	3.39923300	-1.59075900	0.59253200
H	2.37970600	-2.27653700	2.76846200
H	0.98340300	-1.92150800	1.74457900
H	0.79791700	-0.21315300	-3.10375700
Cl	4.18073000	-1.32756000	-4.31163500
C	2.79268600	3.15180500	1.21947800
H	2.32957300	3.47851400	2.14846900
H	3.72398400	2.62037400	1.37829600
H	3.02988700	4.03376800	0.59961900
I	0.08863400	3.32625200	-2.69365900

TS-AcO-Norbornene

Pd	1.59255800	2.94079200	-0.24875500
N	-0.32436600	3.82631300	0.48464400
C	-0.54179900	5.13809300	0.32211500
C	-1.37902700	3.02972000	0.70384800
C	-1.80937600	5.69975100	0.38713400
H	0.33364900	5.74227200	0.11073300
C	-2.68095600	3.50484200	0.77946400
H	-1.17424300	1.96883600	0.80696600
C	-2.90045700	4.86734200	0.61496900
H	-1.93386700	6.76744800	0.24605100
H	-3.49777600	2.81403400	0.95120000
H	-3.90661700	5.27209600	0.65631900
N	0.03525600	-0.59336900	-2.36056100
C	-1.29173900	-0.25018900	-2.09296700
C	-2.05576100	0.29830400	-3.12466600
C	-1.85760600	-0.25477900	-0.82206400
C	-3.30446900	0.84134700	-2.88664800
C	-3.12017200	0.27264400	-0.58700400
C	-3.86986000	0.84046000	-1.61099100
C	-5.20349600	1.51260500	-1.40805100
F	-3.53579400	0.28839400	0.68342800
F	-1.16127000	-0.65496400	0.24663800
F	-1.55349700	0.35156300	-4.35260300
F	-3.96731600	1.38686000	-3.90440300
F	-5.66642300	1.36886100	-0.15948600
F	-6.12969700	1.02376700	-2.23977400
F	-5.10772400	2.83342100	-1.64263700
C	0.67835400	-1.69937600	-1.85903400
O	0.09278800	-2.60589900	-1.29973500
C	2.19535700	-1.73524700	-2.09014500
H	2.58645200	-2.40212400	-1.31899600
H	2.35511800	-2.24616300	-3.04403600
C	2.87045400	-0.38036800	-2.10754000
C	3.59617200	0.08500800	-3.21054000
C	2.64600200	0.53993100	-1.06228700
C	4.02471600	1.40619800	-3.31791300
C	2.91398500	1.89286600	-1.25518900
C	3.63287900	2.33269200	-2.35823000
H	4.59290600	1.71485400	-4.18882000
H	3.82575200	3.38908500	-2.51181400
C	1.75456500	1.28306600	1.27276200
C	2.38643400	0.68141100	2.54849500
C	1.98278000	0.12972800	0.22815600
H	0.69802700	1.47060800	1.46589000
C	3.60604100	-0.06937600	1.99789800
C	1.46492700	-0.48897100	2.98642300
H	2.56573200	1.39165700	3.35570900
C	2.78641700	-0.93212400	1.03453200
H	0.98988700	-0.26443300	0.00826900
H	4.12488800	-0.65892300	2.76083700
H	4.33431000	0.56705400	1.48574900
H	1.70095400	-0.77413300	4.01650000
H	0.40637700	-0.20945400	2.96228800
C	1.80376400	-1.62984800	1.98457200
H	3.37136700	-1.60526300	0.40773500
H	2.28825700	-2.46977000	2.49289200
H	0.92846700	-2.01961700	1.45806500
H	0.56129800	0.18352700	-2.75645800
Cl	3.98347900	-0.98762300	-4.54730500
C	2.81418000	3.04885000	1.51575500
H	2.27705300	3.28303400	2.43256400
H	3.73627700	2.50895200	1.69966500
H	3.09089600	3.99092500	1.01512000
O	1.16949900	4.01971000	-2.03156800
C	0.48061500	3.28266300	-2.82356800
C	0.18844800	3.88107800	-4.18616900
H	-0.47046100	3.22419100	-4.75587600
H	-0.26778700	4.86890500	-4.07525300
H	1.13065500	4.01387900	-4.72756400
O	0.07646000	2.14595100	-2.53497400

70

Pd	0.62896400	1.73415200	-0.25715200
N	-1.07488300	2.88412800	0.62909500
C	-1.66705300	3.86485700	-0.06898100
C	-1.73208300	2.35502600	1.66897000
C	-2.94012100	4.33030300	0.22436800
H	-1.10373000	4.25824400	-0.90957100
C	-3.00619600	2.76579400	2.03694600
H	-1.22282700	1.55613700	2.19744800
C	-3.62783900	3.76103400	1.29209200
H	-3.39392600	5.09593600	-0.39346700
H	-3.50553100	2.28933800	2.87261700
H	-4.63784400	4.08017600	1.52725300
N	-0.68084100	0.44486000	-1.13317400
C	-1.87535400	0.99406900	-1.58310000
C	-1.88429900	1.89685900	-2.64741400
C	-3.09118400	0.79468900	-0.91998100
C	-3.02902900	2.58997400	-3.01714000
C	-4.23458800	1.47862300	-1.29103200
C	-4.23710200	2.38402900	-2.35402900
C	-5.48400100	3.17746500	-2.64063800
F	-5.33964700	1.30250600	-0.56388500
F	-3.13826900	0.01668300	0.15887300
F	-0.74713500	2.17013000	-3.28953400
F	-2.92119000	3.47350600	-4.00942700
F	-5.44416100	3.79516100	-3.82315000
F	-5.66402400	4.13180000	-1.69916900
F	-6.57573200	2.40475400	-2.62780100
C	-0.57810500	-0.91513300	-1.05690200
O	-1.45193100	-1.68920900	-1.41740600
C	0.74787500	-1.42006100	-0.48556400
H	0.74095200	-1.23788400	0.59777900
H	0.77047800	-2.50049700	-0.64003600
C	1.94096500	-0.74675200	-1.11982300
C	2.94227200	-1.51017500	-1.72092600
C	2.02515300	0.65074700	-1.15560100
C	4.00101100	-0.88307700	-2.36868900
H	2.89054500	-2.59444500	-1.69803200
C	3.06917300	1.26103700	-1.85036100
C	4.07089300	0.50028000	-2.45566300
H	3.12049500	2.34419800	-1.92969900
H	4.88589500	0.97700100	-2.99005700
I	2.44721100	3.16697700	1.24735600
C	4.02011300	1.68962400	1.43000200
H	4.32648400	1.43407000	0.41754000
H	4.82056200	2.15002000	2.00587000
H	3.58888500	0.83197900	1.94112800
Cl	5.25460700	-1.85846500	-3.10541800

TS71

Pd	0.76453400	1.71340000	-0.52387500
N	-0.90228800	2.85943100	0.47878900
C	-1.47258700	3.88408100	-0.17165900
C	-1.54223500	2.33910500	1.53249600
C	-2.71161400	4.39782800	0.18155500
H	-0.91843500	4.28030700	-1.01679900
C	-2.77685400	2.80235600	1.96578200
H	-1.05944900	1.50108800	2.02392600
C	-3.38153500	3.83965300	1.26592500
H	-3.15154300	5.19964900	-0.39950300
H	-3.26188100	2.33280600	2.81359800
H	-4.36375700	4.20212200	1.55036700
N	-0.62584100	0.39461900	-1.23912900
C	-1.84632700	0.94361400	-1.61743500
C	-1.91687800	1.83218400	-2.69095800
C	-3.01605600	0.76369000	-0.87257300
C	-3.07569800	2.53512300	-2.99203200
C	-4.17311400	1.45880800	-1.17314000
C	-4.23638000	2.35308400	-2.24335200
C	-5.48871900	3.16490300	-2.44480700
F	-5.22720300	1.30637000	-0.37000800
F	-2.99644100	0.00223500	0.21896700

F	-0.81938600	2.08548200	-3.40724500
F	-3.02569000	3.40521700	-3.99953100
F	-5.51953900	3.78233700	-3.62744900
F	-5.58801500	4.12011700	-1.49346200
F	-6.58759800	2.40778300	-2.35679000
C	-0.51742100	-0.96363300	-1.14453300
O	-1.41791900	-1.74366200	-1.40929700
C	0.85169900	-1.45459100	-0.67475300
H	0.94732200	-1.25206900	0.40137000
H	0.85253500	-2.53651300	-0.79307400
C	1.98283200	-0.80795100	-1.43764200
C	2.94886500	-1.55463700	-2.12382000
C	2.06179900	0.58881700	-1.54782900
C	3.91722100	-0.95880700	-2.92602000
C	3.00439300	1.19980100	-2.36819000
C	3.92968700	0.42117700	-3.06021500
H	4.63869100	-1.57857600	-3.44632900
H	3.02876400	2.27759900	-2.47868600
H	4.66644400	0.89610200	-3.70087800
I	2.50720400	3.56453100	0.31781200
C	2.06601200	1.30461200	1.46214300
H	2.96285800	0.80498200	1.11213400
H	2.18035600	1.84667200	2.39314700
H	1.19008100	0.65631500	1.48648600
Cl	2.98143500	-3.30605100	-2.00926500

72

Pd	0.76064500	1.51413000	-0.38548100
N	-0.88471000	2.82865400	0.52842000
C	-1.02295600	4.09251900	0.10307100
C	-1.88812700	2.27431600	1.22045800
C	-2.17952800	4.82860400	0.31825800
H	-0.17897200	4.51107100	-0.43429100
C	-3.07317600	2.94273500	1.49055800
H	-1.74666900	1.24290600	1.52881100
C	-3.23037800	4.23930900	1.01254300
H	-2.25368300	5.83791800	-0.06987500
H	-3.86381700	2.44035500	2.03621400
H	-4.15873500	4.77686300	1.17364400
N	-0.67390500	0.19649500	-1.03249400
C	-1.87179600	0.78106800	-1.43737900
C	-1.85533500	1.93967000	-2.21181500
C	-3.12333600	0.34844400	-0.98894700
C	-2.99862400	2.66496300	-2.50084300
C	-4.27611200	1.04366600	-1.31346300
C	-4.24581800	2.21383000	-2.07350400
C	-5.52038300	2.99467500	-2.26941600
F	-5.43050400	0.61095000	-0.80972200
F	-3.21597100	-0.66992300	-0.14032200
F	-0.66495900	2.44731800	-2.58854800
F	-2.85511000	3.80529400	-3.17087800
F	-5.40344000	3.94139800	-3.20352300
F	-5.87652000	3.60580600	-1.12144900
F	-6.53274400	2.19821200	-2.62697600
C	-0.51567400	-1.15221700	-1.25601500
O	-1.37697700	-1.84807200	-1.76262600
C	0.82920400	-1.73596000	-0.84631400
H	0.92197200	-1.73988800	0.24468100
H	0.80835900	-2.77672900	-1.16254300
C	1.97780100	-0.99805800	-1.48534700
C	2.93579200	-1.66923300	-2.25962000
C	2.09188500	0.39849600	-1.41325000
C	3.91703900	-0.99707100	-2.97925200
C	3.04840500	1.09087700	-2.15059500
C	3.95353200	0.38709800	-2.94039200
H	4.62945800	-1.56083000	-3.57063200
H	3.11508100	2.16983700	-2.11324200
H	4.70138800	0.92840600	-3.51099400
I	2.55039800	3.34287300	0.46687000
C	1.07129600	0.55802800	1.39225000
H	2.04783300	0.08149600	1.35237000
H	1.01376800	1.33667300	2.14878100

H	0.23986700	-0.14252100	1.43203200
Cl	2.93465200	-3.41888300	-2.37190200

TS73

Pd	0.34778600	0.86192100	0.11929300
N	-0.70966700	2.75368500	-0.08567200
C	-0.40313900	3.48986300	-1.16207500
C	-1.74236000	3.11879200	0.68811500
C	-1.14047900	4.60843900	-1.52226200
H	0.43800100	3.14955400	-1.75541300
C	-2.54100500	4.20885700	0.38063100
H	-1.92539300	2.50819900	1.56522500
C	-2.23991200	4.96273200	-0.74955100
H	-0.86691400	5.16764800	-2.40923400
H	-3.39050900	4.44792200	1.00908000
H	-2.85668300	5.81226100	-1.02376200
N	-0.79501900	0.18015500	-1.43815000
C	-2.12696500	0.59528800	-1.33559300
C	-2.67656800	1.51328700	-2.23546400
C	-2.92521900	0.20731000	-0.26311000
C	-3.93062300	2.05456900	-2.02837400
C	-4.18724800	0.75037700	-0.04902700
C	-4.71461000	1.68828800	-0.93149600
C	-6.02745500	2.39886300	-0.71839200
F	-4.84850500	0.35450700	1.03505100
F	-2.44888600	-0.65693100	0.63882700
F	-1.94890600	1.94801400	-3.25942400
F	-4.37144000	2.98377700	-2.87547900
F	-6.78819900	2.35743700	-1.81771700
F	-5.80934300	3.69890000	-0.43155000
F	-6.73781100	1.88478000	0.28600900
C	-0.48570500	-0.58598200	-2.51924500
O	-1.31867400	-0.95014900	-3.33587400
C	0.94464700	-1.07246500	-2.66808800
H	0.95956600	-2.09617400	-2.26632000
H	1.08906600	-1.18915900	-3.74053300
C	2.08568400	-0.30168400	-2.06452800
C	3.28086900	-0.12980900	-2.78749600
C	2.09832300	0.19298200	-0.75016200
C	4.41942000	0.45026900	-2.24150100
C	3.24366100	0.72533700	-0.16197000
C	4.40028200	0.86324000	-0.91926500
H	5.31245000	0.55214600	-2.84729400
H	3.23913500	1.04092700	0.87132000
H	5.28700700	1.29558200	-0.46754900
I	1.12084100	1.74174600	2.56222100
C	0.99164700	-1.10608500	0.61556900
H	1.83523800	-1.15092600	1.29790900
H	0.04451000	-1.21106300	1.15708400
H	1.04383600	-1.85470500	-0.16901100
Cl	3.41257900	-0.67857600	-4.44708700

74

Pd	0.71473500	1.68705900	-1.21985200
N	-0.70212900	3.16781100	-1.05818500
C	-0.89135500	4.02574400	-2.07064000
C	-1.52474800	3.19373200	0.00172200
C	-1.95164900	4.91953900	-2.07461000
H	-0.17922200	3.97437100	-2.88399100
C	-2.60467900	4.05834200	0.06371200
H	-1.30730700	2.48914900	0.79532800
C	-2.83154500	4.92709100	-0.99895000
H	-2.08402300	5.58463100	-2.91959800
H	-3.26302600	4.03453400	0.92400200
H	-3.68411400	5.59736900	-0.98787100
N	-0.72122900	0.37903500	-1.87728500
C	-2.07646800	0.68435100	-1.72581700
C	-2.73501500	1.48873900	-2.65541100
C	-2.79572500	0.30817900	-0.59431100
C	-4.01687100	1.95525700	-2.42423400
C	-4.09109800	0.75405300	-0.36547900

C	-4.72693400	1.59343900	-1.27882600
C	-6.07758700	2.21914800	-1.03840200
F	-4.67704500	0.38915200	0.77262100
F	-2.20595100	-0.43540200	0.34321400
F	-2.09105100	1.89336200	-3.74939300
F	-4.55753900	2.79489000	-3.30720300
F	-6.85823600	2.13281900	-2.12061900
F	-5.93647200	3.53080600	-0.75094400
F	-6.73365500	1.65955200	-0.02117300
C	-0.42648200	-0.87250200	-2.33080700
O	-1.25767600	-1.71863000	-2.61526800
C	1.05926500	-1.12339300	-2.52051200
H	1.25127300	-2.16389200	-2.24046300
H	1.24275800	-1.05542700	-3.59538700
C	2.02415800	-0.21935800	-1.77307200
C	3.04810700	0.48547200	-2.47436100
C	2.22986500	-0.42972500	-0.37279100
C	4.22040100	0.88895800	-1.86595000
C	3.41022300	0.01317100	0.23117200
C	4.40159600	0.63531300	-0.50800100
H	4.97201800	1.41918600	-2.43807600
H	3.55198700	-0.15344500	1.29397800
H	5.31656900	0.95989000	-0.02413500
I	2.38341500	3.55950900	-0.26368100
C	1.26973400	-1.27711100	0.42386100
H	1.42773500	-2.33841100	0.19308500
H	1.43975700	-1.13991900	1.49463300
H	0.22444900	-1.04766800	0.21148700
Cl	2.87144300	0.81398600	-4.18027700

75

Pd	0.70322500	1.57444100	-0.84199100
N	-0.71995200	3.04116200	-0.46516500
C	-0.84843000	4.05513300	-1.33372900
C	-1.60608700	2.90065500	0.53407900
C	-1.91305100	4.94345200	-1.25316100
H	-0.07044100	4.13449700	-2.08325100
C	-2.69062200	3.74993800	0.67411400
H	-1.44065700	2.07004600	1.21052900
C	-2.85752600	4.77980100	-0.24837000
H	-1.99863700	5.73571100	-1.98745500
H	-3.40323200	3.58839400	1.47419400
H	-3.71603700	5.43990000	-0.18313000
N	-0.67749700	0.37324600	-1.72642500
C	-2.04057300	0.63972400	-1.56558000
C	-2.68313500	1.59429400	-2.35311300
C	-2.78351900	0.06513300	-0.53736200
C	-3.97439700	2.00783100	-2.07270100
C	-4.08645000	0.45818600	-0.26438300
C	-4.70927900	1.44319200	-1.02963600
C	-6.06636100	2.01152600	-0.70054000
F	-4.69553100	-0.10150300	0.77918900
F	-2.20939300	-0.82878600	0.27009600
F	-2.01952500	2.18748200	-3.34330600
F	-4.49744100	2.99070800	-2.80562600
F	-6.80404100	2.19542800	-1.80030600
F	-5.93416900	3.21562700	-0.10262300
F	-6.76606900	1.23370700	0.12724900
C	-0.34836300	-0.81743800	-2.30434200
O	-1.15433400	-1.63446200	-2.71750600
C	1.15089400	-1.03789800	-2.45636500
H	1.34094600	-2.09855500	-2.26544000
H	1.37822600	-0.86860300	-3.51123400
C	2.06045700	-0.19461800	-1.58340900
C	3.05831000	0.65126800	-2.15188200
C	2.19633300	-0.52149100	-0.19602800
C	4.13233000	1.11968400	-1.41581400
C	3.28040700	-0.02399300	0.53220400
C	4.23771500	0.77498100	-0.07024200
H	4.86625800	1.76138700	-1.88905000
H	3.37125600	-0.27905600	1.58305800
H	5.07671900	1.14568700	0.50992400

C	1.26930600	-1.52584300	0.44352600
H	1.39315600	-1.52133600	1.52940400
H	0.21896300	-1.33245900	0.21870500
H	1.50202400	-2.53594000	0.08353300
O	2.16711400	3.97937900	-1.72581500
C	2.50495500	3.72188700	-0.57315800
O	2.03930400	2.73509000	0.13560500
C	3.57240600	4.52688900	0.14471400
H	4.52429100	3.98808300	0.07403000
H	3.68886100	5.50222500	-0.33079300
H	3.33381300	4.64215100	1.20457700
Cl	2.98951100	1.08004600	-3.83787300

76

Pd	-0.39171100	2.45339700	0.30702400
N	-0.01723500	4.10841400	1.49598700
C	1.21900900	4.61832600	1.57972100
C	-1.02817000	4.72249100	2.12372000
C	1.49042300	5.76442200	2.31020000
H	1.98526900	4.09034100	1.02422700
C	-0.83648100	5.87919200	2.86397900
H	-2.00366700	4.26269100	2.02185400
C	0.44469900	6.40989400	2.96116600
H	2.50446200	6.14466700	2.35455200
H	-1.68368000	6.35199400	3.34724800
H	0.62493500	7.31640200	3.53002600
N	-0.73332600	0.76092700	-0.83775400
C	-1.93090100	0.68982700	-1.58566400
C	-2.60434000	1.79671700	-2.09268300
C	-2.53102800	-0.55767700	-1.79355000
C	-3.82280000	1.67692400	-2.75562700
C	-3.73196000	-0.68316300	-2.46497900
C	-4.40671800	0.43219500	-2.96531000
C	-5.73423300	0.22255500	-3.65147000
F	-4.25665600	-1.89848700	-2.61334400
F	-1.94392100	-1.65084200	-1.31177800
F	-2.10361300	3.02295600	-1.93892300
F	-4.39535400	2.80061700	-3.17930900
F	-6.21852000	1.34194500	-4.19456600
F	-6.65058600	-0.23194000	-2.77990000
F	-5.62952200	-0.68672500	-4.63027000
C	0.37340000	0.18113900	-1.47622900
O	0.32780600	-0.25888600	-2.60629200
C	1.63797500	0.12501300	-0.62536100
H	2.14624500	1.08026400	-0.78173400
H	1.37002000	0.08365400	0.43415100
C	2.53071200	-1.02587200	-1.00343600
C	2.41322900	-2.27192200	-0.38476700
C	3.49980400	-0.87757200	-2.01295000
C	3.23016300	-3.34907800	-0.70953900
C	4.32032400	-1.95592200	-2.34013800
C	4.19348700	-3.18106100	-1.69416400
H	3.10201000	-4.29883200	-0.20261100
H	5.06702100	-1.83514500	-3.12022000
H	4.84014500	-4.01046700	-1.96372800
C	3.64060100	0.43150500	-2.74991200
H	4.38586600	0.35021300	-3.54599500
H	2.68628900	0.72260800	-3.19969800
H	3.95533100	1.24211100	-2.08111400
O	-0.00193000	4.98218700	-1.36876700
C	0.85410700	4.15364600	-1.62009400
O	1.02402000	3.01362800	-0.98310500
C	1.88033000	4.32864900	-2.72559200
H	1.71997800	3.56309600	-3.49133100
H	1.78226400	5.31935900	-3.17119600
H	2.89194300	4.19010600	-2.33223400
O	-1.80642300	1.82572100	1.75027500
C	-2.04249500	0.64374100	2.05785900
O	-1.60057200	-0.38238800	1.40425000
H	-1.13292700	-0.07536800	0.54518300
C	-2.88966400	0.31629200	3.24944400
H	-3.16593100	1.22629900	3.78077500

H	-3.78758400	-0.21305300	2.91759900
H	-2.33622200	-0.35703000	3.90966500
Cl	1.18148700	-2.53019300	0.84260300

TS77

Pd	-0.43773100	2.54012500	0.41242400
N	0.04802900	4.19982800	1.54470500
C	1.26741300	4.74920200	1.45602700
C	-0.88434900	4.77921400	2.31277600
C	1.59992500	5.90499100	2.14418500
H	1.96640800	4.23911800	0.80443000
C	-0.62768400	5.94314900	3.02170600
H	-1.84470100	4.28009000	2.35372600
C	0.63525200	6.51738900	2.93644400
H	2.59669900	6.31881000	2.04488800
H	-1.41223100	6.38643600	3.62407500
H	0.86368700	7.43066200	3.47655000
N	-0.88679200	0.79911700	-0.67951500
C	-2.03356700	0.78811300	-1.52109300
C	-2.66341200	1.92379400	-2.01410700
C	-2.60939500	-0.44521200	-1.84275400
C	-3.82016000	1.84255700	-2.78674900
C	-3.74837400	-0.53110800	-2.62037400
C	-4.38347200	0.61289300	-3.10714700
C	-5.63496400	0.43908800	-3.93436100
F	-4.24819200	-1.73448500	-2.89261000
F	-2.05086000	-1.56169700	-1.38469900
F	-2.18555400	3.13962800	-1.75303100
F	-4.35243500	2.98869400	-3.19952700
F	-6.15376000	1.60015200	-4.33914800
F	-6.58079700	-0.20105600	-3.22932200
F	-5.38370100	-0.29484900	-5.02730000
C	0.26792800	0.24069200	-1.29495000
O	0.30905200	-0.03519600	-2.46982100
C	1.42697400	0.01646400	-0.33242500
H	1.91875300	0.98721500	-0.21941000
H	1.03385400	-0.26084400	0.64983600
C	2.40361700	-1.00936100	-0.84017100
C	2.28142600	-2.35941600	-0.50526100
C	3.45875500	-0.62829000	-1.68874500
C	3.17617000	-3.32284800	-0.95766800
C	4.35598200	-1.59325100	-2.14334800
C	4.22243400	-2.92892600	-1.77986900
H	3.04285400	-4.36063400	-0.67362100
H	5.16782400	-1.29311500	-2.80013600
H	4.92969000	-3.66789600	-2.14364500
C	3.61359800	0.81038800	-2.11627200
H	4.40126000	0.90746300	-2.86861700
H	2.68180700	1.19498100	-2.54084200
H	3.87749500	1.45808100	-1.27066500
O	0.04345100	4.97110600	-1.40604300
C	0.81480200	4.06542900	-1.66638700
O	0.96305200	2.96652800	-0.95430200
C	1.73450800	4.08362000	-2.87322400
H	1.41447000	3.30763100	-3.57620400
H	1.68892600	5.05851400	-3.36029200
H	2.76326800	3.85466200	-2.57970200
O	-1.79943000	1.99286200	1.89914400
C	-2.07902400	0.79298100	2.15865400
O	-1.72691900	-0.20136100	1.44261900
H	-1.25925700	0.16306600	0.45530300
C	-2.88128500	0.48421900	3.39108500
H	-3.13810700	1.39873400	3.92534300
H	-3.78861200	-0.05538500	3.10626800
H	-2.29632300	-0.17628800	4.03763700
Cl	0.95014400	-2.89569100	0.50571000

78

N	-0.60624900	-0.35061600	-1.20030700
C	-1.75035700	-0.02058500	-1.93057200
C	-3.00682900	-0.14891400	-1.34550200

C	-1.68965100	0.40523200	-3.25816300
C	-4.17220900	0.14978500	-2.03813200
C	-2.85252700	0.73215300	-3.93834400
C	-4.11223800	0.61421400	-3.35033200
C	-5.32494600	0.96963100	-4.17943500
F	-2.74883300	1.13723600	-5.20096800
F	-0.52961000	0.47047700	-3.89664600
F	-3.08987800	-0.58087600	-0.08425500
F	-5.32468900	-0.00933700	-1.39641000
F	-6.46229900	0.88839600	-3.48613900
F	-5.43318500	0.14859100	-5.23430100
F	-5.22630700	2.21996800	-4.65057500
C	0.47603100	0.50230200	-1.07813900
O	0.51895700	1.58502500	-1.62171800
C	1.60914300	-0.05669700	-0.22081500
H	2.32064000	0.75929200	-0.08685200
H	1.22066900	-0.32254200	0.76665200
C	2.27781100	-1.25044000	-0.86940600
C	1.94988400	-2.56610200	-0.52984200
C	3.25109400	-1.05219000	-1.86971500
C	2.55048300	-3.66841300	-1.12603700
C	3.85252700	-2.15793300	-2.46936800
C	3.51126500	-3.45510500	-2.10416600
H	2.26436600	-4.67038300	-0.82689900
H	4.60209700	-1.99668200	-3.23882500
H	3.99040200	-4.30321700	-2.58276800
C	3.65431400	0.34111100	-2.28830600
H	4.33273900	0.30449000	-3.14449900
H	2.78942800	0.95330900	-2.56036500
H	4.17607000	0.86118400	-1.47516700
H	-0.67632200	-1.13084900	-0.55928000
Cl	0.72225400	-2.89222100	0.69349700

79

Pd	0.60545100	1.68950200	-0.15979600
N	-1.12686400	2.76678200	0.77135300
C	-1.69111400	3.80004000	0.12765500
C	-1.83759500	2.14086400	1.71845700
C	-2.98618900	4.22569200	0.38295500
H	-1.08333700	4.27330300	-0.63749500
C	-3.13717600	2.50559300	2.04326600
H	-1.34979800	1.30217700	2.20396600
C	-3.72775300	3.55737800	1.35282800
H	-3.41364900	5.03916700	-0.19092600
H	-3.67929800	1.95113800	2.80046000
H	-4.75466800	3.84418900	1.55389000
N	-0.68048000	0.46484400	-1.15099800
C	-1.84573800	1.04279800	-1.63165700
C	-1.78921500	2.02362800	-2.62466100
C	-3.10065500	0.80630300	-1.05851500
C	-2.90671900	2.74996600	-3.00943800
C	-4.21819600	1.52301900	-1.44807700
C	-4.15503200	2.50301900	-2.44039400
C	-5.37420700	3.33118300	-2.74689700
F	-5.36324900	1.30210700	-0.79961500
F	-3.21708800	-0.04001700	-0.03802400
F	-0.61344300	2.33666100	-3.17543100
F	-2.73670600	3.70524400	-3.92378000
F	-5.27378100	3.98682100	-3.90552900
F	-5.57285700	4.25761700	-1.78163300
F	-6.48129800	2.58302400	-2.80458400
C	-0.58321200	-0.89744100	-1.08432700
O	-1.43379700	-1.66841000	-1.50003700
C	0.71710100	-1.40082500	-0.44954600
H	0.67123400	-1.20194100	0.62974200
H	0.74289700	-2.48323400	-0.58911900
C	1.92995100	-0.73835600	-1.06065500
C	2.93267400	-1.51294000	-1.64181700
C	2.00525200	0.65899500	-1.12106400
C	3.97869900	-0.88407200	-2.30539800
H	2.88844500	-2.59653200	-1.59711000
C	3.01111600	1.28457300	-1.86758600

C	4.01471900	0.49487200	-2.44389700
H	4.81182100	0.95960400	-3.01673200
I	2.32541300	2.89048500	1.64731100
C	4.16869900	1.78172900	1.39664000
H	4.10905200	1.29883800	0.42186300
H	4.98232800	2.50193400	1.44987800
H	4.21581900	1.05403800	2.20368700
Cl	5.25001900	-1.85277600	-3.02073200
C	3.04879600	2.78029600	-2.08350400
H	2.03744000	3.19218400	-2.15305900
H	3.56341500	3.30086100	-1.26566900
H	3.57704100	3.02381400	-3.01019100

TS80

Pd	0.82907700	1.70505900	-0.46049000
N	-0.79817500	3.00977500	0.45384800
C	-0.93847600	4.25122000	-0.03255400
C	-1.82770700	2.46719600	1.11622400
C	-2.11471800	4.97658400	0.09297200
H	-0.07930700	4.65908200	-0.55496800
C	-3.03618900	3.12451700	1.29761300
H	-1.68740000	1.44994600	1.46942000
C	-3.18985400	4.39717400	0.75885800
H	-2.18765300	5.96580600	-0.34413600
H	-3.84908600	2.62801900	1.81534000
H	-4.13564300	4.92088600	0.84649900
N	-0.58997700	0.36599400	-1.12708700
C	-1.83804000	0.85799000	-1.48004600
C	-1.95469900	1.97276200	-2.31329900
C	-3.02849700	0.39135600	-0.90548300
C	-3.16252400	2.61496800	-2.53620900
C	-4.24198400	1.00319900	-1.16211000
C	-4.34414400	2.12824300	-1.98157400
C	-5.67033700	2.82972500	-2.10266200
F	-5.32274000	0.54479600	-0.52910700
F	-2.99404200	-0.56837900	0.01689300
F	-0.84925800	2.51385500	-2.84536800
F	-3.14266900	3.71751900	-3.28385700
F	-5.68542800	3.74065400	-3.07914200
F	-5.96945100	3.47374900	-0.95351000
F	-6.66491600	1.96768400	-2.34074700
C	-0.38692700	-0.99118300	-1.17039200
O	-1.20648700	-1.79141400	-1.58724900
C	0.97428900	-1.45244900	-0.64853300
H	1.02818600	-1.26525300	0.43124200
H	1.00959500	-2.53173700	-0.78642400
C	2.10107400	-0.77481000	-1.39105400
C	3.10059700	-1.49956000	-2.04917100
C	2.09541200	0.61662000	-1.56490200
C	3.99918800	-0.88238800	-2.91063000
C	2.91008200	1.25345700	-2.50409100
C	3.87102300	0.47435800	-3.15744400
H	4.75910500	-1.47082500	-3.41219300
H	4.52820900	0.94681200	-3.88326400
I	2.70384100	3.25501300	0.67626100
C	1.80963500	1.00180700	1.61548600
H	2.59564300	0.34691400	1.25387000
H	2.01564600	1.46540600	2.57159200
H	0.80936400	0.57258600	1.59593100
Cl	3.25079100	-3.23343700	-1.83046600
C	2.78332400	2.70971700	-2.88727400
H	3.50072900	3.33376400	-2.34390400
H	2.97550700	2.82987100	-3.95814900
H	1.78238900	3.09960200	-2.68461700

81

Pd	0.76360600	1.48107900	-0.32938700
N	-0.87865300	2.80926600	0.57598300
C	-0.90716800	4.09632400	0.20423100
C	-1.96458800	2.28946000	1.16152900
C	-2.03079900	4.89496100	0.36726700

H	0.00183500	4.48578600	-0.24265300
C	-3.12614900	3.01778500	1.37153100
H	-1.90548200	1.24091500	1.43717300
C	-3.16639700	4.34274400	0.94959900
H	-2.01180200	5.92485300	0.02979800
H	-3.98684900	2.54330900	1.82884300
H	-4.07047500	4.93027700	1.06816700
N	-0.62294100	0.21864500	-1.15113900
C	-1.83617700	0.79597200	-1.51062900
C	-1.85407200	1.98973100	-2.23133600
C	-3.07156300	0.32788300	-1.05060900
C	-3.01583900	2.70705000	-2.46205200
C	-4.24178900	1.01870700	-1.31519800
C	-4.24664900	2.21926800	-2.02701200
C	-5.53263900	2.99490500	-2.15610500
F	-5.37532500	0.55055000	-0.79566900
F	-3.12823800	-0.72134000	-0.23570700
F	-0.68454900	2.52999500	-2.61830900
F	-2.90618400	3.87602500	-3.08824900
F	-5.45810100	3.96048300	-3.07509100
F	-5.84629600	3.58176700	-0.98256800
F	-6.55456900	2.20012400	-2.48853100
C	-0.45585400	-1.13250500	-1.36292900
O	-1.30019900	-1.82683500	-1.89982200
C	0.86417300	-1.73577700	-0.88876600
H	0.86130200	-1.82920200	0.20194100
H	0.86940800	-2.75199500	-1.27975300
C	2.06438900	-0.97761900	-1.40047200
C	3.11870000	-1.64134400	-2.03942800
C	2.09693900	0.42364600	-1.41705300
C	4.08982400	-0.95163600	-2.75369300
C	2.96009100	1.14163100	-2.24726600
C	3.96982300	0.41966800	-2.89276100
H	4.89326800	-1.49359100	-3.23925900
H	4.67264600	0.95692400	-3.52430700
I	2.61511400	3.04828700	0.87694300
C	0.86459200	0.39639800	1.40653900
H	1.82196500	-0.11817100	1.41936500
H	0.76824600	1.12722500	2.20494200
H	0.00261100	-0.26098800	1.31954300
Cl	3.24137500	-3.38874700	-1.98861400
C	2.84135700	2.61421700	-2.56845600
H	1.87527100	3.03848200	-2.28425500
H	3.61632300	3.19941700	-2.06636100
H	2.94835000	2.75251800	-3.64942400

TS82

Pd	0.24498300	0.68923200	0.25582600
N	-0.68363700	2.64420400	-0.03872700
C	-0.24402400	3.32119400	-1.10837000
C	-1.74330900	3.10674700	0.63946500
C	-0.86412100	4.47957400	-1.55338600
H	0.60980100	2.89887000	-1.62694800
C	-2.43030100	4.24409100	0.24456400
H	-2.04055500	2.53541400	1.51182600
C	-1.98768200	4.93972900	-0.87624000
H	-0.48264400	4.98752100	-2.43126300
H	-3.30665400	4.56087400	0.79719400
H	-2.51350300	5.82505700	-1.21824600
N	-0.84542100	0.11230300	-1.38776800
C	-2.16727400	0.55633900	-1.30309900
C	-2.67912400	1.49126100	-2.20862200
C	-2.99254100	0.17718300	-0.24787700
C	-3.92499300	2.05727800	-2.02159800
C	-4.24524200	0.74883600	-0.05209100
C	-4.73400200	1.70464800	-0.93808200
C	-6.03873900	2.43805600	-0.75249900
F	-4.93737800	0.35865500	1.01391200
F	-2.55421700	-0.71177900	0.64715400
F	-1.92495900	1.90847800	-3.22067400
F	-4.33427900	2.99597000	-2.87419600
F	-6.78990600	2.38143800	-1.85820700

F	-5.80500500	3.74087000	-0.49414400
F	-6.76546000	1.95730300	0.25649100
C	-0.52827200	-0.66180800	-2.45892300
O	-1.34591200	-1.02399900	-3.29057100
C	0.90864400	-1.13043600	-2.55216600
H	0.95524600	-2.10476900	-2.04913200
H	1.07502500	-1.34114200	-3.60598600
C	1.99183000	-0.23669700	-2.01439500
C	3.05414200	0.13704800	-2.85085200
C	2.06486900	0.19341900	-0.67039500
C	4.15895300	0.82917700	-2.37617900
C	3.20858200	0.79879500	-0.13020300
C	4.23364800	1.12142700	-1.03033700
H	4.96225500	1.09886600	-3.05193000
H	5.12015100	1.61575200	-0.64445000
I	0.40793600	1.29288800	2.90085300
C	1.06515000	-1.24150400	0.64602900
H	1.86497500	-1.24157100	1.38047100
H	0.10919300	-1.47874400	1.12965800
H	1.24315400	-1.95490300	-0.15071700
Cl	3.06315500	-0.26510800	-4.55616400
C	3.47002700	1.13339100	1.31493200
H	2.98746700	2.06923800	1.60894600
H	3.10877000	0.36228700	1.99572700
H	4.54639800	1.24392500	1.47142700

83

Pd	0.77988200	1.67431200	-1.22617500
N	-0.62980900	3.15628700	-0.98718800
C	-0.80405600	4.05983400	-1.96157600
C	-1.45558800	3.14710000	0.07043500
C	-1.85151700	4.96818000	-1.92964500
H	-0.09132100	4.03234200	-2.77577400
C	-2.52505400	4.02174000	0.16587700
H	-1.24808600	2.40901400	0.83559400
C	-2.73582600	4.93982700	-0.85809400
H	-1.97114900	5.67193500	-2.74471200
H	-3.18776200	3.96901100	1.02143200
H	-3.57973300	5.62016500	-0.82050200
N	-0.65334300	0.44882400	-2.03117600
C	-2.00464200	0.73046800	-1.80963700
C	-2.71080500	1.58832800	-2.65182400
C	-2.66959300	0.26649800	-0.67723500
C	-3.98721100	2.01735800	-2.33273500
C	-3.95785200	0.67683900	-0.36075100
C	-4.64093400	1.57038400	-1.18412100
C	-5.98330900	2.16773000	-0.84629800
F	-4.48956400	0.22404500	0.77243000
F	-2.02913500	-0.53219200	0.17744500
F	-2.12142500	2.07567400	-3.74263300
F	-4.57863400	2.90635900	-3.13096900
F	-6.82366500	2.10496900	-1.88470200
F	-5.84112700	3.47172500	-0.52582100
F	-6.57334800	1.56868400	0.18882200
C	-0.37199300	-0.78175100	-2.54694800
O	-1.21364400	-1.60243600	-2.87309200
C	1.11038600	-1.05269000	-2.72960400
H	1.28687300	-2.09108000	-2.43333900
H	1.30076600	-1.00538900	-3.80415500
C	2.08743600	-0.15170600	-1.99301400
C	3.06078700	0.59254600	-2.72547400
C	2.34481300	-0.37589000	-0.60567500
C	4.25073600	0.98784600	-2.15905400
C	3.55834100	0.05541200	-0.02347900
C	4.49674400	0.69293700	-0.81799200
H	4.97540500	1.54032600	-2.74514700
H	5.43446700	1.01606300	-0.37644500
I	2.42583400	3.44786500	-0.05544200
C	1.40750600	-1.22359300	0.22146000
H	1.84932100	-2.21422000	0.38911400
H	1.24488900	-0.76773100	1.20234300
H	0.43068300	-1.35955800	-0.23959900

Cl	2.78781700	0.97316700	-4.40826900
C	3.82576300	-0.15487900	1.44176400
H	3.68612300	-1.19857200	1.74316200
H	4.84795000	0.13737900	1.69456200
H	3.14672600	0.46182600	2.04342200

84

Pd	0.75242900	1.57585000	-0.86711700
N	-0.66396300	3.04557900	-0.47443500
C	-0.78085700	4.07114700	-1.33102100
C	-1.54863800	2.90576500	0.52563100
C	-1.82877100	4.97711900	-1.23275500
H	-0.00526000	4.14781000	-2.08293100
C	-2.61822400	3.77131600	0.68297800
H	-1.39479300	2.06317100	1.18981300
C	-2.76884700	4.81831600	-0.22285100
H	-1.90371400	5.78096500	-1.95553600
H	-3.33105700	3.60769300	1.48220300
H	-3.60976300	5.49925600	-0.13980000
N	-0.62484700	0.42712400	-1.81860500
C	-1.98651800	0.67376200	-1.61511000
C	-2.66828900	1.62557600	-2.36739400
C	-2.68427800	0.07410900	-0.56649700
C	-3.96122300	2.02151900	-2.04786900
C	-3.97856000	0.44990500	-0.25411400
C	-4.64540600	1.43451100	-0.98541000
C	-6.00245600	1.89105200	-0.51278400
F	-4.56949700	-0.11086800	0.80139100
F	-2.06664600	-0.81739900	0.20956700
F	-2.04651500	2.24055900	-3.37142700
F	-4.50211900	2.99742300	-2.77429900
F	-6.61036800	2.70033000	-1.38233000
F	-5.88673500	2.56866300	0.64886500
F	-6.81773700	0.85524400	-0.28749100
C	-0.30263000	-0.73889100	-2.44738600
O	-1.11507800	-1.53591600	-2.88725300
C	1.19431700	-0.96901200	-2.60268700
H	1.37913800	-2.02958000	-2.40748900
H	1.42123800	-0.80740800	-3.65854900
C	2.11403000	-0.12635400	-1.73804500
C	3.08800700	0.73024300	-2.33227100
C	2.27330300	-0.44492200	-0.35292800
C	4.17645000	1.18956400	-1.62231700
C	3.38245700	0.04612600	0.37133100
C	4.31666500	0.83376700	-0.28122400
H	4.90052900	1.83583600	-2.10445300
H	5.17606000	1.20473600	0.27019000
C	1.35630800	-1.44533000	0.31241000
H	1.11402600	-1.13097500	1.33116900
H	0.41411600	-1.58440500	-0.21494100
H	1.85710100	-2.41983000	0.38136600
O	2.23103400	4.00922200	-1.64822300
C	2.55334000	3.71201000	-0.50072600
O	2.07757000	2.70342700	0.16930300
C	3.61356700	4.49103500	0.25567900
H	4.56577400	3.95446400	0.17318100
H	3.73403000	5.48267900	-0.18376600
H	3.36615500	4.56833900	1.31702000
Cl	2.95731500	1.18603700	-4.00810600
C	3.54444800	-0.26397300	1.83497800
H	3.52680700	-1.34136600	2.03279200
H	4.48927900	0.13359500	2.21447900
H	2.73510300	0.19299000	2.41670700

85

Pd	-0.40435600	2.39465500	0.28028500
N	-0.02932800	4.03529100	1.48906500
C	1.20807400	4.54060800	1.58236900
C	-1.04035900	4.64507900	2.12074900
C	1.48062900	5.67738100	2.32687200
H	1.97450300	4.01667000	1.02327800

C	-0.84761200	5.79258000	2.87494000
H	-2.01682000	4.18917600	2.01090100
C	0.43479100	6.31837300	2.98209500
H	2.49564200	6.05404000	2.37882100
H	-1.69491900	6.26224000	3.36108300
H	0.61600300	7.21757500	3.56213900
N	-0.74529700	0.71624500	-0.88443000
C	-1.93617600	0.65779500	-1.64390600
C	-2.60394100	1.77279300	-2.14057100
C	-2.53570900	-0.58583700	-1.87565100
C	-3.81593900	1.66411700	-2.81707900
C	-3.73004900	-0.70009400	-2.56077100
C	-4.39859500	0.42321400	-3.05155500
C	-5.72046200	0.22584400	-3.75207800
F	-4.25449200	-1.91258000	-2.73158700
F	-1.95486600	-1.68657900	-1.40392200
F	-2.10380200	2.99622300	-1.96352200
F	-4.38395200	2.79455300	-3.22889100
F	-6.19277200	1.35163400	-4.29269800
F	-6.64811500	-0.22881400	-2.89259700
F	-5.61161100	-0.67756300	-4.73582200
C	0.36585600	0.14114900	-1.52060600
O	0.32807300	-0.28360700	-2.65677300
C	1.62253400	0.06980300	-0.65933900
H	2.13026300	1.02924700	-0.78619000
H	1.34204500	0.00170400	0.39558800
C	2.52042600	-1.07404400	-1.04992500
C	2.38571600	-2.32606600	-0.44803900
C	3.50434400	-0.90573200	-2.04159700
C	3.20825300	-3.39274300	-0.77847000
C	4.34795800	-1.97486100	-2.38534900
C	4.18664500	-3.20279200	-1.74260500
H	3.07882900	-4.35335100	-0.29271200
H	4.83615200	-4.03284000	-2.00764800
C	3.62658300	0.43644900	-2.72655700
H	4.31496000	0.40404700	-3.57217700
H	2.65239300	0.76408400	-3.10123300
H	3.99442900	1.20550100	-2.03521700
O	0.00387700	4.94396800	-1.36398500
C	0.85396500	4.11218700	-1.62480900
O	1.01608900	2.96392600	-1.00093600
C	1.88066900	4.29206400	-2.72912200
H	1.71156300	3.53826000	-3.50455500
H	1.79150400	5.28936100	-3.16175900
H	2.89138900	4.13820900	-2.33926700
O	-1.82509800	1.75504200	1.71235600
C	-2.07071800	0.57048400	2.00240100
O	-1.63454600	-0.44952400	1.33584000
H	-1.15970800	-0.13400600	0.48341800
C	-2.92349500	0.23290500	3.18721900
H	-3.20002000	1.13814800	3.72651500
H	-3.82094600	-0.29159900	2.84665400
H	-2.37382200	-0.44782600	3.84303300
Cl	1.13456500	-2.60074300	0.75605700
C	5.42114400	-1.83265200	-3.43900700
H	4.99375100	-1.60268200	-4.42173900
H	6.13078700	-1.03451900	-3.19373200
H	5.98933300	-2.76203600	-3.53759100

TS86

Pd	-0.42156500	2.52233000	0.43156900
N	0.08177200	4.17290000	1.57043600
C	1.30372000	4.71569700	1.47629500
C	-0.84204600	4.75397900	2.34767800
C	1.64727000	5.86644400	2.16753900
H	1.99605700	4.20406500	0.81900000
C	-0.57395900	5.91290600	3.06051100
H	-1.80485200	4.25999300	2.39297400
C	0.69158700	6.48054900	2.96922700
H	2.64579700	6.27486000	2.06360300
H	-1.35170100	6.35738500	3.67078100
H	0.92895300	7.38982700	3.51223900

N	-0.88890200	0.79671700	-0.67265900
C	-2.02405600	0.80650700	-1.52899000
C	-2.64335400	1.95315200	-2.01013500
C	-2.60301800	-0.41826500	-1.87802800
C	-3.78907900	1.89040200	-2.80071200
C	-3.73075100	-0.48572400	-2.67352100
C	-4.35305700	0.66927800	-3.15093000
C	-5.59174200	0.51651700	-4.00114900
F	-4.23269700	-1.68197300	-2.97205500
F	-2.05881900	-1.54527600	-1.42780100
F	-2.16572600	3.16275700	-1.72086700
F	-4.31008500	3.04619700	-3.20089800
F	-6.09639900	1.68712700	-4.39622000
F	-6.55331300	-0.12844100	-3.32217800
F	-5.32692800	-0.20190200	-5.10128500
C	0.26681500	0.22344600	-1.27585900
O	0.32159500	-0.03973100	-2.45265800
C	1.39852600	-0.04285200	-0.29198100
H	1.89629500	0.91402100	-0.11125700
H	0.97164500	-0.35537600	0.66433300
C	2.38101500	-1.06417500	-0.80300500
C	2.31852500	-2.39180500	-0.36569300
C	3.37079400	-0.71554600	-1.73912600
C	3.21637400	-3.35370800	-0.80240800
C	4.28521100	-1.68328800	-2.19227000
C	4.19798800	-2.98736700	-1.71143700
H	3.14040100	-4.37250900	-0.43938800
H	4.90423500	-3.73590600	-2.06060800
C	3.46507500	0.68083500	-2.30667600
H	3.27365500	0.65925400	-3.38575700
H	2.74443900	1.37587900	-1.87600800
H	4.46968100	1.09724500	-2.16332600
O	0.09202600	4.94773800	-1.39504200
C	0.84871800	4.02985900	-1.65437700
O	0.98762800	2.93560500	-0.93201200
C	1.76211100	4.02491900	-2.86606200
H	1.47954100	3.19702800	-3.52410600
H	1.67430100	4.97167500	-3.40039900
H	2.80072500	3.85955100	-2.56325500
O	-1.79049000	1.98314100	1.91499900
C	-2.09708800	0.78726400	2.16109600
O	-1.76734100	-0.20693400	1.43386600
H	-1.28806800	0.15670000	0.45676000
C	-2.92919100	0.48665600	3.37540900
H	-3.95265200	0.26753400	3.05423200
H	-2.54038900	-0.40437700	3.87302800
H	-2.93921500	1.33649600	4.05805700
Cl	1.06772900	-2.90799600	0.75625900
C	5.34861300	-1.32612600	-3.19971700
H	4.91037600	-0.92232700	-4.11988700
H	6.03541600	-0.56374100	-2.81198500
H	5.94313600	-2.20376400	-3.46902100

87

N	0.95559800	-1.21528500	-1.49998300
C	-0.11999800	-1.94707100	-2.00514800
C	0.10758900	-3.04838700	-2.82978300
C	-1.44108400	-1.59218400	-1.74558300
C	-0.94310800	-3.77767800	-3.35661400
C	-2.49664500	-2.34514100	-2.24993400
C	-2.26819600	-3.45726900	-3.05744200
C	-3.36949600	-4.29823500	-3.66173100
F	-3.72587900	-1.93675300	-1.95664600
F	-1.72018500	-0.49991400	-1.04273800
F	1.36426700	-3.39024100	-3.12162200
F	-0.66531200	-4.80998400	-4.14799500
F	-3.13532200	-5.60169700	-3.45936400
F	-3.44175500	-4.10260400	-4.98713700
F	-4.56771200	-4.02137800	-3.14466000
C	1.09980200	-0.92968300	-0.15105300
O	0.28165900	-1.25904200	0.67761100
C	2.38748200	-0.19023400	0.19743800

H	2.18552400	0.33969200	1.13165400
H	3.13525100	-0.95231000	0.43420800
C	2.89840000	0.74448800	-0.87305200
C	4.08516600	0.48765900	-1.56903400
C	2.15317500	1.89344100	-1.21541400
C	4.54631000	1.33626900	-2.56670200
C	2.60428000	2.75189500	-2.23137700
C	3.80049000	2.45934900	-2.88772800
H	5.47357700	1.11462500	-3.08281000
H	4.15520700	3.12285900	-3.67149900
H	1.76113300	-1.09806500	-2.09948100
C	1.82205800	3.97809700	-2.63665200
H	0.79657500	3.72709600	-2.92885800
H	1.76045100	4.70749500	-1.82063800
H	2.29693700	4.47543800	-3.48681500
Cl	5.04992500	-0.93933400	-1.22063400
C	0.84662300	2.16564500	-0.50728000
H	0.05057700	1.51237100	-0.88459500
H	0.91943000	1.98762300	0.56954800
H	0.51733400	3.19664100	-0.64355100

Table 1
N1-DMAP-Me
DMAP

C	2.32618900	-6.74980600	-6.78504900
C	1.54454900	-5.60498700	-6.77077100
C	3.45943700	-6.82117500	-5.95093100
C	2.85610200	-4.59807600	-5.23531800
C	3.71437000	-5.68399100	-5.15911200
N	1.77637400	-4.52578700	-6.01852600
H	4.56635000	-5.63512900	-4.49194800
H	3.05712100	-3.72138900	-4.62169500
H	0.66890400	-5.55525800	-7.41604000
H	2.04908000	-7.56700600	-7.43987000
N	4.26519600	-7.93198800	-5.91214900
C	5.48143600	-7.90702200	-5.12745800
H	5.97775100	-8.87550800	-5.20364200
H	6.18371300	-7.13373700	-5.47076700
H	5.26526700	-7.72782000	-4.06746200
C	4.03963800	-9.01074000	-6.85089900
H	4.78169700	-9.79300100	-6.68478000
H	3.04798500	-9.45837400	-6.71168700
H	4.12339500	-8.67657800	-7.89487700

1			
Pd	-0.00858300	1.28654900	0.02799300
O	-1.67427000	1.17276400	1.19883100
O	1.65798700	1.40265500	-1.14074500
C	-1.47989500	1.09137200	2.47298200
C	1.46681000	1.49519600	-2.41456300
O	-0.37824700	1.05750400	3.02961200
O	0.36679900	1.51935800	-2.97495800
C	-2.77040000	1.05778700	3.27845500
H	-3.28728700	2.01733800	3.17309100
H	-3.43971600	0.28536300	2.88894700
H	-2.55522000	0.87387500	4.33238100
C	2.75841800	1.59692800	-3.21246500
H	3.21493100	2.57704500	-3.03744800
H	3.47353800	0.84094200	-2.87711800
H	2.55474100	1.48038800	-4.27829800
C	-0.02707800	-1.36544300	-1.30729800
C	0.13959800	-1.51814700	0.98754200
C	0.00063300	-2.73691900	-1.44766700
C	0.18155800	-2.89573500	0.93925800
C	0.11130000	-3.55974000	-0.30502800
C	-0.16053900	4.09109500	-0.93228700
C	0.01310800	3.93976000	1.36201900
C	-0.20296900	5.46871200	-0.88470600
C	-0.01509100	5.31129700	1.50180300
C	-0.12944800	6.13346900	0.35902300
N	0.03943300	-0.75621200	-0.11300900

N	-0.05671400	3.32977200	0.16833700
H	0.18749000	-0.98111800	1.93009600
H	0.27015300	-3.43835800	1.87139000
H	-0.29487700	6.01078100	-1.81684500
H	-0.21102000	3.55349800	-1.87446600
H	-0.06761900	-3.15337600	-2.44416800
H	-0.10586900	-0.70861400	-2.16839600
H	0.09534300	3.28344400	2.22324200
H	0.05615400	5.72837100	2.49784100
N	0.14925100	-4.92044700	-0.39797100
N	-0.16773900	7.49416200	0.45134300
C	0.23238500	-5.72437000	0.80570200
H	-0.62022200	-5.54221700	1.47241600
H	0.22771500	-6.78065600	0.53461800
H	1.15681000	-5.52180400	1.36146700
C	0.06567500	-5.56060000	-1.69592700
H	0.88054900	-5.23708900	-2.35548300
H	0.14765200	-6.64052700	-1.56885300
H	-0.88920900	-5.34750200	-2.19407800
C	-0.25523200	8.29746200	-0.75245000
H	-1.18198500	8.09529100	-1.30449700
H	-0.24859000	9.35389100	-0.48199300
H	0.59461000	8.11436900	-1.42239200
C	-0.08222500	8.13502200	1.74884500
H	0.87396900	7.92333600	2.24506300
H	-0.16579100	9.21478200	1.62145500
H	-0.89531200	7.81084200	2.41027600

CH₃Pd(I)L₂

Pd	0.12732300	1.34749300	0.00346200
N	0.02426000	-0.89707000	-0.23018100
C	-0.75224700	-1.63102800	0.57854700
C	0.77718800	-1.57224400	-1.11144100
C	-0.81996600	-3.01024900	0.55077500
H	-1.35362400	-1.07310700	1.29055100
C	0.78048900	-2.94864400	-1.22687400
H	1.42288000	-0.96688200	-1.73900100
C	-0.03242600	-3.72659400	-0.37602000
H	-1.47250400	-3.51367200	1.25297600
H	1.42800100	-3.40166600	-1.96672300
I	2.78896800	1.38657500	-0.18639900
N	-2.00887900	1.37808600	0.18306500
C	-2.64087300	2.03981100	1.16450100
C	-2.77879500	0.70091000	-0.68354300
C	-4.01119600	2.04653000	1.32838700
H	-2.00573400	2.59827300	1.84341200
C	-4.15595900	0.65312500	-0.61284700
H	-2.25127000	0.16741900	-1.46678000
C	-4.82970300	1.33727900	0.42272000
H	-4.42936800	2.60844600	2.15360100
H	-4.69205500	0.08679200	-1.36347300
C	0.14153500	3.35246900	0.26408600
H	0.27927900	3.53991000	1.33656800
H	0.95340800	3.82826300	-0.28706300
H	-0.82230200	3.75185100	-0.07320900
N	-6.18835600	1.31510800	0.53938700
N	-0.05503400	-5.09107800	-0.44317000
C	-6.83507700	2.06501600	1.59915500
H	-7.91280100	1.90947200	1.54251700
H	-6.49855400	1.72850500	2.58736200
H	-6.64074700	3.14219600	1.51269800
C	-6.98785400	0.63412500	-0.46051400
H	-8.04370400	0.74134000	-0.21043300
H	-6.83219700	1.05791400	-1.46128400
H	-6.75755600	-0.43800100	-0.49709400
C	-0.86575000	-5.84576000	0.49061900
H	-1.93172000	-5.60922500	0.37869800
H	-0.73814700	-6.91157400	0.29806800
H	-0.57595500	-5.65238200	1.53206700
C	0.82115700	-5.78276800	-1.36805100
H	1.87835100	-5.56473800	-1.16757900
H	0.67229800	-6.85831700	-1.26629900

H	0.60297700	-5.50998700	-2.40820000
---	------------	-------------	-------------

31

Pd	2.17698600	4.25339000	0.46114000
N	-0.21322200	0.16208200	-2.29357100
C	-1.41281500	0.22661000	-2.99919900
C	-1.49192700	0.99906100	-4.15905500
C	-2.57002600	-0.42027400	-2.57163600
C	-2.66954000	1.09976300	-4.87610400
C	-3.74567500	-0.34295900	-3.31231200
C	-3.81778000	0.41069200	-4.48176200
C	-5.07019800	0.55590000	-5.31261500
F	-4.80433100	-0.98923700	-2.83409800
F	-2.58969500	-1.08795600	-1.42573400
F	-0.40720100	1.65947700	-4.57040300
F	-2.68647300	1.86011500	-5.96895600
F	-5.56545800	1.80054400	-5.21486300
F	-6.03352400	-0.29091700	-4.94365100
F	-4.81181100	0.32961800	-6.60823100
C	0.38123200	-1.03959200	-1.93276100
O	-0.15102600	-2.11233400	-2.10904800
C	1.73749200	-0.89588600	-1.24296500
H	1.54804900	-1.09423400	-0.18426300
H	2.35048100	-1.72242700	-1.60796600
C	2.41654500	0.43890300	-1.42867800
C	3.19768600	0.70258800	-2.56046800
C	2.19664200	1.50045200	-0.53018900
C	3.75301200	1.95378100	-2.79768500
C	2.70764900	2.79016700	-0.76888300
C	3.49804800	2.99001900	-1.90477400
H	4.35715400	2.11361500	-3.68462300
H	3.91879700	3.97135300	-2.11687900
C	1.17976600	2.75786700	1.38965300
C	1.69687500	2.55557900	2.82047400
C	1.37862800	1.35928400	0.72279000
C	2.89199300	1.61745900	2.59238300
C	0.70112100	1.62041500	3.55205800
H	1.89427600	3.48246900	3.36389900
C	2.06267500	0.54824700	1.86354800
H	0.40424400	0.90792200	0.48864700
H	3.33410300	1.24128900	3.52214800
H	3.67353600	2.06154600	1.96922600
H	0.90246100	1.61417000	4.62898600
H	-0.33674400	1.94249500	3.41555800
C	0.98575500	0.22781900	2.91612900
H	2.62292800	-0.32292000	1.51498200
H	1.37328100	-0.47404600	3.66224900
H	0.09389400	-0.22593300	2.47100700
H	0.39258500	0.97185500	-2.34629300
H	0.13762600	3.09916800	1.36032400
Cl	3.46900900	-0.55417500	-3.76012200
C	2.32530300	6.32001100	2.79955100
C	0.34124600	6.45468700	1.67548600
C	1.95164300	7.30338500	3.69157800
C	-0.13047400	7.44324100	2.51414300
C	0.68126900	7.91075600	3.57191400
N	1.55138300	5.88373300	1.79179100
H	2.64613200	7.58691100	4.47183800
H	3.29574800	5.84177800	2.89237100
H	-0.27824800	6.08864600	0.86277500
H	-1.12162500	7.84186300	2.34041200
N	0.26386100	8.88604800	4.42523600
C	-1.05497400	9.47046300	4.26779800
H	-1.84399200	8.71542100	4.37422600
H	-1.20697500	10.22672900	5.03817500
H	-1.16632000	9.95621300	3.29022400
C	1.13923300	9.34197000	5.48877200
H	2.07411500	9.75479500	5.08933000
H	0.63871100	10.12957900	6.05241000
H	1.38506200	8.53080500	6.18565700

TS32

Pd	2.50910000	4.18573300	-3.79910500
N	2.29344800	6.35432500	-4.07791100
C	3.12784300	6.94852600	-4.95605300
C	1.47049300	7.16255600	-3.38609700
C	3.17828600	8.30728500	-5.16372100
H	3.82810800	6.31858700	-5.50361800
C	1.44138500	8.53175200	-3.52462600
H	0.80422000	6.68103800	-2.67558700
C	2.32112500	9.16375200	-4.43888900
H	3.91031900	8.67354600	-5.87202000
H	0.74529500	9.09973700	-2.92095200
N	-0.71597100	0.08457400	-1.69557000
C	-2.07399200	0.38053700	-1.55329400
C	-3.03700600	-0.50077300	-2.04396400
C	-2.51738700	1.55610800	-0.95480100
C	-4.38716100	-0.22348500	-1.92543500
C	-3.87509100	1.82190500	-0.80990200
C	-4.83579500	0.93670100	-1.29233200
C	-6.32770900	1.16308400	-1.19000300
F	-4.20631800	2.96701200	-0.22412000
F	-1.64799600	2.47698500	-0.54089800
F	-2.64018500	-1.62377200	-2.64386700
F	-5.26113400	-1.09691600	-2.41444500
F	-6.91742700	0.13785000	-0.56174500
F	-6.87278700	1.25707200	-2.41135200
F	-6.63348600	2.27665300	-0.52285200
C	0.15982800	0.07280400	-0.62129500
O	-0.18323500	0.37708100	0.50029500
C	1.57390300	-0.36090500	-0.98040000
H	2.19424100	-0.10774000	-0.11890000
H	1.57217900	-1.45285500	-1.05125200
C	2.11497800	0.24697200	-2.25579700
C	2.54435400	-0.53780300	-3.33204900
C	2.18586900	1.64675500	-2.40932200
C	3.03816300	0.01765600	-4.51009500
C	2.64347600	2.21278900	-3.60533900
C	3.09112800	1.39788900	-4.64465100
H	3.37571500	-0.63210700	-5.30987900
H	3.48661600	1.82794200	-5.56147600
H	-0.42564000	-0.36887100	-2.55150400
C	1.77201300	4.06199700	-1.91187900
C	2.56804100	4.84320800	-0.87843900
C	1.71386800	2.61685800	-1.36267700
H	0.78462400	4.48479700	-2.15244800
C	1.64907400	4.93818800	0.37306700
C	3.60059700	3.79969000	-0.42178900
H	2.94541100	5.80702300	-1.22486400
C	2.55305000	2.73864000	-0.05732000
H	0.67248900	2.39690400	-1.10682800
C	1.68584000	3.49721500	0.96260100
H	0.63512200	5.26522000	0.11863000
H	2.06041300	5.67148600	1.07358200
H	4.28704400	3.48630900	-1.21082000
H	4.18245500	4.13146900	0.44378900
H	2.95005400	1.79264700	0.31119300
H	0.69535700	3.04756300	1.07154600
H	2.16343300	3.49043000	1.94687200
Cl	2.47396700	-2.29070700	-3.25110300
C	4.54807800	4.19272300	-3.74611300
I	6.44143400	5.65265300	-6.26767300
H	4.79055600	5.10516100	-3.20175800
H	5.01760200	3.29988000	-3.34126100
H	4.69872300	4.29683600	-4.83453900
N	2.34330000	10.51095600	-4.60329400
C	1.47979800	11.35601600	-3.79995300
H	1.67366000	11.22458500	-2.72793200
H	1.66657800	12.40074400	-4.04850700
H	0.41983200	11.14681400	-3.99181300
C	3.27353300	11.10744300	-5.54870500
H	3.10709800	10.72450500	-6.56200500
H	3.12192800	12.18679000	-5.56685700
H	4.31535700	10.91012500	-5.26899200

TS35

Pd	1.83537600	3.48553000	0.05825000
N	0.67010200	4.63251800	1.59052200
C	1.22034100	5.41228400	2.53151200
C	-0.66499100	4.50945400	1.62601800
C	0.50681900	6.06169200	3.51736400
H	2.29921200	5.52670600	2.48595600
C	-1.47509600	5.11864900	2.56196200
H	-1.10612300	3.88466900	0.85592800
C	-0.89867300	5.92662600	3.56657500
H	1.04619400	6.66862000	4.23308300
H	-2.54400700	4.95993200	2.50147200
N	-0.04151200	-0.80751200	-2.66626100
C	-1.42679400	-0.77705600	-2.80863600
C	-1.99684200	-0.64824500	-4.07558500
C	-2.28825700	-0.82653700	-1.71465300
C	-3.36857800	-0.59354900	-4.24235400
C	-3.66835400	-0.80274000	-1.88643400
C	-4.23623400	-0.68643900	-3.15298100
C	-5.72233600	-0.62873100	-3.41652900
F	-4.41478600	-0.85749900	-0.78743300
F	-1.80947900	-0.85342700	-0.47507700
F	-1.19813000	-0.56586500	-5.14027600
F	-3.85642900	-0.46561100	-5.47374000
F	-6.08714300	-1.58055600	-4.28695700
F	-6.06237800	0.55473600	-3.95030400
F	-6.45024700	-0.79529000	-2.31044400
C	0.62329100	-1.76585000	-1.92060800
O	0.04465300	-2.67153400	-1.36048200
C	2.13875400	-1.59753200	-1.88181900
H	2.45133400	-2.02581800	-0.92754900
H	2.55047300	-2.24544600	-2.66138300
C	2.61778000	-0.17504800	-2.04941600
C	3.31906000	0.25084100	-3.18131800
C	2.28175700	0.79827900	-1.08504300
C	3.67814700	1.58151800	-3.36175600
C	2.58453000	2.16008000	-1.26914900
C	3.30197700	2.52543500	-2.41347300
H	4.22709400	1.87499100	-4.25037200
H	3.55834400	3.56510500	-2.59498700
C	1.15085200	1.75889500	0.92423100
C	1.74887800	1.56436200	2.32661200
C	1.54490800	0.45364100	0.17335800
H	0.06259100	1.89416500	0.96091100
C	3.06709200	0.84084500	2.00535300
C	0.94991600	0.44549900	3.03878700
H	1.82226400	2.48225300	2.91678100
C	2.38609900	-0.30464800	1.24135600
H	0.64560900	-0.13006700	-0.05498600
H	3.60300600	0.49489000	2.89647900
H	3.74836600	1.42454200	1.37777900
H	1.20572400	0.40525200	4.10367700
H	-0.12989100	0.61264000	2.96697500
C	1.40788300	-0.84669800	2.29874000
H	3.06276000	-1.05790000	0.83152800
H	1.92096300	-1.53063500	2.98302600
H	0.57813600	-1.39610200	1.84282400
H	0.50770200	-0.17022800	-3.22722600
Cl	3.76551600	-0.88423500	-4.45155600
I	2.75264500	5.90316100	-0.93181900
C	4.05926700	4.27962800	0.60724000
H	3.70371500	3.72834900	1.47736700
H	4.60561800	3.67199000	-0.10643600
H	4.58154100	5.18318100	0.89836200
N	-1.65112600	6.53866100	4.52280500
C	-3.09209500	6.36961600	4.52711100
H	-3.37077800	5.31390300	4.63470000
H	-3.51550500	6.91549600	5.37046500
H	-3.54728800	6.75948000	3.60788400
C	-1.01169000	7.36521100	5.52862100
H	-0.49245300	8.22062800	5.07797000

H	-1.76935800	7.75231800	6.21035800
H	-0.28889700	6.78967100	6.12057300

TS65

Pd	4.73144200	2.51092700	-4.00208400
N	5.06831600	2.58957100	-6.15763500
C	6.17672100	3.09270500	-6.72462600
C	4.12159100	2.13614500	-6.99768200
C	6.38568500	3.16616300	-8.08725600
H	6.93418200	3.45657000	-6.03852400
C	4.23158300	2.16317000	-8.37317000
H	3.22855400	1.73311600	-6.53443100
C	5.39371800	2.69342200	-8.97392700
H	7.31340700	3.59198100	-8.44777300
H	3.41133300	1.77417200	-8.96284500
N	1.15815400	-0.65469700	-2.31877500
C	0.27444400	-0.18573700	-3.29103100
C	-1.11080100	-0.31755300	-3.18889000
C	0.78259100	0.41865900	-4.43966600
C	-1.93255500	0.19756200	-4.18159500
C	-0.03915300	0.90674000	-5.44252400
C	-1.42430900	0.81499400	-5.32489500
C	-2.40074600	1.32605800	-6.35723600
F	0.54855700	1.47025600	-6.49793700
F	2.10957000	0.52475600	-4.57398900
F	-1.66281400	-0.96385500	-2.17346900
F	-3.24795200	0.06138400	-4.03974100
F	-3.23354900	2.22721300	-5.81951300
F	-3.14950600	0.32406800	-6.84056100
F	-1.79141100	1.90829600	-7.39406600
C	1.07356000	-0.24301700	-0.98783300
O	0.10241400	0.32281200	-0.53999700
C	2.31492900	-0.58029100	-0.17661200
H	2.18029900	-0.12327300	0.80798500
H	2.34732700	-1.66499300	-0.02855600
C	3.58825400	-0.10007400	-0.83689300
C	4.81040800	-0.78034100	-0.75999500
C	3.61330100	1.10606300	-1.53603100
C	5.98791600	-0.24851800	-1.28323100
C	4.75292900	1.61176200	-2.17921500
C	5.98110500	0.96302000	-1.97430200
H	6.91573600	-0.79601600	-1.15330200
H	6.91413300	1.36747700	-2.35163500
H	2.09860400	-0.82802600	-2.65301100
C	3.77213300	3.23154200	-2.18955800
C	4.21565400	4.14929000	-1.03427100
C	2.70401100	2.30010800	-1.53914600
H	3.37185000	3.85339700	-3.01331300
C	3.08476100	5.19277900	-0.88931400
C	3.96830200	3.31025100	0.23343300
H	5.21236300	4.57649700	-1.15723300
C	2.52111100	2.94097400	-0.14527000
H	1.76035800	2.21204300	-2.08835300
C	1.89284700	4.33645000	-0.35952000
H	2.85959500	5.69749800	-1.83450700
H	3.36949200	5.96255100	-0.16371000
H	4.63737100	2.45426200	0.34757500
H	4.01853500	3.91613700	1.14456000
H	1.96965800	2.31305700	0.55796300
H	1.05777900	4.29754200	-1.06686000
H	1.50326500	4.73469300	0.58245100
Cl	4.91333500	-2.32251000	0.07727700
N	5.54827500	2.74741700	-10.32802600
C	6.76910000	3.28432700	-10.89625300
H	7.64957100	2.71228500	-10.57614500
H	6.71173700	3.23169800	-11.98389300
H	6.91707100	4.33514200	-10.61612500
C	4.50117800	2.24416500	-11.19577100
H	3.55513100	2.77579800	-11.03396900
H	4.79366100	2.39107800	-12.23586100
H	4.32712900	1.17166000	-11.03965400

TS36

Pd	1.79265200	3.92430800	0.50802600
N	-0.57435500	0.00260400	-1.61485000
C	-1.91195400	0.00821700	-1.22371100
C	-2.91469000	0.24080200	-2.16521100
C	-2.29416600	-0.15468300	0.10675800
C	-4.24714900	0.28370700	-1.79591600
C	-3.63621100	-0.13836300	0.47234700
C	-4.63787800	0.09086200	-0.46926700
C	-6.11408300	0.11855500	-0.14890800
F	-3.91461600	-0.28454200	1.76404500
F	-1.37931500	-0.26596200	1.06335000
F	-2.57424600	0.42783500	-3.43943600
F	-5.16275200	0.49613500	-2.73524800
F	-6.67072500	1.26300400	-0.58376600
F	-6.35724400	0.03478200	1.16173500
F	-6.75341000	-0.89046800	-0.74949600
C	0.30318800	-1.01847700	-1.27104600
O	-0.04208600	-1.97091400	-0.60902300
C	1.72584900	-0.83845500	-1.79399700
H	2.36619000	-1.35156200	-1.07433400
H	1.79811700	-1.40002900	-2.72960100
C	2.13826500	0.60065900	-1.99363600
C	2.25763000	1.16880300	-3.26638700
C	2.29268600	1.43686900	-0.86866400
C	2.49138600	2.52834200	-3.44320200
C	2.52681100	2.81158300	-1.05233900
C	2.61758500	3.35236700	-2.33563200
H	2.56098300	2.94160200	-4.44317100
H	2.76453600	4.41812300	-2.46925500
C	1.83014000	2.11588400	1.50351100
C	2.90135300	1.87916100	2.58208800
C	2.01519400	0.93172100	0.52471600
H	0.83780900	2.10809000	1.95628600
C	4.02962400	1.14957500	1.83222000
C	2.36112600	0.71486100	3.45197100
H	3.18147000	2.76472700	3.15836700
C	3.10795400	0.08279400	1.22738600
H	1.08548200	0.35576100	0.49799900
H	4.77186000	0.72087500	2.51467200
H	4.55273700	1.74751600	1.09045700
H	2.99226000	0.58280300	4.33743300
H	1.33966700	0.89531300	3.80085200
C	2.46592100	-0.51554400	2.49767400
H	3.59438800	-0.65250000	0.58186400
H	3.11167200	-1.28985900	2.92304500
H	1.49524000	-0.97606200	2.28800700
H	-0.29739700	0.64807200	-2.34303600
Cl	2.06344600	0.19217700	-4.71326700
I	1.61466800	6.57655500	-0.44130900
C	3.88933900	3.88970700	0.03693500
H	4.04960100	4.13780300	1.09547700
H	4.56387900	3.08489700	-0.23464500
H	4.05503700	4.76115600	-0.59110400
C	-0.79140800	5.07685600	1.88206900
C	-1.14049300	3.18529500	0.63790600
C	-2.13474900	5.19489600	2.16902800
C	-2.50075100	3.23422400	0.84138500
C	-3.05218000	4.25373800	1.64988100
N	-0.27720600	4.08047800	1.14377500
H	-2.45827100	6.02656100	2.78123400
H	-0.08500200	5.81708000	2.24025600
H	-0.70680400	2.38943900	0.03874800
H	-3.12347800	2.48699800	0.36939100
N	-4.38469100	4.31658200	1.90849200
C	-4.91093400	5.37522000	2.74983700
H	-4.72513600	6.36347800	2.31177100
H	-5.98870900	5.24845200	2.85259200
H	-4.46846300	5.34811000	3.75365300
C	-5.26806900	3.28984900	1.38726600
H	-6.29074300	3.49498600	1.70339700
H	-5.25748100	3.26619100	0.29161700

H	-4.99326600	2.29626100	1.76281500
---	-------------	------------	------------

TS40

Pd	-2.03443000	-1.06240700	-0.92363400
N	-0.63889300	-2.70933200	-0.72158100
C	-0.99156100	-3.89444900	-0.19900500
C	0.66439500	-2.52216000	-0.99515000
C	-0.10092500	-4.91108700	0.06710700
H	-2.04582000	-4.02141100	0.02652500
C	1.63241700	-3.47452900	-0.75680700
H	0.92071300	-1.54842800	-1.40313600
C	1.27473700	-4.72337600	-0.20197900
H	-0.47821900	-5.83118700	0.49427000
H	2.65984100	-3.23298300	-0.99362600
N	0.58722000	1.75052300	0.54610500
C	1.70574100	0.91603500	0.49043800
C	2.66069900	1.10878800	-0.50695800
C	1.86225500	-0.17943100	1.33512400
C	3.73348200	0.24491300	-0.63946100
C	2.94963300	-1.03476600	1.21527300
C	3.91597600	-0.82976200	0.23275400
C	5.10984800	-1.72539000	0.03270600
F	3.00278400	-2.08320200	2.03609300
F	0.93325600	-0.47019900	2.24420800
F	2.54298900	2.12927000	-1.34482300
F	4.61096000	0.46419500	-1.61741900
F	4.97007500	-2.47157400	-1.08575500
F	5.29514600	-2.57791700	1.04901900
F	6.23664400	-1.02151800	-0.10476200
C	0.17074300	2.35601100	1.70951900
O	0.83034300	2.33601300	2.72936600
C	-1.19149700	3.06795900	1.65843100
H	-1.66740200	2.85412600	2.61913400
H	-0.99137800	4.14186100	1.64364800
C	-2.04393200	2.64912100	0.48939500
C	-2.25280400	3.47427600	-0.61577000
C	-2.46121700	1.30121400	0.40733900
C	-2.78486700	2.98731900	-1.80849600
C	-2.87584800	0.79426600	-0.82976800
C	-3.05262600	1.63633600	-1.92811400
H	-2.92547900	3.65761000	-2.64922400
H	-3.35073500	1.22991000	-2.88780100
O	0.10032500	0.43304400	-1.91931200
C	-0.48898200	0.10316600	-2.97553100
C	-0.04379900	0.72336500	-4.28688400
H	1.03070600	0.91879100	-4.26753600
H	-0.30707800	0.08993300	-5.13640800
H	-0.55609200	1.68615800	-4.40128800
O	-1.47366900	-0.70317400	-3.02219900
H	0.04473000	1.76570300	-0.31543400
C	-2.27237800	-1.11380900	1.09971100
C	-3.48478800	-1.73204100	1.81557900
C	-2.27374700	0.35609000	1.57569900
H	-1.34789200	-1.61544100	1.39389100
C	-3.04465400	-1.94020500	3.28461500
C	-4.45462200	-0.54706900	1.98808300
H	-3.89284300	-2.63383000	1.34908900
C	-3.40787500	0.37523000	2.62912400
H	-1.32100100	0.56609000	2.06289800
C	-2.93887900	-0.48027400	3.82644900
H	-2.09960400	-2.48730200	3.35973700
H	-3.80269200	-2.51066400	3.83295900
H	-4.86558400	-0.14938600	1.06101300
H	-5.28369500	-0.78089400	2.66523200
H	-3.74825200	1.37950400	2.89654200
H	-1.92214900	-0.22239600	4.13981900
H	-3.59733000	-0.33057400	4.68772800
Cl	-1.79783400	5.16704400	-0.57775800
C	-4.14429100	-0.80399100	-1.27719100
H	-4.11871200	-0.85671200	-2.36586600
H	-4.90121100	-0.09948300	-0.94875900
H	-4.35303800	-1.77596800	-0.82274800

N	2.19947000	-5.68502600	0.06139600
C	1.79197200	-6.92915200	0.68486200
H	2.66177400	-7.57777700	0.79139300
H	1.36125000	-6.76704100	1.68224500
H	1.05524000	-7.45813500	0.06868200
C	3.61217900	-5.38860400	-0.10632400
H	4.19582600	-6.26908100	0.16404400
H	3.84435800	-5.13708100	-1.14716400
H	3.92761500	-4.55624700	0.53172600

TS67

Pd	0.58430000	3.98740700	-0.69797600
N	0.23389600	-0.76130000	-2.89739300
C	-1.12390400	-1.02234100	-3.10869100
C	-1.65285000	-0.87454400	-4.39036700
C	-2.00041500	-1.36616800	-2.08473800
C	-2.99953100	-1.07111200	-4.63514500
C	-3.34949700	-1.59011500	-2.33578500
C	-3.87636600	-1.44397800	-3.61606900
C	-5.32918700	-1.65845200	-3.96656600
F	-4.11155800	-1.91926500	-1.29664100
F	-1.57768700	-1.44406900	-0.82480500
F	-0.84745600	-0.52597400	-5.39122900
F	-3.45113200	-0.91678900	-5.87781800
F	-5.45688600	-2.63010400	-4.88359400
F	-5.86210000	-0.54409900	-4.48822800
F	-6.07123300	-2.00351800	-2.91182100
C	1.06625600	-1.58916300	-2.18238900
O	0.70949100	-2.65910400	-1.73322600
C	2.50768500	-1.10638100	-2.06056200
H	2.94519400	-1.66867500	-1.22986800
H	3.02708400	-1.44539100	-2.96319000
C	2.72215500	0.37552800	-1.87441300
C	3.80600700	1.06092700	-2.44097200
C	1.87941100	1.14178200	-1.06946200
C	4.06575600	2.40041200	-2.16834700
C	2.06450900	2.51041700	-0.86366300
C	3.21014600	3.13982100	-1.35383100
H	4.93965600	2.87063800	-2.60572700
H	3.43484600	4.18180000	-1.15831100
C	0.70529300	2.14372400	0.57909700
C	1.37009300	1.97512200	1.94698700
C	0.82531600	0.75355200	-0.08910400
H	-0.32575800	2.50467300	0.67696700
C	2.38207300	0.83491100	1.73929600
C	0.29214200	1.23924000	2.78600500
H	1.73783100	2.89096800	2.40784600
C	1.36288400	-0.11120200	1.07729000
H	-0.10541000	0.37524500	-0.51113400
H	2.76175200	0.44506000	2.68928100
H	3.23144500	1.09910100	1.10489000
H	0.61132300	1.19580700	3.83246400
H	-0.67849900	1.74493400	2.76086500
C	0.25387000	-0.18148100	2.14669200
H	1.72907800	-1.08832600	0.75650000
H	0.47934800	-0.95521800	2.88625200
H	-0.71679200	-0.42121700	1.70357800
H	0.57199100	0.13540100	-3.22980400
Cl	4.93843200	0.22251700	-3.48316000
C	1.65825100	4.99061700	0.72330400
H	2.57434500	4.45207500	0.97689400
H	1.89666800	5.98070400	0.32518800
H	1.02930300	5.08408600	1.61555100
I	-1.01443900	2.77105600	-2.69987200
C	-0.96406300	6.58714500	-0.13179300
C	-0.46317000	6.32942600	-2.35197400
C	-1.63129600	7.77047400	-0.36257700
C	-1.09468600	7.50853800	-2.68149300
C	-1.71675400	8.28247100	-1.67690000
N	-0.38023300	5.85764200	-1.09533900
H	-2.08255400	8.27981300	0.47891900
H	-0.89044100	6.19552900	0.87650800

H	-1.11407900	7.80334100	-3.72241100
H	-0.01709600	5.71303800	-3.12328100
N	-2.35943900	9.44854800	-1.95723400
C	-3.02539900	10.18116700	-0.89651700
H	-3.48021200	11.08021500	-1.31280700
H	-3.81856000	9.58479700	-0.42756200
H	-2.31546300	10.49185700	-0.12023500
C	-2.45934200	9.90794400	-3.33061800
H	-1.46752800	10.06367800	-3.77177600
H	-3.01260600	9.19646700	-3.95675600
H	-2.98773900	10.86129200	-3.35230800

TS69

Pd	0.47714600	3.99147800	0.03913000
N	0.36538800	0.04864600	-3.23481300
C	-0.95512500	-0.13118600	-3.65440300
C	-1.32915000	0.28139000	-4.93005200
C	-1.95195600	-0.64716600	-2.82467900
C	-2.64421700	0.19730200	-5.36935000
C	-3.25798600	-0.75428800	-3.27257500
C	-3.63431300	-0.33806600	-4.55021700
C	-5.08897400	-0.44227800	-4.93935900
F	-4.17466400	-1.24131200	-2.43784300
F	-1.68149700	-0.99819000	-1.57054200
F	-0.41717300	0.80269400	-5.74448600
F	-2.91137800	0.65156700	-6.59084100
F	-5.30408500	-0.13077700	-6.21982500
F	-5.83966100	0.38213600	-4.19111800
F	-5.54823500	-1.68675300	-4.74626700
C	1.09624800	-0.96738600	-2.67146200
O	0.66905800	-2.09862300	-2.54455000
C	2.52501700	-0.60377400	-2.28971200
H	2.85377500	-1.36496900	-1.57548200
H	3.13189400	-0.74633900	-3.18955800
C	2.73948900	0.78157200	-1.73719200
C	3.86421600	1.55772100	-2.04098900
C	1.83769700	1.35009200	-0.83777000
C	4.10521700	2.78912400	-1.43889200
C	2.01337400	2.62239800	-0.29840000
C	3.19090900	3.33177300	-0.54004300
H	5.01010900	3.33304200	-1.68705000
H	3.39998900	4.29392800	-0.08926100
C	0.57952400	1.96938500	0.92750300
C	1.18506000	1.47893500	2.24651300
C	0.71694600	0.76851400	-0.04182900
H	-0.45757200	2.29859000	1.07965800
C	2.18101600	0.38339600	1.82479900
C	0.06501400	0.60306500	2.86282700
H	1.55247300	2.26306800	2.90942800
C	1.17360500	-0.35376700	0.92129500
H	-0.19002300	0.52389900	-0.59427300
H	2.50304400	-0.22535500	2.67602200
H	3.06775100	0.75422300	1.30632500
H	0.34811100	0.30257500	3.87708700
H	-0.89216700	1.12992800	2.93291000
C	0.01396400	-0.62495500	1.90301100
H	1.53295500	-1.24709300	0.40699400
H	0.17913100	-1.56051000	2.44538900
H	-0.94319100	-0.71381100	1.38025400
H	0.71252100	1.01113600	-3.29530400
Cl	5.07248900	0.96923300	-3.16731400
C	1.48308200	4.82416900	1.59425300
H	2.30992100	4.19654700	1.93560100
H	1.86026900	5.80677400	1.29333600
H	0.75630900	4.93494300	2.40927500
O	-0.98506000	3.22258900	-1.34982100
C	-0.84264500	3.04730000	-2.60843400
O	0.23144500	2.88209700	-3.21017500
C	-2.15412200	3.09399600	-3.39039300
H	-2.64848200	4.05256300	-3.20044700
H	-1.97277700	2.98071700	-4.46071100
H	-2.83560400	2.31062900	-3.04194400

C	-0.38585600	6.20407700	-1.77633000
C	-0.76886700	6.82554500	0.39753700
C	-0.94253300	7.36777100	-2.25927900
C	-1.35286100	8.01380000	0.01253100
C	-1.46321900	8.32702800	-1.36106100
N	-0.29165900	5.91771400	-0.46518100
H	-0.97040900	7.51703000	-3.33072800
H	0.01058700	5.46087100	-2.46043400
H	-0.67251500	6.58247900	1.45032400
H	-1.71905100	8.68307100	0.78013100
N	-2.03376200	9.48394200	-1.79375200
C	-2.15119300	9.74631300	-3.21666900
H	-2.74659200	8.97462400	-3.72035000
H	-2.64738400	10.70564400	-3.36454000
H	-1.16675600	9.79756600	-3.69777100
C	-2.57153200	10.42911800	-0.83323200
H	-2.97556600	11.29133200	-1.36397300
H	-3.38158700	9.98516400	-0.24047500
H	-1.79456400	10.78947000	-0.14771700

TS44

N	6.61846700	-1.09118200	0.34907200
C	6.91737000	-2.35061200	-0.00154900
C	7.35175100	-0.12114800	-0.21024200
C	7.91751300	-2.68505300	-0.89302600
H	6.32947000	-3.12686500	0.47755400
C	8.37420200	-0.34574000	-1.11163500
H	7.10527800	0.89290400	0.08788100
C	8.69323200	-1.66720900	-1.48889400
H	8.08303800	-3.73143900	-1.11469600
H	8.90769200	0.50798900	-1.51063500
N	0.53173300	-0.69657600	-1.28464500
C	-0.74415600	-0.53363700	-1.82280300
C	-0.90676000	0.05246300	-3.07762400
C	-1.88921800	-0.90630000	-1.12456700
C	-2.16379200	0.23925800	-3.62202200
C	-3.15229800	-0.74480000	-1.68599000
C	-3.31391600	-0.16862400	-2.94410900
C	-4.65120500	0.05626400	-3.61023400
F	-4.19183900	-1.13273700	-0.95581000
F	-1.79749300	-1.38912000	0.10787200
F	0.17583100	0.44663900	-3.75284800
F	-2.26213500	0.80575300	-4.82236000
F	-4.69410000	-0.55334000	-4.80360300
F	-4.85825400	1.36529700	-3.82141000
F	-5.67349100	-0.40247900	-2.88681900
C	0.99187200	-1.92492600	-0.83111300
O	0.29647300	-2.91503600	-0.81599200
C	2.41898500	-1.92763100	-0.29592000
H	2.33996500	-2.21124200	0.74731700
H	2.93045700	-2.75603500	-0.79112600
C	3.19882600	-0.64842300	-0.46112400
C	3.80821200	-0.41558600	-1.69800000
C	3.31807700	0.34593200	0.56232100
C	4.50968300	0.75121700	-1.98220500
C	4.07769100	1.52662900	0.27769700
C	4.62901400	1.71359100	-1.00350200
H	4.95485000	0.89042100	-2.96124300
H	5.16153800	2.63249900	-1.22480800
C	3.55405600	0.02955600	3.06882100
C	2.75783300	-0.85122500	4.02503300
C	2.56414400	0.35980300	1.92846800
H	3.99152000	0.91005600	3.55570800
C	1.97874400	-1.74151800	3.05364800
C	1.62803600	0.03466900	4.61021200
H	3.36127700	-1.36255900	4.77343100
C	1.36090200	-0.56063200	2.26997900
H	2.22664100	1.39711400	2.02164300
H	1.21311600	-2.35563700	3.53895300
H	2.65237100	-2.40054000	2.50034600
H	1.16738200	-0.45455200	5.47465000
H	2.00398300	1.00667200	4.94757600

C	0.62612400	0.15677600	3.42542000
H	0.69171300	-0.79588900	1.44224500
H	-0.31141400	-0.36388800	3.64531200
H	0.37462500	1.19405500	3.18022600
H	1.22198600	0.00468100	-1.51659400
N	7.07779400	2.56292100	2.68516100
C	7.33310900	1.37117500	3.26731500
C	8.03956900	3.03539300	1.86642500
C	8.44488400	0.60205400	3.00158800
H	6.58653300	1.00545100	3.96434800
C	9.20075700	2.35625300	1.55515100
H	7.84875300	4.01022500	1.42798100
C	9.40555300	1.05880300	2.07787000
H	8.51516100	-0.36799300	3.47567500
H	9.90368200	2.81291000	0.86949100
Cl	3.68631800	-1.59484800	-2.99423700
Pd	5.04647200	-0.63068200	1.87607000
Pd	5.10856200	2.46166900	1.69582300
I	6.03843000	-2.37936800	3.66264700
C	3.31266300	3.31893500	0.91547400
H	2.35182900	2.90791400	0.60374500
H	3.16119700	3.80829700	1.88909900
H	3.64193800	4.04606000	0.17032900
N	9.69567500	-1.94613400	-2.37429400
C	10.39654300	-0.86248600	-3.03174300
H	11.12857300	-1.27472400	-3.72712500
H	9.71254400	-0.21904300	-3.60112300
H	10.93774300	-0.23715500	-2.30990000
C	9.94509000	-3.31854900	-2.77192700
H	10.77238800	-3.34227800	-3.48196400
H	10.22350600	-3.93817800	-1.91074100
H	9.06799900	-3.76949100	-3.25454600
N	10.45337200	0.27263800	1.69929100
C	10.40100400	-1.15370600	1.98700000
H	9.44713600	-1.59066900	1.66515600
H	11.20818600	-1.65410000	1.45015300
H	10.53141000	-1.35254100	3.05670500
C	11.41061600	0.77035600	0.73607000
H	11.87024000	1.70139400	1.08596900
H	12.20698700	0.03570300	0.60895900
H	10.95195200	0.95790800	-0.24668200

N1-acridine-Me

acridine

C	-0.25449200	-8.21398100	-5.99812400
C	1.10713200	-8.26558300	-5.99326700
C	1.87891600	-7.06253000	-5.99384000
C	1.20205000	-5.79723600	-5.99964800
C	-0.22908500	-5.78827800	-6.00452000
C	-0.92990300	-6.95698600	-6.00385800
C	3.27244100	-7.05094700	-5.98915100
C	3.18338600	-4.63215200	-5.99551500
C	3.95995800	-5.83894600	-5.98993300
C	5.38648800	-5.74995200	-5.98529300
H	5.96506800	-6.67028500	-5.98118500
C	6.00377000	-4.53526300	-5.98601100
C	5.23370600	-3.33363300	-5.99138000
C	3.87159500	-3.37766500	-5.99596600
H	3.82377200	-7.98939800	-5.98481500
H	-0.83575400	-9.13105000	-5.99763700
H	1.62884100	-9.21919700	-5.98879800
H	-0.72143500	-4.82152000	-6.00891300
H	-2.01584000	-6.93962600	-6.00782100
H	7.08769100	-4.47223800	-5.98233500
H	5.74668600	-2.37645800	-5.99184400
H	3.26672300	-2.47690700	-6.00006900
N	1.84460500	-4.62276400	-6.00031100

CH₃Pd(I)(acridine)₂

Pd	-1.09540400	1.02883800	-0.70079000
I	-3.13488100	2.48893800	-1.56439000

C	-2.09414600	-0.63491100	-1.24879400
H	-3.06343200	-0.67290500	-0.74487700
H	-2.24993200	-0.60402800	-2.33001300
H	-1.47583100	-1.49415600	-0.97110300
C	0.78655300	2.84169800	1.15819500
C	1.24199800	3.16507000	-1.09193000
C	-0.16130300	2.57001800	2.19104100
C	2.14589600	3.10327100	1.52387900
C	2.62163600	3.44480300	-0.81950100
C	0.78014900	3.23663400	-2.44373900
C	0.23318200	2.53327400	3.49656500
H	-1.19295300	2.40008100	1.89816400
C	2.52142800	3.03983200	2.90064100
C	3.05268500	3.37844500	0.50220800
C	3.50029200	3.74197200	-1.90568500
H	-0.27466900	3.06045800	-2.63040600
C	1.64832600	3.54439500	-3.44917900
C	1.59270100	2.75915400	3.85840500
H	-0.49517700	2.32144100	4.27272900
H	3.55910500	3.22722300	3.16422300
H	4.10129000	3.54833100	0.73780700
C	3.02794300	3.78825200	-3.18330500
H	4.54753800	3.93500500	-1.68899100
H	1.28410500	3.61217900	-4.46983000
H	1.88033200	2.71232900	4.90414200
H	3.69731200	4.02347000	-4.00522600
C	0.42892100	-0.46570400	1.48712000
C	1.75181300	-0.07931100	-0.39331600
C	-0.86270700	-0.62343700	2.07698600
C	1.58484400	-0.63674500	2.31470900
C	2.95512800	-0.22693900	0.36661700
C	1.85392900	0.16427800	-1.79550700
C	-0.98365800	-0.91595700	3.40336100
H	-1.73371300	-0.50042600	1.44183900
C	1.41306100	-0.91739400	3.70419900
C	2.83862100	-0.48301000	1.73040100
C	4.21569400	-0.07680600	-0.28797800
H	0.93316400	0.25542800	-2.36369600
C	3.07652700	0.28564000	-2.38769200
C	0.16542800	-1.05281600	4.23484100
H	-1.97080800	-1.04123200	3.83731900
H	2.29942000	-1.02268600	4.32367500
H	3.73371500	-0.56715800	2.34290000
C	4.27505200	0.17686900	-1.62581900
H	5.12214600	-0.17582700	0.30306700
H	3.13951400	0.47704000	-3.45376800
H	0.03856600	-1.27023100	5.29064400
H	5.23432900	0.29102600	-2.12037900
N	0.53318800	-0.13953400	0.18258800
N	0.37636100	2.81607900	-0.12352800

1			
Pd	-0.01038700	1.15447900	0.02837600
O	-1.75764600	1.05176700	1.05227400
O	1.73327400	1.25005600	-1.00317800
C	-1.72529600	1.48816100	2.27490900
C	1.67243400	1.82738300	-2.16498200
O	-0.70981300	1.80478400	2.89216500
O	0.64195500	2.19806200	-2.72419500
C	-3.10453900	1.59096600	2.90449400
H	-3.67298800	2.37874100	2.39906100
H	-3.65205300	0.65386300	2.77011300
H	-3.01674100	1.82753600	3.96595200
C	3.03762400	2.00689300	-2.80809700
H	3.67319700	2.61810000	-2.15983300
H	3.52537800	1.03377100	-2.92084100
H	2.93373000	2.48471900	-3.78339100
C	-0.22352000	-1.52439400	-1.29605200
C	0.34032100	-1.66451000	0.97835200
C	-0.54324500	-0.74296900	-2.44750400
C	-0.18307400	-2.94996100	-1.43026700
C	0.41398700	-3.09355800	0.90726400

C	0.59750900	-1.03253500	2.23271600
C	-0.80785600	-1.35444200	-3.63856300
H	-0.53031000	0.34155000	-2.38254400
C	-0.47153900	-3.54715000	-2.69525500
C	0.14488900	-3.70806200	-0.31104300
C	0.75626600	-3.84051700	2.07579500
H	0.49921800	0.04596900	2.32482000
C	0.91304700	-1.78576300	3.32645700
C	-0.77942600	-2.77174200	-3.77175300
H	-1.03632700	-0.74226900	-4.50546000
H	-0.43658300	-4.63022700	-2.77514400
H	0.19148200	-4.79226200	-0.39000500
C	1.00238700	-3.20508900	3.25478000
H	0.81310400	-4.92277200	1.99748600
H	1.09044500	-1.28811500	4.27473100
H	-0.99584800	-3.22651000	-4.73315000
H	1.25999200	-3.77287800	4.14329200
C	-1.03813400	3.92047600	-0.43262500
C	0.90367900	3.86843000	0.88197200
C	-2.03543200	3.24228000	-1.19557200
C	-1.11506700	5.34559000	-0.32702900
C	0.89789500	5.29405200	1.01040600
C	1.94571500	3.13472900	1.52432700
C	-3.04000500	3.94425000	-1.79246200
H	-1.97484800	2.16670000	-1.29395900
C	-2.18491200	6.04261800	-0.96798100
C	-0.12902900	6.00549300	0.39891900
C	1.93014800	5.93859900	1.75880600
H	1.95368300	2.05622100	1.43913100
C	2.91388800	3.78785500	2.22747400
C	-3.12510200	5.36144800	-1.67887300
H	-3.78889200	3.41270000	-2.37118600
H	-2.22718900	7.12407100	-0.87213800
H	-0.16193100	7.08916600	0.49047100
C	2.91424900	5.20692700	2.34985700
H	1.90668700	7.02149800	1.84431100
H	3.69975700	3.21449400	2.70917900
H	-3.93838000	5.89056200	-2.16534800
H	3.69925200	5.69655200	2.91735700
N	0.03440600	-0.92620100	-0.11179600
N	-0.04968800	3.22820400	0.17250400

31

Pd	2.59225900	3.79145400	0.22869700
N	0.25968400	0.37077200	-2.35987700
C	-0.94399200	1.06275600	-2.42810000
C	-1.28696600	1.71739600	-3.61476100
C	-1.80047600	1.22856100	-1.33890400
C	-2.43258600	2.48477900	-3.71134700
C	-2.96494700	1.98254000	-1.44456600
C	-3.30528800	2.62725100	-2.63085900
C	-4.50589400	3.52489500	-2.79292900
F	-3.70676300	2.10180100	-0.34918700
F	-1.50206100	0.72247600	-0.14735400
F	-0.47314500	1.61573900	-4.66583400
F	-2.69498200	3.09807500	-4.86326300
F	-4.11210700	4.79606600	-3.02594200
F	-5.28803800	3.54862200	-1.71344700
F	-5.25685000	3.14962900	-3.83392400
C	0.45710100	-0.82808100	-1.69063000
O	-0.46218800	-1.51009300	-1.29552300
C	1.92798300	-1.20987400	-1.49178300
H	1.96134500	-1.71587300	-0.52266600
H	2.17733200	-1.96251900	-2.24484100
C	2.87343900	-0.03257200	-1.54657000
C	3.81834500	0.14322500	-2.56308900
C	2.70748000	1.02205100	-0.62789000
C	4.55688900	1.31667800	-2.68206500
C	3.36116800	2.25771800	-0.78532800
C	4.30635500	2.37267900	-1.81063700
H	5.29244800	1.40827800	-3.47441700
H	4.84742200	3.30542700	-1.95878500

C	1.54187900	2.33583800	1.15678200
C	1.95030600	2.16781700	2.62523500
C	1.77536700	0.92759500	0.54308700
C	3.13878500	1.19870200	2.51734400
C	0.87852900	1.27100800	3.29646500
H	2.12573600	3.10430100	3.15981000
C	2.34638100	0.12767800	1.74932100
H	0.81386700	0.49430200	0.25858500
H	3.49490800	0.84094700	3.49025200
H	3.97793800	1.61153300	1.95049100
H	0.99983200	1.28690700	4.38508200
H	-0.13820700	1.61198900	3.07461700
C	1.17742200	-0.14224100	2.71417200
H	2.90538400	-0.76555900	1.45726600
H	1.48313100	-0.83682200	3.50369200
H	0.31488700	-0.58195900	2.20282900
H	1.06935700	0.81994900	-2.76738300
H	0.50684200	2.67860700	1.03996800
Cl	4.09181300	-1.11225600	-3.76701200
C	1.74170000	5.94624800	2.37326300
C	0.14129000	5.62141800	0.71194600
C	3.05211500	5.70447000	2.88726400
C	0.84876500	6.76588600	3.13571400
C	-0.81860800	6.41561200	1.41908200
C	-0.23986200	5.05909800	-0.54477700
C	3.43979800	6.24911600	4.07615600
H	3.71751400	5.06724800	2.30985400
C	1.29496700	7.31959800	4.37512900
C	-0.43343100	6.97726800	2.63402400
C	-2.12420000	6.59685700	0.86496400
H	0.49241600	4.46304200	-1.08236300
C	-1.49087600	5.26732500	-1.04586400
C	2.55397400	7.07012300	4.83265400
H	4.43776800	6.05523000	4.45675900
H	0.60812100	7.94114400	4.94287800
H	-1.13898700	7.58520500	3.19639200
C	-2.45473300	6.03500000	-0.33154900
H	-2.84319700	7.19207900	1.42098600
H	-1.76200800	4.84855900	-2.00856600
H	2.88973500	7.49239700	5.77417400
H	-3.44524400	6.16563700	-0.75370500
N	1.38047300	5.39321500	1.19860100

TS32

Pd	2.71050300	4.06175800	0.36318500
N	-0.04037200	0.35186600	-2.65175600
C	-1.17446900	0.83644700	-3.30932900
C	-1.33536900	0.60966400	-4.67639300
C	-2.15824400	1.57415600	-2.65788500
C	-2.44104700	1.08555100	-5.35707700
C	-3.28576800	2.02736600	-3.33589900
C	-3.44771400	1.79385700	-4.69875100
C	-4.63555300	2.26354400	-5.50908200
F	-4.17565500	2.71579000	-2.63142600
F	-2.02481600	1.90195300	-1.37388900
F	-0.39471900	-0.07345600	-5.33171200
F	-2.54097500	0.84007500	-6.65928400
F	-5.25703300	1.22245300	-6.07803900
F	-4.23651600	3.08337300	-6.49177300
F	-5.53286600	2.91946600	-4.77272500
C	-0.11612900	-0.43760100	-1.51283600
O	-1.16544000	-0.68400200	-0.96085700
C	1.22972600	-0.96854400	-1.04257300
H	1.05377700	-1.43942800	-0.07359000
H	1.51794800	-1.77259300	-1.72672300
C	2.33268200	0.06567100	-0.96788800
C	3.57964100	-0.14239000	-1.57117000
C	2.14320600	1.28570100	-0.28676600
C	4.60812200	0.79511300	-1.51025300
C	3.15756300	2.24700900	-0.27156800
C	4.39763300	2.00021200	-0.85481700
H	5.56171400	0.57844200	-1.97846700

H	5.19673700	2.73548600	-0.80674800
C	1.03836600	3.09975200	1.02907700
C	0.87528600	2.90621100	2.53471400
C	0.88002400	1.67335800	0.43209200
C	1.44184900	1.49599800	2.75729900
C	-0.64343500	2.66155700	2.74744000
H	1.27776500	3.70707700	3.15451000
C	0.54937800	0.83641600	1.69770700
H	0.03310500	1.67138900	-0.25921900
H	1.25184800	1.12185300	3.76797200
H	2.50953400	1.40832500	2.54233900
H	-0.86840400	2.69756900	3.81806000
H	-1.26202000	3.42180600	2.25887100
C	-0.86199700	1.23445200	2.16496100
H	0.68014200	-0.23693000	1.56561200
H	-1.21672800	0.54461000	2.93615900
H	-1.58312500	1.20734000	1.34364300
H	0.82381300	0.33962900	-3.17658800
I	6.77591900	6.07845800	2.38612700
C	3.98738500	3.74822600	1.92118100
H	3.48413900	4.21446200	2.76895500
H	0.34449700	3.83914100	0.60484400
H	4.23089700	2.70259300	2.08735700
H	4.84381800	4.34693000	1.57659900
Cl	3.91751800	-1.62432500	-2.44903900
C	3.44004100	6.74929200	-0.26369200
C	2.43459000	6.83517000	1.84397000
C	3.46534000	6.22913100	-1.59030400
C	4.40823000	7.72526100	0.10367100
C	3.36924900	7.81251800	2.29403400
C	1.39089200	6.43340800	2.72113000
C	4.42838100	6.63816000	-2.47616400
H	2.67956500	5.54384000	-1.90516800
C	5.39225300	8.12335200	-0.84046600
C	4.40005400	8.18896300	1.42575900
C	3.26499100	8.31933800	3.62012800
H	0.65163900	5.72954900	2.35338800
C	1.30867800	6.95666000	3.98284200
C	5.40822800	7.59077100	-2.09964400
H	4.43307200	6.23722200	-3.48530700
H	6.14886700	8.83532200	-0.52658800
H	5.15873000	8.89014200	1.75691500
C	2.26144100	7.90254000	4.44743300
H	4.01121800	9.03055500	3.96042200
H	0.50062600	6.64947600	4.64034900
H	6.16803200	7.89014900	-2.81326500
H	2.18498800	8.29011500	5.45770200
N	2.52227700	6.26696500	0.61708200

TS35

Pd	2.41773800	3.95658100	0.27297700
N	-0.21484500	-0.46896500	-2.85870300
C	-1.37167400	0.10316300	-3.38376300
C	-1.94269500	-0.40066100	-4.54836900
C	-1.96953400	1.22256100	-2.79897700
C	-3.07779700	0.16790000	-5.11383600
C	-3.11748500	1.76726400	-3.34709700
C	-3.69534300	1.26150000	-4.51193000
C	-4.93705300	1.93736600	-5.04453500
F	-3.65493700	2.83642600	-2.75555000
F	-1.42484100	1.80385000	-1.73552700
F	-1.37829700	-1.45183000	-5.14394500
F	-3.54802500	-0.38203600	-6.22795700
F	-5.40642900	1.35794600	-6.15026500
F	-4.68785200	3.22346100	-5.33473600
F	-5.91549600	1.91607800	-4.12808900
C	-0.08374800	-0.80118100	-1.52042200
O	-1.01877600	-0.74556000	-0.74966800
C	1.33765600	-1.17369000	-1.11447300
H	1.29423900	-1.44795900	-0.06041300
H	1.66571700	-2.05263200	-1.67707700
C	2.25873600	0.00555100	-1.35670900

C	3.06441000	0.10121600	-2.49284700
C	2.21152900	1.11848400	-0.49617400
C	3.80198400	1.24100500	-2.78126300
C	2.89187300	2.31260200	-0.80035500
C	3.69946700	2.34423500	-1.94073300
H	4.42087000	1.27484000	-3.67173800
H	4.23602600	3.24865000	-2.21451200
C	1.39507400	2.55591000	1.37064000
C	2.00760300	2.38405100	2.76922000
C	1.41958200	1.11885100	0.77660700
C	3.07384900	1.30368300	2.52152500
C	0.98628900	1.61016200	3.63860700
H	2.34526600	3.31369700	3.23627400
C	2.07846600	0.29692200	1.92244100
H	0.40122600	0.75550800	0.60305600
H	3.54493100	0.93789100	3.44085100
H	3.85208100	1.60310600	1.81180700
H	1.28698500	1.62693600	4.69230600
H	-0.01363500	2.05133400	3.57548000
C	1.04643900	0.16623800	3.05720900
H	2.51069200	-0.65349800	1.59774300
H	1.39198000	-0.54802900	3.81219300
H	0.07766600	-0.18512000	2.68778900
H	0.52797800	-0.71421300	-3.50102800
I	3.79409000	5.98080800	-1.01007200
C	4.82874400	4.29193600	0.63606600
H	4.41461200	3.73544700	1.47476100
H	5.43842500	5.12525000	0.96566700
H	0.37969900	2.96279600	1.42106500
H	5.30920600	3.65075000	-0.09506800
Cl	3.13574600	-1.22466700	-3.66064400
C	1.49127700	6.30121500	2.37602600
C	-0.10180500	5.74220800	0.77503700
C	2.78087600	6.11591000	2.95938800
C	0.62351900	7.27773000	2.96386000
C	-1.03114100	6.69694800	1.30510300
C	-0.51747100	4.95366300	-0.34279200
C	3.16959400	6.84534200	4.04455100
H	3.43942100	5.37969100	2.51828000
C	1.06691800	8.02490700	4.09757800
C	-0.63683300	7.45641600	2.40147500
C	-2.32210800	6.83448000	0.70810500
H	0.17291800	4.22318800	-0.75342100
C	-1.76475700	5.10133800	-0.87464400
C	2.30479800	7.81604300	4.62621800
H	4.15381500	6.68656200	4.47454300
H	0.39234700	8.76069000	4.52682600
H	-1.31965200	8.19028500	2.82458500
C	-2.68200100	6.05606000	-0.34978200
H	-3.00818400	7.56801900	1.12277000
H	-2.07149700	4.46971000	-1.70028000
H	2.63875600	8.38342100	5.48882400
H	-3.66533200	6.15484900	-0.79796800
N	1.12634900	5.56508500	1.30895300

TS65

Pd	4.68835300	3.40930700	-3.65090200
N	0.71612700	-0.77239900	-2.57221300
C	-0.03748600	-0.91094800	-3.73445700
C	-0.24612500	0.13931400	-4.62669900
C	-0.57617200	-2.15516000	-4.06569300
C	-1.00604400	-0.04079900	-5.77728800
C	-1.30162000	-2.33909600	-5.22829800
C	-1.54637000	-1.28141600	-6.10512100
C	-2.34784800	-1.55831900	-7.35559500
F	-1.78248900	-3.55061100	-5.49398700
F	-0.36986200	-3.18748200	-3.24588500
F	0.31540500	1.32630200	-4.42301100
F	-1.15335000	1.01709500	-6.57450800
F	-1.70262700	-2.42943300	-8.14575800
F	-2.57837000	-0.45664200	-8.07322300
F	-3.53576300	-2.09681000	-7.04937200

C	0.53862400	0.25548000	-1.65834400
O	-0.32109900	1.09898900	-1.78259100
C	1.55830400	0.23649100	-0.52563500
H	1.26517700	1.02911000	0.16419800
H	1.51517800	-0.71836100	0.00739000
C	2.93502000	0.49587300	-1.08896700
C	3.88635000	-0.49515500	-1.35140700
C	3.29932900	1.78984100	-1.45034400
C	5.14964600	-0.20189000	-1.85954100
C	4.50405200	2.10404800	-2.09359900
C	5.48296300	1.10478200	-2.21645000
H	5.86656900	-1.00480700	-1.99612700
H	6.47400600	1.31222700	-2.60556400
H	1.31755400	-1.54510100	-2.31475500
C	4.01376500	3.89632500	-1.65144700
C	4.77997900	4.39259400	-0.41414100
C	2.78001900	3.13953800	-1.06387000
H	3.73428400	4.75973300	-2.28973000
C	3.98224000	5.61130500	0.10236800
C	4.43634300	3.35962100	0.67354600
H	5.83919200	4.58736100	-0.59137000
C	2.91555900	3.44916200	0.44729800
H	1.80436700	3.42344700	-1.47041800
C	2.66650000	4.96276800	0.63339800
H	3.80255400	6.35453300	-0.68126400
H	4.52866800	6.11017000	0.91044900
H	4.85914700	2.36712000	0.50347900
H	4.72766000	3.69915200	1.67339100
H	2.29713500	2.81775300	1.09043100
H	1.78117900	5.29867800	0.08354700
H	2.50506700	5.19927100	1.68980000
Cl	3.51563800	-2.18741100	-1.01060400
C	4.18994600	3.31376000	-6.71854300
C	6.29372300	4.18318500	-6.22834200
C	2.94900900	2.75997300	-6.27848400
C	4.40177800	3.48171000	-8.12587500
C	6.58390400	4.38447500	-7.61594800
C	7.28401500	4.54896700	-5.26653000
C	1.98910700	2.40981500	-7.18187200
H	2.79888000	2.62832500	-5.20931200
C	3.37246700	3.09728700	-9.03995500
C	5.61330400	4.02275000	-8.54678800
C	7.84263600	4.94538400	-7.99398200
H	7.05022500	4.38754200	-4.21631200
C	8.47486300	5.08027700	-5.66670900
C	2.19929000	2.57866500	-8.58133500
H	1.04800300	2.00217500	-6.83167000
H	3.54770400	3.23229900	-10.10377700
H	5.80183100	4.16623800	-9.60870700
C	8.76228600	5.28461100	-7.04773900
H	8.04606200	5.09533500	-9.05078900
H	9.21818400	5.35444600	-4.92445400
H	1.41761500	2.28986800	-9.27675800
H	9.71682100	5.71188900	-7.33803500
N	5.12219600	3.66390500	-5.80740500

TS36

Pd	1.62767400	3.95818000	0.17683400
N	-0.51918600	-0.10640400	-1.36133400
C	-1.78042900	-0.01307400	-0.76336300
C	-2.92807900	0.02519700	-1.55025800
C	-1.94351300	0.10296200	0.61585800
C	-4.18097600	0.18756100	-0.98470200
C	-3.20058600	0.25271700	1.18536200
C	-4.34766600	0.29126000	0.39482800
C	-5.72996300	0.53800900	0.94742300
F	-3.25641700	0.40731100	2.50409100
F	-0.88702500	0.13137700	1.42405800
F	-2.81508600	-0.03320400	-2.87470300
F	-5.23112000	0.28064500	-1.79670600
F	-6.62435400	-0.29702600	0.41252700
F	-6.13582800	1.79524500	0.65750200

F	-5.78798000	0.40229900	2.27198200
C	0.39943300	-1.07717300	-1.01321200
O	0.12799500	-1.97635100	-0.24637500
C	1.77990900	-0.93455400	-1.65865600
H	2.47377900	-1.39792600	-0.95316900
H	1.78511300	-1.55616600	-2.55849800
C	2.18572800	0.48494200	-1.98253200
C	2.30799500	0.94900100	-3.29625800
C	2.34470600	1.41046100	-0.93034100
C	2.56213300	2.28735400	-3.58059800
C	2.54435600	2.77007900	-1.22417000
C	2.67119600	3.20293100	-2.54446800
H	2.65127500	2.61355500	-4.61087500
H	2.80855200	4.25565200	-2.76503900
C	1.74359700	2.25546100	1.34033500
C	2.75558900	2.19936900	2.49469700
C	2.07811500	1.01299800	0.49458000
H	0.72361400	2.20852000	1.72030000
C	3.99136000	1.52103800	1.87602800
C	2.24985300	1.05911300	3.41821200
H	2.92320200	3.14535600	3.01648500
C	3.20918900	0.33033500	1.30755700
H	1.21080500	0.35608600	0.50749600
H	4.71964400	1.21549900	2.63521200
H	4.50927800	2.10769000	1.12213900
H	2.80770900	1.06234200	4.36081300
H	1.18856500	1.16823200	3.66192900
C	2.55091300	-0.22860000	2.58794600
H	3.79130000	-0.40219200	0.74254000
H	3.24651500	-0.88454100	3.12025400
H	1.65131400	-0.81050500	2.36591800
H	-0.28470800	0.58218300	-2.06478900
Cl	2.10412200	-0.13643100	-4.65910600
I	1.28163900	6.50934600	-0.93681600
C	3.74531000	4.07296500	-0.14890600
H	3.82258500	4.42290500	0.88987800
H	4.49574300	3.30687200	-0.31209400
H	3.87559500	4.89855700	-0.84383500
C	-1.05202100	4.11721800	1.78802600
C	-1.42342200	3.61807500	-0.45965900
C	-0.16013200	4.48679400	2.83920900
C	-2.44202100	3.97193200	2.09728300
C	-2.83620000	3.52575300	-0.24227200
C	-0.93311100	3.39824600	-1.78319400
C	-0.62017900	4.65254900	4.11229200
H	0.88717600	4.65254600	2.60167000
C	-2.88308700	4.14164600	3.44536300
C	-3.31645900	3.67719400	1.05603000
C	-3.70558300	3.26214600	-1.34560100
H	0.12900400	3.48272900	-1.96887200
C	-1.79603900	3.14021800	-2.80967100
C	-1.99697500	4.46568800	4.42765700
H	0.07114600	4.93930100	4.89838000
H	-3.93920200	4.01089500	3.66281600
H	-4.37850000	3.55869100	1.25478800
C	-3.20236700	3.08087300	-2.59840500
H	-4.77243500	3.19399200	-1.15581900
H	-1.40096300	2.99533500	-3.81064100
H	-2.33390000	4.59703100	5.45060100
H	-3.86443100	2.87216300	-3.43185400
N	-0.57066900	3.90477600	0.54771300

TS40

Pd	1.57072400	3.85173500	0.04345000
N	-0.51749300	-0.15812300	-1.28768200
C	-1.76676400	0.01308600	-0.68584700
C	-2.91547900	0.11005800	-1.46847000
C	-1.91723000	0.14249000	0.69413100
C	-4.15568100	0.32980400	-0.89596600
C	-3.16357300	0.35191400	1.27004300
C	-4.30832700	0.45930000	0.48318700
C	-5.68333300	0.75314900	1.02878800

F	-3.20543400	0.49103600	2.59083800
F	-0.85883800	0.11546000	1.49904300
F	-2.81336200	0.02910200	-2.79278900
F	-5.21376500	0.44369900	-1.69582200
F	-6.53914400	-0.23465000	0.75191100
F	-6.18146600	1.87848200	0.47012000
F	-5.68688800	0.94392000	2.34920700
C	0.36230700	-1.15807400	-0.91416200
O	0.05344900	-2.02626200	-0.12653700
C	1.75005600	-1.08264500	-1.55657200
H	2.42938100	-1.51804000	-0.81958000
H	1.74854700	-1.75788800	-2.41642900
C	2.17709500	0.31062600	-1.95489500
C	2.28258600	0.71330000	-3.28987100
C	2.34370400	1.28530900	-0.94845900
C	2.51665500	2.04019500	-3.63987300
C	2.51741600	2.62917000	-1.31382900
C	2.61986800	3.00831100	-2.65161500
H	2.59478900	2.31620800	-4.68575800
H	2.73948500	4.06179200	-2.90220500
C	1.78294700	2.23786300	1.28759400
C	2.84292100	2.26053900	2.40442500
C	2.11276200	0.95360000	0.49954300
H	0.78255200	2.17193100	1.71729100
C	4.06363300	1.56778400	1.77098800
C	2.40046800	1.17203500	3.41532600
H	3.01954500	3.23757100	2.86319200
C	3.27936900	0.33334100	1.30963800
H	1.25837700	0.28290900	0.56896600
H	4.83256200	1.32214800	2.51185700
H	4.53167100	2.11536000	0.95663100
H	3.00395100	1.23246500	4.32773100
H	1.35081400	1.28351800	3.70530100
C	2.67744400	-0.15719300	2.64466700
H	3.85096300	-0.42475100	0.76756900
H	3.39699900	-0.78109900	3.18384100
H	1.77281700	-0.75354700	2.49118900
H	-0.25874900	0.48789100	-2.02192200
Cl	2.07703000	-0.43976400	-4.59817200
C	3.66804900	4.05238200	-0.32848800
H	3.76239100	4.40870100	0.70678900
H	4.46141300	3.33702000	-0.51636300
H	3.67944400	4.86413100	-1.05553000
C	-1.10187000	4.02415800	1.73361000
C	-1.47434700	3.64165700	-0.53641500
C	-0.20803600	4.32116400	2.80704100
C	-2.49786800	3.90834500	2.02900900
C	-2.89107400	3.58262600	-0.33103600
C	-0.98119000	3.45153400	-1.86469400
C	-0.67226800	4.43570200	4.08447100
H	0.84482200	4.46408000	2.58303200
C	-2.94324900	4.01901300	3.38174800
C	-3.37448400	3.69560000	0.96956700
C	-3.76038400	3.37046400	-1.44571100
H	0.08301800	3.52080800	-2.04344900
C	-1.84400000	3.23524700	-2.90023500
C	-2.05500900	4.26739800	4.38396800
H	0.02185900	4.66237300	4.88769900
H	-4.00325000	3.89969300	3.58667300
H	-4.44144800	3.60769200	1.15763300
C	-3.25282400	3.20031300	-2.69803500
H	-4.82938000	3.32099800	-1.26376700
H	-1.44595400	3.10040500	-3.90138200
H	-2.39417200	4.35127400	5.41117900
H	-3.91407100	3.02326800	-3.53949600
N	-0.61931700	3.85526000	0.48729500
O	1.03323900	5.67814600	-0.95947900
C	1.62615300	6.38990700	-1.84978000
C	0.95145700	7.73202500	-2.11235300
H	-0.03496400	7.56142200	-2.55707400
H	0.79461900	8.26285300	-1.16862100
H	1.55473600	8.33975600	-2.78917900
O	2.63987100	6.07616900	-2.48752900

TS67

Pd	0.56141600	3.98073400	-0.77807100
N	0.16595300	-0.78210700	-2.86510600
C	-1.19831000	-1.04407300	-3.03185500
C	-1.76117800	-0.92087000	-4.29816100
C	-2.04890100	-1.36084200	-1.97377300
C	-3.11940800	-1.10832600	-4.51758600
C	-3.39859500	-1.57388000	-2.19704100
C	-3.96512100	-1.44995100	-3.46521900
C	-5.44969800	-1.68479500	-3.61013700
F	-4.16993300	-1.87589800	-1.15419400
F	-1.59451200	-1.41573800	-0.72406100
F	-0.97944000	-0.59890600	-5.32702500
F	-3.56364000	-0.96726000	-5.76206900
F	-5.87937900	-1.51818600	-4.86275400
F	-6.14381600	-0.84373800	-2.83015300
F	-5.76944600	-2.93353600	-3.23611000
C	1.01970900	-1.59721400	-2.16104300
O	0.67530400	-2.65437500	-1.67396000
C	2.46697200	-1.11754600	-2.10176300
H	2.93321100	-1.66484900	-1.27669800
H	2.95092700	-1.47660200	-3.01595800
C	2.68802400	0.36737300	-1.94988900
C	3.74867800	1.04803500	-2.56373700
C	1.87010400	1.14306700	-1.12859600
C	4.01228900	2.39241300	-2.31672400
C	2.05005000	2.51652900	-0.95458800
C	3.18003600	3.14129400	-1.48687700
H	4.87266500	2.85802200	-2.78497300
H	3.40997600	4.18544800	-1.30843600
C	0.74238000	2.17028700	0.53573100
C	1.44509800	2.04841300	1.88792800
C	0.85837700	0.76588000	-0.10162400
H	-0.29291300	2.50973800	0.65018400
C	2.46971700	0.91939400	1.67842300
C	0.40365300	1.31655800	2.77474100
H	1.80790800	2.98333300	2.31389100
C	1.44756200	-0.05924500	1.06865700
H	-0.08149600	0.36476600	-0.48040300
H	2.88198900	0.55784200	2.62589600
H	3.29684100	1.18170000	1.01470200
H	0.75174600	1.30597100	3.81270400
H	-0.57596800	1.80580300	2.76393700
C	0.37200600	-0.12058200	2.17258700
H	1.82138600	-1.03800300	0.76211900
H	0.63351700	-0.87091200	2.92412700
H	-0.60685500	-0.38871500	1.76519200
H	0.49683700	0.10336800	-3.23201800
Cl	4.84830400	0.20039600	-3.63225700
C	1.69348100	5.06896300	0.53394800
H	2.56429100	4.50153600	0.86961800
H	2.00987000	5.97747900	0.01248300
H	1.06056800	5.33271600	1.38708400
I	-1.14417300	2.75413400	-2.64852100
C	-1.44085500	6.28248400	-0.38864600
C	-0.04676100	6.59598200	-2.23968600
C	-1.87623800	5.48788800	0.71311000
C	-2.09946300	7.53153000	-0.62271800
C	-0.65912800	7.85599000	-2.53500000
C	0.99345900	6.13061000	-3.09862500
C	-2.88772100	5.91567100	1.52215400
H	-1.39548000	4.53128500	0.88127300
C	-3.15170600	7.94666200	0.24950000
C	-1.68209800	8.30149500	-1.70397900
C	-0.20769500	8.61089300	-3.66029200
H	1.43627300	5.15912000	-2.90470800
C	1.39273000	6.87909400	-4.16724500
C	-3.53585700	7.16304500	1.29527000
H	-3.21059900	5.29221400	2.35005300
H	-3.63769800	8.89875200	0.05600800
H	-2.16249700	9.25679500	-1.90347900

C	0.79218500	8.13801200	-4.45473500
H	-0.68405500	9.56508800	-3.86678200
H	2.17487800	6.50352900	-4.81950800
H	-4.33689800	7.47880400	1.95544700
H	1.13092200	8.70945000	-5.31269900
N	-0.43685400	5.85468400	-1.18156900

TS69

Pd	0.34334500	4.00052700	-0.09367300
N	0.34421600	-0.06285000	-3.26624100
C	-0.96801400	-0.30144400	-3.68383900
C	-1.34667700	0.04046400	-4.97871100
C	-1.95299000	-0.81218400	-2.83714000
C	-2.65464900	-0.10839500	-5.42241900
C	-3.25114700	-0.98411800	-3.28727800
C	-3.63179000	-0.63891100	-4.58471700
C	-5.07730900	-0.82338700	-4.97966900
F	-4.15645500	-1.46638900	-2.43769200
F	-1.67928100	-1.09728500	-1.56676400
F	-0.44636800	0.55799000	-5.80962000
F	-2.92615900	0.27565500	-6.66628600
F	-5.87308100	-0.02548900	-4.25043300
F	-5.47301500	-2.08642300	-4.76637700
F	-5.29945300	-0.54591200	-6.26642600
C	1.10231000	-1.03374000	-2.66169100
O	0.70893200	-2.17136800	-2.48991700
C	2.51918900	-0.61380800	-2.29266500
H	2.87063200	-1.34062200	-1.55387200
H	3.12951600	-0.76883600	-3.18796500
C	2.69276000	0.79476500	-1.78639500
C	3.78894200	1.59717800	-2.12301600
C	1.77699900	1.36433000	-0.90182600
C	3.99476800	2.85330500	-1.55946800
C	1.91631000	2.65608500	-0.40099700
C	3.07145500	3.39269100	-0.66831800
H	4.88114600	3.41731400	-1.82897600
H	3.25492200	4.37290100	-0.24665500
C	0.48795000	2.00180000	0.83595500
C	1.08982800	1.56437100	2.17493700
C	0.66596900	0.77798700	-0.09736500
H	-0.56020100	2.30496900	0.96623500
C	2.11855700	0.48468500	1.79490100
C	-0.01486000	0.67686500	2.80261400
H	1.42835700	2.37589500	2.81982600
C	1.14079400	-0.30417100	0.90199800
H	-0.22890200	0.49399300	-0.65108600
H	2.44724400	-0.09110200	2.66610900
H	3.00057800	0.86481100	1.27504300
H	0.26262600	0.41374200	3.82866700
H	-0.98624000	1.18049600	2.84620700
C	-0.02251600	-0.57874400	1.87817700
H	1.52899800	-1.20146900	0.41648200
H	0.16142300	-1.49365000	2.44889700
H	-0.97083200	-0.70804700	1.34793700
H	0.66145300	0.90880900	-3.35770200
Cl	5.00739700	1.01688600	-3.24213300
C	1.37302300	4.89880600	1.41471400
H	2.17472000	4.26312200	1.79751500
H	1.78874900	5.83801400	1.03533200
H	0.65885900	5.11465500	2.21669200
O	-1.07825900	3.21777500	-1.50660700
C	-0.85342800	2.96718800	-2.73972400
O	0.26080800	2.76071000	-3.25298500
C	-2.10848500	2.95332900	-3.60731500
H	-2.61567100	3.91887700	-3.51594500
H	-1.85622400	2.77020900	-4.65317900
H	-2.80812600	2.18948000	-3.25125000
C	-1.31678600	6.59844800	0.21194300
C	0.09081000	6.59435400	-1.65686800
C	-1.93082000	5.90329900	1.29705100
C	-1.67455800	7.96685500	-0.00770100
C	-0.21451700	7.96701800	-1.93507600

C	0.95670300	5.89409300	-2.55089900
C	-2.82286800	6.53857100	2.11049000
H	-1.68682200	4.85575000	1.44373000
C	-2.60465800	8.59865600	0.87331800
C	-1.09048500	8.63195300	-1.08242000
C	0.38365800	8.60468700	-3.06495100
H	1.14114300	4.83384900	-2.40611200
C	1.49282700	6.53737100	-3.62859400
C	-3.16214100	7.90681100	1.90582700
H	-3.28857000	5.99312200	2.92537600
H	-2.85817000	9.64010200	0.69619400
H	-1.32901800	9.67780600	-1.26361000
C	1.21901500	7.91059900	-3.88720200
H	0.15059000	9.64895900	-3.25336600
H	2.12903200	5.98152000	-4.30980000
H	-3.87127700	8.38781100	2.57149100
H	1.66751400	8.39344900	-4.74939500
N	-0.43061300	5.96461000	-0.58106000

TS44

N	0.21274400	-0.64878400	-1.66569800
C	-1.13519000	-0.29979200	-1.60104300
C	-1.70043900	0.49038400	-2.60172900
C	-1.94557700	-0.67227200	-0.53166100
C	-3.02760300	0.87455100	-2.54685500
C	-3.28886400	-0.31142100	-0.49364300
C	-3.85678300	0.46539200	-1.50111400
C	-5.29784700	0.91985900	-1.50867900
F	-3.99178900	-0.70976200	0.56117300
F	-1.44076400	-1.34491300	0.49647900
F	-0.93424700	0.89045300	-3.61875100
F	-3.51101800	1.63661900	-3.52438600
F	-5.88697100	0.61002100	-2.67172200
F	-5.37403500	2.25179000	-1.36210900
F	-6.01855700	0.36453400	-0.53287500
C	0.65083500	-1.95910600	-1.54567800
O	-0.10209200	-2.88227400	-1.32929500
C	2.15911700	-2.15077100	-1.65000500
H	2.44549300	-2.66766700	-0.74042900
H	2.32407000	-2.86443200	-2.46057900
C	2.98158000	-0.90653500	-1.86804400
C	3.19907800	-0.48901700	-3.17900600
C	3.50905100	-0.10768000	-0.79562000
C	3.93090300	0.65558100	-3.49895200
C	4.23339400	1.08507500	-1.12899900
C	4.42737700	1.43228200	-2.48405100
H	4.10084600	0.91241800	-4.53790100
H	4.97937500	2.33414500	-2.72551900
C	4.52862700	-0.72720500	1.38742700
C	4.14082000	-1.83585500	2.35917500
C	3.20964600	-0.28284900	0.72372900
H	5.08892900	0.08092100	1.87100800
C	3.04394000	-2.57217500	1.58466100
C	3.32024400	-1.15750300	3.48333000
H	4.97382100	-2.44134200	2.72163600
C	2.20498000	-1.30289400	1.31892300
H	2.91759600	0.71838300	1.06188500
H	2.49915900	-3.30668700	2.18710800
H	3.44450500	-3.07797700	0.70378200
H	3.17939500	-1.84387700	4.32517800
H	3.81854000	-0.26185500	3.86956500
C	1.96945100	-0.84009400	2.77647100
H	1.26688100	-1.42480500	0.78017900
H	1.14906400	-1.41535200	3.21674800
H	1.69422400	0.21786400	2.83593600
H	0.83863800	0.01289100	-2.10523900
Cl	2.53231900	-1.38580800	-4.53011600
Pd	5.57438000	-1.14428900	-0.30509700
Pd	5.65900900	1.76445100	0.06513100
I	7.02872600	-1.45210700	-2.67999000
C	3.76006100	2.79647600	-0.15963400
H	2.72804800	2.44319900	-0.18658500

H	3.92666300	3.23831900	0.83189500
H	3.89675500	3.55817000	-0.92833500
C	8.69298100	2.19935300	0.57799300
C	7.46117400	2.87041700	2.43751100
C	8.74479100	1.55603000	-0.69337100
C	9.91943000	2.64096100	1.17458900
C	8.63794000	3.35047600	3.09827300
C	6.21426000	2.95035100	3.12865400
C	9.93951400	1.35825700	-1.32005300
H	7.82630200	1.18412200	-1.14368100
C	11.14832200	2.44040200	0.47330800
C	9.85743000	3.23274900	2.43299800
C	8.52438000	3.91372400	4.40660200
H	5.33235200	2.56087200	2.62910600
C	6.14793100	3.48507700	4.38190200
C	11.15793900	1.81301000	-0.73655700
H	9.95359400	0.83245400	-2.26949600
H	12.06984600	2.78722400	0.93277800
H	10.76860300	3.59033500	2.90829000
C	7.31518100	3.98142300	5.03121200
H	9.42426300	4.28333600	4.89070900
H	5.19295800	3.53417000	4.89601900
H	12.09465100	1.64894400	-1.25959100
H	7.23327500	4.40962800	6.02501800
C	6.42557500	-3.96963600	0.45642100
C	7.64318900	-2.34999200	1.61720800
C	5.46491300	-4.31836300	-0.54067000
C	7.06537500	-5.02510100	1.18354600
C	8.32972800	-3.34833400	2.37819100
C	7.95677000	-0.98045600	1.85290200
C	5.15185000	-5.62518500	-0.77197100
H	5.02307100	-3.52286600	-1.13264400
C	6.70815700	-6.38160300	0.91034300
C	8.01257200	-4.68356600	2.14388400
C	9.29663700	-2.94340200	3.34864600
H	7.44431900	-0.22993100	1.26215400
C	8.88368700	-0.63138800	2.78960500
C	5.77379500	-6.67460400	-0.03594500
H	4.42584200	-5.87246900	-1.53991900
H	7.20103200	-7.16944800	1.47319900
H	8.50990500	-5.46581300	2.71338200
C	9.56482000	-1.62292900	3.55205600
H	9.81098900	-3.71280000	3.91790100
H	9.10897600	0.41780100	2.95504600
H	5.50607500	-7.70571100	-0.24250300
H	10.29965600	-1.31960200	4.29075700
N	7.50206600	2.33905400	1.19901300
N	6.71043800	-2.67410700	0.69963600

N1-L1-Me

L1			
C	6.00650600	-2.97317100	-5.20622300
C	6.64019900	-3.59110900	-3.13630800
C	7.22354100	-3.37702000	-5.77230500
C	7.91370400	-3.99584200	-3.54259600
C	6.46649600	-3.78526900	-1.64996200
C	8.19217200	-3.90504000	-4.90646100
C	8.73673600	-4.42682100	-2.34691700
H	5.90762100	-4.71218900	-1.46477900
C	7.91705500	-3.89076800	-1.14738800
H	9.74925900	-4.01156600	-2.35107600
H	8.01968600	-4.52093700	-0.25997900
N	5.69290400	-3.09392300	-3.91838000
C	7.47150200	-3.29702100	-7.25933900
H	8.17392400	-2.48225200	-7.47963100
H	7.95933400	-4.21536300	-7.60057900
C	6.15596800	-3.06804000	-8.00102900
H	5.57193600	-3.99499400	-8.03842100
H	6.33680200	-2.74783100	-9.03231400
C	5.34777100	-2.01331100	-7.26401500
H	5.91328300	-1.07198400	-7.20256700
O	5.00959600	-2.43919300	-5.95112200

H	4.39281600	-1.81041400	-7.75290500
H	8.83606100	-5.51922700	-2.29521300
H	8.28097100	-2.89110700	-0.88621500
H	5.90271600	-2.96838700	-1.19251100
O	9.35570000	-4.27078200	-5.50392100
C	10.09181100	-5.34877100	-4.95636800
H	9.42757400	-6.16568600	-4.65343900
H	10.75257900	-5.69679900	-5.75244600
H	10.70011000	-5.03837800	-4.10149400

CH₃Pd(I)(L1)₂

Pd	-0.42681000	1.16825400	-0.07398500
I	-1.92598800	2.97191000	-1.34614300
C	-1.60297000	-0.29097500	-0.81283900
H	-2.64411500	-0.08637300	-0.55176000
H	-1.50477000	-0.33170100	-1.90224500
H	-1.27625900	-1.23371300	-0.36024500
C	0.42504400	3.46378400	1.96828600
C	2.21988200	2.81433300	0.73362200
C	-1.01644800	3.45020100	2.39255500
C	1.18262900	4.32221700	2.76522000
C	3.09823500	3.59585500	1.48745900
C	-0.97493500	4.09432800	3.78958900
H	-1.42671300	2.43674700	2.38529400
C	0.30465200	4.96383800	3.82012900
C	2.55076200	4.39953600	2.49845700
C	4.58658900	3.55652400	1.24113900
C	3.97889700	2.16774900	-0.72456800
H	-1.87360700	4.67401100	4.01398700
H	0.07607100	6.00691500	3.56682800
C	4.94429800	2.30703400	0.43937800
H	4.90535900	4.45749600	0.70051100
H	4.17029900	1.26459700	-1.30801100
H	4.86943200	1.41649300	1.07546000
C	1.89101600	-0.82263000	-0.11233400
C	1.39920300	-0.11433900	1.99782700
C	1.58184500	-1.10088300	-1.55753100
C	3.18130700	-1.22790900	0.22973100
C	2.68546500	-0.39958900	2.45140200
H	1.10198900	-0.24180700	-2.03324700
C	3.83633000	-1.89542300	-0.96748400
C	3.58820400	-0.98111400	1.54543300
C	3.11824600	-0.01070500	3.84421300
C	0.71400200	0.49033900	4.18286900
C	2.95452900	-1.44653600	-2.15533000
H	3.81265500	-2.98735600	-0.85171500
C	2.12488100	0.98825600	4.43414600
H	3.19381100	-0.89881600	4.48523100
H	-0.04313300	1.17594300	4.56685100
H	2.89784400	-2.20847300	-2.93638800
H	2.24260700	1.96890000	3.95824700
N	0.90458100	2.73486700	0.96190600
N	1.01544500	-0.26434500	0.72274500
H	5.11798500	3.56942700	2.19721600
H	5.97011100	2.36370100	0.06014900
H	4.04845400	3.03706700	-1.39204700
H	0.56027500	-0.49529800	4.64284000
H	2.28655300	1.11579300	5.50913000
H	4.12220400	0.42292600	3.80136600
O	2.63343900	2.03725700	-0.28526300
O	0.43943700	0.39144000	2.78846100
O	3.45139400	5.15891900	3.16494800
O	4.79933200	-1.23148200	2.08913700
C	3.03564100	6.38263300	3.74691000
H	3.94581100	6.96808700	3.88685900
H	2.35505600	6.92413900	3.08187200
H	2.55668600	6.23047500	4.71814100
C	5.90595200	-1.57853600	1.28152100
H	6.75142300	-1.65610300	1.96627100
H	5.75822000	-2.54021500	0.78126600
H	6.11394900	-0.79930100	0.53997900
H	0.76003100	4.96517200	4.81485300

H	-0.89372400	3.31347200	4.55471800
H	-1.60829700	4.03159600	1.67591800
H	0.87637100	-1.93828800	-1.62198000
H	3.38834000	-0.54854900	-2.60880200
H	4.87901000	-1.61594200	-1.13023100

1

Pd	-0.02491400	1.27634700	0.01403400
O	-2.03031200	1.07356400	0.25843100
O	1.98751600	1.47287600	-0.20673100
C	-2.46955100	0.94054200	1.46865300
C	2.45131000	1.67670800	-1.39709100
O	-1.79856900	0.97306100	2.49990000
O	1.79964000	1.70682200	-2.44104000
C	-3.97851600	0.72987600	1.52187600
H	-4.48642300	1.58849000	1.07164800
H	-4.25339400	-0.15344200	0.93665900
H	-4.30744300	0.60688900	2.55523500
C	3.95986400	1.89642300	-1.40643500
H	4.20601600	2.78861800	-0.82131800
H	4.46339600	1.04835000	-0.93257100
H	4.31976300	2.01816400	-2.42959200
C	0.30633800	3.98957200	1.16576300
C	-0.30581100	4.02215800	-1.04623900
C	0.62996900	3.30939100	2.46254800
C	0.55784100	5.35877600	1.20323100
C	-0.05333300	5.38775400	-1.14491500
C	0.72005600	4.49119900	3.44082400
H	-0.12026500	2.55450500	2.72265500
C	1.09281500	5.72131600	2.58034400
C	0.40085100	6.06266000	0.00168000
C	-0.24161800	6.11286200	-2.45617400
C	-0.50717100	3.80036300	-3.36558000
H	-0.26138400	4.65662200	3.89845500
H	0.67242800	6.63747800	3.00101300
C	-0.98694700	5.23912700	-3.46884000
H	-0.77576400	7.05328000	-2.28736100
H	-0.83301900	5.61408000	-4.48591000
C	0.36417700	-1.49654000	0.98964400
C	-0.22582700	-1.41537100	-1.22673600
C	0.31254400	-2.88770100	1.00309800
C	-0.29569400	-2.80114300	-1.34464400
C	-0.52742600	-0.70781500	-2.51438900
C	0.48738600	-1.39180100	3.32164500
C	0.60305100	-3.65733200	2.27041000
C	-0.01851800	-3.54989000	-0.19215000
C	-0.60198600	-3.15766000	-2.79099300
H	-1.21531400	0.12711100	-2.35254400
C	-1.12054600	-1.82730500	-3.38672000
C	1.18543800	-2.74167700	3.35182800
H	-0.32552000	-4.12126300	2.62767900
H	-1.34001900	-3.95324300	-2.91233400
H	-0.86278600	-1.72272800	-4.44354700
H	2.25515400	-2.58040900	3.17622600
N	-0.10662200	3.33011000	0.08511300
N	0.09163700	-0.77227000	-0.10465600
O	-0.77278400	3.28895900	-2.06017100
O	0.69061800	-0.76551000	2.05793700
H	-1.04587600	3.13526900	-4.04124600
H	-2.06434300	5.26068700	-3.26824200
H	0.74324100	6.39127600	-2.85314100
H	-0.59247000	-1.47894300	3.49179100
H	1.07790900	-3.19891800	4.34078600
H	1.28965500	-4.48176300	2.05394000
H	0.89640900	-0.69240300	4.05094500
H	0.56745900	3.69750900	-3.55442800
O	0.65082100	7.37108400	-0.21409400
O	-0.01356100	-4.89366400	-0.07227900
C	-0.47484300	-5.72546800	-1.11757500
H	-0.35348100	-6.74559600	-0.75080100
H	-1.53359100	-5.54281300	-1.32868000
H	0.11440000	-5.59878900	-2.03054200

C	0.90039400	8.25188900	0.86287500
H	1.01243700	9.23837500	0.41097900
H	0.05908400	8.26895500	1.56338500
H	1.82126600	7.99388700	1.39426500
H	1.43769500	4.32294400	4.24789800
H	2.18280800	5.85227000	2.54011400
H	1.59037600	2.79019500	2.34392600
H	0.39668000	-0.27174200	-2.91350300
H	-2.21297200	-1.80563000	-3.30906000
H	0.31398500	-3.48365500	-3.30160000

31			
Pd	2.09607700	3.42164000	-0.19214700
N	-0.45750900	-0.97179800	-2.30502000
C	-1.84531200	-0.87926500	-2.23319000
C	-2.60377800	-0.85645100	-3.40472700
C	-2.52436400	-0.76039800	-1.02204900
C	-3.98097300	-0.73777800	-3.36511500
C	-3.91223400	-0.67079800	-0.98276800
C	-4.66742900	-0.65454400	-2.15289600
C	-6.17207000	-0.53106800	-2.19254800
F	-4.47745800	-0.56280800	0.21575100
F	-1.85977900	-0.68328900	0.12651500
F	-1.98165200	-0.93974100	-4.58125000
F	-4.65313100	-0.71885700	-4.51381500
F	-6.71825000	-1.56950900	-2.84065200
F	-6.53751400	0.58455700	-2.84323800
F	-6.71869700	-0.48338200	-0.97590200
C	0.28648800	-1.86622700	-1.55441400
O	-0.22750000	-2.67350500	-0.81009600
C	1.79282800	-1.76333400	-1.76406900
H	2.23843300	-2.13047200	-0.83686600
H	2.05657200	-2.48701100	-2.54110500
C	2.29007400	-0.38065000	-2.11676500
C	2.86087300	-0.07739700	-3.35789200
C	2.12753300	0.67904100	-1.20262100
C	3.26181700	1.21337000	-3.68691400
C	2.48920300	1.99984500	-1.51988900
C	3.06827200	2.24147900	-2.77041100
H	3.70978600	1.40428500	-4.65650800
H	3.36897200	3.24933900	-3.05197100
C	1.23655100	1.88092600	0.80995600
C	1.83299500	1.72150500	2.21419700
C	1.50908500	0.49492100	0.15035300
H	0.16942500	2.13467200	0.82891000
C	3.12335400	0.94585200	1.90920100
C	0.99002300	0.65792900	2.96877900
H	1.93905400	2.65394700	2.77239000
C	2.39465300	-0.21833300	1.21718000
H	0.56341600	-0.05138200	0.06182500
H	3.66237900	0.62190500	2.80771700
H	3.80191400	1.49671000	1.25150600
H	1.20499300	0.68887000	4.04273600
H	-0.08439700	0.83257500	2.84593000
C	1.44880800	-0.68846600	2.33466500
H	3.03961500	-1.00175700	0.81267100
H	1.98891200	-1.30210500	3.06392100
H	0.61852900	-1.28639400	1.94614700
H	0.02066100	-0.42173600	-3.00609200
Cl	3.08568200	-1.32703700	-4.58201000
C	2.50460700	5.18065800	2.30653300
C	0.37399200	5.41269600	1.53523900
C	2.20948100	5.84954400	3.49075000
C	-0.06301100	6.07793300	2.67958900
C	0.89135600	6.30418600	3.68044900
N	1.61018600	4.95688600	1.33285100
O	0.71269300	6.93446900	4.85622600
C	-0.54345500	7.47119000	5.22618700
H	-0.36491500	8.01119200	6.15657700
H	-0.92336300	8.16659500	4.47219100
H	-1.27489100	6.67815900	5.40797400
O	3.72492200	4.68854200	2.03043600

C	-1.99134100	5.53341900	1.35441300
H	-2.36121300	4.58542600	1.75996900
H	-2.80037600	5.98464400	0.77507600
C	-0.72809600	5.26923800	0.52141700
H	-0.59256800	6.02496900	-0.26416200
H	-0.71176600	4.29153200	0.03237500
C	-1.53219800	6.43644100	2.52150600
H	-2.13425800	6.25913900	3.41453700
H	-1.64504300	7.49658000	2.25824600
C	3.27007000	6.08565300	4.53943700
H	3.20607300	7.11604400	4.90221800
H	3.07215400	5.44530300	5.40887100
C	4.66077100	5.79612600	3.97412400
H	5.39299800	5.68205500	4.77955200
H	4.99452000	6.62448100	3.33867200
C	4.61499000	4.53114600	3.13458700
H	4.28088700	3.67070600	3.73034400
H	5.57960600	4.29233900	2.68583600

TS32

Pd	0.67309400	3.09695600	0.86780000
N	0.93170300	-2.42290100	-2.98976300
C	-0.09553500	-3.34569900	-2.78320400
C	0.03369000	-4.29139900	-1.76813400
C	-1.23919700	-3.40432700	-3.58084200
C	-0.94722300	-5.23652500	-1.51068600
C	-2.23253600	-4.33363400	-3.30366700
C	-2.11838100	-5.25848200	-2.26592100
C	-3.23210000	-6.25970700	-2.05905000
F	-3.30514400	-4.35039600	-4.08782200
F	-1.38134100	-2.61491300	-4.63427900
F	1.15206600	-4.29120000	-1.03125700
F	-0.72567900	-6.09628800	-0.52231500
F	-4.41936400	-5.64277600	-2.00084700
F	-3.08608800	-6.95626000	-0.92952900
F	-3.27923700	-7.13414100	-3.07401400
C	0.71230100	-1.05651700	-3.13049000
O	-0.39878400	-0.58020100	-3.17710700
C	1.99615000	-0.25833900	-3.27840500
H	2.85289300	-0.81637000	-2.88149500
H	2.16660100	-0.19266100	-4.35761700
C	1.96984400	1.13327700	-2.68795300
C	2.48926400	2.21453100	-3.41210600
C	1.49294200	1.39758500	-1.38885700
C	2.54093800	3.50543600	-2.89879300
C	1.51588200	2.70278700	-0.87491600
C	2.05248300	3.74786900	-1.62279100
H	2.96362500	4.30556400	-3.49608600
H	2.10181600	4.75727700	-1.22019900
C	0.54003600	1.06795600	0.89366900
C	1.41882400	0.38735300	1.94392700
C	0.92358000	0.37260700	-0.44504300
H	-0.52862900	1.01815300	1.13247600
C	2.68391700	0.02989400	1.15086000
C	0.79363100	-1.01185000	2.16499200
H	1.55475600	0.95153200	2.86589100
C	1.92274600	-0.71219000	0.04291900
H	0.03364700	-0.08695400	-0.88567100
H	3.36759400	-0.61640700	1.71053000
H	3.23433400	0.89981500	0.78455400
H	1.25736300	-1.49709600	3.03079200
H	-0.28338600	-0.95603300	2.35303100
C	1.13172100	-1.76364400	0.84481500
H	2.54248500	-1.13916800	-0.74776500
H	1.74431800	-2.64815000	1.03847000
H	0.23581200	-2.09609500	0.31039500
H	1.85157000	-2.72228600	-2.70062100
Cl	3.14297700	1.99105900	-5.02847300
I	4.47990700	4.96688600	3.44561600
C	2.59766300	3.57776500	1.76397800
H	2.44514300	4.63585500	1.58204600
H	3.39844500	3.10662600	1.20894900

H	2.36944200	3.18504800	2.74573400
C	-0.24376400	3.15641600	3.89544500
C	0.10018900	5.21340700	2.97704000
C	0.19506200	3.58377000	5.14802400
C	0.50842200	5.77622100	4.17403200
C	0.62269100	4.91703900	5.27543500
N	-0.22639400	3.92534900	2.79536000
O	1.08375500	5.25059900	6.48748000
C	2.08117000	6.26719400	6.60472900
H	2.53354900	6.11437400	7.58483400
H	2.84183500	6.14969600	5.82636300
H	1.63451800	7.26394400	6.56523400
O	-0.67795600	1.90365700	3.65939500
C	0.11807800	7.56393200	2.63635400
H	-0.91309500	7.88148800	2.82431900
H	0.62104600	8.36368300	2.08823900
C	0.10246100	6.23186400	1.86420800
H	1.01154500	6.13635300	1.25225200
H	-0.75829300	6.12014300	1.19731500
C	0.81205400	7.24563400	3.97981400
H	0.43211300	7.87921200	4.78560200
H	1.89592600	7.39938600	3.90663800
C	0.31622700	2.61843600	6.30111000
H	1.25903600	2.80462300	6.82271200
H	-0.48249900	2.79928000	7.03203600
C	0.25072600	1.18045700	5.79101700
H	0.09245900	0.47735500	6.61445800
H	1.19316300	0.90726300	5.30121700
C	-0.88276000	1.05521400	4.79002400
H	-1.84201200	1.31972000	5.25430900
H	-0.96116000	0.04991300	4.37342500

TS35

Pd	2.03963400	3.24235000	0.20358900
N	-0.05635000	-0.48262700	-2.25645800
C	-1.33984100	-0.01200400	-2.01219200
C	-2.02196400	0.64656600	-3.03870900
C	-1.95803400	-0.05340100	-0.76137300
C	-3.25970400	1.22728200	-2.83258600
C	-3.21688100	0.50316300	-0.56671900
C	-3.88357200	1.17903600	-1.58525700
C	-5.22951600	1.83850900	-1.41247500
F	-3.72577500	0.41947300	0.66133800
F	-1.34459900	-0.57385500	0.29652500
F	-1.44739900	0.73498300	-4.23873300
F	-3.85295800	1.83389200	-3.85694600
F	-6.19501700	1.14533800	-2.02904600
F	-5.22327800	3.07413800	-1.94220300
F	-5.57617100	1.96628700	-0.12788900
C	0.50177800	-1.63610500	-1.72546900
O	-0.16308600	-2.49929100	-1.19753400
C	2.02686700	-1.71425600	-1.86188300
H	2.36715900	-2.25053200	-0.97195000
H	2.25294700	-2.35446000	-2.71945100
C	2.67543300	-0.35642000	-1.99692500
C	3.29735400	0.07611400	-3.17066400
C	2.49797400	0.58989800	-0.96631900
C	3.70754400	1.39523200	-3.33526300
C	2.80392900	1.95022500	-1.14657300
C	3.43515100	2.32554000	-2.33812300
H	4.19674400	1.69487700	-4.25613200
H	3.69385200	3.36483100	-2.52240500
C	1.58252500	1.49474700	1.17312700
C	2.38836400	1.32986200	2.47179600
C	1.92677100	0.21342000	0.36496900
H	0.50741600	1.57614300	1.37291600
C	3.67508100	0.66078900	1.96065200
C	1.74840200	0.18063400	3.28724200
H	2.51285200	2.25391700	3.04091600
C	2.93868700	-0.51322000	1.29507800
H	1.03526600	-0.41013800	0.25776300
H	4.34726000	0.33758400	2.76394600

H	4.23379900	1.27684700	1.24871700
H	2.16377600	0.14952500	4.30118800
H	0.66415000	0.30262900	3.38014200
C	2.14390100	-1.09221200	2.48011500
H	3.57005600	-1.24129900	0.77841400
H	2.77466200	-1.75715700	3.07970200
H	1.27608600	-1.67078700	2.14688300
H	0.54475500	0.12219300	-2.80044200
Cl	3.56097800	-1.03082900	-4.51334300
I	2.54007800	5.69611400	-0.96409600
C	4.20214000	4.31551600	0.47579000
H	4.00024500	3.71433500	1.35932100
H	4.76442800	3.81405200	-0.30424300
H	4.58161000	5.29414700	0.74254400
C	1.12428900	4.86766700	2.80719900
C	-0.59741800	4.37345200	1.40286300
C	0.28322100	5.52701500	3.69870500
C	-1.55379700	4.97539000	2.22025700
C	-1.08983400	5.57714300	3.39617900
N	0.70769100	4.30368200	1.66782800
O	-1.81183100	6.24198800	4.31809200
C	-3.22006600	6.34560300	4.22139700
H	-3.52054000	6.98653600	5.05095400
H	-3.52884100	6.80758700	3.27962300
H	-3.69599400	5.36654100	4.33313200
O	2.45265400	4.75121600	3.01105500
C	-2.71088100	3.80004000	0.47559800
H	-2.96680200	2.82784900	0.90742600
H	-3.34879700	3.95562600	-0.39639600
C	-1.21286500	3.83281300	0.13894300
H	-0.98585800	4.52016000	-0.68674900
H	-0.80386300	2.85683000	-0.14042100
C	-2.91521500	4.88909000	1.54980700
H	-3.73339200	4.62469700	2.22183000
H	-3.17092700	5.84935000	1.08288500
C	0.82623000	6.19888000	4.93721900
H	0.36140200	7.18234700	5.05323500
H	0.54193800	5.62122000	5.82660000
C	2.34652000	6.32766100	4.85345800
H	2.77498000	6.55465900	5.83457500
H	2.62458800	7.13984000	4.17211800
C	2.93048700	5.03000200	4.32592400
H	2.66784100	4.18720600	4.98017400
H	4.01641700	5.07099100	4.22683500

TS65

Pd	4.71875900	2.92345800	-3.67999800
N	0.84897900	1.32336500	-2.65726100
C	0.15209800	1.34068300	-3.85974800
C	-1.10824600	1.92200700	-4.00706100
C	0.76160400	0.81235200	-4.99738600
C	-1.73042600	1.93263700	-5.24710700
C	0.14236500	0.83862200	-6.23604300
C	-1.12157500	1.40652500	-6.38692200
C	-1.84125400	1.53477000	-7.70589200
F	0.81081800	0.32315400	-7.26700500
F	1.97687600	0.27789100	-4.88885500
F	-1.70870900	2.51326600	-2.98436200
F	-2.92858500	2.50425900	-5.34574300
F	-2.06103000	2.83128000	-7.99515900
F	-3.03314400	0.92761800	-7.67170200
F	-1.14950700	1.01499000	-8.72342000
C	0.33513600	0.83568400	-1.46498500
O	-0.81788800	0.48974100	-1.33805800
C	1.34082000	0.81554000	-0.30285600
H	1.18292800	1.74716800	0.25368100
H	1.04551000	-0.00921000	0.34716900
C	2.76960200	0.72751000	-0.76580100
C	3.46791900	-0.46872800	-0.96543200
C	3.41010400	1.88005300	-1.21694000
C	4.74143900	-0.49470900	-1.53517700
C	4.59538300	1.86700300	-1.96504600

C	5.32203200	0.66793600	-2.04317100
H	5.25619200	-1.44560200	-1.62601700
H	6.29664800	0.61503900	-2.51669200
H	1.85807000	1.37874900	-2.73983300
C	4.50567100	3.77264600	-1.69136800
C	5.46880000	4.18987900	-0.56714800
C	3.20934500	3.33706600	-0.93932400
H	4.35271700	4.62453300	-2.38013200
C	4.98503300	5.58488200	-0.10821600
C	5.02687800	3.34216100	0.64002000
H	6.52477900	4.14428400	-0.83921700
C	3.53964400	3.72829000	0.52127100
H	2.27930100	3.78840700	-1.30260300
C	3.62013700	5.27019500	0.57963900
H	4.88784900	6.28865500	-0.94138800
H	5.69459900	6.01648300	0.60635600
H	5.22313900	2.27301300	0.53829500
H	5.47205700	3.69412600	1.57675800
H	2.86742500	3.28615200	1.26186700
H	2.77426300	5.74093700	0.06716400
H	3.60858800	5.61919900	1.61704500
Cl	2.74927200	-1.99503700	-0.48532300
C	3.68957300	3.47556400	-6.56881000
C	5.93685800	3.10402600	-6.53942800
C	3.70921700	3.79525600	-7.92606400
C	6.09703600	3.39047400	-7.89340400
C	7.25206400	2.78899600	-5.88130600
C	1.40808300	4.08800900	-6.40915100
C	2.44019100	4.13830900	-8.66870900
C	4.94637500	3.77446600	-8.59352900
C	7.56951200	3.29471900	-8.25799800
H	7.58319000	3.66389100	-5.30617400
C	8.17240200	2.50102600	-7.07734600
C	1.22078600	3.69747000	-7.86363000
H	0.57447500	3.76843100	-5.78103800
H	2.40308700	5.21910600	-8.85860300
H	8.01556900	4.29656700	-8.32049300
H	9.21597500	2.76480100	-6.88904500
H	1.10733700	2.61232900	-7.93581500
N	4.78563400	3.14829900	-5.86797600
O	2.55782100	3.45919000	-5.84045800
O	4.86231100	4.15062600	-9.88458000
C	5.95927500	4.00950000	-10.76607400
H	6.24643800	2.95855300	-10.87374700
H	5.60747300	4.38539400	-11.72753300
H	6.81971300	4.60166400	-10.44120500
H	7.76687300	2.79385400	-9.20776200
H	8.13680300	1.43129400	-7.31076400
H	7.16501300	1.95732200	-5.17582800
H	1.52236900	5.17571300	-6.30929500
H	0.30353900	4.14898600	-8.25160900
H	2.44862800	3.65644000	-9.65050700

TS36

Pd	0.59010600	3.64436700	0.45057500
N	-0.11777400	-0.44373000	-2.60329300
C	-1.49341200	-0.63698800	-2.69926000
C	-2.13567000	-0.48797900	-3.92541900
C	-2.28381200	-0.90397000	-1.58100900
C	-3.51421400	-0.60249300	-4.04785300
C	-3.65327300	-1.05438200	-1.71179400
C	-4.30016400	-0.90506900	-2.93784400
C	-5.80857100	-0.95633900	-2.96660000
F	-4.36699200	-1.25626700	-0.60531500
F	-1.75109000	-0.92900800	-0.36270200
F	-1.40693800	-0.20177300	-5.00472300
F	-4.04150700	-0.41832200	-5.25247500
F	-6.29861900	-0.97791100	-4.20654000
F	-6.32171200	0.12234200	-2.34626700
F	-6.26692400	-2.04007500	-2.32987600
C	0.73252000	-1.31357500	-1.94002800
O	0.34531100	-2.34574200	-1.43850600

C	2.18931900	-0.85423700	-1.89203400
H	2.60584000	-1.29546200	-0.98479300
H	2.70778500	-1.31981900	-2.73491300
C	2.34571600	0.64758300	-1.91834800
C	2.75701300	1.33133300	-3.06716600
C	1.93256900	1.40386900	-0.80237300
C	2.73238500	2.72016300	-3.14368100
C	1.90960700	2.80612600	-0.88134800
C	2.30179200	3.45717700	-2.05156200
H	3.03813300	3.21834500	-4.05686800
H	2.25144100	4.53852300	-2.11494000
C	0.54837100	1.75771200	1.26726300
C	1.11283500	1.56082900	2.67901800
C	1.32729900	0.74009900	0.40560700
H	-0.52497000	1.55855300	1.24762100
C	2.58564800	1.20005700	2.42357600
C	0.57178800	0.19100600	3.16993300
H	0.91311200	2.38706300	3.36497400
C	2.26911800	0.06373900	1.43970200
H	0.61544300	-0.00958000	0.04657000
H	3.09077100	0.83516000	3.32489200
H	3.18212300	2.00326700	1.99778700
H	0.77355400	0.06358500	4.23893400
H	-0.50958200	0.10017200	3.02693100
C	1.37768700	-0.83958500	2.31750100
H	3.13371300	-0.44251000	1.00269200
H	1.99477300	-1.48002400	2.95572400
H	0.73611000	-1.49211600	1.71672600
H	0.28676900	0.30170200	-3.15378000
Cl	3.27206500	0.45517200	-4.50015000
I	0.19847000	6.25691600	-0.63167300
C	2.69564100	3.97933500	0.63358000
H	2.48034700	4.19552700	1.68829700
H	3.52794200	3.28603000	0.57025000
H	2.90002700	4.89397400	0.08268000
C	-1.71745300	4.63839600	2.13208200
C	-2.51210400	3.47471700	0.33427700
C	-2.97664400	5.13814100	2.43680300
C	-3.82349100	3.89835200	0.53160300
C	-4.04880900	4.77893600	1.59919900
N	-1.47847600	3.82899300	1.09381100
O	-5.21094600	5.35862000	1.94856800
C	-6.41932500	5.04960500	1.27892000
H	-7.17299700	5.69730200	1.72760000
H	-6.35241700	5.26186500	0.20842500
H	-6.70033100	4.00387700	1.43819900
O	-0.61751800	4.92322200	2.84999500
C	-3.82913700	2.22201500	-1.17991000
H	-4.05506700	1.30078900	-0.63442200
H	-4.03456000	2.04336900	-2.23813000
C	-2.37602600	2.63298800	-0.90340600
H	-1.95976100	3.25984700	-1.70383100
H	-1.69546800	1.78707300	-0.76425700
C	-4.69210400	3.35864600	-0.59420500
H	-5.66641400	2.98191600	-0.27820300
H	-4.86639800	4.13916900	-1.34626100
C	-3.17803200	6.07753200	3.60117300
H	-3.40424600	7.07838100	3.21239800
H	-4.05493600	5.77008600	4.17970400
C	-1.93141100	6.12514900	4.48775900
H	-1.89736500	5.25031000	5.14748800
H	-1.94388000	7.01649800	5.12304000
C	-0.68326000	6.12676800	3.62114000
H	0.23380500	6.13448100	4.21126000
H	-0.66870600	6.97496500	2.92565700

TS40

Pd	0.28968500	3.32035900	0.18098000
N	0.21927000	0.11092400	-2.68026800
C	-1.15305800	0.03603800	-2.91897600
C	-1.70607500	0.70124700	-4.01079700
C	-2.02182000	-0.59825500	-2.03742200

C	-3.07452100	0.72428100	-4.20901900
C	-3.39278000	-0.60216100	-2.25430300
C	-3.94850200	0.07300500	-3.33801100
C	-5.42809300	0.15818800	-3.61527900
F	-4.15191100	-1.20786700	-1.34032200
F	-1.55948200	-1.14978300	-0.91582600
F	-0.91304200	1.33426500	-4.86804100
F	-3.55641100	1.38040000	-5.26359400
F	-5.74098600	-0.44218500	-4.77114300
F	-5.82014100	1.44031500	-3.71223500
F	-6.16671100	-0.40723600	-2.65412000
C	0.97902200	-1.00041100	-2.38835000
O	0.54715900	-2.13066700	-2.48597100
C	2.41486300	-0.73962700	-1.90847400
H	2.52680400	-1.32794200	-0.99375600
H	3.08047800	-1.18986400	-2.64745300
C	2.72555300	0.71607200	-1.68757400
C	3.41086000	1.47114900	-2.64083600
C	2.12538400	1.39020700	-0.60064400
C	3.44562900	2.86305300	-2.59082900
C	2.10113400	2.79272900	-0.59179400
C	2.75579400	3.52002400	-1.59013500
H	3.96612700	3.41788000	-3.36358500
H	2.69097100	4.60222900	-1.60339000
C	0.36603200	1.57761900	1.19854000
C	0.81449900	1.45142200	2.65980200
C	1.31349100	0.62859800	0.42964900
H	-0.68206900	1.28521800	1.07800300
C	2.31541000	1.11944500	2.55129800
C	0.27027500	0.08766700	3.15157400
H	0.53666800	2.29523800	3.29676200
C	2.11481200	-0.04434700	1.56964100
H	0.70562300	-0.11662300	-0.08913200
H	2.74312000	0.79639600	3.50700700
H	2.93395600	1.91974500	2.14768700
H	0.42590000	-0.01696300	4.23099900
H	-0.80176500	-0.02483600	2.96074300
C	1.13482700	-0.94100700	2.35723000
H	3.02346800	-0.55281300	1.23579400
H	1.68151000	-1.60379200	3.03519100
H	0.53345100	-1.57171200	1.69440500
H	0.58426400	1.05749400	-2.61729000
Cl	4.20797900	0.69977000	-3.99880600
C	2.17885900	4.01153000	1.02625200
H	1.70917200	4.01627700	2.01164100
H	3.19246800	3.63391800	1.12210200
H	2.18875700	5.00940400	0.58744400
C	-1.73749900	4.82449500	1.90713400
C	-2.87668800	3.25527900	0.70358700
C	-2.90812300	5.35057000	2.44769200
C	-4.11713300	3.70790500	1.14866600
C	-4.12557200	4.76989200	2.05718700
N	-1.70376800	3.78593700	1.06025300
O	-5.21253600	5.33994600	2.61651400
C	-6.42209100	4.60968900	2.73787400
H	-7.02587200	5.16167500	3.45934300
H	-6.96036000	4.55528000	1.78852900
H	-6.23651700	3.59981600	3.11757800
O	-0.51840100	5.30406800	2.21864400
C	-4.50237200	2.16837300	-0.65734800
H	-4.93989800	1.18254900	-0.82100100
H	-4.59884700	2.73016600	-1.59110300
C	-3.01907900	2.10079900	-0.25084400
H	-2.32561600	2.19347000	-1.09255300
H	-2.79073200	1.15949200	0.26799400
C	-5.22752300	2.92180700	0.48151100
H	-5.69383000	2.21695500	1.18118300
H	-6.02215800	3.55951600	0.08529000
C	-2.87223100	6.48703800	3.44091700
H	-3.23529700	7.40515200	2.96138500
H	-3.56793700	6.27817300	4.25918900
C	-1.45395400	6.69544600	3.97068400
H	-1.20444500	5.92715000	4.71164900

H	-1.35853100	7.67019400	4.45915100
C	-0.47018000	6.59731200	2.81811600
H	0.56507000	6.71906800	3.14045400
H	-0.68955700	7.34809400	2.04768600
O	-0.00580500	4.87017600	-1.38135800
C	-0.41758100	4.14134400	-2.33876700
C	-0.71038700	4.82258200	-3.66201100
H	-1.67360000	5.34006400	-3.59108200
H	0.05236000	5.57329300	-3.88366000
H	-0.76616600	4.08399300	-4.46335400
O	-0.60948000	2.90244900	-2.23538200

TS67

Pd	0.70956100	4.07775000	-0.82257500
N	-0.34664400	5.89215500	-1.21616300
C	-1.45725000	6.15639400	-0.51506100
C	-0.11772700	6.61562200	-2.31124900
C	-2.37007400	7.13957600	-0.87888200
C	-0.95388600	7.62104100	-2.78713400
C	-2.12396200	7.86816200	-2.05685100
N	0.08244000	-0.68011200	-2.84964600
C	-1.29481800	-0.91170000	-2.92333200
C	-1.93590100	-0.78807600	-4.15527300
C	-2.08078900	-1.19811100	-1.81178600
C	-3.30444900	-0.94854500	-4.26887800
C	-3.45365100	-1.38427400	-1.93037300
C	-4.09262400	-1.26125600	-3.16088400
C	-5.57805600	-1.43299400	-3.36825600
F	-4.12628200	-1.65285600	-0.81431300
F	-1.54570300	-1.25093500	-0.59428000
F	-1.21738700	-0.49526700	-5.23700300
F	-3.86568100	-0.81746900	-5.46870000
F	-6.22794800	-1.73027600	-2.24039500
F	-5.82428900	-2.41784900	-4.24584300
F	-6.12165200	-0.31142000	-3.86366000
C	0.96223100	-1.50290300	-2.18753700
O	0.62699200	-2.54592600	-1.66437100
C	2.41928100	-1.05283200	-2.22499300
H	2.92623100	-1.60677200	-1.42872300
H	2.83669700	-1.42481500	-3.16669500
C	2.68155200	0.42776700	-2.09491500
C	3.72519000	1.07806900	-2.76912800
C	1.93111100	1.22779200	-1.23367800
C	4.03856400	2.41547600	-2.54523900
C	2.16057800	2.59628800	-1.07568300
C	3.27308800	3.18893800	-1.67449200
H	4.88270200	2.85613600	-3.06436600
H	3.53699200	4.22782600	-1.51373900
C	0.95436900	2.29474300	0.49841700
C	1.76321900	2.14587400	1.78935400
C	0.97261400	0.88633600	-0.14221200
H	-0.04999900	2.68511700	0.70371500
C	2.71826400	0.97248000	1.50685500
C	0.77012100	1.46307500	2.76471500
H	2.19940300	3.06618600	2.17666300
C	1.60963700	0.03847200	0.98496200
H	-0.00456000	0.52073300	-0.45703000
H	3.18742000	0.59587100	2.42137200
H	3.50007600	1.19591100	0.77731000
H	1.20651700	1.43312700	3.76843700
H	-0.18295900	1.99700100	2.83714700
C	0.62158900	0.03006900	2.16985000
H	1.91317200	-0.95781600	0.65776600
H	0.90332900	-0.73349900	2.90065000
H	-0.39842700	-0.18923900	1.84108300
H	0.40721400	0.19216500	-3.25234600
Cl	4.74187100	0.19486700	-3.89144400
C	1.89198700	5.16768200	0.43129000
H	2.12876900	6.10953700	-0.07213700
H	1.30419500	5.36519900	1.33233700
H	2.80799600	4.62639600	0.68017600
I	-1.10105100	2.87141700	-2.65438700

C	-0.41133200	8.13130100	-4.11292700
C	1.04589600	7.61813700	-4.12057200
C	1.03915300	6.36345000	-3.23378100
H	-0.44696700	9.21612300	-4.22998900
H	1.69735600	8.37787800	-3.67464400
H	1.97641900	6.20246800	-2.69228100
H	0.83148800	5.44810400	-3.80404800
H	1.40900100	7.42103200	-5.13184400
H	-0.97757300	7.69202100	-4.94438600
O	-3.09639500	8.75205900	-2.34435800
C	-2.97823100	9.65523800	-3.42733100
H	-3.91294800	10.21671800	-3.43844200
H	-2.14411200	10.34752400	-3.27453300
H	-2.86230100	9.13171600	-4.38019300
C	-3.60149300	7.40345400	-0.04595600
C	-3.49153100	6.71350700	1.31451600
H	-2.83248100	7.28337800	1.97971700
C	-2.91443300	5.32033700	1.13360700
H	-2.79060100	4.79675600	2.08244200
H	-3.74005100	8.48200900	0.07644200
O	-1.60032900	5.38632600	0.57627700
H	-4.48647900	7.04112700	-0.58419600
H	-4.47174200	6.64779600	1.79678900
H	-3.54068900	4.71078800	0.47011300

TS69

Pd	0.70421900	3.97593600	-0.24358500
N	-0.37960000	5.67398800	-1.00509600
C	-1.52231100	6.00611400	-0.39062400
C	-0.21229000	6.07783000	-2.26554600
C	-2.51063600	6.78364300	-0.98294800
C	-1.14366400	6.82401200	-2.98585400
C	-2.31333000	7.20080900	-2.31330200
N	0.09090000	-0.04407100	-2.95564000
C	-1.29469500	-0.14685900	-3.10208800
C	-1.88445300	0.21572000	-4.31276900
C	-2.13791200	-0.51550100	-2.05722000
C	-3.25975600	0.22026200	-4.46155300
C	-3.51859000	-0.53674400	-2.21647700
C	-4.10698600	-0.16788900	-3.42414700
C	-5.59642600	-0.09100100	-3.64996900
F	-4.24837800	-0.88807900	-1.16047600
F	-1.64268500	-0.81464900	-0.85994100
F	-1.12151000	0.59281800	-5.33169500
F	-3.77202400	0.61842800	-5.62568900
F	-6.30252400	-0.59739400	-2.63645400
F	-5.95109900	-0.75666400	-4.75800300
F	-5.98157800	1.18685400	-3.81052000
C	0.85697700	-1.07593300	-2.47646500
O	0.40647500	-2.17713700	-2.22790600
C	2.34715100	-0.77320000	-2.33984900
H	2.72297500	-1.45452200	-1.57062800
H	2.81857700	-1.07974200	-3.27839800
C	2.69067100	0.65650300	-2.01705900
C	3.67169000	1.39914800	-2.68427500
C	2.02236000	1.32572800	-0.99274500
C	4.00346300	2.70035800	-2.31191300
C	2.25501000	2.66444000	-0.68736400
C	3.30831900	3.34966400	-1.29460300
H	4.79759500	3.21608300	-2.84092200
H	3.56845400	4.36961300	-1.03791400
C	1.20057500	2.18045600	0.91819500
C	2.14273100	1.91913500	2.09858600
C	1.16576100	0.84415400	0.13092300
H	0.21723400	2.50794600	1.28823800
C	3.06815000	0.79185100	1.60623800
C	1.26564000	1.12837500	3.10116400
H	2.61348200	2.80801200	2.52035200
C	1.91552200	-0.09917100	1.10321800
H	0.16813100	0.49707100	-0.13911400
H	3.62185400	0.33042600	2.43038900
H	3.77946500	1.09215500	0.83411600

H	1.80656000	0.99523000	4.04378900
H	0.32587700	1.64058600	3.33205400
C	1.05092700	-0.23555400	2.37550100
H	2.19525200	-1.05457800	0.65505600
H	1.39813800	-1.07066800	2.99114800
H	0.00043200	-0.42167000	2.13127200
H	0.46825200	0.89177400	-3.13038300
Cl	4.57943700	0.68997500	-4.00584600
C	1.91331600	5.19081300	0.82997700
H	1.31635800	5.52496800	1.68499800
H	2.81455800	4.67677100	1.17429200
H	2.18096100	6.05053100	0.20775200
C	-0.62551400	7.03055600	-4.40036100
C	0.47604200	5.95586000	-4.52146700
C	0.99878600	5.74607000	-3.09391000
H	-0.20246800	8.03755600	-4.51782700
H	1.25781400	6.23906700	-5.23029000
H	1.81234500	6.43998800	-2.83956600
H	1.34377500	4.72371100	-2.92664200
H	0.03254900	5.01173100	-4.85376000
H	-1.38720200	6.90371900	-5.17203500
O	-3.33001400	7.94092600	-2.79003300
C	-3.29411500	8.49975200	-4.09104200
H	-4.13628000	9.19123100	-4.13297500
H	-2.36530000	9.04927400	-4.26665300
H	-3.42375700	7.72788500	-4.85497700
C	-3.76150900	7.16294200	-0.22801900
C	-3.61764400	6.83128800	1.25771300
H	-3.00997200	7.59087900	1.76283500
C	-2.93568200	5.48315000	1.41514500
H	-2.79086300	5.21000800	2.46090200
H	-3.96588400	8.22868400	-0.36971100
O	-1.62051200	5.51665100	0.85751100
H	-4.61997700	6.62972300	-0.65584600
H	-4.59599500	6.81152400	1.74768900
H	-3.50222600	4.68764100	0.91409500
O	-0.92006100	2.86848200	-1.18041800
C	-1.04776000	2.91353900	-2.45269600
O	-0.13450600	2.76595900	-3.28482300
C	-2.46676600	3.19837800	-2.93538000
H	-2.73795200	4.21889600	-2.63931000
H	-2.54190400	3.10491700	-4.02073100
H	-3.17884700	2.52174400	-2.45243000

TS44

N	0.46462200	-0.88293600	-1.36280000
C	-0.88547200	-0.53811700	-1.40585400
C	-1.42847900	0.01393600	-2.56577200
C	-1.72164500	-0.68333600	-0.30179400
C	-2.75939600	0.38346100	-2.62694800
C	-3.06839900	-0.34060000	-0.37508100
C	-3.61335700	0.19802600	-1.53846200
C	-5.05750800	0.61781900	-1.68411800
F	-3.79743000	-0.51674600	0.72160900
F	-1.24057800	-1.11752900	0.85712100
F	-0.63924500	0.19549500	-3.62660900
F	-3.22299700	0.91119600	-3.75697300
F	-5.61974100	0.01915300	-2.74357900
F	-5.14731600	1.94268900	-1.87720700
F	-5.79381000	0.31522500	-0.61358700
C	0.90394900	-2.13175500	-0.95606200
O	0.14781700	-2.99882000	-0.57599800
C	2.41442300	-2.32900600	-0.98395300
H	2.68202400	-2.68668900	0.00657700
H	2.59407800	-3.17194800	-1.65422600
C	3.23721100	-1.13340600	-1.40485300
C	3.63666600	-1.05726500	-2.75018200
C	3.58766400	-0.06800300	-0.53420600
C	4.35082700	0.01341500	-3.26520500
C	4.25999700	1.06274000	-1.08062600
C	4.63123600	1.07762000	-2.43253800
H	4.65862900	0.01703700	-4.30428900

H	5.14724300	1.94227200	-2.83660800
C	4.59829500	-0.00589300	1.82343200
C	4.29526500	-0.99454400	2.94962200
C	3.28310500	0.03387000	0.97254900
H	4.85898900	0.98516200	2.21386100
C	3.40079700	-2.02568800	2.25359900
C	3.29239500	-0.29973100	3.89805000
H	5.18116500	-1.37695600	3.45475500
C	2.39364100	-0.97856500	1.73712200
H	2.83267200	1.02689400	1.09165300
H	2.94550300	-2.74829700	2.93989100
H	3.94215700	-2.57006500	1.47431700
H	3.17504600	-0.87116400	4.82586500
H	3.61961600	0.70902900	4.17172000
C	1.98188500	-0.29987900	3.06288700
H	1.51719700	-1.34133200	1.20620900
H	1.20082300	-0.89069000	3.55190700
H	1.57604000	0.70395900	2.90130000
H	1.11159900	-0.30470400	-1.88191200
Cl	3.22823600	-2.33287400	-3.88982200
Pd	6.20388300	-0.28855600	0.62363800
Pd	5.41973200	2.30819400	-0.00033300
I	8.43668500	-0.43975600	-1.12192000
C	3.44432100	2.84953700	-0.58305800
H	2.48133700	2.35120100	-0.47768000
H	3.52218700	3.59212300	0.22957900
H	3.48960300	3.35097500	-1.55064200
C	8.33831000	3.09212100	0.00616300
C	7.60420500	2.59550900	2.11158700
C	8.19273900	3.50219300	-1.43204700
C	9.65870400	2.81104900	0.31803900
C	8.88861400	2.27752900	2.54458700
C	9.63397800	3.88194500	-1.81902000
H	7.84445900	2.63150800	-2.00324400
C	10.53747300	3.03786900	-0.89033300
C	9.92134300	2.31872700	1.59684300
C	9.15246300	1.83645300	3.96146200
C	6.66659600	1.81193300	4.12645700
H	9.84611700	3.70108200	-2.87540900
H	10.78233800	2.07900400	-1.36287300
C	7.95430400	2.16393900	4.85311600
H	9.35314700	0.75748100	3.96088700
H	5.78042300	2.05341000	4.71646000
H	8.00787200	1.61953600	5.80268100
C	7.43915800	-2.45810400	2.51253000
C	6.56603100	-3.30675700	0.58524600
C	7.99472200	-3.68671200	2.86480900
C	7.01438600	-4.59699400	0.85455000
C	5.83973700	-3.25555700	-0.72435000
C	7.90475700	-1.62767900	4.65888900
C	8.83947000	-3.85075100	4.10632900
C	7.77952800	-4.77774900	2.00635200
C	6.52977200	-5.54411800	-0.22794800
H	5.00516500	-2.55617800	-0.70428000
C	5.43649200	-4.71912300	-0.94504900
C	9.14618500	-2.49453800	4.73846400
H	8.05207900	-0.64753800	5.11347900
H	8.31250100	-4.49191400	4.82445400
H	6.12976100	-6.48090800	0.16975600
H	4.46850500	-4.90861900	-0.46576400
H	9.95638200	-1.98926700	4.19994400
N	7.31044900	2.95306200	0.85202100
N	6.75032900	-2.24994300	1.38160700
H	5.34117700	-4.97698900	-2.00228800
H	7.33902400	-5.79906400	-0.92352300
H	6.53306200	-2.88953700	-1.49268900
O	8.34752300	-5.92985300	2.41863200
C	8.67781100	-6.93069300	1.46903600
H	9.40767300	-7.57492700	1.96136400
H	7.80526400	-7.52764800	1.19035300
H	9.12779000	-6.48947700	0.57435300
H	7.05013100	-2.11549100	5.14900000
H	9.45937600	-2.61013200	5.78078700

H	9.76242200	-4.37968400	3.84975600
O	7.56504300	-1.36553900	3.29795400
H	11.47502900	3.55079400	-0.65393200
H	9.79899700	4.94689800	-1.62028700
H	7.46857200	4.31240900	-1.56318700
H	7.94146400	3.23357600	5.09256300
H	6.63794100	0.74928900	3.85599100
H	10.05924500	2.31706900	4.34071800
O	6.53204700	2.57729000	2.93038600
O	11.12430400	1.89104600	2.03324500
C	11.93751100	1.16240400	1.11752900
H	12.60643800	0.55845100	1.73299800
H	11.32125000	0.50925900	0.49094000
H	12.53432900	1.83109900	0.49039800

N1-L2-Me

L2

C	6.04047100	-3.10322800	-5.21224700
C	6.57126800	-3.70557900	-3.07944400
C	7.07348600	-3.92232100	-5.78217200
C	7.65089200	-4.51529400	-3.50796200
C	6.30131300	-3.61525000	-1.69514600
C	7.89640000	-4.60567500	-4.91593300
C	8.41514300	-5.20409000	-2.53716900
H	5.47293700	-2.98727600	-1.38350100
C	7.06417200	-4.29916300	-0.78192700
C	8.14737400	-5.11885200	-1.18588600
H	9.23744300	-5.82803700	-2.87353200
H	6.82303300	-4.20040100	0.27059000
N	5.78900700	-2.99957900	-3.93920700
C	9.04164900	-5.45206900	-5.40977300
H	9.20879500	-5.34286900	-6.48180700
H	9.97157200	-5.17313800	-4.90330800
H	8.86381500	-6.51373300	-5.20168600
C	9.01432600	-5.89570500	-0.18386000
C	10.47176100	-5.40629300	-0.28306300
H	11.10608600	-5.94881000	0.42807200
H	10.88337400	-5.56323900	-1.28546300
H	10.53979000	-4.33662600	-0.05730000
C	8.95642800	-7.40014200	-0.51032300
H	9.56746200	-7.96869300	0.20075100
H	7.92781000	-7.77201300	-0.45255800
H	9.33400000	-7.61163200	-1.51588900
C	8.54429600	-5.70519100	1.26541300
H	8.60050100	-4.65644100	1.57716800
H	7.51586800	-6.05476600	1.40871800
H	9.18691200	-6.28422000	1.93747600
C	7.20870600	-4.02076100	-7.28845300
H	8.09456700	-3.46138200	-7.61994800
H	7.36952900	-5.06220000	-7.58517800
C	5.97207900	-3.47345600	-7.99612400
H	5.13507600	-4.17700800	-7.90661100
H	6.17166600	-3.32969300	-9.06314300
C	5.56112300	-2.15680100	-7.35844200
H	6.41326200	-1.45956600	-7.38784300
C	4.35312900	-1.51204600	-8.01046300
H	3.50065100	-2.19826400	-7.98709900
H	4.07573300	-0.59806700	-7.47892300
H	4.57394800	-1.26089200	-9.05267900
O	5.21014300	-2.36973600	-5.99152400

CH₃Pd(I)(L2)₂

Pd	-0.82648000	1.05835200	-0.61622100
I	-2.88527600	2.52442600	-1.44596300
C	-1.87455200	-0.60802000	-1.02821400
H	-2.82209400	-0.59947300	-0.48264400
H	-2.07132800	-0.63588800	-2.10309700
H	-1.25897300	-1.46316900	-0.73039700
C	1.08861700	2.92999400	1.08859400
C	1.53796600	3.22357600	-1.14499300

C	2.42298500	3.28078000	1.47261300
C	2.88751900	3.55085800	-0.88635500
C	1.05513400	3.29380000	-2.47454800
C	0.46189200	2.54454400	3.38337200
C	2.75597000	3.37081100	2.94560400
C	3.33663400	3.52133000	0.47255100
C	3.72671400	3.91975100	-1.97195700
H	0.01067700	3.05684800	-2.65332000
C	1.88898600	3.67943500	-3.48988300
C	1.48687900	3.59667600	3.76251200
H	3.23884000	2.44115200	3.28087400
C	3.25756300	3.99472500	-3.26444800
H	4.75975800	4.16805700	-1.76039700
H	1.48332100	3.73948600	-4.49558100
H	1.07633200	4.59569800	3.56997300
C	1.98674600	-0.06546100	-0.63025800
C	1.01521800	-0.39181000	1.43758700
C	3.30958800	-0.17845300	-0.09954900
C	2.27427100	-0.49834400	2.06544600
C	-0.15659100	-0.58589600	2.20656200
C	2.82941600	0.37602700	-2.84148300
C	4.48168800	-0.11560300	-1.05454000
C	3.44668900	-0.32629500	1.26146700
C	2.32548900	-0.78121300	3.45649900
H	-1.11753300	-0.48483300	1.71218100
C	-0.06490800	-0.88374900	3.53959200
C	4.04240000	-0.45837800	-2.47604500
H	4.91495500	0.89468900	-1.04427400
C	1.18742700	-0.97920100	4.20555100
H	3.29768100	-0.85717500	3.92778200
H	-0.98349800	-1.03191100	4.09955000
H	3.79145700	-1.52357400	-2.55571300
C	4.78979700	3.77758600	0.77723400
H	5.42949900	3.15699300	0.14054100
H	5.05709100	4.82344000	0.58452600
H	5.04116600	3.54997400	1.81399800
C	4.14231600	4.37994900	-4.45335900
C	5.57863000	4.71551100	-4.02970900
H	6.16834400	4.98638600	-4.91215300
H	5.60927700	5.56375200	-3.33671000
H	6.07158100	3.85999000	-3.55329300
C	3.54752600	5.61360300	-5.15877400
H	4.17589400	5.90432100	-6.00887600
H	2.54013500	5.42232200	-5.54120200
H	3.48916100	6.46251200	-4.46912300
C	4.19801900	3.19633700	-5.43866100
H	4.63630400	2.31396700	-4.95674000
H	3.20289600	2.92203600	-5.80340800
H	4.81508800	3.45107200	-6.30839200
C	4.80012100	-0.32377200	1.92241400
H	5.59569500	-0.03219200	1.23602700
H	4.81261500	0.38454000	2.75785000
H	5.04626400	-1.31141300	2.32963200
C	1.21430700	-1.25367900	5.71140000
C	0.48516200	-2.57738100	6.01001100
H	0.49456200	-2.77891400	7.08735600
H	-0.56041800	-2.55145500	5.68725200
H	0.97395300	-3.41484600	5.50049600
C	0.50075000	-0.09590100	6.43715100
H	1.01174000	0.85504200	6.24418400
H	-0.53923400	0.01032800	6.11169300
H	0.49740300	-0.26781400	7.51975200
C	2.64323400	-1.35665200	6.26141600
H	3.20184400	-2.17194300	5.78799100
H	3.20073500	-0.42365100	6.11959100
H	2.60910500	-1.55862100	7.33726400
N	0.68189800	2.83802100	-0.15478000
N	0.89840100	-0.09435000	0.10859800
O	0.14182700	2.63434900	1.98819100
O	1.74965300	0.10240600	-1.93260400
H	3.46544400	4.18359300	3.12726600
H	1.70071100	3.52491300	4.83415200
H	0.89818500	1.55533100	3.55740900

H	4.85063200	-0.25437100	-3.18603000
H	5.26832200	-0.80524600	-0.73443200
C	-0.85835200	2.65718300	4.11654000
H	-1.55244000	1.89395700	3.75453900
H	-0.70434900	2.51338800	5.19072900
H	-1.30975400	3.63986700	3.94854400
H	3.08018100	1.43601700	-2.73672000
C	2.27395300	0.11641100	-4.22560300
H	3.01476400	0.39020800	-4.98295000
H	2.01601500	-0.94048500	-4.34689700
H	1.37360800	0.71620700	-4.38221600

1

Pd	-0.02244500	1.22638300	0.07145600
O	-1.97182500	0.95451300	0.55230600
O	1.93881800	1.46481600	-0.40851200
C	-2.30957900	0.93888000	1.80067700
C	2.25517200	1.94294300	-1.56520900
O	-1.55812400	1.06200900	2.76749900
O	1.47634700	2.20793900	-2.48461300
C	-3.80987900	0.75539800	1.99610400
H	-4.33405500	1.64172100	1.62427000
H	-4.16718700	-0.10102300	1.41680400
H	-4.03800600	0.61659900	3.05440400
C	3.75275700	2.16929400	-1.71962200
H	4.09991100	2.87143300	-0.95523500
H	4.28680700	1.22714200	-1.56357200
H	3.97622200	2.56187300	-2.71310300
C	0.43719200	3.97892100	1.21765800
C	-0.52816400	3.93263600	-0.89720100
C	0.77905800	3.29292600	2.40379100
C	0.69539300	5.36074100	1.11348400
C	-0.23911500	5.31363700	-1.12352600
C	1.37472000	3.96908100	3.43432100
H	0.51535100	2.24343800	2.49021000
C	1.31794400	6.02017500	2.20470200
C	0.35204700	6.02809900	-0.10804000
C	-0.53002200	5.86220400	-2.50236200
C	-1.50797300	3.64699500	-3.08578700
C	1.67031400	5.35583300	3.35771100
H	1.61666200	3.41755700	4.33839600
H	1.52228900	7.07936800	2.11107500
C	-0.52560400	4.72011100	-3.51627800
H	-1.50013100	6.37836000	-2.52124700
H	0.47194700	4.26937400	-3.57637600
C	0.30386200	-1.54096700	0.97709000
C	-0.11652000	-1.46231000	-1.30457700
C	0.16235900	-2.96047000	1.02305300
C	-0.29182700	-2.86097000	-1.35847900
C	-0.20943800	-0.70024300	-2.49083400
C	0.35758700	-1.37548800	3.34472500
C	0.35972100	-3.67021200	2.34880300
C	-0.16662900	-3.61201700	-0.14480400
C	-0.57697600	-3.46147500	-2.61223400
H	-0.02661400	0.37044600	-2.44506500
C	-0.48109800	-1.32188100	-3.67974100
C	0.98315300	-2.75890200	3.40867600
H	-0.61257900	-4.03227400	2.70964500
C	-0.67770700	-2.72574100	-3.77139000
H	-0.71115300	-4.53544400	-2.64564700
H	-0.53690700	-0.71080700	-4.57641400
H	2.06180200	-2.65413600	3.23944700
N	-0.15037000	3.29135300	0.18967100
N	0.13707100	-0.83216500	-0.11782200
O	-1.20278400	3.18299500	-1.75969900
O	0.62908900	-0.82118400	2.04853400
H	-2.52096600	4.07095500	-3.03792800
H	-0.80332700	5.08411400	-4.51081500
H	0.22852900	6.59846100	-2.78164400
H	-0.73338300	-1.43310600	3.45017000
H	0.84519000	-3.19130300	4.40497800
H	0.98974700	-4.55510700	2.21114600

C	-1.49474100	2.41845600	-3.97603100
H	-0.47485800	2.02893600	-4.03690800
H	-2.14738100	1.64361500	-3.56316800
H	-1.84838700	2.68041800	-4.97912100
C	0.90651000	-0.38294500	4.34701400
H	1.98088100	-0.23795000	4.19217200
H	0.38557400	0.56894900	4.22449000
H	0.74159300	-0.75163500	5.36463600
C	0.64632800	7.49930000	-0.24375300
H	0.19515300	8.05424300	0.58562200
H	1.72583000	7.68638500	-0.21242300
H	0.25389500	7.92118700	-1.16924100
C	-0.39005600	-5.10126500	-0.17912600
H	-1.37614100	-5.32875700	-0.59788100
H	0.35510400	-5.59269700	-0.81525100
H	-0.33858900	-5.55491000	0.81082700
C	2.35363900	6.04406000	4.54345900
C	2.60719000	7.53568600	4.28662400
H	3.26318900	7.69276700	3.42289200
H	1.67230400	8.08183200	4.11725100
H	3.09650500	7.98113800	5.15965700
C	3.71061500	5.36421300	4.81021500
H	3.59345900	4.30080900	5.04197200
H	4.36539700	5.44608100	3.93576400
H	4.21219200	5.83898500	5.66192700
C	1.45937700	5.91589200	5.79185700
H	1.93877900	6.39532100	6.65367800
H	0.48939100	6.39723600	5.62614600
H	1.27313600	4.86925100	6.05279000
C	-0.97506600	-3.35327400	-5.13658300
C	0.19458100	-3.06000400	-6.09603200
H	0.00084100	-3.50705500	-7.07826000
H	0.34366900	-1.98552000	-6.24196200
H	1.12912300	-3.47881100	-5.70696000
C	-1.15549300	-4.87480400	-5.05209000
H	-0.25124600	-5.36959400	-4.67991200
H	-1.99402300	-5.14882800	-4.40179300
H	-1.36466300	-5.27697900	-6.04925400
C	-2.27227500	-2.74426900	-5.70327000
H	-3.11742200	-2.93838100	-5.03388100
H	-2.18888800	-1.66059200	-5.83420600
H	-2.50013900	-3.18286800	-6.68188200

31

Pd	2.60236000	3.92901700	0.27780300
N	-0.07467000	0.43409900	-1.82186900
C	-1.30050300	0.92386900	-2.24387700
C	-1.34467100	2.18933300	-2.83446100
C	-2.52446200	0.28342400	-2.02634800
C	-2.52876500	2.77557600	-3.24715500
C	-3.70482900	0.86119200	-2.47236500
C	-3.74384100	2.11322200	-3.08491800
C	-5.07877700	2.65633600	-3.53033400
F	-4.83999400	0.20018400	-2.26029200
F	-2.59982300	-0.85334300	-1.34935000
F	-0.19929300	2.86770800	-2.98310300
F	-2.45150200	3.99208400	-3.78825400
F	-5.91937500	2.77292600	-2.48942600
F	-5.65573700	1.83682200	-4.41903900
F	-4.97905100	3.86189600	-4.09960500
C	0.34972900	-0.89081600	-1.88387700
O	-0.32716000	-1.77835900	-2.34853700
C	1.72684600	-1.13115400	-1.25191100
H	1.54167600	-1.36717700	-0.19786100
H	2.12058000	-2.03453600	-1.71842300
C	2.67235500	0.04031900	-1.37676000
C	3.53791800	0.17027100	-2.46796400
C	2.58698500	1.12487300	-0.48218100
C	4.28534500	1.32319500	-2.67775200
C	3.24779300	2.34444900	-0.73147500
C	4.11752300	2.40939400	-1.82455800
H	4.95867700	1.37767700	-3.52699200

H	4.66173500	3.32717100	-2.03954600
C	1.61590900	2.53240500	1.34976700
C	2.18071300	2.41184300	2.77264100
C	1.75646400	1.09190600	0.77326900
C	3.32658500	1.40531000	2.57982400
C	1.17341600	1.57775000	3.60283600
H	2.44258400	3.36693400	3.23389200
C	2.42911600	0.32783500	1.94954100
H	0.76493700	0.66184000	0.58772100
H	3.77712700	1.07576200	3.52329400
H	4.10782600	1.77089400	1.90799300
H	1.41880200	1.62917800	4.66965200
H	0.14719100	1.94210300	3.48531600
C	1.36662700	0.13478500	3.04815300
H	2.92994100	-0.59423400	1.64149900
H	1.73696800	-0.54055900	3.82671500
H	0.43924800	-0.29587200	2.65521000
H	0.65312800	1.12863800	-1.69195900
C	1.96814300	6.15270100	2.32678500
C	0.19480700	5.83738400	0.88212100
C	1.22150900	7.03162100	3.17011400
C	-0.65111600	6.64378600	1.67713400
C	-0.32250900	5.25621200	-0.29510800
C	3.75567700	6.06676300	3.90558300
C	1.90549300	7.67264400	4.36221000
C	-0.10095500	7.25065500	2.85374200
C	-1.99820400	6.81180200	1.27795700
H	0.33490200	4.64449500	-0.90615800
C	-1.63456900	5.44720100	-0.65047200
C	3.42256100	7.49096400	4.31470400
H	1.66727900	8.74045000	4.40186800
C	-2.51537400	6.22193800	0.14177100
H	-2.64532600	7.42845600	1.89293900
H	-1.98678800	4.99410900	-1.56901800
H	3.86466200	7.71508800	5.29054500
N	1.49470700	5.58940900	1.24169500
O	3.24679200	5.83211300	2.58461200
C	-3.99066900	6.42137700	-0.23138500
C	-4.39695500	5.57547400	-1.44548600
H	-4.24227200	4.50702400	-1.25905200
H	-5.46197100	5.71636300	-1.65549000
H	-3.84674200	5.85201400	-2.34994800
C	-4.23139000	7.90592300	-0.56334700
H	-5.28232700	8.07144100	-0.82740800
H	-3.99255000	8.55281500	0.28799300
H	-3.61174900	8.22123600	-1.40993800
C	-4.88304100	6.00609700	0.95398800
H	-5.93957500	6.13868200	0.69491700
H	-4.72387900	4.95288900	1.20941100
H	-4.68522700	6.60431600	1.84950400
C	-0.98478700	8.11482800	3.71369600
H	-0.47816100	8.47288000	4.60994700
H	-1.33897400	8.98782700	3.15381700
H	-1.86886500	7.55430200	4.03601900
H	3.87124400	8.17369200	3.58273200
H	1.51494300	7.23031300	5.28850100
H	3.25357300	5.35996500	4.58313700
C	5.23651700	5.75486900	3.84359200
H	5.68215500	5.84282000	4.83907200
H	5.39196700	4.73699200	3.47555600
H	5.74483700	6.45009000	3.16803900
H	0.58069800	2.89425200	1.33768200
Cl	3.68479700	-1.12199400	-3.65113300

TS32

Pd	2.46181700	3.78086300	0.23166500
N	-0.31073500	0.72175400	-2.11150000
C	-1.36995700	1.36361800	-2.74351100
C	-1.09326600	2.30582800	-3.73662300
C	-2.70422800	1.18236000	-2.38332900
C	-2.10178100	3.00158300	-4.37563700
C	-3.72117400	1.86220500	-3.04883100

C	-3.44312500	2.78527200	-4.05438000
C	-4.49677500	3.55928000	-4.81381300
F	-4.96291300	1.63190000	-2.63890400
F	-3.03477000	0.41399300	-1.35320200
F	0.18418500	2.54579200	-4.05104000
F	-1.77258000	3.87823400	-5.31822400
F	-4.47952000	3.23321600	-6.11233600
F	-4.26327700	4.87825500	-4.72695400
F	-5.72879800	3.33925500	-4.35294700
C	-0.26455400	-0.64088100	-1.83800100
O	-1.17275300	-1.39333100	-2.10083800
C	1.00584300	-1.11017800	-1.11744100
H	0.69395400	-1.31918800	-0.08935000
H	1.27020300	-2.07090300	-1.56132700
C	2.15544900	-0.13382000	-1.14843000
C	3.17388500	-0.21250500	-2.10566100
C	2.14935100	0.99116800	-0.30133900
C	4.14938000	0.77297700	-2.23129500
C	3.05329800	2.04406700	-0.50539300
C	4.07711400	1.91527700	-1.44166700
H	4.93300700	0.66001400	-2.97240200
H	4.80980600	2.70558000	-1.58108400
C	1.34179900	2.56877500	1.46036600
C	1.83948700	2.30854400	2.87884800
C	1.17047900	1.16219700	0.82997700
C	2.61750000	0.99136400	2.74065800
C	0.57858500	1.82425400	3.64554500
H	2.35209700	3.13558000	3.37129000
C	1.47241400	0.23959400	2.04764200
H	0.13909800	1.03068500	0.48132600
H	2.88753900	0.56485400	3.71050700
H	3.51943100	1.06178300	2.12911900
H	0.80698300	1.78250600	4.71457400
H	-0.27434700	2.49896400	3.51869400
C	0.32444300	0.40382600	3.06098400
H	1.68518800	-0.79537900	1.77013500
H	0.39091100	-0.36135500	3.83990700
H	-0.65991300	0.30764400	2.59047800
H	0.57414700	1.21216400	-2.12245800
I	5.33757800	4.50276000	4.39049900
C	4.14233800	3.83560500	1.44991700
H	3.72066300	4.45395000	2.23488600
C	1.76187300	6.61138000	1.42511800
C	-0.06554900	5.54390400	0.48034400
C	0.92930100	7.48185200	2.19945200
C	-0.97045800	6.30843700	1.24147200
C	-0.57479500	4.61445400	-0.45581800
C	3.77254400	7.50380400	2.42273400
C	1.59061500	8.54729500	3.04770500
C	-0.43234500	7.28851300	2.14367500
C	-2.36138300	6.08232500	1.07976000
H	0.11867800	4.05610800	-1.08367700
C	-1.92516200	4.42744000	-0.58867800
C	3.02389500	8.81135900	2.59101200
H	1.01589600	9.47705700	2.99886200
C	-2.85981100	5.15250600	0.19321500
H	-3.04732800	6.66998600	1.67700900
H	-2.28250400	3.70777600	-1.31804000
H	3.54573300	9.43206900	3.32519700
N	1.29174200	5.65804500	0.64209400
O	3.08627500	6.69158100	1.42889900
C	-4.35416900	4.87595300	0.00738700
C	-4.73806000	5.16765600	-1.45456400
H	-4.13923600	4.57981100	-2.15357300
H	-5.79085900	4.92327200	-1.63240700
H	-4.58309700	6.22454100	-1.69643700
C	-5.22670500	5.74665200	0.92023100
H	-6.28273900	5.51651100	0.74515200
H	-5.01977300	5.56095300	1.98041900
H	-5.08551300	6.81468400	0.71922500
C	-4.63614700	3.39641000	0.33527100
H	-5.69602400	3.17031400	0.17533500
H	-4.05795500	2.71226600	-0.29226700

H	-4.39234000	3.17757500	1.38072100
C	-1.37753900	8.09290300	2.99545800
H	-0.85577900	8.72943000	3.70950200
H	-2.01726600	8.73012900	2.37397200
H	-2.03365900	7.42804300	3.56671100
H	3.02814100	9.35313600	1.63640500
H	1.59568400	8.22866300	4.09841400
H	3.77670000	6.92266300	3.35372800
C	5.19212900	7.65526300	1.92523100
H	5.76999000	8.23306400	2.65208700
H	5.66642500	6.67464100	1.83905400
H	5.21383700	8.17043600	0.95861500
H	0.43563400	3.17920800	1.42805300
H	4.45509000	2.85135200	1.77406500
H	4.87239000	4.35134300	0.82068000
Cl	3.24080600	-1.56042600	-3.22056000

TS35

Pd	2.29073900	4.03009000	0.14067900
N	-0.18296000	-0.48386200	-2.69730700
C	-1.34992000	0.07726300	-3.20864800
C	-1.88554400	-0.38609200	-4.40710900
C	-1.99063900	1.15183400	-2.58464200
C	-3.02411300	0.17756300	-4.97065600
C	-3.14241000	1.68681100	-3.13303700
C	-3.68332500	1.22481000	-4.33218600
C	-4.92938700	1.89754100	-4.85772100
F	-3.72608600	2.71245500	-2.50482100
F	-1.48502600	1.70261700	-1.48709000
F	-1.27967700	-1.39154400	-5.03969800
F	-3.45651900	-0.33112700	-6.11914000
F	-5.35710300	1.36708600	-6.00409300
F	-4.70690300	3.20373800	-5.07202900
F	-5.92826400	1.80339300	-3.96809700
C	-0.03622500	-0.84921600	-1.36840000
O	-0.97133500	-0.85250100	-0.59615400
C	1.40024400	-1.18220600	-0.97831800
H	1.38165000	-1.42408800	0.08467600
H	1.72977200	-2.07415700	-1.51928600
C	2.29444900	0.00369600	-1.27850900
C	3.09290000	0.06744400	-2.42189200
C	2.21453200	1.15666900	-0.47501500
C	3.79341300	1.21444000	-2.76967200
C	2.84121100	2.36068600	-0.84951600
C	3.64940700	2.35736500	-1.99041900
H	4.41177500	1.22180700	-3.66124100
H	4.15313200	3.26462500	-2.31282300
C	1.36744500	2.64796400	1.33670100
C	2.03055300	2.57998600	2.72154600
C	1.44529900	1.18656800	0.81243300
C	3.13536900	1.53428000	2.49574900
C	1.07520300	1.81353100	3.66668000
H	2.34646200	3.55055000	3.11527600
C	2.16745900	0.45575700	1.98166300
H	0.44139200	0.76864700	0.68200500
H	3.64932200	1.23800400	3.41759400
H	3.87653900	1.83400000	1.74798300
H	1.41389400	1.89248600	4.70643500
H	0.05588200	2.21087400	3.62156900
C	1.17314500	0.34608000	3.15282400
H	2.62866600	-0.49402600	1.69685300
H	1.56511500	-0.31836000	3.93043800
H	0.20759800	-0.05683200	2.83055700
H	0.57012500	-0.67855700	-3.34483100
I	3.51221100	6.04107700	-1.31527900
C	4.63181500	4.59890600	0.51106000
H	4.21266000	4.16781900	1.41694300
H	5.18539100	5.50376100	0.72753600
C	1.52402600	6.35546600	2.16037500
C	-0.24645500	5.77874600	0.80344200
C	0.78530400	7.38796600	2.81176600
C	-1.08958900	6.72450100	1.42714500

C	-0.78227000	4.95509600	-0.21495300
C	3.30300600	6.57474500	3.73987000
C	1.47229300	8.25441300	3.84894300
C	-0.53478100	7.55446800	2.45142500
C	-2.44564800	6.81275300	1.01474100
H	-0.13549200	4.22801600	-0.69677000
C	-2.10068400	5.05306200	-0.56701300
C	2.98660100	8.05610700	3.83900900
H	1.24316200	9.30897900	3.66547600
C	-2.97255600	5.99420100	0.04196700
H	-3.07933000	7.54680200	1.49632500
H	-2.48256900	4.37491600	-1.32148800
H	3.43402000	8.47888900	4.74413000
N	1.05551200	5.60947500	1.19072600
O	2.79687100	6.07063900	2.49776300
C	-4.44425700	6.03439200	-0.37973900
C	-4.54654000	6.21153700	-1.90738900
H	-4.10657300	5.36995700	-2.45002700
H	-5.59914300	6.27708900	-2.20576800
H	-4.04183700	7.12878300	-2.23010700
C	-5.20715700	7.18514900	0.29048900
H	-6.24403200	7.19227700	-0.06223200
H	-5.23354800	7.07582000	1.38073600
H	-4.76599600	8.15896000	0.04866900
C	-5.11043400	4.70550400	0.02829000
H	-6.16710300	4.70632100	-0.26432500
H	-4.63129400	3.84808900	-0.45258400
H	-5.05429500	4.56024400	1.11282200
C	-1.40984300	8.58473200	3.11593300
H	-0.89538500	9.12194500	3.91302300
H	-1.76593000	9.32054800	2.38628200
H	-2.29292500	8.10929400	3.55614700
H	3.43751400	8.56149800	2.97625100
H	1.07998500	8.01745900	4.84706300
H	2.79452200	6.03273100	4.55145900
C	4.78352700	6.25211700	3.75689000
H	5.22301100	6.55672000	4.71140900
H	4.94456500	5.17796600	3.62752900
H	5.29813800	6.78377500	2.94976000
H	0.33450500	3.00587200	1.40144400
H	5.15474700	3.89220000	-0.12402000
Cl	3.19527400	-1.31097400	-3.52604600

TS65

Pd	4.68657800	3.57845100	-3.62821800
N	0.72201300	-1.03987700	-2.52085800
C	0.12379400	-1.23989300	-3.76807900
C	0.46416300	-0.45135500	-4.86447400
C	-0.82550400	-2.24221500	-3.95627500
C	-0.16481800	-0.61732200	-6.09196600
C	-1.42629700	-2.43015300	-5.19027700
C	-1.11832000	-1.61542900	-6.28006500
C	-1.83351600	-1.87254300	-7.58689600
F	-2.32860400	-3.39925300	-5.31887500
F	-1.15797300	-3.03067700	-2.93686400
F	1.42039400	0.46182100	-4.75022100
F	0.20247800	0.19422100	-7.08450200
F	-1.60298000	-3.12221000	-8.01316200
F	-1.45006700	-1.03870200	-8.55653100
F	-3.15779200	-1.73511300	-7.43555700
C	0.71859400	0.19567500	-1.89946000
O	0.09718600	1.13971400	-2.34042800
C	1.61848400	0.27545400	-0.67472900
H	1.24080600	1.09093800	-0.05584900
H	1.59190800	-0.65017400	-0.09271700
C	3.01250800	0.58983600	-1.16676100
C	4.00229800	-0.36917700	-1.40637100
C	3.34956400	1.89954100	-1.49148900
C	5.27173300	-0.02929900	-1.86728000
C	4.56555700	2.26238000	-2.09022300
C	5.57610000	1.29246300	-2.19671000
H	6.01776700	-0.80795000	-1.98846800

H	6.57207100	1.53614500	-2.55092200
H	1.20412400	-1.81375500	-2.08386200
C	4.02483800	4.02299300	-1.61430200
C	4.74426200	4.49393900	-0.33886200
C	2.78729700	3.22746900	-1.08766500
H	3.75262000	4.90369900	-2.23121800
C	3.91183100	5.68500000	0.18653200
C	4.38248200	3.42600700	0.70859400
H	5.80532800	4.70860700	-0.47750500
C	2.86797200	3.49740900	0.43476200
H	1.82111100	3.50080100	-1.52194400
C	2.58892400	5.00162200	0.65369400
H	3.74682600	6.44786200	-0.58135100
H	4.42251200	6.16792400	1.02724400
H	4.82661600	2.44523200	0.52547800
H	4.63466700	3.74166800	1.72692800
H	2.24062500	2.83926000	1.04232400
H	1.71799300	5.33960700	0.08217500
H	2.38801200	5.20715300	1.71003800
C	3.92531200	3.67941100	-6.55521100
C	6.21626000	3.90862300	-6.40888900
C	3.95293700	3.60604300	-7.98490500
C	6.36175800	3.81730600	-7.81161000
C	7.36570700	4.08913000	-5.61251600
C	1.60282000	3.11793300	-6.51093900
C	2.64520400	3.48816900	-8.74340100
C	5.18027800	3.64611100	-8.60573500
C	7.65929000	3.91063500	-8.36649500
H	7.22957700	4.15590200	-4.53541600
C	8.60880800	4.18052400	-6.18893200
C	1.44018000	3.80032500	-7.85700400
H	1.75299300	2.04276700	-6.65804800
H	2.64974000	4.16400700	-9.60475400
C	8.78709100	4.09295700	-7.59095500
H	7.76513100	3.84160000	-9.44442800
H	9.46565400	4.32439800	-5.54054400
H	0.51768600	3.45970800	-8.33774800
N	4.99307700	3.81412700	-5.80233400
C	5.31600500	3.52002400	-10.10070500
H	5.72137700	4.44130800	-10.53512800
H	6.00742600	2.70939000	-10.35443800
H	4.36600100	3.30641800	-10.59074900
C	10.16688400	4.19981200	-8.25646500
C	10.45979900	2.90540500	-9.03909200
H	9.71424900	2.72716700	-9.82109000
H	11.44237500	2.96683600	-9.52156300
H	10.45912400	2.03785600	-8.37020000
C	10.17478700	5.39882400	-9.22413400
H	9.96121900	6.33155400	-8.69087900
H	11.15604500	5.49522800	-9.70372200
H	9.42627500	5.28610600	-10.01536900
C	11.29235600	4.40535300	-7.23238100
H	11.16015400	5.33337200	-6.66509800
H	11.35696400	3.57187700	-6.52417200
H	12.25381600	4.47172800	-7.75299100
O	2.77913000	3.62985900	-5.86507800
H	1.35009200	4.88108000	-7.69195000
H	2.54568900	2.47020800	-9.14409200
C	0.45451000	3.34678200	-5.55021200
H	-0.45841100	2.90318400	-5.96026000
H	0.66028400	2.88218800	-4.58337000
H	0.28821800	4.41836400	-5.40020100
Cl	3.68308300	-2.07500300	-1.07274000

TS36

Pd	1.62533600	3.97615700	0.47395000
N	-0.49715000	-0.37743900	-2.10466400
C	-1.86127400	-0.56371800	-1.86223900
C	-2.72605900	-0.92258800	-2.89472100
C	-2.39874500	-0.39091200	-0.59004400
C	-4.07378100	-1.12591500	-2.65655100
C	-3.75119400	-0.60657900	-0.34958700

C	-4.61398900	-0.97830900	-1.37842200
C	-6.09583500	-1.21791800	-1.20421300
F	-4.18724300	-0.40650800	0.88988000
F	-1.62696700	0.00525900	0.41499000
F	-2.24090900	-1.07652400	-4.12599000
F	-4.85664100	-1.47211100	-3.67406700
F	-6.41563700	-2.47139800	-1.55094600
F	-6.80349700	-0.39074700	-1.99079800
F	-6.50559800	-1.02756500	0.05096900
C	0.45988200	-1.13781000	-1.45210300
O	0.16590700	-1.97049400	-0.62158700
C	1.89617600	-0.82877200	-1.86048500
H	2.52364900	-1.25692000	-1.07762200
H	2.10893600	-1.38260300	-2.77973800
C	2.16860000	0.64614000	-2.04879800
C	2.30357500	1.22614600	-3.31408500
C	2.19999100	1.48963300	-0.92188800
C	2.45184000	2.59791200	-3.48279200
C	2.37457400	2.87465300	-1.09170900
C	2.48990500	3.42365100	-2.36902800
H	2.53581100	3.01726800	-4.47917300
H	2.59380600	4.49610000	-2.49253300
C	1.45444400	2.13863000	1.38586300
C	2.30014400	1.90250100	2.64201500
C	1.84231500	0.97542400	0.44721700
H	0.38871000	2.12201700	1.61702800
C	3.60172900	1.30075000	2.08744400
C	1.69075100	0.65499600	3.33777500
H	2.39160700	2.77205800	3.29684000
C	2.89760300	0.19728300	1.28324200
H	0.96222800	0.33646700	0.33079400
H	4.24200000	0.88906700	2.87585500
H	4.19784200	1.98217600	1.48603500
H	2.11577400	0.53658400	4.34047000
H	0.60473700	0.73502200	3.44817900
C	2.11698100	-0.52128900	2.40376500
H	3.54953800	-0.45608300	0.69801900
H	2.76924000	-1.22359000	2.93244800
H	1.26768400	-1.08899600	2.01204800
H	-0.22783900	0.13016200	-2.93664700
Cl	2.23314000	0.23780100	-4.76829700
I	1.55726400	6.66300100	-0.49589300
C	3.72459800	3.88921700	0.04926400
H	3.84263900	4.20606500	1.09580000
H	4.37440700	3.04013600	-0.13761300
H	3.95533600	4.71331600	-0.62088400
C	-0.30932000	5.17533400	2.37884200
C	-1.52560200	4.11994800	0.71690500
C	-1.45807200	5.83235800	2.90880900
C	-2.73451500	4.65485400	1.21590300
C	-1.55419300	3.29287900	-0.42326400
C	1.20069700	6.27956900	3.92338100
C	-1.22522300	6.86254700	3.99017700
C	-2.67749000	5.54107700	2.34451300
C	-3.93736300	4.33992100	0.54544700
H	-0.62085700	2.88773400	-0.80242600
C	-2.74498400	3.02444300	-1.05378700
C	0.19470600	7.41459400	3.86343800
H	-1.94417300	7.67997600	3.89226100
C	-3.97287300	3.54806700	-0.58510900
H	-4.86400900	4.75280700	0.92909400
H	-2.72607200	2.39943400	-1.93950600
H	0.40892500	8.12323800	4.66953300
N	-0.33323200	4.39838000	1.32494600
O	0.91136800	5.29518100	2.90915500
C	-5.31198900	3.25457600	-1.27419100
C	-5.12529600	2.47576400	-2.58311200
H	-4.65070800	1.50539400	-2.41479800
H	-6.09994200	2.28360300	-3.04235700
H	-4.51800200	3.03776200	-3.30157900
C	-6.02882500	4.57549600	-1.61293700
H	-6.97597200	4.36851300	-2.12426500
H	-6.26050700	5.15857700	-0.71585400

H	-5.41202600	5.19801100	-2.26992700
C	-6.19029300	2.42627200	-0.31762500
H	-7.12734200	2.13754900	-0.80550700
H	-5.67765400	1.51564500	0.00385100
H	-6.43956100	2.99560400	0.58457300
C	-3.95368100	6.14231900	2.87048000
H	-4.38915600	6.83200900	2.13820300
H	-4.69410500	5.35980200	3.06559000
H	-3.80265700	6.68623000	3.80333100
H	0.31026600	7.94226600	2.90848300
H	-1.36996700	6.42455900	4.98759600
H	1.11173400	5.76370100	4.88921000
C	2.63481900	6.70986100	3.68360600
H	2.94834900	7.41972200	4.45574900
H	3.30287000	5.84377100	3.71642200
H	2.72320100	7.17996900	2.69919700

TS40

Pd	1.49480700	3.69815100	0.62371300
N	-0.18733500	-0.26117500	-2.13979500
C	-1.57042300	-0.43263100	-2.08212200
C	-2.35611000	-0.22905900	-3.21587600
C	-2.21193500	-0.80097400	-0.90197500
C	-3.72425500	-0.43508500	-3.18114600
C	-3.58195500	-1.03774300	-0.87716800
C	-4.36579900	-0.85478100	-2.01491400
C	-5.84592400	-1.15495800	-2.07695900
F	-4.11578400	-1.40000900	0.28440200
F	-1.52689900	-0.91028500	0.23056700
F	-1.77269700	0.15008700	-4.35131200
F	-4.42331000	-0.24639600	-4.29683300
F	-6.07317300	-2.23543100	-2.83738900
F	-6.52194000	-0.13314500	-2.62419000
F	-6.37664300	-1.38678700	-0.87505600
C	0.68427900	-1.25733600	-1.72866300
O	0.29468600	-2.31499100	-1.28444400
C	2.16651000	-0.92756900	-1.87718000
H	2.65648900	-1.42009300	-1.03490400
H	2.51582300	-1.43617100	-2.77981800
C	2.48563800	0.54548100	-1.92443200
C	2.81292700	1.19556900	-3.11895000
C	2.34630800	1.32148800	-0.75550400
C	2.96929900	2.57674800	-3.18725200
C	2.53387200	2.71093900	-0.82455100
C	2.82229200	3.33466500	-2.03796400
H	3.18791900	3.05048700	-4.13750500
H	2.91377800	4.41354600	-2.08096700
C	1.27983000	1.85036800	1.46355400
C	1.99514200	1.55978500	2.79249900
C	1.79239800	0.73288900	0.51900200
H	0.19639500	1.79111800	1.59580700
C	3.34919200	0.97744700	2.35169000
C	1.32719900	0.28931600	3.37910300
H	2.02225100	2.40376700	3.48639700
C	2.73411300	-0.09097700	1.43641900
H	0.94039600	0.10397400	0.24191000
H	3.90735600	0.53611200	3.18530500
H	4.00214900	1.67667300	1.83387300
H	1.66239700	0.12288300	4.40879000
H	0.23589300	0.37071400	3.39790700
C	1.83037400	-0.84674900	2.43374600
H	3.44517300	-0.72788400	0.90372400
H	2.41148600	-1.59052200	2.98818400
H	1.01454300	-1.37468100	1.92974200
H	0.17544300	0.52417400	-2.66385600
Cl	2.98878400	0.29402000	-4.61609500
C	3.63228100	3.71245400	0.54814200
H	3.58563900	3.87296300	1.63241000
H	4.39359600	2.96784100	0.33781900
H	3.82965600	4.64527900	0.02380400
C	-0.26731000	5.37435100	2.26431500
C	-1.66534300	4.09156300	0.94441200

C	-1.29371800	6.30912800	2.57622200
C	-2.77425100	4.89895200	1.27944000
C	-1.84832400	3.00556000	0.05847300
C	1.49300100	6.70539000	3.28644900
C	-0.86406300	7.54595800	3.32796700
C	-2.56052300	6.05012000	2.10640400
C	-4.04492700	4.57390900	0.73997800
H	-0.98450800	2.42217900	-0.24241100
C	-3.09329800	2.72267900	-0.43432300
C	0.57968700	7.86795900	2.94007100
H	-1.50789700	8.39218200	3.07617900
C	-4.23244800	3.50253900	-0.10132500
H	-4.88675200	5.20295000	1.00018500
H	-3.20438000	1.88344300	-1.11410500
H	0.93740300	8.76202000	3.46018200
N	-0.42502600	4.35097500	1.45911000
O	0.95931500	5.45641100	2.79446200
C	-5.60262400	3.11120300	-0.66068700
C	-5.51232900	2.92105900	-2.18683500
H	-4.84584700	2.10116200	-2.46757100
H	-6.49994000	2.68511000	-2.59646600
H	-5.14563500	3.83321000	-2.66956900
C	-6.67227800	4.17696600	-0.38415400
H	-7.62478400	3.86017900	-0.82211700
H	-6.83995600	4.32171300	0.68891100
H	-6.40383000	5.14231000	-0.82820800
C	-6.04088300	1.79767500	0.01300400
H	-6.97571800	1.42975900	-0.42257500
H	-5.28575800	1.01516000	-0.09936500
H	-6.19454200	1.94915600	1.08713400
C	-3.72662800	6.94402300	2.43697300
H	-4.13424000	7.40611700	1.53091500
H	-4.53271500	6.36371300	2.89828400
H	-3.45850000	7.73810500	3.13425100
H	0.64023700	8.05940400	1.86120400
H	-0.93754800	7.39666200	4.41405200
H	1.54288800	6.59476900	4.37712500
C	2.88427500	6.83655700	2.69384100
H	3.34902800	7.77267900	3.02116000
H	3.51831500	6.00549500	3.01789800
H	2.80577400	6.81640100	1.60218600
O	1.63633200	5.73236500	-0.15533700
C	0.71572100	5.96936000	-1.03050900
C	0.51112200	7.44710800	-1.34978100
H	0.05730700	7.56717800	-2.33575200
H	-0.17713000	7.86881900	-0.60623900
H	1.45156700	8.00136900	-1.29138500
O	0.00215000	5.11602800	-1.55998600

TS67

Pd	0.83743600	4.05251600	-0.87149900
N	-0.22225100	5.88791600	-1.23551100
C	-1.38738400	5.98473600	-0.64056200
C	0.14504900	6.83676200	-2.14876100
C	-2.32814300	7.02733100	-0.88688200
C	-0.70869400	7.91966600	-2.45713000
C	-1.98451200	7.99324000	-1.80561200
N	-0.02481300	-0.76395400	-2.64110300
C	-1.41201800	-0.91485800	-2.73129000
C	-2.02118700	-0.82877900	-3.98273900
C	-2.23618300	-1.08126600	-1.62263400
C	-3.39505600	-0.91108000	-4.11717600
C	-3.61520100	-1.19031500	-1.76086700
C	-4.22197000	-1.10941500	-3.01104100
C	-5.71117200	-1.20274900	-3.23963800
F	-4.32438400	-1.34157800	-0.64478300
F	-1.73130400	-1.08591600	-0.39067900
F	-1.26627300	-0.64778500	-5.06343900
F	-3.92455400	-0.81613200	-5.33440300
F	-5.99820600	-2.18589600	-4.10584200
F	-6.18594300	-0.06062700	-3.75911000
F	-6.39271300	-1.44724400	-2.11737000

C	0.78944700	-1.59304900	-1.90643200
O	0.37980300	-2.57674600	-1.32427100
C	2.27150500	-1.23514000	-1.94053600
H	2.73228200	-1.77506000	-1.10745400
H	2.67975600	-1.67987200	-2.85443400
C	2.62018100	0.23240500	-1.88327900
C	3.72241800	0.77916200	-2.55658000
C	1.89660100	1.12366700	-1.09236600
C	4.11345300	2.10502700	-2.39579300
C	2.20829600	2.48283500	-1.00081500
C	3.37377300	2.97125500	-1.59260700
H	4.99823400	2.46289400	-2.91080000
H	3.70107500	3.99830400	-1.47693400
C	0.96391400	2.33985900	0.55985900
C	1.74161400	2.19885400	1.87082600
C	0.89002200	0.90506600	-0.01152700
H	-0.00924500	2.81235400	0.73371800
C	2.60225700	0.93874400	1.67216000
C	0.67931600	1.65155400	2.85953200
H	2.24390900	3.10147900	2.21706000
C	1.43173000	0.07035400	1.17355500
H	-0.10368800	0.59742700	-0.33552900
H	3.02222000	0.57612300	2.61592300
H	3.41444100	1.05715000	0.95114500
H	1.09616700	1.63524500	3.87183400
H	-0.22590900	2.26721000	2.88663500
C	0.42001300	0.20824300	2.33121000
H	1.65700600	-0.96428000	0.90800400
H	0.61493100	-0.53943600	3.10552400
H	-0.60723900	0.06105800	1.98444700
H	0.36088900	0.06062200	-3.08887300
Cl	4.71571200	-0.22775300	-3.59217400
C	2.02866800	5.13628700	0.38339300
H	2.92920600	4.57832200	0.65180500
H	2.29271500	6.06662600	-0.12731700
H	1.43804500	5.35783500	1.27755600
I	-0.99295400	2.85014300	-2.68359600
C	-0.27553200	8.86724800	-3.41273400
C	0.93664800	8.76487300	-4.06567400
C	1.75765900	7.65659100	-3.74868700
C	1.37754200	6.71929000	-2.82017800
C	1.34568500	9.82881900	-5.09361500
H	-0.92935600	9.70193400	-3.64234100
C	-2.92103200	9.11806300	-2.15819600
H	-3.12736100	9.11758800	-3.23393600
H	-3.87676500	9.04587700	-1.63938200
H	-2.47471300	10.08785800	-1.91093900
C	-3.65954800	7.00555200	-0.15926800
C	-3.71917500	5.94426100	0.94417700
H	-3.22607100	6.30488900	1.85502900
C	-3.00935200	4.68051400	0.49007900
H	-3.86866900	7.98982400	0.27234200
O	-1.63083100	5.01274500	0.24758400
H	-4.45324200	6.80904300	-0.89159900
H	-4.76127900	5.72507100	1.19728800
H	-3.42737600	4.32008600	-0.45930300
C	-2.99522900	3.55368500	1.50123700
H	-4.01824800	3.23532500	1.72271700
H	-2.44776000	2.69675100	1.09710100
H	-2.51819500	3.87744300	2.43251500
C	0.27735900	9.91357200	-6.20074200
H	0.56829100	10.65877500	-6.94990100
H	0.15904800	8.94801200	-6.70383200
H	-0.69955200	10.20716900	-5.80286100
C	1.46514300	11.19398400	-4.38915300
H	1.75738700	11.96784100	-5.10845400
H	0.51643000	11.49948000	-3.93537200
H	2.22130100	11.15953000	-3.59730200
C	2.69435100	9.51028900	-5.75466000
H	3.50949600	9.48094300	-5.02306800
H	2.67000800	8.55320500	-6.28742200
H	2.93656500	10.28924400	-6.48529800
H	2.70999800	7.52600300	-4.24943400

H	2.00725600	5.86122800	-2.60437900
---	------------	------------	-------------

TS69

Pd	0.93754900	4.01489200	-0.43218700
N	-0.18052400	5.79317300	-0.93399100
C	-1.30038800	5.99221400	-0.27343500
C	0.07908500	6.53132100	-2.05425300
C	-2.29156800	6.94285500	-0.66139100
C	-0.84044500	7.49068900	-2.52744600
C	-2.06144900	7.68019800	-1.80241000
N	-0.12383300	0.00492000	-2.66985500
C	-1.51311700	0.05412300	-2.84660100
C	-2.03879500	0.58905000	-4.01942300
C	-2.40556600	-0.32269600	-1.84797300
C	-3.40251300	0.75752400	-4.17639000
C	-3.77580700	-0.16475300	-2.00906400
C	-4.29984500	0.38020100	-3.17890000
C	-5.76423900	0.66783700	-3.39528000
F	-4.55545600	-0.52194800	-0.99353700
F	-1.95661200	-0.78581000	-0.68650400
F	-1.21781900	1.00500600	-4.98161300
F	-3.84877300	1.32240300	-5.29779100
F	-6.19822400	0.12930200	-4.54364500
F	-5.97316700	1.99485700	-3.47273700
F	-6.53843000	0.19797900	-2.41542900
C	0.51254600	-1.15067000	-2.28697700
O	-0.05532200	-2.22346400	-2.23841700
C	2.00628800	-1.04792300	-1.97615300
H	2.17529800	-1.73467000	-1.14007800
H	2.52583200	-1.48755300	-2.83225700
C	2.55054200	0.32032000	-1.66503000
C	3.72431000	0.84706700	-2.22416200
C	1.88840100	1.15511300	-0.76777800
C	4.22516800	2.09778700	-1.87065100
C	2.29714400	2.46477300	-0.51005900
C	3.51916800	2.92636400	-0.99826000
H	5.15831300	2.43674700	-2.30746400
H	3.91116000	3.90833400	-0.75659600
C	0.94658500	2.27706100	0.94394500
C	1.65738100	2.00211500	2.26911700
C	0.82587000	0.90164700	0.25096300
H	-0.01846600	2.77464200	1.09592300
C	2.47022700	0.72210500	2.00359800
C	0.53357100	1.42786400	3.16897600
H	2.18255800	2.85450100	2.70080300
C	1.28599500	-0.04682700	1.38620000
H	-0.17417700	0.68622700	-0.12428800
H	2.82757200	0.26397500	2.93153000
H	3.32104800	0.85632900	1.33204100
H	0.90761500	1.30653500	4.19095100
H	-0.34205000	2.08248000	3.21416700
C	0.23128500	0.04699000	2.51091300
H	1.48745900	-1.06632900	1.05050700
H	0.35646000	-0.76887800	3.22908600
H	-0.78555300	-0.01649100	2.11149000
H	0.33694000	0.91187400	-2.63600600
Cl	4.65574700	-0.08980600	-3.37689600
C	2.01468600	5.10431100	0.89097000
H	2.87931700	4.54673900	1.26207500
H	2.34160200	6.01803500	0.38410800
H	1.34656600	5.35833500	1.71952900
C	-0.52425600	8.21369300	-3.70687600
C	0.64201600	8.00390200	-4.40680800
C	1.54244800	7.02546600	-3.90696600
C	1.27724800	6.31184300	-2.76943600
C	0.99472800	8.76070800	-5.69077600
H	-1.23449000	8.95103600	-4.05884800
C	-3.06946700	8.67548200	-2.31295300
H	-3.34856400	8.44116000	-3.34574500
H	-3.98316300	8.68719200	-1.71871500
H	-2.65057200	9.68816000	-2.30921000
C	-3.55381000	7.07343500	0.17041000

C	-3.48156500	6.28225800	1.47905100
H	-2.90784700	6.83226500	2.23506200
C	-2.79794800	4.94930100	1.23250000
H	-3.75164400	8.12850900	0.38700500
O	-1.44572200	5.22419600	0.80884900
H	-4.40349500	6.71015000	-0.42224500
H	-4.48830200	6.12523200	1.87884000
H	-3.27632100	4.39814400	0.41443900
C	-2.68353500	4.04449100	2.43840200
H	-3.67955700	3.81766000	2.83059500
H	-2.20911500	3.10623400	2.13926400
H	-2.09306400	4.51929200	3.22943500
C	1.12226000	7.75104500	-6.84829800
H	1.37881900	8.27169200	-7.77815300
H	1.90150100	7.00608200	-6.65747400
H	0.17843200	7.21740400	-7.00323500
C	-0.07382500	9.79492300	-6.06990000
H	0.22381800	10.30925000	-6.98979000
H	-1.04618700	9.32508500	-6.25591600
H	-0.19780100	10.55589100	-5.29077900
C	2.33385300	9.49828800	-5.49893500
H	2.26613400	10.22512700	-4.68203900
H	3.15189900	8.80811800	-5.26903300
H	2.60216200	10.03698400	-6.41503900
H	2.46846900	6.82716900	-4.43821800
H	1.96987500	5.55704400	-2.40761500
O	-0.25706800	3.01804600	-1.97777400
C	-1.52331000	3.03423000	-1.72356400
O	-2.04899400	2.66276100	-0.66732100
C	-2.38984000	3.62931700	-2.83007100
H	-1.99214500	3.39275100	-3.81957800
H	-3.42774300	3.29962000	-2.74214100
H	-2.36187000	4.72196900	-2.72529400

TS44

N	0.78369200	-1.20245800	-1.09038600
C	-0.59060000	-1.01092700	-0.96087800
C	-1.31078500	-0.38166500	-1.97198400
C	-1.28091500	-1.39488300	0.18946000
C	-2.67644600	-0.15464400	-1.86450900
C	-2.64888900	-1.19614700	0.28196600
C	-3.37518300	-0.57364200	-0.73423600
C	-4.85930500	-0.37746900	-0.53254400
F	-3.26901000	-1.58422500	1.39338700
F	-0.63310200	-1.91779900	1.22337500
F	-0.66551500	0.02341700	-3.06809800
F	-3.27733700	0.45719300	-2.87997900
F	-5.45044500	0.19366600	-1.58392300
F	-5.09376700	0.40011400	0.53537800
F	-5.46722200	-1.55205800	-0.31506300
C	1.38581500	-2.43681000	-0.90866000
O	0.76181400	-3.42944900	-0.59970400
C	2.89510300	-2.45507000	-1.08199600
H	3.30387800	-2.79715600	-0.13578400
H	3.09983800	-3.26420500	-1.78379600
C	3.55376600	-1.17959900	-1.55083600
C	3.71261700	-1.00639200	-2.93673200
C	3.99316200	-0.14178600	-0.68939900
C	4.32865100	0.10166800	-3.49697100
C	4.55557200	1.03590700	-1.26857300
C	4.73217100	1.12069600	-2.65709600
H	4.45844700	0.17311700	-4.57065000
H	5.17441500	2.01475600	-3.08471900
C	5.27272200	-0.16856200	1.53206900
C	5.09149900	-1.16260300	2.67788000
C	3.87287100	-0.10471700	0.84650300
C	4.12446700	-2.19064800	2.08181200
C	4.19533500	-0.46600100	3.72939100
H	6.02340800	-1.53809000	3.09809800
C	3.07000900	-1.13970900	1.67894000
H	3.43971100	0.88270100	1.04985900
H	3.74121900	-2.91056900	2.81370800

H	4.57117400	-2.73918800	1.25020500
H	4.18835800	-1.03276800	4.66763200
H	4.55246500	0.54363900	3.95850000
C	2.79724400	-0.47892300	3.04942100
H	2.14893700	-1.50145600	1.22676400
H	2.08718400	-1.08755400	3.61852000
H	2.36020800	0.51978600	2.94546200
H	1.31388700	-0.49282500	-1.57808300
Pd	6.74926900	-0.32334300	0.15526100
Pd	5.83919100	2.24706100	-0.29746800
I	8.88932500	-0.12577700	-1.62778800
C	3.77616300	2.76750300	-0.60574400
H	2.83893300	2.24786400	-0.40887200
H	3.93499700	3.48109800	0.21855500
C	8.62569400	3.37155300	0.03636200
C	7.68701800	3.02072800	2.11806700
C	9.95298400	3.40528400	0.56933100
C	8.95032800	3.01831600	2.74278100
C	6.52836900	2.91534900	2.92077600
C	9.42554300	3.60487300	-2.22139700
C	11.10268300	3.65429500	-0.38166300
C	10.11202300	3.17765400	1.91644900
C	9.01680900	2.85478600	4.15019300
C	6.63165100	2.76120300	4.27775500
C	10.62518700	4.34363000	-1.65856200
H	11.86942000	4.26887300	0.09932300
C	7.89061200	2.70489000	4.92928000
H	11.42678900	4.35585700	-2.40384100
C	6.67125800	-3.40970000	-0.07325100
C	7.83200100	-2.64093300	1.76849100
C	6.16747300	-3.16789000	-1.36613000
C	6.61530400	-4.71869000	0.45581300
C	7.86436800	-3.93266100	2.37966600
C	5.55874400	-4.17727700	-2.06977600
C	5.93046200	-5.71451500	-0.27896700
C	7.23469000	-4.96658400	1.72438100
C	8.53429400	-4.09220500	3.73122600
C	9.36878400	-1.77556600	3.36466900
C	5.37405300	-5.46715300	-1.51778700
C	8.81440800	-2.74369300	4.39519300
H	7.90635000	-4.69884900	4.39091500
H	7.89344100	-2.31541400	4.81114900
N	7.55088000	3.13986700	0.76167800
N	7.21218600	-2.37785300	0.64608000
C	11.47560300	3.09609000	2.55112100
H	12.27914000	3.12338100	1.81560700
H	11.63176100	3.91774900	3.25992800
H	11.57762200	2.15965000	3.11016200
H	10.34752800	5.38574700	-1.45279500
H	11.56796700	2.69358600	-0.63870800
O	8.36135400	3.60176400	-1.24936600
O	8.38112600	-1.56519900	2.34964800
H	9.52461900	-2.86571200	5.21941400
H	9.47938200	-4.63794500	3.60754600
C	7.19052500	-6.35909000	2.29622400
H	7.57745900	-7.08253800	1.57101400
H	7.78074000	-6.45862500	3.20724400
H	6.15890900	-6.64889900	2.52749600
H	9.99425900	2.83312700	4.61613600
H	5.71891600	2.68602300	4.86207500
H	5.55946000	2.97005700	2.43325500
H	5.82629900	-6.70043100	0.16111900
H	5.19478700	-3.95578700	-3.06622600
H	6.29273900	-2.17997700	-1.79828400
C	4.54681600	-6.54757600	-2.22562900
C	3.25914900	-6.78098300	-1.40899800
H	2.63002500	-7.53445400	-1.89759500
H	3.48782700	-7.13683800	-0.39831600
H	2.67367000	-5.85922900	-1.31297600
C	4.14754600	-6.13198900	-3.64909500
H	5.02405100	-5.92578400	-4.27376100
H	3.58435500	-6.94404100	-4.12134100
H	3.50536000	-5.24455800	-3.65163400

C	5.34698300	-7.85987700	-2.31776300
H	4.76303100	-8.61968900	-2.84978800
H	6.28659700	-7.70782000	-2.85985100
H	5.58817400	-8.26681700	-1.33030600
C	7.93865600	2.48499100	6.44448500
C	7.24298900	3.66345500	7.15256400
H	7.26412500	3.52007300	8.23929300
H	7.74707300	4.60806800	6.92131900
H	6.19513700	3.75902800	6.84946000
C	7.20464100	1.17482700	6.79441600
H	7.69050500	0.31423500	6.32097800
H	7.21343700	1.01467700	7.87887300
H	6.15950400	1.18918500	6.46879400
C	9.37601900	2.38266200	6.97189800
H	9.36026000	2.20607000	8.05279300
H	9.91822400	1.55130800	6.50665100
H	9.93925600	3.30616400	6.79723600
H	5.59075900	0.80701300	1.91846500
H	3.69759700	3.30915500	-1.54898300
Cl	3.07495800	-2.19278300	-4.07043700
H	9.68097800	2.55573700	-2.40470200
C	8.83800000	4.22212500	-3.47283300
H	9.57535100	4.19370800	-4.28095900
H	7.95599500	3.65786100	-3.78798100
H	8.54814400	5.26334700	-3.29540300
H	10.25440700	-2.21390600	2.88274400
C	9.69529300	-0.39890100	3.89845100
H	10.47726800	-0.45865400	4.66269100
H	10.03574800	0.24495200	3.08302500
H	8.80324300	0.05988000	4.33351600

Table 2
N1-L2-Et
CH₃CH₂I

I	4.01388300	4.78110500	-1.72504300
C	2.02484500	5.12387100	-2.56878000
H	1.33794600	4.94531200	-1.74171300
H	2.01317700	6.18251800	-2.82720000
C	1.74429300	4.23085700	-3.76088600
H	2.45968800	4.40425500	-4.56922000
H	1.78169300	3.17271700	-3.48823000
H	0.73885000	4.45154700	-4.14005700

CH ₃ CH ₂ Pd(I)(L2) ₂	-0.84339300	1.05061100	-0.58457400
Pd	-0.84339300	1.05061100	-0.58457400
I	-2.89612700	2.60048800	-1.29486700
C	-1.94497100	-0.58689400	-1.03967600
H	-2.71864800	-0.64926300	-0.26501800
H	-2.44053800	-0.36983400	-1.98902600
C	1.09255500	2.93005800	1.13427500
C	1.53188800	3.22900200	-1.09936400
C	2.43090200	3.27261300	1.51288000
C	2.88502200	3.54670400	-0.84762700
C	1.04111400	3.30893500	-2.42564300
C	0.47621600	2.54084700	3.43064200
C	2.77161000	3.35651300	2.98443200
C	3.34104300	3.50992500	0.50885900
C	3.71957000	3.91633600	-1.93666100
H	-0.00595900	3.07907400	-2.59811000
C	1.87050600	3.69548100	-3.44426900
C	1.50756300	3.58750800	3.80788200
H	3.24988200	2.42250800	3.31450600
C	3.24252800	4.00121000	-3.22567600
H	4.75546400	4.15738200	-1.73044200
H	1.45898800	3.76340000	-4.44708900
H	1.10112300	4.58897300	3.61940300
C	1.99282700	-0.03812000	-0.61190700
C	1.04125800	-0.37294000	1.46130300
C	3.32091000	-0.14308400	-0.09302600
C	2.30550400	-0.47416900	2.07907200

C	-0.12350200	-0.58258400	2.23659700
C	2.81120900	0.38944900	-2.83662800
C	4.48234600	-0.07197700	-1.05997200
C	3.47050300	-0.29150800	1.26653300
C	2.36846900	-0.76444700	3.46798400
H	-1.08853300	-0.48445100	1.74906000
C	-0.02060500	-0.88960000	3.56673800
C	4.03144200	-0.43497700	-2.47289500
H	4.89991800	0.94504400	-1.06497600
C	1.23715000	-0.97748400	4.22340000
H	3.34437800	-0.83444100	3.93261200
H	-0.93394800	-1.05004200	4.13186000
H	3.78543700	-1.50247400	-2.53653000
C	4.79739500	3.75539900	0.80680100
H	5.42961300	3.13083600	0.16640900
H	5.07166500	4.79943100	0.61399400
H	5.05216200	3.52467000	1.84207600
C	4.12297300	4.38382300	-4.41866900
C	5.56292000	4.71233400	-4.00194400
H	6.14931100	4.98212900	-4.88693800
H	5.60069500	5.55915700	-3.30756200
H	6.05455600	3.85386300	-3.52950800
C	3.53079000	5.62063300	-5.12065800
H	4.15658600	5.90888700	-5.97350100
H	2.52078700	5.43444100	-5.49864400
H	3.47964600	6.46937900	-4.43024800
C	4.16813200	3.20016900	-5.40460900
H	4.60553600	2.31588500	-4.92531500
H	3.16961200	2.93008900	-5.76325600
H	4.78110100	3.45233700	-6.27799600
C	4.82877300	-0.27678900	1.91718800
H	5.61580300	0.02565500	1.22561600
H	4.83977200	0.42992100	2.75407000
H	5.08926200	-1.26254500	2.32003800
C	1.27653200	-1.25840700	5.72777900
C	0.56043000	-2.58928600	6.02571500
H	0.57958800	-2.79551100	7.10203500
H	-0.48776600	-2.57051000	5.71101800
H	1.05224400	-3.42047500	5.50885900
C	0.55869900	-0.10917400	6.46290100
H	1.06143100	0.84636400	6.27097400
H	-0.48400600	-0.00912200	6.14424700
H	0.56338900	-0.28569800	7.54476000
C	2.71006700	-1.35165400	6.26740100
H	3.27230200	-2.16019100	5.78669500
H	3.25868400	-0.41338700	6.12566100
H	2.68527100	-1.55830400	7.34262300
N	0.67912700	2.84450300	-0.10669000
N	0.91138500	-0.07326200	0.13471600
O	0.14858100	2.63680600	2.03791200
O	1.74185400	0.12500500	-1.91316000
H	3.48711100	4.16426500	3.16502100
H	1.72602700	3.51212700	4.87835800
H	0.91062700	1.54988300	3.59885200
H	4.83158300	-0.23557700	-3.19329800
H	5.28249900	-0.74685400	-0.74219200
C	-0.83948700	2.65377600	4.17183300
H	-1.53660500	1.89232100	3.81176900
H	-0.67961200	2.50718400	5.24482800
H	-1.29071100	3.63731600	4.00850700
H	3.05900300	1.45131400	-2.74839700
C	2.24194600	0.10992400	-4.21119100
H	2.97407400	0.37501900	-4.98002400
H	1.98528800	-0.94922100	-4.31565600
H	1.33841900	0.70539600	-4.36656600
C	-1.13389600	-1.87193300	-1.13558200
H	-1.78557200	-2.69551200	-1.46329800
H	-0.32152700	-1.78078800	-1.86401100
H	-0.69198500	-2.16113800	-0.17654700

1
Pd

-0.02244500 1.22638300 0.07145600

O	-1.97182500	0.95451300	0.55230600
O	1.93881800	1.46481600	-0.40851200
C	-2.30957900	0.93888000	1.80067700
C	2.25517200	1.94294300	-1.56520900
O	-1.55812400	1.06200900	2.76749900
O	1.47634700	2.20793900	-2.48461300
C	-3.80987900	0.75539800	1.99610400
H	-4.33405500	1.64172100	1.62427000
H	-4.16718700	-0.10102300	1.41680400
H	-4.03800600	0.61659900	3.05440400
C	3.75275700	2.16929400	-1.71962200
H	4.09991100	2.87143300	-0.95523500
H	4.28680700	1.22714200	-1.56357200
H	3.97622200	2.56187300	-2.71310300
C	0.43719200	3.97892100	1.21765800
C	-0.52816400	3.93263600	-0.89720100
C	0.77905800	3.29292600	2.40379100
C	0.69539300	5.36074100	1.11348400
C	-0.23911500	5.31363700	-1.12352600
C	1.37472000	3.96908100	3.43432100
H	0.51535100	2.24343800	2.49021000
C	1.31794400	6.02017500	2.20470200
C	0.35204700	6.02809900	-0.10804000
C	-0.53002200	5.86220400	-2.50236200
C	-1.50797300	3.64699500	-3.08578700
C	1.67031400	5.35583300	3.35771100
H	1.61666200	3.41755700	4.33839600
H	1.52228900	7.07936800	2.11107500
C	-0.52560400	4.72011100	-3.51627800
H	-1.50013100	6.37836000	-2.52124700
H	0.47194700	4.26937400	-3.57637600
C	0.30386200	-1.54096700	0.97709000
C	-0.11652000	-1.46231000	-1.30457700
C	0.16235900	-2.96047000	1.02305300
C	-0.29182700	-2.86097000	-1.35847900
C	-0.20943800	-0.70024300	-2.49083400
C	0.35758700	-1.37548800	3.34472500
C	0.35972100	-3.67021200	2.34880300
C	-0.16662900	-3.61201700	-0.14480400
C	-0.57697600	-3.46147500	-2.61223400
H	-0.02661400	0.37044600	-2.44506500
C	-0.48109800	-1.32188100	-3.67974100
C	0.98315300	-2.75890200	3.40867600
H	-0.61257900	-4.03227400	2.70964500
C	-0.67770700	-2.72574100	-3.77139000
H	-0.71115300	-4.53544400	-2.64564700
H	-0.53690700	-0.71080700	-4.57641400
H	2.06180200	-2.65413600	3.23944700
N	-0.15037000	3.29135300	0.18967100
N	0.13707100	-0.83216500	-0.11782200
O	-1.20278400	3.18299500	-1.75969900
O	0.62908900	-0.82118400	2.04853400
H	-2.52096600	4.07095500	-3.03792800
H	-0.80332700	5.08411400	-4.51081500
H	0.22852900	6.59846100	-2.78164400
H	-0.73338300	-1.43310600	3.45017000
H	0.84519000	-3.19130300	4.40497800
H	0.98974700	-4.55510700	2.21114600
C	-1.49474100	2.41845600	-3.97603100
H	-0.47485800	2.02893600	-4.03690800
H	-2.14738100	1.64361500	-3.56316800
H	-1.84838700	2.68041800	-4.97912100
C	0.90651000	-0.38294500	4.34701400
H	1.98088100	-0.23795000	4.19217200
H	0.38557400	0.56894900	4.22449000
H	0.74159300	-0.75163500	5.36463600
C	0.64632800	7.49930000	-0.24375300
H	0.19515300	8.05424300	0.58562200
H	1.72583000	7.68638500	-0.21242300
H	0.25389500	7.92118700	-1.16924100
C	-0.39005600	-5.10126500	-0.17912600
H	-1.37614100	-5.32875700	-0.59788100
H	0.35510400	-5.59269700	-0.81525100

H	-0.33858900	-5.55491000	0.81082700
C	2.35363900	6.04406000	4.54345900
C	2.60719000	7.53568600	4.28662400
H	3.26318900	7.69276700	3.42289200
H	1.67230400	8.08183200	4.11725100
H	3.09650500	7.98113800	5.15965700
C	3.71061500	5.36421300	4.81021500
H	3.59345900	4.30080800	5.04197200
H	4.36539700	5.44608100	3.93576400
H	4.21219200	5.83898500	5.66192700
C	1.45937700	5.91589200	5.79185700
H	1.93877900	6.39532100	6.65367800
H	0.48939100	6.39723600	5.62614600
H	1.27313600	4.86925100	6.05279000
C	-0.97506600	-3.35327400	-5.13658300
C	0.19458100	-3.06000400	-6.09603200
H	0.00084100	-3.50705500	-7.07826000
H	0.34366900	-1.98552000	-6.24196200
H	1.12912300	-3.47881100	-5.70696000
C	-1.15549300	-4.87480400	-5.05209000
H	-0.25124600	-5.36959400	-4.67991200
H	-1.99402300	-5.14882800	-4.40179300
H	-1.36466300	-5.27697900	-6.04925400
C	-2.27227500	-2.74426900	-5.70327000
H	-3.11742200	-2.93838100	-5.03388100
H	-2.18888800	-1.66059200	-5.83420600
H	-2.50013900	-3.18286800	-6.68188200

1a'			
C	1.49372500	-0.12281600	-0.39841800
C	1.28010600	0.48523500	0.83326100
C	0.68986000	1.74472100	0.89890900
C	0.29559200	2.41770800	-0.26011500
C	0.51669100	1.80401600	-1.50869900
C	1.11278900	0.54299800	-1.55973000
H	1.95563800	-1.10521300	-0.45945400
H	1.57325300	-0.01756200	1.75138200
H	0.53770900	2.22885500	1.85726000
H	1.27867500	0.07527400	-2.52883900
C	-0.35432900	3.78826300	-0.20557000
H	-1.23164000	3.80707300	-0.86002100
H	0.36182300	4.52719800	-0.59415400
C	-0.77543400	4.24447600	1.19682800
O	0.10632700	4.53559900	2.01873200
N	-2.10837900	4.32093800	1.34318600
C	-2.62043700	4.50999400	2.58003200
C	-3.69977900	5.40784900	2.76624300
C	-2.25806900	3.79250900	3.74546900
C	-4.31817900	5.58709000	3.98298400
C	-2.87769600	3.97997500	4.96788800
C	-3.93202100	4.88425000	5.13061600
C	-4.64328000	5.14934300	6.41522900
F	-4.12940300	6.13610000	1.72513000
F	-5.31899900	6.48072300	4.07215400
F	-2.44372500	3.23856300	5.99827400
F	-1.31487700	2.84294500	3.68063900
F	-4.50918400	6.43347900	6.81548600
F	-5.97366500	4.93233600	6.31242000
F	-4.21028500	4.38634100	7.43043100
C	0.11905800	2.49795100	-2.78825200
H	-0.96665700	2.64320500	-2.84773800
H	0.57330400	3.49347400	-2.86247000
H	0.42937700	1.91778300	-3.66395800

31			
Pd	2.60895600	3.94087700	0.27579800
N	-0.09987900	0.43909500	-1.78934500
C	-1.30904300	0.93152800	-2.25306600
C	-1.34011800	2.20521000	-2.82556100
C	-2.53441600	0.27748500	-2.09328900
C	-2.51420100	2.79108200	-3.26728900

C	-3.70389300	0.85697100	-2.56379900
C	-3.73020800	2.12064200	-3.15332600
C	-5.05449800	2.66956300	-3.62220900
F	-4.84176500	0.18653400	-2.40014700
F	-2.61919900	-0.87645500	-1.44658100
F	-0.19488600	2.89110000	-2.92913200
F	-2.42630000	4.01531100	-3.78917700
F	-5.91873100	2.77181600	-2.59931700
F	-5.61081100	1.86219500	-4.53523700
F	-4.94244700	3.88282800	-4.17242100
C	0.34346700	-0.87695700	-1.89255000
O	-0.29724200	-1.74659900	-2.43926800
C	1.69424700	-1.11908200	-1.21110000
H	1.47745600	-1.32531000	-0.15657500
H	2.08626900	-2.04352600	-1.63824000
C	2.64914700	0.04781600	-1.35460100
C	3.48289800	0.13080100	-2.48347100
C	2.57238200	1.12910800	-0.46028300
C	4.21755300	1.29944400	-2.68451500
C	3.23319200	2.34562500	-0.72849000
C	4.07830400	2.39809300	-1.83939500
H	4.87836400	1.36474200	-3.54667400
H	4.61946200	3.31369700	-2.07371500
C	1.63719000	2.55607100	1.37716100
C	2.22392000	2.44096600	2.79185800
C	1.76024400	1.11039700	0.80789400
C	3.35895100	1.42423000	2.58786100
C	1.22446400	1.62067800	3.64486000
H	2.50121800	3.39703000	3.24216300
C	2.44279600	0.34946500	1.98004000
H	0.76177900	0.68661200	0.64171600
H	3.82281500	1.09862700	3.52644200
H	4.13063200	1.77889300	1.89946600
H	1.48778200	1.67695400	4.70731600
H	0.19930500	1.99262100	3.54178300
C	1.39675000	0.17247300	3.09686600
H	2.93148200	-0.57869900	1.67048400
H	1.77318200	-0.50089900	3.87445400
H	0.45945500	-0.25255500	2.72135600
H	0.62085300	1.13242900	-1.61391200
C	1.96887700	6.17848800	2.32355500
C	0.19794000	5.84828300	0.88096100
C	1.21291300	7.04573400	3.17133600
C	-0.65669600	6.64229600	1.67916300
C	-0.31416400	5.26394100	-0.29696000
C	3.75730600	6.10587800	3.90121000
C	1.89037100	7.68943000	4.36580200
C	-0.11219800	7.25114200	2.85731600
C	-2.00632300	6.79563600	1.28206700
H	0.34951300	4.65963300	-0.90847100
C	-1.62868000	5.44052000	-0.65023400
C	3.40933700	7.52450300	4.31741200
H	1.64045300	8.75441500	4.41013800
C	-2.51772300	6.20285800	0.14471700
H	-2.65960500	7.40315900	1.89969500
H	-1.97650800	4.98582400	-1.56947000
H	3.84914200	7.74886500	5.29428300
N	1.50112800	5.61388400	1.23716400
O	3.25178600	5.87269400	2.57933100
C	-3.99545700	6.38617500	-0.22757900
C	-4.39314900	5.54069400	-1.44519800
H	-4.22764800	4.47279600	-1.26388600
H	-5.45958400	5.67193600	-1.65451900
H	-3.84574700	5.82688400	-2.34831700
C	-4.25339200	7.86902700	-0.55442000
H	-5.30610000	8.02368300	-0.81820600
H	-4.02206200	8.51554700	0.29924800
H	-3.63707200	8.19432100	-1.39965100
C	-4.88319700	5.95686300	0.95623000
H	-5.94117500	6.08014700	0.69821200
H	-4.71340700	4.90418100	1.20700500
H	-4.69065400	6.55300500	1.85424700
C	-1.00485200	8.10253200	3.72105300

H	-0.50157600	8.46297200	4.61826300
H	-1.36915700	8.97360100	3.16464300
H	-1.88250800	7.53118700	4.04206800
H	3.85037800	8.21538500	3.58841700
H	1.50502400	7.23899200	5.29038400
H	3.26261600	5.39072300	4.57555700
C	5.24130600	5.80933100	3.83826800
H	5.68605200	5.89709800	4.83420100
H	5.40648200	4.79483100	3.46521200
H	5.74244000	6.51267200	3.16573000
C	3.56979900	-0.99806200	-3.48372900
H	2.59173100	-1.23558500	-3.91918300
H	4.24176300	-0.73397400	-4.30547300
H	3.95241100	-1.91997500	-3.02865900
H	0.60294500	2.92164600	1.38245600

TS32

Pd	2.47964800	3.74791300	0.19317100
N	-0.43655200	0.68697900	-1.98931700
C	-1.42207300	1.35994000	-2.69831100
C	-1.03757700	2.33492800	-3.62245200
C	-2.78672100	1.18455400	-2.47841700
C	-1.97034000	3.07431800	-4.32346800
C	-3.72587100	1.91723700	-3.19942900
C	-3.33932100	2.87340400	-4.13585600
C	-4.30113900	3.70483100	-4.95240500
F	-5.00413300	1.70342700	-2.90979300
F	-3.22214900	0.37400500	-1.52235900
F	0.26708900	2.56840200	-3.80058400
F	-1.54160800	3.98172300	-5.19527800
F	-4.16241500	3.44204000	-6.25861500
F	-4.05804500	5.01371200	-4.77861000
F	-5.57616300	3.48782500	-4.62589700
C	-0.40075400	-0.68501300	-1.77088700
O	-1.27495100	-1.43373000	-2.14405600
C	0.82656300	-1.15348600	-0.97659200
H	0.49009700	-1.25826000	0.06030900
H	1.04770200	-2.16249000	-1.32916300
C	2.00819400	-0.21572700	-1.08709200
C	2.93491700	-0.36732800	-2.13392200
C	2.06140700	0.92566600	-0.26898800
C	3.88384400	0.63424700	-2.34191800
C	2.95485900	1.97212800	-0.56045300
C	3.88169600	1.80482700	-1.58723300
H	4.61008200	0.51708500	-3.14261800
H	4.58857700	2.59268200	-1.83538400
C	1.36642500	2.58978100	1.45744700
C	1.93583200	2.38291000	2.86457400
C	1.15565000	1.15025800	0.91051400
C	2.71356600	1.06363500	2.73289300
C	0.73604100	1.93084500	3.73561200
H	2.47571500	3.23217600	3.28690500
C	1.52910900	0.28233800	2.14615500
H	0.10294600	1.00193900	0.63893600
H	3.05420100	0.67607900	3.69762800
H	3.56669100	1.10964100	2.05154600
H	1.02894900	1.92520700	4.79038900
H	-0.12424500	2.60122000	3.63680300
C	0.44569800	0.48980800	3.22148600
H	1.72568700	-0.76464000	1.90093800
H	0.55480500	-0.24607500	4.02412600
H	-0.56488200	0.38156700	2.81268500
H	0.44446500	1.17628600	-1.88407000
I	5.92630500	4.34889700	3.81110000
C	4.36830000	3.92577400	1.40859200
H	3.82990400	4.64375500	2.00894400
C	1.74458400	6.60953300	1.47146500
C	-0.04767200	5.53252300	0.48352900
C	0.88906100	7.43918100	2.26410000
C	-0.97511700	6.25797600	1.25840700
C	-0.53823900	4.62005500	-0.48137000
C	3.73087000	7.56447200	2.47923600

C	1.51296000	8.49890400	3.14546300
C	-0.46775000	7.21959400	2.19282700
C	-2.36193200	6.01658100	1.08011900
H	0.16992500	4.08375800	-1.10950000
C	-1.88485300	4.41669200	-0.62693700
C	2.92583600	8.83351000	2.68065900
H	0.90213700	9.40633800	3.13387000
C	-2.83904300	5.10602600	0.16488100
H	-3.05998400	6.57859400	1.68760600
H	-2.22753800	3.70767700	-1.37350600
H	3.43037400	9.46525100	3.41772300
N	1.30771400	5.66908200	0.65779200
O	3.07536800	6.72423100	1.49437200
C	-4.32833000	4.81724200	-0.04231900
C	-4.70317100	5.14393800	-1.49918900
H	-4.09293300	4.58020100	-2.20768300
H	-5.75246600	4.89490900	-1.69173100
H	-4.55577500	6.20815500	-1.71193000
C	-5.21870300	5.65474900	0.88458600
H	-6.27065200	5.41670300	0.69558700
H	-5.01768000	5.44620500	1.94168500
H	-5.08819900	6.72885300	0.71031300
C	-4.59824100	3.32692800	0.24372000
H	-5.65547500	3.09571700	0.07304700
H	-4.01099300	2.66504400	-0.39917700
H	-4.35681800	3.08166100	1.28387500
C	-1.43660900	7.97733500	3.06166400
H	-0.93612400	8.59657400	3.80557700
H	-2.07987000	8.62569400	2.45555600
H	-2.08830600	7.28177100	3.60028700
H	2.89507000	9.38908800	1.73460600
H	1.54211100	8.14750600	4.18564000
H	3.78080700	6.98268900	3.40879000
C	5.13062500	7.81324100	1.96062300
H	5.66531100	8.46577400	2.65713400
H	5.68780100	6.87657000	1.90077200
H	5.09571300	8.29412700	0.97745400
H	0.44519000	3.17877500	1.46474400
H	4.45823400	2.91880700	1.78008000
C	2.89212200	-1.56545100	-3.05157800
H	1.92953400	-1.64473300	-3.57096800
H	3.67322200	-1.49832100	-3.81359100
H	3.04267700	-2.50359800	-2.50477600
C	5.27198900	4.40996800	0.31198000
H	6.03620700	5.08132700	0.70973400
H	5.77135800	3.57566400	-0.18261900
H	4.71383700	4.99651200	-0.43618700

TS35

Pd	2.93104900	3.71980000	0.15958500
N	-0.39768500	0.43258700	-1.67165400
C	-1.51365900	1.03421900	-2.23639700
C	-1.35816900	2.27080500	-2.86508700
C	-2.80975600	0.52223900	-2.14210800
C	-2.42443500	2.95924800	-3.41757400
C	-3.87210500	1.20513300	-2.71773400
C	-3.71392800	2.43481500	-3.35663400
C	-4.93605400	3.11574800	-3.92077900
F	-5.08745400	0.67407000	-2.60939400
F	-3.06277800	-0.58817000	-1.46395500
F	-0.13718700	2.81667200	-2.91610200
F	-2.16114300	4.13431500	-3.98825100
F	-5.84383200	3.33991500	-2.95670100
F	-5.52342900	2.35380700	-4.85315400
F	-4.65247300	4.29481400	-4.48240800
C	-0.06971800	-0.91618900	-1.78205500
O	-0.78395200	-1.72671400	-2.32849500
C	1.26973700	-1.26313300	-1.12478800
H	1.08322300	-1.38261300	-0.05235700
H	1.55048400	-2.24439200	-1.51106600
C	2.32018500	-0.20396800	-1.39122500
C	3.03133800	-0.23358400	-2.60176200

C	2.44373100	0.89950100	-0.52688800
C	3.84980300	0.84997600	-2.91663500
C	3.20341100	2.02905500	-0.89655200
C	3.91756700	1.97184900	-2.09555000
H	4.40931700	0.83660600	-3.84966800
H	4.51553400	2.81970300	-2.41766600
C	1.89417000	2.43076300	1.36835100
C	2.60882900	2.22980100	2.71638000
C	1.76128200	0.98448800	0.80971900
C	3.56273900	1.06364900	2.40268700
C	1.61948200	1.55702200	3.69530100
H	3.06524500	3.13818800	3.11936700
C	2.44241600	0.13003700	1.91446100
H	0.70337300	0.70004700	0.73682500
H	4.08147600	0.67523100	3.28694100
H	4.29594600	1.29391300	1.62305600
H	2.02073600	1.55925500	4.71567900
H	0.65537100	2.07565700	3.71939800
C	1.50887200	0.10540300	3.13980800
H	2.76078600	-0.85903200	1.57266800
H	1.85758200	-0.62628400	3.87644900
H	0.48233500	-0.16546100	2.87006000
H	0.38721900	1.05412300	-1.50437200
I	4.40249000	5.60312700	-1.24232400
C	5.37186900	4.05802600	0.72044600
H	4.77755400	3.58754400	1.49944800
H	5.74992500	5.01671400	1.05195600
C	2.33765800	5.95334600	2.37693700
C	0.61873900	5.73968900	0.85790700
C	1.61327100	6.89121500	3.17675900
C	-0.21329000	6.59769100	1.61337300
C	0.11698300	5.19097100	-0.34234700
C	4.03316900	5.78756400	4.05030200
C	2.28212000	7.51908700	4.38388600
C	0.32075400	7.18439100	2.80542800
C	-1.53081600	6.84131800	1.16012700
H	0.76365700	4.55506400	-0.93941700
C	-1.16662400	5.45630600	-0.75164900
C	3.78325000	7.24112300	4.41013200
H	2.11031500	8.60020900	4.38567400
C	-2.03541100	6.27869200	0.00548300
H	-2.16517100	7.49606500	1.74816300
H	-1.50348200	5.02569200	-1.68674300
H	4.19683400	7.46182300	5.39927000
N	1.88169600	5.41106500	1.27743400
O	3.58221900	5.55548400	2.70965700
C	-3.48207300	6.56385500	-0.42143800
C	-3.90032400	5.73209900	-1.64073600
H	-3.80896700	4.65832600	-1.44137800
H	-4.94983000	5.92852600	-1.88160600
H	-3.31090200	5.97066400	-2.53089600
C	-3.61873600	8.05665400	-0.77517800
H	-4.64580300	8.28135000	-1.08571300
H	-3.37737100	8.69653700	0.08069900
H	-2.94547700	8.32548000	-1.59628600
C	-4.43936200	6.21682900	0.73498500
H	-5.47677500	6.40249200	0.43437900
H	-4.34782400	5.16054900	1.01050300
H	-4.24227400	6.81683800	1.62939600
C	-0.54535000	8.10864100	3.62027500
H	-0.05594000	8.44750300	4.53340500
H	-0.82484000	8.99427100	3.03824000
H	-1.47294500	7.60394200	3.91090400
H	4.30828400	7.87084300	3.68161600
H	1.82511300	7.12710600	5.30243900
H	3.44696200	5.13535500	4.71533000
C	5.49135400	5.37735700	4.08637300
H	5.88554800	5.48311400	5.10156700
H	5.60584400	4.33380000	3.77828500
H	6.08307600	6.00956900	3.41622900
C	6.34576600	3.15525900	0.03632400
H	5.86416000	2.26097600	-0.36116500
H	6.89740300	3.65389800	-0.76255600

H	7.06643000	2.83749200	0.80718500
C	2.89692300	-1.38847500	-3.56600700
H	1.85444400	-1.55779600	-3.86006600
H	3.47187400	-1.20053800	-4.47715300
H	3.26359400	-2.32615500	-3.13009600
H	0.91709000	2.91087000	1.49776200

TS65

Pd	4.72308600	3.59537900	-3.63065500
N	0.67040100	-1.06180000	-2.54057900
C	0.01164800	-1.22672200	-3.75921600
C	0.40599300	-0.51443400	-4.88955300
C	-1.04603900	-2.12379400	-3.89220200
C	-0.27631200	-0.64509400	-6.09269400
C	-1.69973800	-2.28252600	-5.10198500
C	-1.34203500	-1.53321100	-6.22358700
C	-2.11008500	-1.75379800	-7.50655000
F	-2.69981100	-3.15679500	-5.17524900
F	-1.42639700	-2.84265900	-2.83443500
F	1.46376200	0.28421200	-4.83434500
F	0.15265400	0.08834300	-7.11963500
F	-1.93644800	-3.00667700	-7.95175200
F	-1.73287300	-0.92275600	-8.48079900
F	-3.42307400	-1.57434400	-7.30934200
C	0.82347400	0.19330900	-1.95817400
O	0.33766700	1.18551500	-2.45615000
C	1.71510800	0.21341800	-0.72937700
H	1.33287500	0.99539100	-0.06931400
H	1.67974500	-0.73904500	-0.19111500
C	3.11753700	0.55234100	-1.20150600
C	4.11298700	-0.41881600	-1.41313800
C	3.41408200	1.87432800	-1.50995200
C	5.37202500	-0.00280000	-1.86100400
C	4.62608500	2.26863400	-2.09485300
C	5.65713600	1.32307100	-2.19228600
H	6.15323800	-0.75146300	-1.97694100
H	6.65012400	1.59046700	-2.53920300
H	0.83851200	-1.88372200	-1.98010300
C	4.02867100	4.02262500	-1.62768300
C	4.72174200	4.51471100	-0.34562700
C	2.81257200	3.18715600	-1.11224300
H	3.73177400	4.89678200	-2.24324900
C	3.84906100	5.67835400	0.17617000
C	4.38589300	3.43412200	0.69744100
H	5.77692600	4.76243900	-0.47450800
C	2.87225200	3.45876700	0.41100300
H	1.84225600	3.43377900	-1.55298300
C	2.54421800	4.95288300	0.63074400
H	3.66660900	6.43765700	-0.59136000
H	4.33763300	6.17462300	1.02249700
H	4.86046200	2.46796600	0.51325900
H	4.62050100	3.75531700	1.71854600
H	2.26087400	2.78097000	1.01391600
H	1.66820700	5.26443300	0.05168500
H	2.32798000	5.15102000	1.68575000
C	3.97197700	3.62083300	-6.56569000
C	6.25265000	3.92673400	-6.41283300
C	4.00866700	3.53119800	-7.99450100
C	6.40838200	3.81940200	-7.81345100
C	7.39217600	4.15262300	-5.61347100
C	1.66752900	2.98640200	-6.52639500
C	2.70840000	3.36509300	-8.75702300
C	5.23676700	3.60234900	-8.61072100
C	7.70580900	3.94088100	-8.36323000
H	7.24737000	4.23017700	-4.53816600
C	8.63541200	4.26919300	-6.18495300
C	1.49081600	3.65174400	-7.87927200
H	1.84814500	1.91421800	-6.66473200
H	2.69692500	4.03022700	-9.62670600
C	8.82384300	4.16466500	-7.58455500
H	7.81941500	3.85913300	-9.43946500
H	9.48469800	4.44623400	-5.53471200

H	0.58041600	3.28044100	-8.36046200
N	5.03037200	3.80365400	-5.80991400
C	5.38326000	3.46245500	-10.10354300
H	5.76964200	4.38769100	-10.54673200
H	6.09462000	2.66514400	-10.34436500
H	4.44095500	3.22120800	-10.59574400
C	10.20411000	4.29856900	-8.24417800
C	10.52876400	3.00952400	-9.02320800
H	9.79160500	2.81361700	-9.80879400
H	11.51230500	3.09144900	-9.50077000
H	10.54329000	2.14334600	-8.35268400
C	10.19089600	5.49569600	-9.21411700
H	9.95695400	6.42474500	-8.68296900
H	11.17133600	5.61105000	-9.69139100
H	9.44637900	5.36626900	-10.00666300
C	11.32054600	4.52915200	-7.21555700
H	11.16960300	5.45775700	-6.65398900
H	11.39540000	3.70079700	-6.50234800
H	12.28345500	4.60956200	-7.73160500
O	2.82464900	3.53824400	-5.88063600
H	1.36989600	4.73100000	-7.72446400
H	2.64060400	2.33986100	-9.14572600
C	0.51071200	3.19032400	-5.57024000
H	-0.39170800	2.72872100	-5.98399300
H	0.72394400	2.73180000	-4.60188700
H	0.32202800	4.25845000	-5.42192600
C	3.86773700	-1.88424600	-1.14360200
H	3.47898200	-2.06435200	-0.13364800
H	3.14980700	-2.31014000	-1.85666200
H	4.79462800	-2.45648600	-1.24154800

TS36

Pd	1.32851400	4.00744700	-0.09595900
N	-0.22994900	-0.34320400	-2.25780300
C	-1.60433200	-0.38878200	-2.48304400
C	-2.11491100	-0.23668700	-3.77163600
C	-2.51053700	-0.57253600	-1.44159200
C	-3.47492000	-0.31863600	-4.01479800
C	-3.87252900	-0.69416600	-1.69297700
C	-4.38276300	-0.56560100	-2.98369600
C	-5.83988900	-0.75578700	-3.33892900
F	-4.66701600	-0.89186100	-0.64682400
F	-2.08766600	-0.61764300	-0.18407700
F	-1.27201500	-0.02966400	-4.78316300
F	-3.90600700	-0.18574400	-5.26611100
F	-6.00055900	-1.86892000	-4.06835000
F	-6.29507200	0.27114900	-4.07282000
F	-6.62442600	-0.85845700	-2.26497400
C	0.43743800	-1.34261700	-1.56678100
O	-0.13088300	-2.31747900	-1.12582800
C	1.94067400	-1.11924100	-1.40204600
H	2.16111900	-1.40321300	-0.37041500
H	2.43571200	-1.86630200	-2.02905300
C	2.40343400	0.28208000	-1.72275500
C	2.93167200	0.57911700	-2.99294800
C	2.15238600	1.30723100	-0.79418000
C	3.17647200	1.91284500	-3.31990300
C	2.42916200	2.64016000	-1.15185500
C	2.92669900	2.93833100	-2.41687400
H	3.55621300	2.15916200	-4.30797500
H	3.09231300	3.97030200	-2.70492700
C	0.79740600	2.37327200	1.03711900
C	1.15712500	2.32852100	2.52679200
C	1.36511800	1.05514300	0.46847500
H	-0.28549900	2.42095200	0.91192200
C	2.50765100	1.59528900	2.55482200
C	0.24564100	1.23699600	3.15016100
H	1.10402800	3.29429300	3.03410000
C	2.02145300	0.40034700	1.71780500
H	0.51087200	0.43212900	0.17750100
H	2.79346300	1.29102900	3.56839600
H	3.33800600	2.14713400	2.12375500

H	0.30316000	1.27563300	4.24346400
H	-0.80478300	1.36756000	2.87184000
C	0.85374900	-0.09331900	2.60157100
H	2.77185000	-0.36222700	1.49424200
H	1.23045300	-0.71813400	3.41763500
H	0.13106200	-0.69052500	2.03658000
H	0.31478700	0.36347700	-2.73466100
I	1.42798900	6.38421200	-1.72677900
C	3.46780100	3.79360400	0.27355500
H	3.16201200	4.30438900	1.19799000
H	3.88006700	2.82964400	0.54561100
C	-0.55879900	5.84963400	1.28625600
C	-1.82040900	4.55866300	-0.15651900
C	-1.61430800	6.78142500	1.49890600
C	-2.95398500	5.37337400	0.05109200
C	-1.91892600	3.44967600	-1.02799700
C	1.03369600	7.13949900	2.59148500
C	-1.28121400	8.02293700	2.29340200
C	-2.82454900	6.52434600	0.89727600
C	-4.15708800	5.04911000	-0.62408000
H	-1.03527000	2.84375400	-1.20608700
C	-3.10760000	3.15827200	-1.64404300
C	0.20834900	8.32959300	2.13860500
H	-1.86587300	8.87231400	1.93164400
C	-4.26303500	3.96299500	-1.46325700
H	-5.01503300	5.69241500	-0.47617300
H	-3.15520800	2.29250400	-2.29867400
H	0.48969200	9.20355500	2.73469600
N	-0.63731800	4.82539200	0.47198600
O	0.62672600	5.94111200	1.90003800
C	-5.56865600	3.58677900	-2.16972000
C	-5.30152500	3.30418000	-3.66032600
H	-4.64225000	2.44470500	-3.81237000
H	-6.24230600	3.07811500	-4.17274200
H	-4.84335300	4.17316100	-4.14467100
C	-6.61922800	4.70301700	-2.08248300
H	-7.51701000	4.40387300	-2.63379800
H	-6.92498100	4.89866100	-1.04868900
H	-6.25123300	5.63788000	-2.52028500
C	-6.13999300	2.32985600	-1.48918400
H	-7.03950300	1.98142700	-2.00704400
H	-5.41413100	1.51330100	-1.48622100
H	-6.39872600	2.53962900	-0.44549700
C	-4.01402300	7.42573700	1.09752700
H	-4.28756600	7.92129900	0.15910200
H	-4.88271800	6.84691300	1.42807800
H	-3.83159000	8.19518700	1.84809100
H	0.43786800	8.54584400	1.08765500
H	-1.52887200	7.88952100	3.35567600
H	0.85085100	6.95451000	3.65869000
C	2.52082000	7.28652100	2.32934400
H	2.91410900	8.15604000	2.86582100
H	3.05805900	6.39672500	2.67193300
H	2.69656700	7.41216300	1.25625700
C	3.17638900	-0.49957100	-4.02209400
H	2.25335300	-1.03396200	-4.27907000
H	3.57214400	-0.06763000	-4.94500600
H	3.89871400	-1.24527600	-3.67018200
C	4.48867700	4.61243300	-0.48788600
H	4.96293800	4.03514400	-1.28485300
H	4.06467200	5.52281900	-0.91367000
H	5.26991600	4.90158100	0.22809500

TS40

Pd	1.29480100	3.88200000	0.06781000
N	-0.21743400	-0.28826200	-2.28299900
C	-1.58649200	-0.32633700	-2.54419400
C	-2.07624600	-0.05224900	-3.82021200
C	-2.50652300	-0.63803200	-1.54610400
C	-3.43030800	-0.13766900	-4.09636500
C	-3.86123200	-0.75750500	-1.83317400
C	-4.35068400	-0.50714100	-3.11420700

C	-5.79626300	-0.69425100	-3.51429300
F	-4.66992900	-1.07793700	-0.82870800
F	-2.10185400	-0.81285800	-0.29399000
F	-1.22276300	0.27220300	-4.78918300
F	-3.84335700	0.11249300	-5.33626500
F	-5.91897200	-1.74207100	-4.34196100
F	-6.26357000	0.38227200	-4.16430100
F	-6.59780000	-0.90710900	-2.46911600
C	0.44144700	-1.36172000	-1.70627600
O	-0.12606400	-2.39501600	-1.42445000
C	1.93160300	-1.14746800	-1.44271200
H	2.08983900	-1.47667300	-0.41279700
H	2.46177100	-1.86992000	-2.06944200
C	2.41843200	0.26280500	-1.67118000
C	2.97081300	0.62244400	-2.91504400
C	2.16512600	1.23718900	-0.69042800
C	3.22806700	1.96907700	-3.16967800
C	2.47114800	2.58216100	-0.97069700
C	2.97276900	2.94485000	-2.21607800
H	3.61238100	2.26447700	-4.14242400
H	3.13058800	3.99096100	-2.44813500
C	0.77082800	2.23518200	1.15262100
C	1.15490200	2.13938600	2.63803600
C	1.33688100	0.93142100	0.53718100
H	-0.31723400	2.27240100	1.05321200
C	2.49502400	1.38380600	2.62201400
C	0.24034600	1.04927200	3.25323500
H	1.13087400	3.09191400	3.17335100
C	1.97486500	0.22204900	1.76216800
H	0.49069400	0.32326400	0.19682400
H	2.79752300	1.05078100	3.62182100
H	3.32589400	1.92882400	2.18209800
H	0.33247600	1.04547600	4.34513400
H	-0.81496600	1.21155900	3.01261500
C	0.80258400	-0.27238300	2.63939000
H	2.70689500	-0.55081600	1.51261700
H	1.16776300	-0.94544400	3.42184000
H	0.05485600	-0.82102200	2.05755900
H	0.32481100	0.49410300	-2.62794100
C	3.43395400	3.70480900	0.47038500
H	3.09537700	4.09351400	1.44085600
H	3.95419500	2.77234200	0.65895100
C	-0.53887500	5.88493500	1.26964800
C	-1.84974200	4.52418000	-0.05738900
C	-1.56577700	6.86021000	1.41796500
C	-2.95361300	5.39282000	0.08561000
C	-1.98670400	3.36148500	-0.85072600
C	1.18458400	7.27909000	2.27435200
C	-1.17195300	8.12136800	2.14662600
C	-2.78699500	6.60047100	0.84077900
C	-4.17137700	5.06193100	-0.56237500
H	-1.12063000	2.72734300	-1.00318000
C	-3.18256900	3.07389300	-1.44991800
C	0.29157000	8.42262600	1.82090100
H	-1.79770900	8.96274300	1.84092400
C	-4.31244800	3.92513200	-1.32291300
H	-5.00735500	5.74166400	-0.45759800
H	-3.25769000	2.17640400	-2.05727000
H	0.62570200	9.34067600	2.31451400
N	-0.65397200	4.79655600	0.54948300
O	0.63454300	5.99416600	1.90785600
C	-5.61650200	3.55302100	-2.03211800
C	-5.34256500	3.36086300	-3.53612500
H	-4.64237100	2.54344800	-3.73037200
H	-6.27315100	3.12314700	-4.06193100
H	-4.92123600	4.27356700	-3.97094700
C	-6.69311600	4.63626900	-1.88101400
H	-7.60176000	4.32427600	-2.40681600
H	-6.96150600	4.80045400	-0.83123900
H	-6.36994800	5.59088400	-2.31175100
C	-6.15978200	2.24889000	-1.42028900
H	-7.05342900	1.91299100	-1.95644500
	-5.42226800	1.44383800	-1.46209100

H	-6.42188000	2.39750600	-0.36697700
C	-3.95292900	7.54363200	0.97985500
H	-4.25341100	7.93903200	0.00308400
H	-4.81853600	7.02129600	1.40067100
H	-3.73338000	8.38750300	1.63423500
H	0.40445700	8.56699400	0.73898900
H	-1.29751200	8.00296500	3.23181700
H	1.22734000	7.26929300	3.37035200
C	2.58053500	7.33695300	1.68040000
H	3.05309700	8.29837500	1.90879800
H	3.20516300	6.53766000	2.09089500
H	2.51068100	7.19998800	0.59663500
C	3.21767600	-0.40379700	-3.99549000
H	2.29265700	-0.91543600	-4.28867300
H	3.62695200	0.07068800	-4.89133300
H	3.92949200	-1.17331700	-3.67451900
C	4.32697200	4.70268500	-0.23915300
H	4.93402800	4.22185900	-1.01059000
H	3.74901900	5.51115400	-0.69142700
H	5.00932400	5.13622900	0.50340400
O	1.62135000	5.72961900	-1.05563500
C	0.84792200	5.77189800	-2.08894900
O	0.17957300	4.82665700	-2.51219100
C	0.77144600	7.13663000	-2.76491100
H	1.76467300	7.58715700	-2.84884800
H	0.30964800	7.05141200	-3.75033700
H	0.15830300	7.80271900	-2.14582000

TS67

Pd	0.72707400	4.08104800	-0.14391200
N	-0.24522800	5.92300100	-0.70805000
C	-1.11337700	6.41119200	0.14358800
C	-0.12898900	6.48651700	-1.94881000
C	-1.94775700	7.53639900	-0.12465800
C	-0.92043200	7.59502200	-2.32172300
C	-1.85583000	8.11742100	-1.36956000
N	-0.18392400	-0.36467600	-2.75467600
C	-1.06992400	-0.33841400	-3.83523500
C	-0.95143500	0.66006700	-4.80171200
C	-2.10002900	-1.26262300	-3.97134700
C	-1.84208500	0.73425000	-5.85737100
C	-2.97657700	-1.20449300	-5.05006200
C	-2.86739800	-0.20031100	-6.00929500
C	-3.78447300	-0.06438400	-7.20077600
F	-3.93134600	-2.12897200	-5.10834300
F	-2.28073000	-2.20482200	-3.05494300
F	0.03618400	1.54730900	-4.71254600
F	-1.69088600	1.70733900	-6.75517900
F	-3.09016500	-0.14761800	-8.34688500
F	-4.40052300	1.12740900	-7.19418700
F	-4.73112600	-1.00472300	-7.23774700
C	0.61874400	-1.44292300	-2.47238000
O	0.58985900	-2.47883900	-3.10553600
C	1.54914100	-1.23051400	-1.27391500
H	0.96192900	-1.43286900	-0.37103500
H	2.31578000	-2.00571400	-1.34581000
C	2.12780000	0.16115200	-1.22063700
C	3.12432500	0.57530500	-2.12658300
C	1.61556800	1.10356300	-0.33840900
C	3.60709600	1.88252700	-2.05336700
C	2.00798900	2.44432800	-0.36854600
C	3.07643200	2.83138000	-1.17576300
H	4.40574700	2.18371700	-2.72690600
H	3.47515200	3.83976400	-1.17499800
C	0.98499300	2.45507800	1.36190900
C	1.94176800	2.38781900	2.55400600
C	0.80714000	0.98061600	0.90979600
H	0.04945800	2.95782900	1.63650800
C	2.77483800	1.12138700	2.29740600
C	1.04879200	1.90203600	3.72375900
H	2.48261900	3.30916700	2.76879800
C	1.55015400	0.22370400	2.04128600

H	-0.23234500	0.66498300	0.78539400
H	3.33926000	0.81344200	3.18389400
H	3.46210500	1.19775700	1.45238900
H	1.60534400	1.96314600	4.66475300
H	0.14416600	2.50798500	3.83928300
C	0.74339100	0.42188400	3.34210400
H	1.76213000	-0.82094900	1.80104900
H	1.08740100	-0.26728800	4.11933500
H	-0.32529000	0.23997600	3.18993200
H	-0.05408700	0.51662600	-2.26397200
C	2.19979100	5.16659600	0.79467900
H	1.72079500	5.48012600	1.72932000
H	3.00921000	4.46906900	1.02656500
I	-1.54570400	2.81610300	-1.34014700
C	-0.76081900	8.13137600	-3.62048200
C	0.13208200	7.60905200	-4.53430500
C	0.89889300	6.48889600	-4.13264400
C	0.77499400	5.94053500	-2.88062000
C	0.24924600	8.22839300	-5.93404200
H	-1.37159100	8.98167900	-3.90529900
C	-2.72374700	9.28335600	-1.76225900
H	-3.30475900	9.03811500	-2.65788700
H	-3.42892900	9.56407000	-0.97997300
H	-2.11325600	10.16218400	-1.99910600
C	-2.89346500	8.02655700	0.95487000
C	-2.60791700	7.38108900	2.31255200
H	-1.73453300	7.84672100	2.78575200
C	-2.31616100	5.90152000	2.13074100
H	-2.82396800	9.11503000	1.04954400
O	-1.13978800	5.76655000	1.31910600
H	-3.92614200	7.80243600	0.65693600
H	-3.46058600	7.51892400	2.98492700
H	-3.14233400	5.41426200	1.59527600
C	-2.01940700	5.15457500	3.41469200
H	-2.88681200	5.18793000	4.08080500
H	-1.79026400	4.10757800	3.19611100
H	-1.16260800	5.60312000	3.92804000
C	-1.10168900	8.08848400	-6.66171700
H	-1.03866300	8.52572300	-7.66513900
H	-1.38222900	7.03478100	-6.76300200
H	-1.90644800	8.60042900	-6.12347700
C	0.61594100	9.71946400	-5.80856900
H	0.70764500	10.17187200	-6.80285700
H	-0.14453800	10.28226200	-5.25728200
H	1.57135100	9.84409900	-5.28716600
C	1.32768300	7.54225500	-6.78498000
H	2.31835600	7.61793900	-6.32248100
H	1.10290900	6.48369100	-6.95482800
H	1.38294000	8.02762400	-7.76520800
C	2.72586000	6.35788200	0.01222800
H	1.96333500	7.12791300	-0.12973900
H	3.56776400	6.81636700	0.54987900
H	3.09426900	6.07505800	-0.98077800
H	1.35006300	5.06352300	-2.59769800
H	1.59827500	6.03354200	-4.82396400
C	3.67793800	-0.38322800	-3.14969300
H	4.11195900	-1.27286000	-2.67838100
H	2.89569100	-0.73498100	-3.83210100
H	4.45779100	0.09208400	-3.75082900

TS69

Pd	0.75716100	4.12487200	0.43961600
N	-0.14685300	5.91442400	-0.39741100
C	-1.00302200	6.54455100	0.36622500
C	-0.11074300	6.18897000	-1.73921400
C	-1.90520600	7.54464500	-0.09917700
C	-1.00945600	7.11680900	-2.31434300
C	-1.92038500	7.80837300	-1.45183200
N	-0.00699600	0.34107100	-3.23184300
C	-0.76700700	0.58159200	-4.37425900
C	-0.38461900	1.60955300	-5.23827300
C	-1.95692100	-0.08570800	-4.64457000

C	-1.16849000	1.95008600	-6.32323300
C	-2.73486600	0.24601400	-5.74985900
C	-2.36116500	1.28197100	-6.60285200
C	-3.15730000	1.72358500	-7.80594300
F	-3.86131300	-0.43823600	-5.93112000
F	-2.40246700	-1.01708300	-3.80892300
F	0.75487400	2.26426400	-5.02541800
F	-0.76095600	2.93909800	-7.12459500
F	-2.46139000	1.53495200	-8.93754200
F	-3.44172400	3.03472100	-7.72810800
F	-4.31475600	1.07149500	-7.93198800
C	0.49892800	-0.88279900	-2.87886300
O	0.32509000	-1.89614100	-3.52629500
C	1.30320800	-0.86826200	-1.57181600
H	0.60195800	-1.11974900	-0.76746400
H	2.01235400	-1.69800800	-1.64546200
C	1.97712000	0.45005400	-1.28236200
C	3.00224500	0.94247100	-2.11447800
C	1.54199600	1.25889800	-0.23932200
C	3.58291900	2.17740100	-1.82188500
C	2.03144400	2.55268800	-0.05165500
C	3.12249300	2.99898000	-0.79170300
H	4.40038000	2.53170200	-2.44524800
H	3.58542300	3.96557100	-0.63190000
C	1.06630900	2.34847200	1.68513500
C	2.08128800	2.01206100	2.78340400
C	0.75425400	0.98738400	1.00144900
H	0.18425800	2.83695600	2.12496400
C	2.78191400	0.73863400	2.27765500
C	1.22156000	1.41253300	3.92270000
H	2.71673600	2.84286100	3.09336500
C	1.46831700	-0.00097400	1.95847400
H	-0.31076900	0.77801600	0.87211300
H	3.35577900	0.24471600	3.06883600
H	3.43231600	0.89157900	1.41460900
H	1.83914100	1.25282200	4.81280600
H	0.39250400	2.06705900	4.21215500
C	0.74179500	0.05602500	3.32007700
H	1.57282200	-1.00719500	1.54467100
H	1.03783500	-0.78542200	3.95405600
H	-0.34586500	0.01159600	3.20158100
H	0.19319500	1.19669000	-2.69898600
C	2.27228600	5.15107900	1.33807400
H	1.83058900	5.42197100	2.30564000
H	3.10007700	4.45811900	1.51917100
C	-0.98195400	7.30284700	-3.71700700
C	-0.11399100	6.61015000	-4.53700700
C	0.78753400	5.70760100	-3.92421100
C	0.79742100	5.50290300	-2.56828400
C	-0.16502700	6.80985400	-6.05822000
H	-1.68238000	8.00362200	-4.15896400
C	-2.88603900	8.79799400	-2.04815200
H	-3.50947500	8.30996400	-2.80514800
H	-3.55298300	9.23370300	-1.30385900
H	-2.35078800	9.61522200	-2.54447400
C	-2.80769400	8.24492700	0.89767700
C	-2.39137600	7.96188600	2.34142000
H	-1.50167600	8.54591100	2.60832100
C	-2.05892900	6.48830600	2.50423000
H	-2.79622700	9.32536800	0.72148800
O	-0.94790800	6.16760600	1.65631800
H	-3.84388700	7.91407400	0.74685800
H	-3.19198200	8.24594600	3.03177700
H	-2.91099000	5.87477800	2.17856200
C	-1.64032900	6.09128400	3.90531600
H	-2.46446900	6.25363700	4.60655500
H	-1.36182200	5.03388200	3.93143400
H	-0.78018800	6.68630500	4.22901100
C	-1.54158100	6.35598800	-6.58225100
H	-1.60785500	6.51958100	-7.66431100
H	-1.70092300	5.29022700	-6.39408100
H	-2.35814700	6.91155500	-6.10860800
C	0.04941000	8.29863100	-6.39030600

H	0.03619400	8.44904200	-7.47605900
H	-0.73380500	8.93155300	-5.95965800
H	1.01421700	8.64968800	-6.00756000
C	0.91492900	5.99520700	-6.78555200
H	1.92395300	6.28440400	-6.46985000
H	0.79074700	4.92060000	-6.62216200
H	0.84007300	6.17385400	-7.86363400
C	2.74701600	6.38558000	0.58714900
H	1.96715400	7.14980100	0.53327300
H	3.61830500	6.82843800	1.08953400
H	3.04588600	6.15521400	-0.44233900
H	1.45532900	4.76237100	-2.12994100
H	1.47184800	5.12761900	-4.53072600
C	3.46018600	0.16625400	-3.32228300
H	3.62674800	-0.89309500	-3.09951600
H	2.70443600	0.21532100	-4.11515400
H	4.39010100	0.57773900	-3.72476200
O	-1.12262700	3.16205400	-0.15454800
C	-1.24351100	2.75585300	-1.35504100
O	-0.36498300	2.84144100	-2.23550600
C	-2.56267700	2.07966600	-1.70987100
H	-2.93444800	2.47700600	-2.65929400
H	-2.38571900	1.00733100	-1.85524900
H	-3.31272500	2.21280600	-0.92806600

TS44

N	0.73060000	-1.19805300	-1.22810200
C	-0.64751100	-0.99498500	-1.25275200
C	-1.23527500	-0.32195400	-2.32330100
C	-1.47437100	-1.42025000	-0.21687800
C	-2.59815900	-0.09385500	-2.36289400
C	-2.85014500	-1.21655100	-0.27198700
C	-3.43694000	-0.54340800	-1.34141500
C	-4.91779400	-0.27131500	-1.46603400
F	-3.56948400	-1.66278200	0.75218100
F	-0.95863700	-1.99864300	0.86015800
F	-0.45910500	0.10799500	-3.32124600
F	-3.10800200	0.55161400	-3.40919500
F	-5.41537200	-0.85679600	-2.56509100
F	-5.14807000	1.04598200	-1.57426100
F	-5.61582400	-0.71680200	-0.42022500
C	1.30238400	-2.44921400	-1.07015000
O	0.64398000	-3.45101600	-0.88192400
C	2.82026800	-2.46757600	-1.13500600
H	3.16095600	-2.84749600	-0.17626100
H	3.06769900	-3.26295200	-1.84042400
C	3.50766900	-1.17783400	-1.52833500
C	3.67487500	-0.97293600	-2.91814300
C	3.93055900	-0.19638700	-0.60155600
C	4.33033100	0.16524100	-3.37317400
C	4.53248800	0.99721400	-1.10636600
C	4.74819500	1.13713800	-2.48136400
H	4.49247200	0.30402000	-4.43869300
H	5.23284300	2.03222000	-2.85924000
C	5.13476500	-0.32662300	1.66245000
C	4.90063200	-1.37322600	2.75335400
C	3.76027100	-0.22069800	0.92826000
C	3.94423400	-2.36053300	2.07540700
C	3.97397200	-0.72064000	3.80591900
H	5.81117100	-1.78287900	3.18868900
C	2.91637500	-1.27906400	1.68617200
H	3.32644900	0.75838100	1.16177700
H	3.52945300	-3.10974300	2.75946200
H	4.41234700	-2.87379100	1.23332100
H	3.92314200	-1.33685600	4.71116700
H	4.33286800	0.27067700	4.10413200
C	2.60262500	-0.67716500	3.07478100
H	2.00654400	-1.60619500	1.18470000
H	1.86153900	-1.29727000	3.58969000
H	2.18681900	0.33322500	3.00093000
H	1.32711500	-0.46364500	-1.58765600
Pd	6.66006900	-0.45317000	0.33102300

Pd	5.85111100	2.12621800	-0.07312300
I	8.88647400	-0.32397000	-1.37832700
C	3.78002200	2.71663000	-0.28967400
H	2.84463400	2.16134200	-0.22334800
H	3.93819100	3.15856800	0.70698500
C	8.64487300	3.19279600	0.05642300
C	7.93469800	2.83851900	2.22476100
C	10.01620500	3.28616500	0.44767900
C	9.25072700	2.93855400	2.72127800
C	6.87177600	2.67840200	3.14223600
C	9.19850200	3.38890900	-2.27587500
C	11.05650100	3.53831700	-0.62073200
C	10.31709700	3.11154100	1.77780700
C	9.46107400	2.87921700	4.12269800
C	7.11299900	2.62620400	4.49008300
C	10.43420300	4.16885900	-1.86576200
H	11.84590100	4.19180700	-0.23737700
C	8.42615400	2.72758500	5.01937700
H	11.15589500	4.16923300	-2.68890200
C	6.57706500	-3.54168000	0.06355000
C	7.70543900	-2.78161300	1.92719100
C	6.09327400	-3.28863500	-1.23494000
C	6.51932600	-4.85491000	0.58106700
C	7.74038200	-4.07844100	2.52738300
C	5.50254100	-4.29628700	-1.95477000
C	5.84400200	-5.84577700	-0.16973900
C	7.12545500	-5.11040700	1.85529200
C	8.39479600	-4.23966900	3.88633400
C	9.19461200	-1.90150100	3.56313400
C	5.30636900	-5.58936000	-1.41509000
C	8.63607400	-2.89240700	4.56982100
H	7.77106100	-4.86694500	4.53058600
H	7.69857900	-2.48641500	4.97075200
N	7.66003600	2.92557900	0.88750600
N	7.10115200	-2.51421000	0.79802700
C	3.67872900	3.80188900	-1.35240900
H	4.61460700	4.35748700	-1.46911600
H	3.40958000	3.38411300	-2.32671400
H	2.89846500	4.51969700	-1.06714200
C	11.73991500	3.10563200	2.27259900
H	12.46239000	3.05958600	1.45764500
H	11.95548200	4.00059100	2.86882000
H	11.91514700	2.23500600	2.91288600
H	10.15466600	5.21225000	-1.66928600
H	11.52575500	2.58337000	-0.89166500
O	8.24218300	3.40380000	-1.19866000
O	8.22988100	-1.70477500	2.52454600
H	9.33077400	-3.01081000	5.40771000
H	9.35307200	-4.76367300	3.76965700
C	7.08293800	-6.50815900	2.41443900
H	7.47646700	-7.22430500	1.68552700
H	7.66884300	-6.61269900	3.32777700
H	6.05124100	-6.80375800	2.63830700
H	10.47651200	2.96793800	4.48861700
H	6.26829300	2.51868900	5.16473600
H	5.86132300	2.62374600	2.74863200
H	5.73195300	-6.83393100	0.26350200
H	5.17325000	-4.07545800	-2.96282700
H	6.22110100	-2.29598600	-1.65529300
C	4.48123900	-6.65858300	-2.14210200
C	3.16964100	-6.86855800	-1.35792900
H	2.54194900	-7.61583100	-1.85793900
H	3.36829400	-7.22106600	-0.33992200
H	2.59640200	-5.93705400	-1.28311100
C	4.12173100	-6.23987700	-3.57568000
H	5.01463400	-6.03467900	-4.17713300
H	3.56814600	-7.04873100	-4.06431000
H	3.47801900	-5.35282800	-3.59277800
C	5.26170400	-7.98369400	-2.21546100
H	4.67779500	-8.73465900	-2.75993500
H	6.21594400	-7.84740900	-2.73577700
H	5.47329100	-8.39348900	-1.22261100
C	8.63142300	2.69784000	6.53787000

C	7.93643900	3.92570500	7.15828300
H	8.07931000	3.93626200	8.24532600
H	8.35005700	4.85339300	6.74814800
H	6.85903900	3.92256100	6.96205700
C	8.01975400	1.41376500	7.13089700
H	8.52085300	0.52321000	6.73743500
H	8.13371700	1.41270300	8.22121100
H	6.95125700	1.32419000	6.91029400
C	10.11658800	2.73474700	6.92303400
H	10.21697700	2.68334100	8.01259200
H	10.66322600	1.88487000	6.49806100
H	10.60125700	3.65956900	6.59112300
C	3.11690700	-1.94090500	-3.93659800
H	3.26328400	-1.55278600	-4.94798400
H	3.59783200	-2.92454600	-3.89291700
H	2.04083000	-2.10263200	-3.79965300
H	5.43480700	0.62789900	2.10972600
H	9.45342800	2.33788000	-2.45082700
C	8.47142400	3.95607500	-3.47706400
H	9.11804300	3.91146600	-4.35899500
H	7.56991500	3.37082300	-3.67881700
H	8.18454300	4.99870700	-3.30229700
C	9.47032400	-0.51914200	4.11142800
H	10.21589800	-0.56136300	4.91240300
H	9.83776500	0.13305300	3.31514100
H	8.54869600	-0.07856600	4.50225100
H	10.10275500	-2.31466500	3.10133400

N2-L2-Et

N2			
C	-0.42069600	1.83372200	0.07902200
C	1.01794000	1.44572800	-0.21794800
C	0.98075600	3.65166900	0.23288000
C	-0.43960500	3.14808600	0.34460000
H	-1.32578300	3.75487400	0.49262600
C	1.75319900	2.41216100	0.73042300
H	2.83113700	2.47145300	0.54171800
H	1.57421800	2.19404900	1.78715100
C	1.35716600	2.08397100	-1.59903100
H	2.35033200	1.76501000	-1.93110300
H	0.63740900	1.78803900	-2.36641300
C	1.32806600	3.60774000	-1.29146400
H	2.30614300	4.06872200	-1.46247600
H	0.59445600	4.15096200	-1.89285300
H	1.24917700	0.38401500	-0.13713500
H	1.19271400	4.60701900	0.71525700
C	-1.62362600	0.99736400	-0.06240200
O	-2.75206500	1.34268200	0.21172300
O	-1.32117600	-0.22495600	-0.54324300
C	-2.43197500	-1.10119700	-0.71175200
H	-3.15439200	-0.67912500	-1.41531300
H	-2.01736200	-2.03026200	-1.10265700
H	-2.93220400	-1.27657700	0.24408600

31

Pd	2.46013200	3.85294900	0.31704400
N	-0.35672700	0.11828000	-1.46094200
C	-1.49752000	0.62031900	-2.08206900
C	-1.52234000	1.95793900	-2.48692900
C	-2.65165800	-0.13337700	-2.27403800
C	-2.65378600	2.50891900	-3.05323500
C	-3.78363700	0.42179600	-2.86512200
C	-3.81020200	1.75665300	-3.26171000
C	-5.01028300	2.43886500	-3.86843700
F	-4.84683400	-0.36604000	-2.99907600
F	-2.71339400	-1.38944500	-1.85320500
F	-0.43505600	2.71376200	-2.33795000
F	-2.62300600	3.79589100	-3.42081400
F	-5.47825600	3.39562200	-3.04405200
F	-6.01649000	1.59890300	-4.11448500
F	-4.69134900	3.03671800	-5.02534900

C	0.33409100	-0.99105700	-1.91225700
O	-0.08547900	-1.70373100	-2.80186000
C	1.68240800	-1.21443900	-1.21760000
H	1.51104200	-1.43056900	-0.15874800
H	2.11400500	-2.10839600	-1.67041100
C	2.55495700	0.01346600	-1.40027200
C	3.22819100	0.20882000	-2.62033700
C	2.52919800	1.04127800	-0.44894800
C	3.83983600	1.43932000	-2.85952400
C	3.04605800	2.31010500	-0.75336600
C	3.72548600	2.49373400	-1.95506900
H	4.37238000	1.59053400	-3.79602700
H	4.14925600	3.46382800	-2.21321200
C	1.61376000	2.35535700	1.47845100
C	2.27155400	2.34901700	2.86863900
C	1.92722800	0.93374900	0.92062400
C	3.58170900	1.59990300	2.56868100
C	1.54123600	1.32342300	3.77529600
H	2.36466200	3.33731900	3.31924400
C	2.87712200	0.35181800	2.00814900
H	1.00746800	0.33778800	0.92118000
H	4.16413500	1.37801500	3.47114900
H	4.21400800	2.11525000	1.84122500
H	1.85928000	1.45259500	4.81560900
H	0.45542200	1.45137900	3.75483200
C	2.00391300	-0.05222400	3.21059300
H	3.52552800	-0.44302200	1.63105300
H	2.59649800	-0.60338700	3.94867300
H	1.16518200	-0.69327800	2.91795300
H	0.09443600	0.78673600	-0.84254500
C	1.98213000	6.16665000	2.31937000
C	0.29017300	6.07886600	0.75275000
C	1.28903200	7.12170100	3.12525300
C	-0.50428500	6.97901800	1.49732900
C	-0.22499200	5.53835800	-0.44323900
C	3.62423200	5.84130500	4.01855600
C	1.95606100	7.65526000	4.37873700
C	0.02973300	7.50380100	2.72022000
C	-1.79495800	7.30041600	1.01611700
H	0.37540600	4.82159200	-0.99575600
C	-1.48535900	5.87021900	-0.87651000
C	3.43974100	7.28964200	4.43621900
H	1.84516900	8.74319300	4.42967200
C	-2.30761200	6.76470400	-0.14959500
H	-2.40688100	7.98323300	1.59631400
H	-1.85028300	5.40642100	-1.78455400
H	3.83140000	7.44357800	5.44673000
N	1.52196100	5.67406200	1.19680300
O	3.19185500	5.69260500	2.65932200
C	-3.73604900	7.10867000	-0.59306600
C	-4.08613700	6.48975400	-1.95358300
H	-4.06527000	5.39697900	-1.93097200
H	-5.10030400	6.78803200	-2.24009700
H	-3.40455000	6.82915000	-2.74134700
C	-3.89503800	8.63651600	-0.70641200
H	-4.91135700	8.88516100	-1.03275500
H	-3.72256500	9.14132900	0.24994400
H	-3.19072900	9.04766200	-1.43776500
C	-4.72428600	6.56196300	0.45551200
H	-5.75677800	6.77566100	0.15576200
H	-4.61762400	5.47640500	0.55966400
H	-4.55953300	7.01408600	1.43982900
C	-0.80860800	8.45212300	3.53601000
H	-0.32249500	8.74992000	4.46503300
H	-1.03702100	9.36024400	2.96678300
H	-1.76394600	7.98450500	3.79831800
H	4.02268300	7.92206800	3.75555500
H	1.44903800	7.24721000	5.26333400
H	2.98832800	5.19422200	4.64139600
C	5.05397100	5.34299100	4.05614600
H	5.43264300	5.35913600	5.08266500
H	5.10411200	4.31825900	3.67693900
H	5.69483100	5.97553200	3.43370700

C	3.27430200	-0.87454700	-3.67223000
H	2.27035600	-1.19302700	-3.97365800
H	3.79941200	-0.52392000	-4.56542200
H	3.79879200	-1.76724300	-3.30886200
C	0.15971500	2.67073000	1.39714700
O	-0.61189300	2.20867600	0.57140000
O	-0.25888800	3.52141000	2.35330700
C	-1.64709800	3.84319700	2.32601400
H	-1.78921500	4.58843400	3.10906100
H	-1.93117100	4.25505400	1.35534700
H	-2.24883200	2.95315900	2.53006200

TS32

Pd	1.06869500	3.36986700	-0.58321900
N	0.19367800	-1.50888200	-1.26190300
C	-1.18645000	-1.58825700	-1.43257200
C	-1.73125200	-1.54610300	-2.71242400
C	-2.07054500	-1.62051800	-0.35282000
C	-3.10430400	-1.54737300	-2.92516900
C	-3.43835900	-1.64556200	-0.56635000
C	-3.98673000	-1.61008300	-1.84902900
C	-5.49101200	-1.56602500	-1.98260600
F	-4.23995600	-1.63777200	0.49491700
F	-1.61921700	-1.55413400	0.89436500
F	-0.91260000	-1.47529900	-3.76361500
F	-3.52820200	-1.49253300	-4.18353400
F	-5.89623900	-1.62637200	-3.25243400
F	-5.97027800	-0.42672800	-1.45714600
F	-6.05899900	-2.58406800	-1.32585400
C	0.90038100	-2.28909600	-0.36687500
O	0.41799900	-3.25965000	0.17387800
C	2.33581300	-1.83171100	-0.09194200
H	2.41086400	-1.80735900	0.99932700
H	2.99010100	-2.64539200	-0.41376600
C	2.72804300	-0.50730600	-0.70563200
C	3.60537100	-0.44584500	-1.80364400
C	2.11874600	0.67089400	-0.23696600
C	3.85503200	0.79100600	-2.40343300
C	2.31471400	1.87947500	-0.91286200
C	3.20896400	1.94748400	-1.97629600
H	4.55299000	0.84458200	-3.23513900
H	3.39952000	2.88807800	-2.48947800
C	0.57327500	2.16361100	1.05366900
C	1.02252700	2.67174600	2.42775500
C	1.20684300	0.73658200	0.95075200
C	2.41822700	2.04095800	2.56099600
C	0.25279000	1.87365300	3.51564900
H	0.96406000	3.75029600	2.56971200
C	1.93081500	0.60811900	2.32069700
H	0.41360400	-0.01324600	0.87630200
H	2.84778300	2.19797600	3.55403700
H	3.14119700	2.37220700	1.81465200
H	0.47215700	2.32382600	4.48844800
H	-0.82832200	1.90502900	3.37728600
C	0.85514000	0.44300900	3.40977000
H	2.70519200	-0.16191100	2.33009100
H	1.30868100	0.13107900	4.35528500
H	0.10949200	-0.31161000	3.13807300
H	0.67729200	-0.75766100	-1.73521000
I	3.45602800	6.49074300	2.70477500
C	2.52451100	4.66203000	0.34426600
H	1.82787900	5.06762400	1.06844300
C	-0.05251600	5.53490400	-2.08866600
C	-0.43067500	6.26121500	0.06344500
C	-0.12036400	6.83544200	-2.64588600
C	-0.36907900	7.61167100	-0.35595500
C	-0.61154900	5.96565800	1.42656500
C	0.85555900	4.65260200	-4.13114000
C	0.02232200	7.00978600	-4.14390900
C	-0.24890800	7.88537300	-1.75568300
C	-0.37857800	8.62249600	0.63397200
H	-0.74505000	4.93154600	1.72398900

C	-0.59564200	6.97592400	2.35407700
C	0.00087800	5.66577700	-4.87423400
H	-0.78138300	7.64724800	-4.52736000
C	-0.43272900	8.33258200	1.98157600
H	-0.28780500	9.65658300	0.31918600
H	-0.68084000	6.71106000	3.40045100
H	0.37138600	5.78280200	-5.89735100
N	-0.22700900	5.23837000	-0.82477600
O	0.28903600	4.44238200	-2.82441500
C	-0.28437800	9.45358200	3.01687600
C	-0.27388000	8.91070400	4.45300000
H	0.55115900	8.20602600	4.60487500
H	-0.13661500	9.74116200	5.15369200
H	-1.21778900	8.41674100	4.71239500
C	-1.44937700	10.44978200	2.87059000
H	-1.35044100	11.25463100	3.60806400
H	-1.46896900	10.91011300	1.87638700
H	-2.41389900	9.95514800	3.03259500
C	1.05789300	10.17293600	2.77537200
H	1.20552000	10.95100200	3.53355000
H	1.89049000	9.46342000	2.83272100
H	1.08842000	10.65784300	1.79322200
C	-0.22692200	9.31503300	-2.22424800
H	-0.19466400	9.40190600	-3.31071000
H	-1.11069300	9.85305700	-1.86620300
H	0.65310900	9.82914900	-1.82171500
H	-1.02126200	5.27249900	-4.93617700
H	0.96454900	7.52829000	-4.36404700
H	1.86791800	5.05927100	-3.98594500
C	0.92947700	3.28653500	-4.78149900
H	1.41828600	3.36394700	-5.75725700
H	1.50265900	2.59442200	-4.15712900
H	-0.07528100	2.87614500	-4.92359100
H	3.26878800	3.99722800	0.76237000
C	4.26957500	-1.68508500	-2.35554500
H	3.53347300	-2.41935100	-2.70318600
H	4.91005900	-1.43382100	-3.20524500
H	4.89720900	-2.17946500	-1.60542700
C	2.97358800	5.55008100	-0.78756900
H	2.34049500	6.43571100	-0.87658600
H	3.99992500	5.87856600	-0.60164100
H	2.98036600	5.01793500	-1.75116200
C	-0.89998200	2.24244200	0.75104700
O	-1.71851000	2.89243200	1.36186900
O	-1.22128600	1.53927400	-0.36054700
C	-2.56795800	1.70408700	-0.80882600
H	-2.77809400	2.76176000	-0.98472700
H	-2.63765700	1.13990000	-1.73870200
H	-3.27193400	1.31450300	-0.06964800

TS35

Pd	2.57220500	3.77009400	-0.00430900
N	-0.47959600	0.21885600	-1.52568200
C	-1.66869900	0.73316400	-2.02308100
C	-1.64018800	1.92963200	-2.74096700
C	-2.91551400	0.15338500	-1.78487800
C	-2.79466200	2.51709000	-3.23043900
C	-4.06849100	0.74234900	-2.28477100
C	-4.04164300	1.93865400	-3.00157100
C	-5.34669100	2.52118400	-3.48738400
F	-5.23411800	0.15278700	-2.03196100
F	-3.02653200	-0.93637600	-1.03961800
F	-0.46641000	2.52778000	-2.95896000
F	-2.65845000	3.65111000	-3.92079700
F	-5.19311600	3.72477600	-4.04876700
F	-6.21046200	2.66371100	-2.46987500
F	-5.92304700	1.72052100	-4.39330100
C	-0.05513500	-1.09084000	-1.68888400
O	-0.74322700	-1.94725200	-2.20095900
C	1.35792800	-1.34393600	-1.14928900
H	1.27671700	-1.50023700	-0.06868800
H	1.67985500	-2.29182400	-1.58313700

C	2.29243600	-0.19911400	-1.48295600
C	2.91445300	-0.16267100	-2.74043900
C	2.37881700	0.90991700	-0.62192900
C	3.61741000	0.98639200	-3.09832200
C	2.99381000	2.10455300	-1.04106500
C	3.63899200	2.11157400	-2.27933500
H	4.11709300	1.02330000	-4.06379900
H	4.14002600	3.00469500	-2.63781200
C	1.76898400	2.35428000	1.34863600
C	2.65985000	2.27063300	2.60970600
C	1.83204400	0.90341300	0.77479300
C	3.76425000	1.30211300	2.14777400
C	1.97200900	1.40907300	3.69683000
H	2.97903000	3.24530000	2.97988100
C	2.78053300	0.18266300	1.77270500
H	0.84235600	0.43731500	0.81984800
H	4.44627300	1.01477500	2.95627900
H	4.34710900	1.65332200	1.29187500
H	2.54746400	1.46653600	4.62810300
H	0.96069100	1.75179300	3.91765300
C	2.02704300	-0.02631200	3.09862500
H	3.22436200	-0.72658500	1.35764200
H	2.57761900	-0.71066400	3.75264400
H	1.03157400	-0.45598500	2.94007400
H	0.23221600	0.90964000	-1.31597900
I	3.82151400	5.69954000	-1.53700100
C	4.96312700	4.36464700	0.51767400
H	4.44013100	3.85659800	1.32222000
H	5.20771600	5.38108600	0.79795900
C	1.81763400	6.02374200	2.08961300
C	0.24383600	5.82217000	0.42066400
C	1.02173400	6.94464400	2.83222300
C	-0.65403600	6.66688300	1.10683900
C	-0.15781800	5.26159000	-0.81412300
C	3.35930700	5.82543500	3.90217800
C	1.56568800	7.53468800	4.11714300
C	-0.23331400	7.23772400	2.34903300
C	-1.93976900	6.89811400	0.55244500
H	0.53012700	4.61921300	-1.35323900
C	-1.40960100	5.50159800	-1.31344200
C	3.05939800	7.26454500	4.28224800
H	1.38659100	8.61435200	4.14149600
C	-2.34539500	6.32223200	-0.63015000
H	-2.62082200	7.54042400	1.09635200
H	-1.68582400	5.03256500	-2.25121000
H	3.36941200	7.45439700	5.31482200
N	1.46395500	5.49314300	0.94747500
O	3.03390800	5.63290300	2.51882800
C	-3.76324900	6.47456800	-1.18828000
C	-3.71649000	6.85613700	-2.67968400
H	-3.25424600	6.07659500	-3.29028900
H	-4.73434400	7.00091700	-3.05907800
H	-3.15949700	7.78745100	-2.82893300
C	-4.57031800	7.54759700	-0.44474500
H	-5.56242800	7.64024600	-0.89922300
H	-4.71885400	7.29412700	0.61087200
H	-4.08329300	8.52782900	-0.50169100
C	-4.48217200	5.12145100	-1.02945200
H	-5.48483600	5.15974700	-1.46804200
H	-3.92989000	4.32170600	-1.53132600
H	-4.57591300	4.85142900	0.02855100
C	-1.17842900	8.13666900	3.10148500
H	-0.76046100	8.48968300	4.04423800
H	-1.44623300	9.01366100	2.50145200
H	-2.10657100	7.60235800	3.33174700
H	3.64846400	7.92248900	3.63145500
H	1.02420200	7.10601600	4.97077900
H	2.72504300	5.14501300	4.48881800
C	4.81618300	5.43460700	4.05234900
H	5.12232000	5.52718900	5.09863500
H	4.97442100	4.39853300	3.73745200
H	5.45078000	6.08742400	3.44374400
C	6.03027000	3.56789900	-0.15645900

H	5.64472500	2.63378200	-0.56810300
H	6.54334000	4.12450500	-0.94217500
H	6.76304500	3.31081100	0.62549300
C	0.38814900	2.84519100	1.62250600
O	0.04296100	3.51037900	2.58089500
O	-0.49907800	2.47918600	0.66275000
C	-1.84591800	2.88145400	0.89226300
H	-1.90718800	3.95060400	1.10413900
H	-2.38748000	2.65078200	-0.02593300
H	-2.27108400	2.32367900	1.73174800
C	2.80562200	-1.31820800	-3.70655400
H	1.76089200	-1.55373100	-3.94135100
H	3.31413300	-1.08682000	-4.64665400
H	3.25748200	-2.23166200	-3.30085500

TS65

Pd	4.94766400	2.65336800	-3.68862600
N	0.50574800	-1.09344600	-2.39648600
C	-0.01373100	-1.40154400	-3.65538100
C	0.53622700	-0.85998900	-4.81872800
C	-1.08341700	-2.27960900	-3.78986500
C	-0.02183900	-1.14802900	-6.05244100
C	-1.61860400	-2.59674600	-5.03234900
C	-1.09970800	-2.02365100	-6.19092200
C	-1.63815100	-2.28080200	-7.57944000
F	-2.64358200	-3.44137500	-5.06008900
F	-1.60874000	-2.83224100	-2.69399600
F	1.60803200	-0.08202900	-4.75537000
F	0.51680900	-0.59150200	-7.13849000
F	-0.66985000	-2.73726600	-8.38665900
F	-2.10933600	-1.14665300	-8.11859700
F	-2.62683300	-3.17574300	-7.59021200
C	0.60665600	0.21935100	-1.95093000
O	0.21748500	1.15065300	-2.62174500
C	1.32075000	0.38043900	-0.62090400
H	0.93621400	1.29601600	-0.16658200
H	1.10572000	-0.45432100	0.05339900
C	2.80283000	0.50691500	-0.92075700
C	3.71406000	-0.55238800	-0.74595200
C	3.27743500	1.70022400	-1.45413800
C	5.06423300	-0.34406300	-1.04993100
C	4.59805400	1.84532900	-1.89690200
C	5.53481000	0.84496200	-1.60975100
H	5.76998300	-1.14974700	-0.85947100
H	6.59125300	0.96722600	-1.82710300
H	0.57104800	-1.84054800	-1.72147500
C	4.15539200	3.74564600	-1.84051700
C	4.75624700	4.31330200	-0.52847800
C	2.79179800	3.11892600	-1.39585500
C	4.00761300	5.63971300	-0.24623300
C	4.13441600	3.44468900	0.57798600
H	5.84191300	4.40629000	-0.54629100
C	2.69040600	3.61990700	0.06786900
H	1.92662300	3.37732300	-2.00846800
C	2.55350700	5.15893800	0.03634900
H	4.07891000	6.35703000	-1.06466000
H	4.44255300	6.11478000	0.63976300
H	4.48301800	2.41101600	0.60645100
H	4.28118900	3.88920400	1.56831700
H	1.91329200	3.11862700	0.65129300
H	1.85402100	5.48194200	-0.74176000
H	2.18201800	5.53934900	0.99344100
C	4.13782200	2.97909900	-6.60669800
C	6.43559600	3.14692700	-6.47516400
C	4.13732800	3.17113900	-8.02561600
C	6.55353700	3.29333600	-7.87556800
C	7.60170000	3.17341500	-5.68300100
C	1.75350400	2.63339600	-6.56984900
C	2.80799900	3.24886700	-8.74658000
C	5.35271000	3.29383400	-8.65879500
C	7.84293600	3.45225300	-8.43429900
H	7.48689800	3.07670200	-4.60575500

C	8.83646300	3.32974700	-6.26256600
C	1.67498700	3.55771300	-7.77172900
H	1.70919400	1.58952000	-6.90393700
H	2.84354600	4.02144700	-9.52047400
C	8.98819800	3.47158300	-7.66331000
H	7.92892900	3.57289100	-9.50933800
H	9.70752700	3.34737800	-5.61755200
H	0.70370800	3.44018600	-8.26261100
N	5.22328100	2.97202000	-5.86670100
C	5.45570700	3.43466500	-10.15509400
H	5.85889800	4.41677700	-10.42830800
H	6.13580600	2.67888300	-10.56208400
H	4.49403200	3.31197300	-10.65377700
C	10.35854500	3.65792600	-8.33042600
C	10.58283900	2.54169900	-9.36869000
H	9.82263500	2.55991200	-10.15624200
H	11.56181100	2.66005700	-9.84793600
H	10.55026800	1.55558300	-8.89288200
C	10.39818300	5.02849200	-9.03348900
H	10.23644700	5.83858100	-8.31414000
H	11.37222900	5.18311500	-9.51272800
H	9.62741200	5.10755700	-9.80745800
C	11.51147900	3.60475200	-7.31768000
H	11.43722100	4.40363900	-6.57165900
H	11.54734100	2.64332400	-6.79311900
H	12.46533900	3.73165900	-7.84113100
O	3.01235400	2.81283300	-5.90309900
H	1.74634500	4.59538000	-7.42112100
H	2.60252800	2.29819400	-9.25754400
C	0.68105100	2.88474200	-5.52943800
H	-0.30334100	2.66769500	-5.95788900
H	0.82931200	2.25334200	-4.65210400
H	0.69947100	3.92886800	-5.20348000
C	4.19259900	4.77884400	-2.93602600
O	5.10872400	5.56513300	-3.12533600
O	3.00151100	4.90235500	-3.58798400
C	3.02236200	5.83469600	-4.65565000
H	2.01781900	5.82347500	-5.08182300
H	3.27220400	6.83724200	-4.29833700
H	3.75646800	5.53713100	-5.41121800
C	3.27997700	-1.89182500	-0.19956100
H	2.75191400	-1.80046500	0.75728900
H	2.61615600	-2.41957500	-0.89652300
H	4.14403700	-2.54091200	-0.03246600

TS36

Pd	0.52898100	3.46304100	-0.42104300
N	1.07487700	-2.74323800	-0.13959400
C	-0.23958400	-3.22092500	-0.13126600
C	-1.13908700	-2.73469000	0.81330800
C	-0.70096400	-4.18606700	-1.02623800
C	-2.46168300	-3.14216500	0.84887900
C	-2.03518600	-4.56821000	-1.00924300
C	-2.94487400	-4.05565200	-0.08508500
C	-4.37504400	-4.53822400	-0.13816100
F	-2.43556700	-5.48001800	-1.89100900
F	0.12033900	-4.78172600	-1.87747900
F	-0.70511700	-1.85612000	1.72552300
F	-3.24141900	-2.61472500	1.79277500
F	-4.44602600	-5.85199500	0.12189000
F	-4.89665000	-4.34035300	-1.35620200
F	-5.16078000	-3.91074600	0.74158300
C	1.62715600	-2.17936700	-1.28968300
O	1.12917800	-2.33569700	-2.37992600
C	2.89111700	-1.35206500	-1.05711000
H	3.14738100	-1.30088800	0.00533000
H	3.71278700	-1.87571300	-1.55497200
C	2.69160000	0.02988300	-1.65404600
C	2.96920200	0.24795900	-3.01431300
C	2.10732400	1.04050900	-0.87661900
C	2.60994300	1.46925400	-3.58139100
C	1.77329400	2.26011900	-1.48107300

C	2.00971500	2.47388000	-2.83156300
H	2.79776100	1.64026200	-4.63815900
H	1.74482800	3.41835200	-3.29360100
C	0.49567500	1.78337100	0.91257200
C	0.77893600	2.07252300	2.40255400
C	1.63273600	0.80701600	0.53026600
C	2.29894400	2.25651100	2.41766400
C	0.67192900	0.74992200	3.21638200
H	0.18404300	2.88305200	2.81906300
C	2.59493500	0.89096300	1.75878000
H	1.19566100	-0.19507800	0.53253500
H	2.70311800	2.30107500	3.43612800
H	2.64420900	3.13429600	1.88471000
H	0.65262100	0.98102000	4.28669900
H	-0.23535200	0.18707300	2.99552800
C	1.97250900	-0.02296000	2.83516500
H	3.64239600	0.67827200	1.52780900
H	2.64451900	-0.12352000	3.69385400
H	1.76092700	-1.03404000	2.47020400
H	1.40102100	-2.37577300	0.74284200
I	0.02937300	5.65706200	-2.11971500
C	2.63438400	3.99594100	-0.30818000
H	2.28526700	4.72533800	0.43300800
H	3.20729100	3.21048600	0.16868500
C	-1.44840900	4.80401600	1.43109900
C	-2.62830100	3.70012000	-0.21982000
C	-2.63231500	5.26863500	2.07148800
C	-3.85882700	4.03622500	0.38120500
C	-2.62355900	2.94784400	-1.41513900
C	-0.06574500	5.70460400	3.16982200
C	-2.50449400	6.20882900	3.25229000
C	-3.83999900	4.84116400	1.56480300
C	-5.05826700	3.56753000	-0.21437900
H	-1.67580700	2.71214900	-1.88807100
C	-3.80315400	2.52402000	-1.96459000
C	-1.09940700	6.80379300	3.34012400
H	-3.23651500	7.01763500	3.16616900
C	-5.05830500	2.81134900	-1.36482500
H	-5.99782600	3.82053200	0.26046700
H	-3.76425100	1.94556300	-2.88223800
H	-0.95567800	7.30295600	4.30362300
N	-1.44316100	4.05672100	0.35684500
O	-0.21789300	5.10592200	1.87638100
C	-6.33695400	2.27058100	-2.01035100
C	-6.47277300	2.84743900	-3.43254400
H	-5.62129100	2.57761600	-4.06533500
H	-7.37984000	2.46094200	-3.91153100
H	-6.53761900	3.94049400	-3.40431100
C	-7.59451100	2.64565800	-1.21481300
H	-8.47895900	2.23074100	-1.70968600
H	-7.56569000	2.24027100	-0.19680700
H	-7.72973500	3.73147700	-1.15391600
C	-6.25227900	0.73304500	-2.08089400
H	-7.16200500	0.32365100	-2.53494700
H	-5.40141200	0.39649500	-2.68158700
H	-6.14670300	0.30153600	-1.07903500
C	-5.14294100	5.21206800	2.22250000
H	-5.72834300	4.31278800	2.44187100
H	-4.99897000	5.74559000	3.16241000
H	-5.74884300	5.84263600	1.56195800
H	-0.94782600	7.54982500	2.55049600
H	-2.73376400	5.67379200	4.18401500
H	-0.23817400	4.91885000	3.92101900
C	1.37356600	6.17324400	3.23716100
H	1.58283400	6.61009500	4.21830600
H	2.05368100	5.33093700	3.07783800
H	1.56219000	6.92622400	2.46552300
C	3.60949000	-0.81257900	-3.87642400
H	2.98314900	-1.70853200	-3.91938700
H	3.74971000	-0.44530500	-4.89675000
H	4.59635100	-1.10423100	-3.49496300
C	3.45244000	4.65942100	-1.39310000
H	3.97546900	3.93184400	-2.01589900

H	2.86087900	5.31961300	-2.02714800
H	4.20645800	5.27524000	-0.88171000
C	-0.83710600	1.13379400	0.64818800
O	-1.06022400	0.33799100	-0.24225300
O	-1.77778200	1.48663200	1.54512500
C	-3.04524500	0.85085700	1.39354400
H	-3.69924600	1.32867300	2.12322400
H	-3.43549600	0.99352600	0.38363200
H	-2.95926600	-0.21736900	1.60220700

TS40

Pd	0.46086400	3.33310800	-0.48769100
N	0.92447300	-2.73252100	-0.24306900
C	-0.42670100	-3.09062400	-0.28091500
C	-1.27932000	-2.64328600	0.72937100
C	-0.97632400	-3.89114300	-1.27894100
C	-2.62845100	-2.92391100	0.70879300
C	-2.34784000	-4.13601700	-1.31927300
C	-3.20304000	-3.64841200	-0.33571600
C	-4.69505300	-3.87290400	-0.31631900
F	-2.79591800	-4.88652900	-2.31985100
F	-0.21384400	-4.47136900	-2.19433000
F	-0.76750000	-1.93523600	1.74410700
F	-3.39202100	-2.47215000	1.70674500
F	-5.05122400	-4.63017100	0.73349700
F	-5.14302800	-4.47402100	-1.41894600
F	-5.34735200	-2.70423200	-0.20206200
C	1.54031900	-2.11968600	-1.33674000
O	1.06095500	-2.15358000	-2.44502500
C	2.85264300	-1.40102400	-1.02031400
H	3.06586900	-1.40637900	0.05283100
H	3.65388400	-1.96863000	-1.50264200
C	2.77830800	0.01058800	-1.57507600
C	3.16799100	0.26006000	-2.90123200
C	2.18073400	1.02099900	-0.80755500
C	2.91277000	1.51629400	-3.44891200
C	1.93558300	2.27220300	-1.39383600
C	2.28719700	2.51434400	-2.71507100
H	3.17795800	1.70816800	-4.48512600
H	2.06116700	3.46620200	-3.17632000
C	0.48441500	1.75032900	0.92464600
C	0.78926900	2.07290900	2.40770500
C	1.61212300	0.75090300	0.55789200
C	2.32016100	2.17148600	2.42662900
C	0.61036400	0.78531500	3.26355100
H	0.24025100	2.92924800	2.79712600
C	2.54168100	0.77843900	1.80747400
H	1.15186700	-0.23817700	0.50637400
H	2.71964500	2.22669400	3.44669600
H	2.72882000	3.00127600	1.86323000
H	0.62679900	1.04732200	4.32710900
H	-0.33434400	0.27401400	3.07523100
C	1.85020500	-0.08168200	2.88426100
H	3.57885100	0.50124100	1.59845300
H	2.51221900	-0.23106300	3.74374400
H	1.56293100	-1.07322800	2.51841600
H	1.26146700	-2.45841400	0.66905200
C	2.53581900	4.00927200	-0.22764100
H	2.08200700	4.52641700	0.62412500
H	3.28188400	3.30595500	0.12236200
C	-1.48098400	4.83101800	1.29911100
C	-2.68748900	3.63157700	-0.26360600
C	-2.65592100	5.30593700	1.95070900
C	-3.90698900	3.96620500	0.36436400
C	-2.70113900	2.80542300	-1.40922400
C	-0.09664300	5.74511400	3.02048800
C	-2.52151700	6.29092200	3.09516700
C	-3.86999100	4.83359500	1.50088000
C	-5.11094800	3.41196500	-0.14356000
H	-1.77286900	2.60437600	-1.93668000
C	-3.88537600	2.29548400	-1.86890000
C	-1.10825700	6.86552400	3.18463000

H	-3.24114300	7.10670000	2.97246000
C	-5.12398800	2.56428100	-1.22845900
H	-6.03970200	3.65926900	0.35511700
H	-3.85717700	1.65421600	-2.74414000
H	-0.96070400	7.36770900	4.14603200
N	-1.48921000	4.04163400	0.25447000
O	-0.24679100	5.16534200	1.71945700
C	-6.39331100	1.87823800	-1.73984900
C	-6.61556300	2.22942700	-3.22285200
H	-5.77789600	1.91000300	-3.85037000
H	-7.51822900	1.73254000	-3.59682500
H	-6.74053800	3.30990300	-3.35363100
C	-7.64151300	2.29965000	-0.95294000
H	-8.52030300	1.78378600	-1.35422000
H	-7.56076600	2.03684600	0.10799600
H	-7.82535400	3.37734100	-1.03212800
C	-6.21751900	0.35365100	-1.58755700
H	-7.11104800	-0.17035100	-1.94624100
H	-5.36034300	-0.01763500	-2.15796000
H	-6.06139200	0.08256400	-0.53786400
C	-5.16018500	5.21043200	2.18048000
H	-5.70703800	4.31129300	2.48404000
H	-5.00258500	5.81515200	3.07389100
H	-5.81020100	5.77210900	1.50017900
H	-0.93896600	7.60503000	2.39237700
H	-2.77003600	5.79325100	4.04230700
H	-0.29940000	4.95829400	3.76296500
C	1.35250200	6.17661800	3.11639700
H	1.55218600	6.61240600	4.09999600
H	2.01410100	5.31618100	2.97629200
H	1.57856100	6.92141600	2.34673100
C	3.79967400	-0.80929800	-3.75823500
H	3.11296900	-1.65193500	-3.88654100
H	4.04165800	-0.41541900	-4.74907100
H	4.73005800	-1.19102400	-3.31917000
C	3.10405000	4.99039800	-1.22402500
H	3.76001700	4.50439100	-1.94918500
H	2.31271800	5.53035100	-1.74566900
H	3.70279700	5.71557600	-0.65541000
C	-0.85685700	1.10145600	0.71304900
O	-1.10523500	0.26194200	-0.13000400
O	-1.78401900	1.52366200	1.59553900
C	-3.05573400	0.88572500	1.51177800
H	-3.70173100	1.43241600	2.19897000
H	-3.45318400	0.93594600	0.49649400
H	-2.97355200	-0.15912300	1.81673200
O	0.26403700	4.94653700	-1.86554500
C	-0.28297400	4.71545900	-3.01444100
C	-0.49300600	5.97507400	-3.84697400
H	-1.13315900	6.67561800	-3.30136300
H	0.46670100	6.47527600	-4.01461000
H	-0.95137800	5.72607300	-4.80548400
O	-0.60939300	3.61088400	-3.44704600

TS67

Pd	0.74946000	3.50411200	-0.98907600
N	-0.06218600	5.01543700	-2.33207900
C	-1.03788400	5.77900300	-1.90083700
C	0.31466800	5.08522800	-3.64780500
C	-1.75310400	6.69856500	-2.72896300
C	-0.32912200	5.96348400	-4.54689100
C	-1.40547800	6.77245600	-4.05793800
N	0.04158600	-2.21696900	-1.49291600
C	-1.29789200	-2.08416400	-1.86895600
C	-2.17379600	-1.49069900	-0.96208600
C	-1.83181200	-2.53121500	-3.07701900
C	-3.50376200	-1.25804100	-1.25640200
C	-3.16300500	-2.27548000	-3.37887500
C	-4.02440200	-1.63128800	-2.49301800
C	-5.45946800	-1.41742000	-2.90618000
F	-3.62672800	-2.70744600	-4.54938500
F	-1.11522100	-3.23756200	-3.94008800

F	-1.69957400	-1.12150500	0.23767600
F	-4.24459800	-0.66067200	-0.32439600
F	-6.14317500	-0.68159100	-2.02475800
F	-6.09982900	-2.59250300	-3.03022800
F	-5.53150600	-0.79721500	-4.09031500
C	1.12145900	-1.88545000	-2.30636900
O	1.04703000	-1.75449000	-3.50453600
C	2.42131800	-1.66384400	-1.53542600
H	2.33024100	-1.99216400	-0.49495700
H	3.19152100	-2.27973300	-2.00451700
C	2.77117800	-0.19196300	-1.60254100
C	3.70193800	0.31735800	-2.52414100
C	2.10109500	0.70848700	-0.78520000
C	4.00715700	1.68102700	-2.48791700
C	2.29276500	2.08457700	-0.88224200
C	3.33869600	2.58344100	-1.65824700
H	4.77170000	2.06357900	-3.15972600
H	3.59881100	3.63480500	-1.69236800
C	1.25391300	2.06472800	0.82152900
C	2.27241700	2.24227300	1.97622900
C	1.33242500	0.54337100	0.47853000
C	3.30053900	1.12175200	1.74561700
C	1.59411300	1.68527600	3.25686300
H	2.64679500	3.25889900	2.09061900
C	2.23692700	0.01342500	1.62373100
H	0.36389600	0.05041800	0.40841800
H	3.94611700	0.98318800	2.61867100
H	3.92866700	1.24529400	0.86301800
H	2.26264800	1.86314100	4.10518300
H	0.64346600	2.16328000	3.49643400
C	1.46837600	0.16407700	2.95399800
H	2.62137400	-0.99365500	1.44329100
H	1.92715100	-0.44053600	3.74220400
H	0.42518400	-0.15208900	2.85470800
H	0.19207000	-2.10012000	-0.50118900
C	1.93344200	4.93236100	-0.08559900
H	1.29828200	5.22562800	0.75394600
H	2.81407900	4.40515900	0.29185300
I	-1.10757900	1.79277900	-2.32639300
C	0.10609000	5.99814000	-5.89190500
C	1.12641600	5.19748400	-6.36334300
C	1.73429700	4.31136500	-5.44375800
C	1.34335100	4.25263400	-4.12944700
C	1.54293400	5.27328900	-7.83847500
H	-0.38975200	6.67939600	-6.57525800
C	-2.13605000	7.67341200	-5.01863300
H	-2.50984600	7.09477800	-5.86977300
H	-2.99124700	8.17030600	-4.56090400
H	-1.46644200	8.44504700	-5.41575500
C	-2.84886800	7.54046100	-2.10992100
C	-2.73546000	7.57105200	-0.58927900
H	-1.89143500	8.20101200	-0.28078800
C	-2.50829100	6.17080800	-0.04793000
H	-2.80395400	8.56279000	-2.49704800
O	-1.28799300	5.64010500	-0.59279400
H	-3.82862500	7.13585700	-2.39747800
H	-3.64183900	7.99532700	-0.14560200
H	-3.32048300	5.50629400	-0.37524700
C	-2.36441900	6.12013700	1.45918800
H	-3.31297700	6.39957000	1.92908400
H	-2.07177300	5.11993000	1.78327000
H	-1.58969100	6.82031000	1.78878900
C	0.34166800	4.88990600	-8.72388000
H	0.62187500	4.92857200	-9.78329500
H	-0.00271300	3.87576200	-8.49558800
H	-0.50219400	5.57218800	-8.57711300
C	1.99129600	6.70916700	-8.17162900
H	2.29354700	6.77877800	-9.22323300
H	1.18792900	7.43517800	-8.00832000
H	2.84344400	7.00576900	-7.54998200
C	2.70345100	4.32254800	-8.16527300
H	3.59920400	4.55758800	-7.57904000
H	2.43634600	3.27537000	-7.98631500

H	2.96657600	4.41951100	-9.22415900
C	2.34776100	6.10925900	-0.94886900
H	1.50199500	6.75246300	-1.20345300
H	3.08010300	6.72290200	-0.40519900
H	2.81921800	5.79702100	-1.88870100
C	-0.11266300	2.59269600	1.25510700
O	-1.05732500	1.66267100	1.13708800
O	-0.30497700	3.67899200	1.76754200
C	-2.39970100	2.08723200	1.35190900
H	-3.01057100	1.20741600	1.15941300
H	-2.53389500	2.44838900	2.37514200
H	-2.64900800	2.87534400	0.63658400
H	2.51992700	3.64011300	-5.77116600
H	1.79683100	3.53550000	-3.45618500
C	4.38313100	-0.58329100	-3.52316500
H	5.02579800	-1.32473200	-3.03185800
H	3.63806700	-1.12448700	-4.11517000
H	5.01143800	-0.00435700	-4.20555700

TS69

Pd	1.21921400	4.11480000	-0.20758700
N	0.51107700	5.40338600	-1.85080800
C	-0.34489000	6.32365000	-1.49096700
C	0.43658100	4.87915600	-3.11320700
C	-1.30846100	6.91236300	-2.35905200
C	-0.53987900	5.32887700	-4.03088500
C	-1.40690000	6.39891500	-3.63433400
N	-0.46548600	-0.98565400	-3.03427300
C	-1.21268000	-1.03019500	-4.20526600
C	-2.58244700	-0.75458300	-4.16081500
C	-0.70480800	-1.45598100	-5.43926700
C	-3.38673200	-0.78914800	-5.28934300
C	-1.50470500	-1.46300500	-6.57033800
C	-2.85482900	-1.12036100	-6.53358600
C	-3.64894500	-1.14420600	-7.81300700
F	-0.94735600	-1.83049100	-7.72310700
F	0.54534900	-1.89366800	-5.56054400
F	-3.14473100	-0.46314200	-2.98397400
F	-4.67383300	-0.49241900	-5.13165000
F	-3.80847500	-2.39748100	-8.26449400
F	-3.01775700	-0.45419600	-8.78003700
F	-4.86358000	-0.60715400	-7.67346100
C	0.84569600	-0.50117000	-3.03048100
O	1.36573200	0.00159300	-4.00376000
C	1.58645700	-0.74305700	-1.71357000
H	0.86277700	-0.94589100	-0.92148300
H	2.17132900	-1.65920800	-1.87225800
C	2.45421300	0.43471800	-1.35217100
C	3.66131700	0.73080600	-2.01334300
C	2.01110500	1.32063800	-0.37487300
C	4.33826100	1.91563700	-1.69774000
C	2.59468200	2.57633400	-0.22560400
C	3.81277200	2.87295600	-0.83006100
H	5.28669000	2.12082000	-2.18783900
H	4.33493800	3.80917100	-0.67794600
C	1.53765200	2.55801800	1.46784300
C	2.59353600	2.26568600	2.56713900
C	1.19879600	1.15551500	0.87038600
C	3.26738100	0.95828000	2.11143700
C	1.79955100	1.71138000	3.78000200
H	3.23578300	3.11513500	2.80352700
C	1.93701100	0.22000800	1.86510500
H	0.14197500	0.93911100	0.73298800
H	3.84503000	0.50715000	2.92505000
H	3.91348600	1.04392000	1.23790700
H	2.49406300	1.56047900	4.61264000
H	1.01610100	2.38199500	4.13974200
C	1.25579900	0.35192300	3.24564900
H	2.01960400	-0.80660700	1.49891400
H	1.54220700	-0.47540300	3.90230700
H	0.16562000	0.34971300	3.15814700
H	-0.97739100	-0.61160400	-2.22165500

C	2.61105200	5.41050100	0.50318300
H	2.00762300	5.94483900	1.24094000
H	3.37734200	4.82952000	1.02468800
C	-0.67162400	4.64839400	-5.26450700
C	0.10161900	3.55238100	-5.59157600
C	1.10863600	3.16348800	-4.67506600
C	1.28230900	3.81223700	-3.47799900
C	-0.19974200	2.74682200	-6.86271400
H	-1.44866800	4.96907800	-5.95039400
C	-2.43681100	6.90686100	-4.60806500
H	-3.17914300	6.12753500	-4.81659700
H	-2.97048400	7.78121700	-4.23478400
H	-1.97094900	7.17694000	-5.56130600
C	-2.20234900	8.01898300	-1.83103500
C	-1.78694600	8.48462600	-0.43241000
H	-0.92751800	9.16392200	-0.48713200
C	-1.38743200	7.28642300	0.41293300
H	-2.19309800	8.87158700	-2.51878000
O	-0.24510300	6.66825000	-0.19486500
H	-3.23825300	7.65683400	-1.79833300
H	-2.60785300	9.02882800	0.04548500
H	-2.20036900	6.54507400	0.41228900
C	-0.98179000	7.60345200	1.83713400
H	-1.83635100	8.00753500	2.38889600
H	-0.62830900	6.69471200	2.33375700
H	-0.17623700	8.34501100	1.84728800
C	-1.59838200	2.12033600	-6.70575300
H	-1.85126200	1.51520400	-7.58302000
H	-1.62556200	1.47307200	-5.82234700
H	-2.37454100	2.88395600	-6.58488000
C	-0.17979800	3.66479900	-8.09773800
H	-0.39420300	3.08323400	-9.00172500
H	-0.93059000	4.45956800	-8.03255700
H	0.80187700	4.13586900	-8.21910600
C	0.80863600	1.60968100	-7.08402900
H	1.82553000	1.99461400	-7.22430600
H	0.82187300	0.90306800	-6.24847400
H	0.53596000	1.05204700	-7.98727100
C	3.20037500	6.33601800	-0.54269700
H	2.44404700	7.01422500	-0.94438100
H	3.99600500	6.94472000	-0.08990200
H	3.64030600	5.79227900	-1.38584700
C	0.39601100	3.37876000	2.05970400
O	-0.76479800	2.72382800	2.01349300
O	0.52214700	4.46393200	2.59993300
C	-1.91702500	3.47883500	2.36749400
H	-2.74655000	2.77353300	2.33958200
H	-1.80988200	3.91760800	3.36239700
H	-2.07108100	4.26887800	1.62714800
H	1.73816400	2.30815900	-4.88566100
H	2.03922900	3.47351000	-2.77932900
C	4.27449600	-0.23194400	-2.99985100
H	4.40902200	-1.22394900	-2.55054800
H	3.63500000	-0.34823200	-3.87758200
H	5.25839000	0.11783800	-3.32562500
O	-0.68999300	3.15143000	-0.83006500
C	-1.19594700	2.15509700	-1.43399900
C	-2.11834700	2.50083000	-2.60131600
H	-2.98309000	1.83584100	-2.62658600
H	-2.43788100	3.54426900	-2.55342000
H	-1.55596600	2.36115500	-3.53305200
O	-0.99607600	0.95107900	-1.16965200

TS44

N	0.63820300	-1.10524700	-1.36632300
C	-0.72786600	-0.87388800	-1.51600600
C	-1.20082700	-0.16133300	-2.61710400
C	-1.65543000	-1.31614600	-0.57728200
C	-2.55052300	0.09009700	-2.77950100
C	-3.01649900	-1.08736000	-0.75603600
C	-3.48855300	-0.37178000	-1.85436100
C	-4.94723000	-0.07412300	-2.11189100

F	-3.83669900	-1.55223900	0.18015000
F	-1.25301800	-1.93722300	0.52359800
F	-0.32722500	0.28077700	-3.52544900
F	-2.94952400	0.77040300	-3.85177800
F	-5.35774000	-0.66158600	-3.24547200
F	-5.14182500	1.24600300	-2.25117300
F	-5.74286700	-0.49543600	-1.12754500
C	1.16368100	-2.37820100	-1.21500800
O	0.46377400	-3.36523300	-1.13485200
C	2.68244000	-2.44060200	-1.14633800
H	2.91864400	-2.98272000	-0.23936500
H	2.97919100	-3.12279200	-1.94544000
C	3.41974800	-1.12165700	-1.27830800
C	3.70097900	-0.75250600	-2.61761900
C	3.76969600	-0.26857000	-0.19533800
C	4.35026300	0.44516000	-2.88289700
C	4.40953700	0.96703200	-0.51457700
C	4.68532700	1.29388100	-1.84629900
H	4.57980400	0.72334000	-3.90822500
H	5.17341200	2.23511800	-2.07342700
C	4.68494500	-0.64052400	2.24019500
C	4.41303300	-1.98178200	2.99218500
C	3.42852800	-0.47777700	1.30131800
C	3.62335600	-2.78608600	1.96152900
C	3.31547300	-1.75815000	4.05708400
H	5.30873000	-2.44356500	3.40161000
C	2.56765500	-1.68414100	1.74105500
H	2.89930900	0.43398600	1.58982500
H	3.20229700	-3.71193100	2.36938900
H	4.22105200	-3.02484400	1.08164100
H	3.17011800	-2.68690800	4.62064200
H	3.55813300	-0.98087400	4.78574500
C	2.07396100	-1.43360900	3.18633700
H	1.72675700	-1.90807600	1.08905300
H	1.23553500	-2.09820400	3.41686600
H	1.72620700	-0.40471000	3.32163500
H	1.27896300	-0.36693900	-1.62760200
Pd	6.39703700	-0.49511800	1.07137100
Pd	5.76697100	2.05178800	0.53611000
I	8.69975000	-0.29940100	-0.50033800
C	3.68379400	2.60811700	0.50502600
H	2.74270800	2.06410700	0.44596800
H	3.82541100	2.85388500	1.56294200
C	8.43050700	3.30382900	-0.06156300
C	8.34748500	2.96020900	2.21546900
C	9.84128600	3.53458400	-0.04126800
C	9.72179400	3.24549300	2.35970400
C	7.59175300	2.66063300	3.35967800
C	8.32519300	3.70681100	-2.44246200
C	10.56409200	3.69814200	-1.36025300
C	10.47909700	3.52529100	1.17589800
C	10.28566600	3.21288300	3.65580800
C	8.16726000	2.64506100	4.60458400
C	9.72692800	3.13222100	-2.50217000
H	10.78678100	4.75819700	-1.54774300
C	9.54293700	2.92008300	4.78368500
H	9.66285300	2.04115900	-2.41664100
C	6.62765600	-3.50753300	0.40515300
C	7.54275100	-2.89865500	2.44029300
C	6.09685500	-3.12209400	-0.84613900
C	6.80387700	-4.87794600	0.68730900
C	7.84164700	-4.25108400	2.78661000
C	5.71109400	-4.07439400	-1.74887300
C	6.36304700	-5.83232300	-0.26670000
C	7.42455200	-5.24146800	1.92578100
C	8.57804600	-4.52383000	4.08233500
C	8.20419400	-2.10752500	4.59580700
C	5.80455000	-5.46253500	-1.46907600
C	9.20288500	-3.25064800	4.65075700
H	7.88165400	-4.94867700	4.81844200
H	9.52515800	-3.41358500	5.68429000
N	7.72148300	2.98482800	0.99818200
N	6.93528100	-2.55045800	1.32998300

C	3.63920900	3.84319600	-0.38263800
H	4.58127900	4.40249600	-0.37701400
H	3.40618800	3.58509300	-1.42013400
H	2.85320300	4.51961100	-0.02062000
C	4.87636000	0.39312500	3.31428800
O	5.72779600	0.33263100	4.18077900
O	3.92491200	1.35613500	3.34877600
C	3.97107200	2.24616000	4.45642000
H	4.82651400	2.92391400	4.38289100
H	3.04262600	2.81649900	4.41191600
H	4.03712300	1.69308900	5.39664100
C	11.95645800	3.78777500	1.29828800
H	12.14744900	4.57154700	2.03887100
H	12.47960100	2.88449500	1.63287000
H	12.40448900	4.11044600	0.35835100
H	8.37337300	4.80369300	-2.50983500
H	10.17898300	3.37664800	-3.46880400
H	11.52156500	3.17133200	-1.32372800
O	7.70426300	3.39051800	-1.18457900
O	7.83819500	-1.86764600	3.23124000
H	7.28606900	-2.38101100	5.13581300
H	10.08700200	-2.96408800	4.06794300
H	9.35895300	-5.27377700	3.92013300
C	7.61983300	-6.69970400	2.24807300
H	6.66060600	-7.22795000	2.22204200
H	8.27558800	-7.17724600	1.51121800
H	8.05393400	-6.85454800	3.23610600
H	11.34515900	3.42248000	3.76220600
H	7.53750500	2.39113900	5.44956300
H	6.54612300	2.42245800	3.22326000
H	6.47619200	-6.88277800	-0.02918100
H	5.32258200	-3.74499600	-2.70776000
H	6.01969100	-2.06497000	-1.07602900
C	5.28616600	-6.46668500	-2.50152700
C	3.80040200	-6.17168600	-2.78934300
H	3.39814600	-6.90541300	-3.49749200
H	3.20328200	-6.21519900	-1.87205200
H	3.66059100	-5.17973500	-3.23282000
C	6.09881100	-6.32721600	-3.80299000
H	7.16124800	-6.52264700	-3.62199000
H	5.73973400	-7.04205800	-4.55276900
H	6.01152600	-5.32311100	-4.23124800
C	5.40323400	-7.91578800	-2.01063800
H	5.00557400	-8.59659700	-2.77091700
H	6.44654900	-8.19816500	-1.82936000
H	4.83400000	-8.07778900	-1.08839100
C	10.21377100	2.91292300	6.16433300
C	10.76306700	4.32054800	6.46621500
H	11.24004600	4.34202800	7.45338000
H	11.50954500	4.62850200	5.72661400
H	9.95761700	5.06301600	6.45840600
C	9.23413000	2.52896400	7.28241600
H	8.81145600	1.53015800	7.12665300
H	9.75871200	2.52288500	8.24422600
H	8.40803300	3.24443200	7.36184000
C	11.37385500	1.89970900	6.17594500
H	11.86686400	1.89870400	7.15539500
H	11.00805200	0.88739200	5.97566700
H	12.13090300	2.13855800	5.42201600
C	3.27038500	-1.60058000	-3.79483800
H	2.18963900	-1.78627500	-3.79772300
H	3.51485700	-1.09396100	-4.73211900
H	3.76635800	-2.57827700	-3.81724600
C	8.73041000	-0.78674700	5.11450700
H	7.96302000	-0.02102000	4.99076300
H	8.99283600	-0.87767400	6.17436300
H	9.61746700	-0.48370700	4.54863300
C	7.40195700	3.16021700	-3.51417700
H	6.41093300	3.61894800	-3.44123900
H	7.81056500	3.37887500	-4.50588200
H	7.30281600	2.07635500	-3.39812800

Table 3**N2-L2-Ar₂****Ar₂I**

C	-2.36859700	1.83082600	-0.19658200
C	-2.80069800	3.15544300	-0.18663300
C	-3.29573100	0.78670400	-0.29796800
C	-4.15526700	3.45296200	-0.28918600
H	-2.07749100	3.95803000	-0.09704300
C	-4.65702900	1.10866200	-0.37976400
C	-5.08880500	2.42711600	-0.38425300
H	-4.47513300	4.49053200	-0.28806400
H	-5.37537400	0.29976000	-0.44650100
H	-6.14817100	2.64972500	-0.46016800
C	-2.91106800	-0.65895400	-0.37472700
O	-1.89635100	-1.09260900	-0.86171400
O	-3.87031800	-1.44397200	0.14655200
C	-3.61175200	-2.84457200	0.06243000
H	-4.47360900	-3.32902500	0.52023800
H	-3.50379600	-3.15398000	-0.98026200
H	-2.69629500	-3.09684800	0.60306500
I	-0.27193500	1.53886600	0.04051800

Ar₂Pd(I)(L2)₂

Pd	-0.90273500	1.41392100	-0.31257000
I	-2.68918200	3.35529900	-0.70439700
C	0.55801500	3.02786200	1.98468400
C	1.84941300	2.89917200	0.08236300
C	1.64200700	3.54729200	2.76287800
C	3.00813000	3.30375400	0.77992000
C	1.92660400	2.67956900	-1.31253500
C	-0.84441400	2.91752700	3.92312900
C	1.38007700	3.98340500	4.19029300
C	2.87981600	3.62915600	2.16771200
C	4.23775000	3.39304200	0.07606800
H	1.02400900	2.41355700	-1.85428900
C	3.12680300	2.80730000	-1.95885600
C	-0.11532600	4.13739500	4.45533500
H	1.79930800	3.24751800	4.89069900
C	4.32555300	3.13833500	-1.27362000
H	5.12564200	3.67703300	0.62773200
H	3.15176700	2.64159500	-3.03259100
H	-0.50826100	5.02908200	3.95212500
C	1.31664100	-0.76250400	-0.33318300
C	0.22441800	-0.65191500	1.69875300
C	2.29629300	-1.67539500	0.17465000
C	1.16958800	-1.50351500	2.31020400
C	-0.86575600	-0.18409800	2.46763200
C	2.49756300	-0.56097300	-2.39841600
C	3.34468800	-2.23281900	-0.76701100
C	2.24157100	-2.00907600	1.50818400
C	1.01701500	-1.82836100	3.68392800
H	-1.58113000	0.48109400	1.99545700
C	-0.98964500	-0.53635300	3.78418800
C	2.97527400	-1.99065500	-2.22719900
H	4.31483000	-1.76223500	-0.55572400
C	-0.03513700	-1.35918900	4.43661600
H	1.75764000	-2.47150300	4.14296500
H	-1.84394700	-0.15899600	4.33942900
H	2.17136300	-2.66792300	-2.54053800
C	4.09841700	4.07074700	2.93576900
H	4.88807600	3.31486500	2.86380000
H	4.50322700	5.00349700	2.52650300
H	3.89170600	4.22838100	3.99465400
C	5.63977100	3.19110100	-2.05741800
C	6.83858600	3.54029100	-1.16556600
H	7.75425300	3.55868500	-1.76671400
H	6.72547500	4.52808400	-0.70498100
H	6.97936900	2.80063900	-0.36891800
C	5.53466500	4.25572800	-3.16601600
H	6.46908200	4.30247200	-3.73790400
H	4.72416100	4.03553200	-3.86788100

H	5.34630500	5.24478900	-2.73504300
C	5.89666700	1.80961300	-2.69221500
H	5.96237200	1.03462300	-1.91937700
H	5.09856900	1.52694500	-3.38726900
H	6.83931200	1.81480300	-3.25217800
C	3.27340700	-2.90618800	2.14113700
H	4.08604200	-3.15576100	1.45895900
H	3.71698300	-2.42021300	3.01663000
H	2.81922300	-3.84302500	2.48395000
C	-0.20837100	-1.66269300	5.92704800
C	-1.55944500	-2.36627300	6.15693300
H	-1.69900300	-2.57913500	7.22320100
H	-2.40286900	-1.75027000	5.82911400
H	-1.60255500	-3.31383700	5.60933400
C	-0.17977300	-0.33528100	6.71103700
H	0.77424500	0.18304800	6.56049600
H	-0.98379200	0.33956400	6.39777700
H	-0.30272700	-0.52246300	7.78414400
C	0.90481100	-2.56732400	6.47158000
H	0.92043900	-3.53895900	5.96526400
H	1.89239400	-2.10418500	6.36495200
H	0.73992200	-2.75275000	7.53836500
N	0.65314800	2.70653900	0.71663200
N	0.34232400	-0.26018700	0.39181800
O	-0.65617600	2.82440800	2.50863300
O	1.31880000	-0.35672900	-1.60574900
H	1.88759400	4.93268400	4.38957800
H	-0.30481700	4.24891800	5.52784200
H	-0.41424300	2.01101000	4.37428100
H	3.83755800	-2.17677400	-2.87550000
H	3.47168400	-3.30605600	-0.59396100
C	-2.34436900	2.94042200	4.13766700
H	-2.80915100	2.06327500	3.67860900
H	-2.57146400	2.94363600	5.20896000
H	-2.78138300	3.82947100	3.67386800
C	-2.11141100	0.15581500	-1.23879000
C	-2.12906700	-0.01959600	-2.63539900
C	-2.93417400	-0.67383100	-0.46790300
C	-2.93587200	-1.01288500	-3.21399000
C	-3.72668700	-1.65773500	-1.04735200
H	-2.96830500	-0.54807700	0.60934300
C	-3.72609700	-1.83603400	-2.42912100
H	-2.93683200	-1.12830500	-4.29192900
H	-4.35223800	-2.28441700	-0.41645000
H	-4.34371300	-2.60169800	-2.88900600
C	-1.31408400	0.84515000	-3.52612800
O	-0.44596000	1.62215800	-3.18546500
O	-1.63183100	0.68531800	-4.82801700
C	-0.92674400	1.52134100	-5.73456400
H	-1.36476000	1.32737400	-6.71407800
H	-1.04718300	2.57303100	-5.46348300
H	0.14000200	1.27720500	-5.74428300
C	2.12508500	-0.19868100	-3.82042100
H	1.70199600	0.80739400	-3.85448100
H	3.01311500	-0.24789500	-4.45952600
H	1.37163300	-0.89373500	-4.20661300
H	3.26239700	0.13527000	-2.02682300

1

Pd	-0.02184900	1.22608400	0.07083100
O	-1.97059500	0.94934000	0.55148800
O	1.93876300	1.46964000	-0.40916600
C	-2.30765500	0.92861700	1.79995000
C	2.25365800	1.94868200	-1.56586800
O	-1.55590900	1.04990700	2.76680900
O	1.47392000	2.21216400	-2.48494600
C	-3.80747100	0.74144400	1.99559500
H	-4.33361500	1.62820600	1.62759200
H	-4.16349000	-0.11339000	1.41316500
H	-4.03466400	0.59812000	3.05349500
C	3.75068300	2.17848600	-1.72073500
H	4.09629400	2.88197800	-0.95688600

H	4.28701800	1.23773300	-1.56412800
H	3.97302400	2.57098800	-2.71449900
C	0.43050000	3.97864900	1.21974000
C	-0.53360600	3.93204000	-0.89567900
C	0.77270800	3.29247900	2.40567500
C	0.68604900	5.36105200	1.11675700
C	-0.24697400	5.31374800	-1.12087300
C	1.36626900	3.96905600	3.43714300
H	0.51090700	2.24241800	2.49119500
C	1.30653600	6.02090000	2.20890200
C	0.34228900	6.02859100	-0.10455700
C	-0.53800700	5.86275500	-2.49950900
C	-1.51234300	3.64648700	-3.08471000
C	1.65931800	5.35641300	3.36170900
H	1.60855800	3.41736600	4.34102600
H	1.50895500	7.08054500	2.11618300
C	-0.53143100	4.72134300	-3.51418900
H	-1.50885200	6.37752300	-2.51855200
H	0.46679200	4.27207300	-3.57419300
C	0.31354300	-1.54104300	0.97410300
C	-0.11087600	-1.46176500	-1.30682100
C	0.17549100	-2.96092900	1.01925800
C	-0.28282600	-2.86079900	-1.36147500
C	-0.20728700	-0.69909200	-2.49241300
C	0.37027000	-1.37695400	3.34166400
C	0.37643600	-3.67113600	2.34422800
C	-0.15374400	-3.61243400	-0.14856100
C	-0.56853000	-3.46107300	-2.61521800
H	-0.02679300	0.37196500	-2.44610300
C	-0.47909200	-1.32053300	-3.68138600
C	0.99884900	-2.75906800	3.40406600
H	-0.59445300	-4.03604400	2.70598100
C	-0.67264100	-2.72477800	-3.77372000
H	-0.70043000	-4.53530600	-2.64916300
H	-0.53746100	-0.70898100	-4.57756600
H	2.07711000	-2.65186400	3.23389300
N	-0.15495800	3.29064200	0.19083900
N	0.14299200	-0.83185000	-0.11999000
O	-1.20655800	3.18184200	-1.75897400
O	0.63914700	-0.82134100	2.04546500
H	-2.52592900	4.06900300	-3.03654800
H	-0.80934100	5.08559200	-4.50858200
H	0.21961200	6.60031600	-2.77788800
H	-0.72044500	-1.43671100	3.44830900
H	0.86278400	-3.19241400	4.40022400
H	1.00865800	-4.55424100	2.20512900
C	-1.49742100	2.41870200	-3.97597100
H	-0.47698100	2.03071500	-4.03730300
H	-2.14889800	1.64259200	-3.56365500
H	-1.85158700	2.68099000	-4.97878900
C	0.91842900	-0.38399300	4.34396200
H	1.99235600	-0.23687200	4.18808500
H	0.39563700	0.56704000	4.22274300
H	0.75526900	-0.75364300	5.36152000
C	0.63399600	7.50040400	-0.23914000
H	0.18100400	8.05404600	0.59012000
H	1.71312500	7.68942100	-0.20665500
H	0.24168600	7.92208800	-1.16477500
C	-0.37343700	-5.10221800	-0.18376600
H	-1.36059100	-5.33176800	-0.59890600
H	0.37046800	-5.59088300	-0.82346600
H	-0.31683200	-5.55695700	0.80539600
C	2.34058700	6.04504300	4.54841000
C	2.59171500	7.53727800	4.29276700
H	3.24799500	7.69610000	3.42956600
H	1.65599500	8.08193300	4.12319700
H	3.07971700	7.98296400	5.16641400
C	3.69855600	5.36736200	4.81563100
H	3.58308100	4.30363300	5.04673900
H	4.35373800	5.45083500	3.94163400
H	4.19881100	5.84250800	5.66791200
C	1.44567100	5.91449000	5.79609600
H	1.92376100	6.39395300	6.65862700

H	0.47508200	6.39452900	5.63011400
H	1.26081100	4.86736900	6.05606800
C	-0.97026400	-3.35209700	-5.13896000
C	0.19817500	-3.05653200	-6.09918500
H	0.00422300	-3.50310400	-7.08159200
H	0.34573200	-1.98173900	-6.24439500
H	1.13358800	-3.47440100	-5.71119200
C	-1.14823500	-4.87395000	-5.05505900
H	-0.24274300	-5.36758100	-4.68437600
H	-1.98546900	-5.14959100	-4.40378000
H	-1.35811500	-5.27590600	-6.05216200
C	-2.26890800	-2.74490700	-5.70429400
H	-3.11318600	-2.94067500	-5.03429100
H	-2.18740700	-1.66104300	-5.83486500
H	-2.49688100	-3.18346100	-6.68290100

TS35

Pd	1.01671700	3.67394500	0.52870300
N	0.25950300	-0.91297600	-2.76928200
C	-0.68636000	-1.16027300	-3.76265800
C	-0.38009000	-1.88849300	-4.90940400
C	-1.96843100	-0.61975700	-3.65939300
C	-1.33071500	-2.10554200	-5.90095900
C	-2.89987300	-0.80445700	-4.66489500
C	-2.61027500	-1.56444400	-5.79866600
C	-3.68748300	-1.73133200	-6.84175800
F	-4.10553300	-0.25143100	-4.52441700
F	-2.30329300	0.08823800	-2.58614000
F	0.84947600	-2.35705600	-5.09854400
F	-0.95323600	-2.81580800	-6.96116800
F	-4.02840100	-0.54342600	-7.36792300
F	-4.79662700	-2.26018800	-6.30276800
F	-3.31572000	-2.52388200	-7.84953000
C	0.99083200	-1.91095100	-2.16798100
O	0.83001600	-3.08929600	-2.41372500
C	2.01963900	-1.43213600	-1.13979400
H	1.60330600	-1.67359400	-0.15791400
H	2.88365500	-2.09022200	-1.26814600
C	2.39481600	0.02649600	-1.24556700
C	3.28002200	0.44327800	-2.25339100
C	1.79242400	0.97749400	-0.40703500
C	3.56469300	1.80190900	-2.36727800
C	1.99161400	2.34845700	-0.62274100
C	2.91399400	2.75285000	-1.58443600
H	4.28398800	2.13360600	-3.11343300
H	3.12073000	3.80224600	-1.75441500
C	0.29698300	1.88377800	1.38893300
C	0.73664000	1.83866400	2.86795400
C	0.95514600	0.61375800	0.77268600
C	2.18141900	1.33233500	2.72719600
C	0.06893300	0.62699300	3.56762500
H	0.59558200	2.77904200	3.39972500
C	1.78610500	0.05656400	1.96585100
H	0.17591700	-0.10119400	0.48819100
H	2.65633400	1.11952100	3.69196700
H	2.82068000	2.00838500	2.15265200
H	0.23546600	0.69180800	4.64838900
H	-1.01243300	0.59578500	3.41248800
C	0.80702000	-0.59843600	2.95576200
H	2.61117900	-0.58959500	1.65471400
H	1.35075000	-1.15840600	3.72410500
H	0.12585000	-1.29761700	2.45940100
H	0.33533500	0.05274600	-2.46197500
I	1.44954300	6.03835200	-0.95233100
C	2.27011000	5.46727500	2.70363800
C	0.08438000	5.87116000	3.26700800
C	2.75221300	6.59151500	3.43857100
C	0.44496600	6.98436800	4.05870200
C	-1.27130300	5.47317200	3.22313500
C	4.51876800	4.77308800	2.13987000
C	4.22923200	6.91889600	3.37976600
C	1.82820200	7.34677000	4.12643100

C	-0.57389100	7.69490000	4.74605100
H	-1.51873500	4.57790500	2.66504700
C	-2.22292500	6.17974800	3.90847100
C	4.88957100	6.24428900	2.17979800
H	4.37072300	8.00110500	3.30654200
C	-1.89814000	7.32466600	4.68382300
H	-0.28707500	8.55620200	5.33642100
H	-3.25456800	5.84154400	3.86045300
H	5.97792700	6.34909400	2.23107800
N	1.00591000	5.14512300	2.56779200
O	3.09392400	4.63715100	2.04214100
C	-3.01436300	8.07128500	5.42033700
C	-4.05652000	8.56558900	4.39856600
H	-4.50819900	7.73701400	3.84340200
H	-4.86471300	9.10103200	4.91030400
H	-3.59913400	9.24726300	3.67321800
C	-2.49035100	9.28700400	6.19674000
H	-3.32432000	9.78889800	6.69909200
H	-1.76760700	8.99612000	6.96734400
H	-2.01544500	10.01810500	5.53269000
C	-3.68735000	7.11294900	6.42218300
H	-4.49211800	7.62900000	6.95884900
H	-4.12587700	6.24238900	5.92366200
H	-2.96241100	6.74870700	7.15821200
C	2.23571400	8.53479700	4.95804100
H	3.31739200	8.66003800	5.01008200
H	1.80521000	9.45822300	4.55415800
H	1.86920900	8.42551100	5.98423200
H	4.55143200	6.71249700	1.24668000
H	4.72615800	6.59657700	4.30504000
H	4.82589200	4.28752200	3.07732800
C	5.09186800	4.02497800	0.95278100
H	6.18345800	3.98863100	1.02474100
H	4.70485600	3.00317300	0.91436100
H	4.81158100	4.52489000	0.02065100
C	-1.17580000	1.88998900	1.13844600
O	-1.73805600	1.32116700	0.22853500
O	-1.86599300	2.57227500	2.08550600
C	-3.28227300	2.46257000	2.00690300
H	-3.64291100	2.73982300	1.01559000
H	-3.59310800	1.43674400	2.22564400
H	-3.67226100	3.14257400	2.76639300
C	-0.47354900	4.48215000	-0.88465300
C	-0.84796200	3.66591700	-1.96051900
C	-1.44688400	5.11442300	-0.10737100
C	-2.20857000	3.40603500	-2.14937300
C	-2.79469700	4.87814200	-0.35288100
H	-1.15484800	5.80360400	0.67426200
C	-3.18242900	4.01151200	-1.36752600
H	-2.48866700	2.70454800	-2.92722900
H	-3.53475600	5.38384700	0.26112800
H	-4.23160600	3.80889600	-1.55491400
C	0.04969100	3.04121400	-2.97641100
O	-0.02967400	1.88332000	-3.33181900
O	0.85122400	3.92826600	-3.55854200
C	1.61963100	3.44081500	-4.65852700
H	2.14156300	2.52321600	-4.38495300
H	0.96269900	3.24662100	-5.51080700
H	2.32581300	4.23607600	-4.89480500
C	3.89033300	-0.54456600	-3.21599700
H	4.47238600	-1.31762100	-2.70038600
H	3.11775600	-1.05853800	-3.80063100
H	4.55920500	-0.04010300	-3.91940400

TS65

Pd	6.26151000	2.85435200	-0.90374600
N	0.97746800	0.11515000	-2.71517100
C	0.28620100	-0.19086500	-3.89489300
C	-0.02459500	0.81810700	-4.81458200
C	-0.09287200	-1.49770400	-4.21414600
C	-0.68092700	0.52616100	-6.00139000
C	-0.77817200	-1.78464600	-5.39421600

C	-1.07609800	-0.77875700	-6.31800900
C	-1.80124500	-1.01070800	-7.62189500
F	-1.10705400	-3.06249500	-5.61600500
F	0.22498100	-2.50905100	-3.40119900
F	0.30338900	2.08787900	-4.54198900
F	-0.95735400	1.53002500	-6.84578600
F	-1.06849300	-0.56256800	-8.66424300
F	-2.97512700	-0.34409400	-7.64647900
F	-2.06799300	-2.30700700	-7.84630600
C	0.47882100	-0.21957400	-1.46461800
O	-0.57685900	-0.81000100	-1.31910700
C	1.32376000	0.24770600	-0.26748100
H	0.93018900	1.22688800	0.02896400
H	1.07847800	-0.44161900	0.54409200
C	2.80905100	0.33525600	-0.52774400
C	3.60017100	-0.83941800	-0.63865600
C	3.39290900	1.55777200	-0.84820000
C	4.88568600	-0.74381900	-1.18359800
C	4.71786600	1.65573900	-1.33671200
C	5.43143700	0.47215900	-1.62335600
H	5.45829600	-1.65783000	-1.32695700
H	6.36551200	0.47474100	-2.17785400
H	1.80455600	0.70063600	-2.81607200
C	4.00919200	3.28884400	-2.15999900
C	4.19208800	4.78180400	-1.78514400
C	2.78059200	2.85682700	-1.29587600
C	2.92836100	5.54325700	-2.30086100
C	3.91059800	4.75588900	-0.26432500
H	5.12905200	5.23598800	-2.10386600
C	2.52240400	4.09517600	-0.39063500
H	1.89301500	2.67836100	-1.91413500
C	1.80373400	5.12545400	-1.29588800
H	2.68613300	5.29438000	-3.33834000
H	3.11070300	6.62271600	-2.26849300
H	4.64312700	4.15985900	0.29414500
H	3.85868100	5.75838600	0.17547000
H	2.00150700	3.87084500	0.54413200
H	0.92691600	4.70130100	-1.79632500
H	1.46236500	5.98375500	-0.70786200
C	8.67004400	3.82450100	0.72804800
C	8.85441500	4.59355700	-1.44627700
C	9.92540200	4.39490300	1.11431600
C	10.09339300	5.23574900	-1.15970300
C	8.32753500	4.68359200	-2.75398900
C	8.19420500	3.16385100	3.00731900
C	10.43449000	4.16552100	2.52748000
C	10.62604300	5.12343600	0.16766000
C	10.74785800	5.94234200	-2.19995100
H	7.38241400	4.18661000	-2.95941300
C	8.99653700	5.38247700	-3.73695000
C	9.69425800	3.01711300	3.21952200
H	7.86611800	4.14631900	3.37992800
H	11.50733200	3.95088100	2.51027700
C	10.23110600	6.03435600	-3.48409500
H	11.69270200	6.42413300	-1.97554400
H	8.55386600	5.42688200	-4.72499700
H	9.92089200	3.00713700	4.29075800
N	8.15517300	3.90376300	-0.48550500
C	11.93552700	5.79839200	0.49716000
H	12.75757900	5.37372400	-0.09084000
H	11.88969000	6.86618600	0.25773800
H	12.19837400	5.71077400	1.55053400
C	10.99367400	6.81557700	-4.57251800
C	11.19031900	8.28119500	-4.11736800
H	11.76814100	8.34669900	-3.19056300
H	11.72824000	8.84944600	-4.88442400
H	10.22648700	8.77129800	-3.94523700
C	12.37642600	6.16009500	-4.80255400
H	12.26812600	5.12176800	-5.13284100
H	12.93398500	6.70506900	-5.57263600
H	12.98225800	6.15833600	-3.89136200
C	10.24051100	6.83053300	-5.91699100
H	10.10107600	5.82205000	-6.31977700

H	9.25699700	7.30388700	-5.82893700
H	10.81552100	7.40098500	-6.65333300
O	7.90193200	3.11946900	1.59131100
H	10.01134500	2.05088300	2.80803200
H	10.31437800	5.08360100	3.11989500
C	7.35735100	2.06715800	3.64439500
H	7.46705300	2.09484700	4.73286600
H	6.30138400	2.19947400	3.39581100
H	7.67446900	1.08409900	3.28363100
C	3.93017800	2.87865800	-3.58617900
O	3.20913700	1.99013800	-4.02339400
O	4.77182300	3.57848400	-4.38569100
C	4.77194400	3.18941700	-5.76842000
H	5.46252000	3.87090100	-6.26553100
H	5.11062700	2.15576400	-5.87798400
H	3.77030600	3.27908900	-6.19566500
C	3.02582000	-2.19618200	-0.30151800
H	2.64434200	-2.23585300	0.72579300
H	2.18967900	-2.46105800	-0.96073000
H	3.78498000	-2.97611300	-0.40430500

TS36

Pd	2.54935200	3.24449600	0.60908000
N	-0.41171800	-0.34638900	-2.22551300
C	-1.76131000	-0.35283900	-1.88363300
C	-2.67150100	0.33968900	-2.67666900
C	-2.22862000	-0.93646800	-0.70475700
C	-4.00920700	0.45246200	-2.32500300
C	-3.57087000	-0.84589500	-0.36968900
C	-4.48580600	-0.14967600	-1.16189300
C	-5.92060700	-0.07582400	-0.69503300
F	-3.97836100	-1.41511200	0.76087300
F	-1.39379500	-1.53832000	0.12722200
F	-2.23571000	0.94129000	-3.78453400
F	-4.80120200	1.14591100	-3.13662000
F	-5.99680900	0.53381500	0.49831700
F	-6.43991900	-1.30276400	-0.55327200
F	-6.70312500	0.59859100	-1.54033200
C	0.40862900	-1.45692400	-2.19661000
O	-0.00677100	-2.57729100	-1.99782500
C	1.89320200	-1.15988300	-2.42740900
H	2.40925500	-1.71674000	-1.64244800
H	2.16790600	-1.65224500	-3.36364400
C	2.24755900	0.31070000	-2.43668000
C	2.42152100	0.98347300	-3.65686400
C	2.23390100	1.03864800	-1.22924300
C	2.60797100	2.36994100	-3.64601000
C	2.30157100	2.44050300	-1.26344100
C	2.53388500	3.10117200	-2.47532400
H	2.76838000	2.89316000	-4.58431300
H	2.60630400	4.18075000	-2.51040500
C	2.17013000	1.31059300	1.31837300
C	3.47085600	0.99129700	2.08359300
C	2.18825900	0.33730400	0.10326200
C	4.44127600	0.64594800	0.94559200
C	3.30154800	-0.40421800	2.74802300
H	3.76843000	1.76581900	2.78392400
C	3.53262100	-0.43317500	0.34850400
H	1.34047300	-0.35516200	0.15942300
H	5.38823600	0.23727900	1.31478400
H	4.66127200	1.47511000	0.26658800
H	4.15107700	-0.57644300	3.41712500
H	2.39593700	-0.48690600	3.35429900
C	3.32072300	-1.38083800	1.54220200
H	3.92102500	-0.91765000	-0.54784000
H	4.14709300	-2.09437200	1.61840100
H	2.39347700	-1.95505200	1.45003500
H	-0.02395200	0.53141500	-2.54554700
I	4.67044400	4.93572700	-0.25585400
C	3.69222000	4.66664800	3.17760100
C	1.45562300	5.13791500	2.88334200
C	3.94680400	5.91762900	3.82287300

C	1.59348700	6.39373900	3.51734200
C	0.16740100	4.72378000	2.49326600
C	5.97290000	3.93458600	3.53616600
C	5.37252100	6.25119400	4.20861300
C	2.89225400	6.78318400	3.98280800
C	0.45953600	7.23096900	3.62398700
H	0.03813600	3.74419000	2.05518000
C	-0.91531800	5.55508700	2.63111800
C	6.36236600	5.39526900	3.42346500
H	5.57316600	7.30703600	4.00713300
C	-0.78707100	6.85602800	3.16475100
H	0.58546800	8.21227800	4.07020300
H	-1.87871800	5.19247200	2.29231400
H	7.37736200	5.53155000	3.81017700
N	2.53676600	4.32407400	2.64950300
O	4.63844500	3.73689700	3.03941900
C	-1.95912100	7.84326900	3.22213600
C	-3.24911400	7.24459600	2.64331400
H	-3.58156800	6.36724700	3.20926600
H	-4.05089200	7.98950400	2.68662500
H	-3.12320300	6.95208900	1.59464900
C	-1.59474900	9.08950600	2.39154200
H	-2.42275800	9.80810400	2.39435300
H	-0.71074600	9.59659400	2.79203800
H	-1.38098400	8.81337200	1.35292600
C	-2.22793700	8.25398500	4.68164900
H	-3.05627100	8.97052400	4.72977500
H	-2.49336500	7.38166800	5.28903100
H	-1.35182400	8.72693800	5.13760900
C	3.06258400	8.12707100	4.64101200
H	4.04756500	8.25079500	5.09114600
H	2.91810000	8.93527400	3.91401200
H	2.32050700	8.26429700	5.43407700
H	6.35618900	5.67891600	2.36479800
H	5.52087400	6.09878500	5.28697300
H	5.96283600	3.63865200	4.59561600
C	6.85161600	2.99169300	2.73741500
H	7.88580300	3.05446900	3.09067100
H	6.50648700	1.95969900	2.85202300
H	6.81325800	3.25732500	1.67683100
C	2.37812000	0.25408700	-4.97810300
H	1.41309000	-0.24245500	-5.13509100
H	2.52775700	0.95151000	-5.80616800
H	3.15727400	-0.51381900	-5.04644700
C	0.95783600	1.19171500	2.20502100
O	-0.03983600	0.55065500	1.94674600
O	1.12082300	1.82506400	3.37255900
C	0.01918100	1.75122300	4.27248000
H	0.32352300	2.31920700	5.15078600
H	-0.87179800	2.19807500	3.82365800
H	-0.19437100	0.71195300	4.53521900
C	0.69958300	3.36825000	-0.42971000
C	0.34369600	4.69510900	-0.72408700
C	-0.32614000	2.42338300	-0.31683400
C	-1.01033400	5.03613000	-0.84240800
C	-1.66363300	2.78257600	-0.40980100
H	-0.09825600	1.38635500	-0.12512000
C	-2.01774700	4.10009100	-0.67860500
H	-1.26215700	6.07249900	-1.04898900
H	-2.42435600	2.02060800	-0.26794000
H	-3.05949400	4.39151400	-0.76663700
C	1.25207300	5.87883000	-0.93063200
O	1.33841600	6.60079800	0.18766000
O	1.71152300	6.21030000	-1.99701400
C	2.08675800	7.81419500	0.10254700
H	1.98036600	8.27856100	1.08324100
H	3.13403800	7.59037500	-0.11183600
H	1.67710500	8.46039300	-0.67823200

TS40

Pd	2.48474700	3.10038800	0.83440600
N	-0.30171200	-0.30253100	-2.29349000

C	-1.66009800	-0.31292000	-1.99075400
C	-2.53440100	0.46396400	-2.75068000
C	-2.17247900	-0.97845700	-0.87952200
C	-3.87052200	0.56896700	-2.41512600
C	-3.52525700	-0.89481200	-0.56057500
C	-4.39732100	-0.11435700	-1.31748200
C	-5.86407500	0.06500300	-1.00756900
F	-3.93696400	-1.55919900	0.51284500
F	-1.37189400	-1.66233900	-0.07758600
F	-2.05662500	1.14593300	-3.79217000
F	-4.65949400	1.33885700	-3.16157900
F	-6.13329200	1.35537200	-0.74813100
F	-6.26230200	-0.64770000	0.04724200
F	-6.62122000	-0.29903400	-2.05205700
C	0.50899200	-1.42070300	-2.31970800
O	0.07697300	-2.54893900	-2.23249700
C	2.00573200	-1.12270200	-2.45711100
H	2.47635500	-1.72394200	-1.67596200
H	2.32769300	-1.56571400	-3.40283800
C	2.36518200	0.34344000	-2.36215000
C	2.63393300	1.08385300	-3.52524000
C	2.26486400	0.99833300	-1.11820900
C	2.82468400	2.46511700	-3.41968100
C	2.30888000	2.40112200	-1.07553300
C	2.64535500	3.12902400	-2.21936600
H	3.06544900	3.03906000	-4.31025000
H	2.70315500	4.20937800	-2.18331400
C	2.11021400	1.15228000	1.42971900
C	3.38327300	0.78378500	2.23443500
C	2.17468500	0.22776300	0.17434600
C	4.39388000	0.50474700	1.11432800
C	3.19782100	-0.63905200	2.82308500
H	3.65676400	1.52802300	2.97852300
C	3.51279200	-0.54641900	0.43044400
H	1.33084500	-0.47170300	0.16631700
H	5.32816700	0.07588400	1.49395600
H	4.63532600	1.37653300	0.49877200
H	4.02233200	-0.84941800	3.51259800
H	2.26965000	-0.75519900	3.38949800
C	3.26002300	-1.55290600	1.56871600
H	3.93855900	-0.98882400	-0.47126400
H	4.08383500	-2.27045800	1.63746600
H	2.33661700	-2.12062000	1.41623900
H	0.10654700	0.59361800	-2.52394600
C	3.75246900	4.55074800	3.18977000
C	1.50789000	5.05230700	3.03747400
C	4.09248100	5.86302300	3.63950300
C	1.72618800	6.36849200	3.50329200
C	0.19053000	4.64753300	2.74384500
C	6.03996800	3.80540300	3.39541600
C	5.55598200	6.21088100	3.81549400
C	3.06920900	6.76712400	3.80383200
C	0.62635400	7.25427200	3.57433900
H	0.01709900	3.63045500	2.41851200
C	-0.85191900	5.53399600	2.82945900
C	6.44599100	5.22716900	3.05883200
H	5.74306600	7.22435600	3.44806400
C	-0.65189300	6.87900800	3.21380100
H	0.80741400	8.27728600	3.88877500
H	-1.84179700	5.18113500	2.56522600
H	7.49711700	5.38088000	3.32243200
N	2.54099500	4.17322200	2.85031000
O	4.66820700	3.59155400	3.02697400
C	-1.77980100	7.91733400	3.18291500
C	-3.12393900	7.30069900	2.76943200
H	-3.44953500	6.52594700	3.47258600
H	-3.89524200	8.07813000	2.75320900
H	-3.07582800	6.85964200	1.76744800
C	-1.41294600	8.99945100	2.14792500
H	-2.21774600	9.73899800	2.06110000
H	-0.49842700	9.53248800	2.43063000
H	-1.24684000	8.54751400	1.16359700
C	-1.94973500	8.56080500	4.57084300

H	-2.74480600	9.31514800	4.54607100
H	-2.21664300	7.80688900	5.31938300
H	-1.03261200	9.05648900	4.90578400
C	3.32959300	8.17298300	4.27757800
H	4.34636100	8.30649300	4.64822000
H	3.16626100	8.89397200	3.46727000
H	2.64719700	8.43786900	5.09120900
H	6.35031100	5.36359400	1.97604200
H	5.82364700	6.20622200	4.88139300
H	6.10703700	3.65422200	4.48305600
C	6.83436200	2.74315000	2.66263300
H	7.89579500	2.82843900	2.91719300
H	6.48629000	1.74580800	2.94711300
H	6.69810000	2.87081100	1.58531300
C	2.69938300	0.42863000	-4.88374800
H	1.75022400	-0.05351700	-5.14626600
H	2.91828000	1.16848700	-5.65796000
H	3.48015100	-0.33933100	-4.92829700
C	0.87473100	0.96689500	2.26713300
O	-0.08692100	0.28541900	1.97494600
O	0.96411900	1.60385600	3.44472700
C	-0.15773300	1.45826100	4.30868700
H	0.08832500	2.02818700	5.20410100
H	-1.05978700	1.86075500	3.83939500
H	-0.32443600	0.40573200	4.55181900
C	0.68627200	3.29890700	-0.27512000
C	0.31306800	4.63103200	-0.54043800
C	-0.33103400	2.34214400	-0.18209200
C	-1.04741700	4.95443100	-0.63861600
C	-1.67371900	2.68493900	-0.26230900
H	-0.09243800	1.30193700	-0.02256100
C	-2.04450700	4.00391400	-0.49352200
H	-1.31455800	5.99215400	-0.81634500
H	-2.42362900	1.90921100	-0.13903200
H	-3.08996500	4.28584600	-0.56808000
C	1.19406900	5.83672200	-0.74997700
O	1.09841600	6.65614700	0.30015900
O	1.75785900	6.11656100	-1.78267500
C	1.90714000	7.82525100	0.25337600
H	1.58783100	8.43189600	1.10135400
H	2.95451900	7.53389800	0.35822100
H	1.76213900	8.36301500	-0.68661600
O	3.34820400	4.98041100	0.25718400
C	4.57656600	4.80285300	-0.08406200
C	5.25347000	6.04605900	-0.63720500
H	4.63335800	6.47072200	-1.43265900
H	5.33516700	6.80263500	0.15281500
H	6.25029300	5.81117600	-1.01461600
O	5.18603500	3.73277900	0.02412000

TS67

Pd	0.79622700	4.11982800	-0.22337300
N	-0.30082400	5.96469300	-0.92111000
C	-1.53120300	6.16880900	-0.49101100
C	0.14872400	6.70639400	-1.99346800
C	-2.46509300	7.03844700	-1.13438200
C	-0.71020300	7.57183400	-2.70698800
C	-2.06362000	7.69694700	-2.27310700
N	-0.56214600	-0.10294900	-2.80792500
C	-1.31424800	0.05169100	-3.97201600
C	-0.80361300	0.82986900	-5.00927500
C	-2.59739700	-0.46136200	-4.11209000
C	-1.56445700	1.13369700	-6.12078700
C	-3.35368500	-0.18386900	-5.24710400
C	-2.85528000	0.62401100	-6.26816000
C	-3.63770600	1.01068100	-7.50081000
F	-4.58348500	-0.68668300	-5.29345000
F	-3.14883500	-1.16178800	-3.13188700
F	0.42765000	1.33499500	-4.89462300
F	-1.04122800	1.91995100	-7.06047800
F	-2.96099600	0.69428900	-8.61350100
F	-3.84871200	2.33714000	-7.52359700

F	-4.82767800	0.41252300	-7.56911200
C	-0.10742500	-1.32278600	-2.34794800
O	-0.48268000	-2.38123400	-2.80327300
C	0.91116600	-1.20765500	-1.20690300
H	0.34845000	-1.28517600	-0.26976900
H	1.54227700	-2.09794100	-1.27530800
C	1.68844300	0.08519100	-1.25353300
C	2.62956500	0.33987400	-2.26687100
C	1.37975600	1.11682000	-0.36689400
C	3.26847300	1.58388500	-2.30625200
C	1.88956500	2.40278600	-0.54927300
C	2.91679600	2.63201100	-1.46046500
H	4.02931100	1.75894900	-3.06209300
H	3.39435200	3.59913100	-1.55248500
C	1.25552200	2.48850700	1.47046100
C	2.56690200	2.29539400	2.28007800
C	0.86459700	1.05182900	1.03209600
C	3.16074500	0.97910500	1.75433000
C	2.11916500	1.79540400	3.68444900
H	3.20389500	3.17765000	2.29582700
C	1.84369400	0.19368800	1.88957100
H	-0.18088700	0.78243200	1.18826200
H	3.93733500	0.60139800	2.42671600
H	3.572444000	1.02617000	0.74646300
H	3.01320100	1.71127300	4.30976600
H	1.43335300	2.46356300	4.20777400
C	1.50697700	0.39773200	3.38212100
H	1.86886700	-0.85139100	1.57115300
H	1.96808600	-0.38401100	3.99316300
H	0.42821800	0.37345200	3.56334000
H	-0.09544600	0.73131300	-2.47121100
I	2.96477700	5.68172600	0.73813900
C	-0.20613000	8.29852200	-3.81783500
C	1.10305100	8.20046200	-4.22532900
C	1.94425600	7.32505300	-3.49210300
C	1.48895300	6.59782800	-2.42698400
C	1.67207300	8.97433500	-5.41704900
H	-0.88143600	8.96290200	-4.34119300
C	-3.01464600	8.56405600	-3.05586000
H	-2.95334500	8.33188200	-4.12318900
H	-4.05216900	8.42753300	-2.75096200
H	-2.76388700	9.62476800	-2.93591400
C	-3.86141800	7.20530300	-0.57399100
C	-3.97896100	6.62192900	0.82537200
H	-3.51672600	7.28810900	1.56439200
C	-3.27053300	5.28207900	0.88376200
H	-4.13264900	8.26573900	-0.55772400
O	-1.86430400	5.48161800	0.61631900
H	-4.57987400	6.70549800	-1.23770700
H	-5.03013000	6.49847900	1.10475100
H	-3.64729900	4.61466000	0.09710500
C	-3.40416700	4.61159100	2.23408900
H	-4.44199400	4.29033300	2.36927700
H	-2.74689100	3.74589600	2.32102900
H	-3.15818600	5.31148500	3.03975200
C	2.14811200	7.97243700	-6.48668100
H	2.58919300	8.50455900	-7.33755000
H	2.90428900	7.28480500	-6.09383400
H	1.30843400	7.37441900	-6.85903400
C	0.63397800	9.90569200	-6.05698500
H	1.08845900	10.43896600	-6.89883400
H	-0.22709700	9.35016400	-6.44578200
H	0.27103600	10.65583400	-5.34534300
C	2.86405900	9.83101600	-4.94822900
H	2.54996300	10.54847700	-4.18262800
H	3.66702700	9.21952900	-4.52503700
H	3.28167400	10.39064900	-5.79317400
C	0.23262300	3.22812900	2.31244800
O	0.68397200	4.38736500	2.76113500
O	-0.82538000	2.72917500	2.65161100
C	-0.17327800	5.18193900	3.57322300
H	0.48620100	5.85543500	4.11869100
H	-0.84020700	5.75202800	2.92390500

H	-0.75333800	4.55659500	4.25567300
H	2.98605300	7.21131000	-3.77603100
H	2.15935800	5.94148600	-1.89293300
C	2.94380300	-0.70277800	-3.30815600
H	3.15615000	-1.68073200	-2.86285000
H	2.09784000	-0.83588900	-3.99346900
H	3.80947900	-0.40945900	-3.90800500
C	-0.81535300	3.16097500	-1.07728900
C	-1.12511100	3.29311600	-2.44758600
C	-1.75703300	2.51820300	-0.27293100
C	-2.36959700	2.86559800	-2.93932800
C	-2.96491400	2.04317800	-0.77938600
H	-1.57755500	2.40083200	0.78646500
C	-3.29011300	2.23700900	-2.11651200
H	-2.59361900	3.01621200	-3.98927900
H	-3.65887700	1.53893300	-0.11202900
H	-4.23683800	1.88904700	-2.51836100
C	-0.14472200	3.83309500	-3.43123500
O	1.04540700	3.94528400	-3.24078800
O	-0.72044800	4.15831100	-4.60020100
C	0.17310900	4.62670800	-5.60919500
H	0.90305600	3.85327400	-5.85657200
H	-0.45421800	4.84582300	-6.47277500
H	0.69103600	5.52501500	-5.26672200

TS69

Pd	0.75435800	4.09781900	-0.58021100
N	-0.31013800	5.96584200	-1.17437000
C	-1.58483400	6.12389900	-0.87718800
C	0.27939700	6.86639100	-2.03326200
C	-2.42707100	7.10875000	-1.47771500
C	-0.46740800	7.88841200	-2.66072200
C	-1.86840400	7.96717200	-2.39690900
N	-0.47653900	-0.58105100	-2.57054900
C	-1.54973300	-0.62301800	-3.45593500
C	-1.47713900	0.08958200	-4.64788000
C	-2.75034100	-1.25758700	-3.14442300
C	-2.56820900	0.20414200	-5.49560800
C	-3.82897000	-1.17209800	-4.00939600
C	-3.76578200	-0.44192600	-5.19749000
C	-5.02211100	-0.29255800	-6.01928600
F	-4.96861700	-1.76133200	-3.65316600
F	-2.90236700	-1.88111300	-1.98413300
F	-0.35285500	0.74461500	-4.94283800
F	-2.42923300	0.96556200	-6.57805400
F	-4.79508800	0.26243600	-7.21207300
F	-5.90784000	0.48822700	-5.37301600
F	-5.61039000	-1.47565400	-6.23132900
C	0.11984700	-1.69774100	-2.02432100
O	-0.25952300	-2.82712100	-2.24815100
C	1.28606400	-1.38108100	-1.08323400
H	0.88646900	-1.48438100	-0.06790200
H	2.01493300	-2.18499900	-1.21739400
C	1.87547400	-0.00920800	-1.28695400
C	2.72397100	0.27460500	-2.37385500
C	1.48934200	1.04817300	-0.46708200
C	3.23351700	1.56802500	-2.52147900
C	1.87743300	2.35992200	-0.73947900
C	2.84615100	2.62896800	-1.70489400
H	3.93450600	1.76789800	-3.32731000
H	3.26408800	3.62279000	-1.83738900
C	1.22361300	2.57676400	1.20708600
C	2.50496100	2.63443700	2.06835700
C	0.99787700	1.06372300	0.93917500
C	3.27736200	1.36316400	1.68419300
C	2.07452700	2.22276500	3.50552500
H	3.00880500	3.59516600	2.00619200
C	2.06803900	0.42918800	1.87830300
H	-0.00851800	0.69331900	1.14267000
H	4.07779900	1.15167700	2.40025600
H	3.70306400	1.36599900	0.68085000
H	2.94236400	2.32852800	4.16391200

H	1.28037200	2.83889000	3.93069900
C	1.67169700	0.72939100	3.33911800
H	2.23731500	-0.62917500	1.66605600
H	2.22409100	0.08538400	4.02989800
H	0.60325800	0.56847800	3.51274900
H	-0.01956400	0.31528300	-2.45452300
C	0.19110700	8.78976700	-3.53795000
C	1.53925400	8.70312500	-3.79990000
C	2.25790600	7.65634600	-3.16763400
C	1.65462000	6.75945500	-2.32810900
C	2.27274800	9.65458100	-4.74775900
H	-0.39702200	9.57117200	-4.00224000
C	-2.69803800	8.98886600	-3.12933900
H	-2.53329700	8.90547400	-4.20833200
H	-3.76622900	8.86777200	-2.95072800
H	-2.41799200	10.00661100	-2.83348900
C	-3.89636300	7.16548500	-1.11343000
C	-4.20837800	6.34374700	0.13049200
H	-3.88966300	6.87747600	1.03475900
C	-3.47104900	5.01862000	0.08117400
H	-4.20416200	8.20345800	-0.95289100
O	-2.05196500	5.27934700	0.05645100
H	-4.48900600	6.78796000	-1.95756600
H	-5.28558700	6.16878700	0.21629400
H	-3.70853200	4.47723100	-0.84436700
C	-3.75773900	4.14016300	1.28073200
H	-4.78470400	3.76699900	1.21345600
H	-3.07118900	3.29494500	1.32459300
H	-3.65799700	4.70500500	2.21370500
C	2.86987900	8.83910500	-5.91129900
H	3.40794900	9.49955300	-6.60129900
H	3.57485100	8.08046400	-5.55701800
H	2.07947600	8.32853500	-6.47363100
C	1.34322700	10.72405600	-5.33636600
H	1.91286100	11.37718400	-6.00614600
H	0.53063900	10.27864500	-5.92185400
H	0.90350400	11.35404300	-4.55482600
C	3.40562600	10.36378100	-3.98135700
H	3.00349500	10.94867200	-3.14697900
H	4.12936500	9.65096700	-3.57380100
H	3.94682300	11.04418900	-4.64907600
C	0.07117400	3.28182300	1.90578100
O	0.37940800	4.50577600	2.32279400
O	-0.97167500	2.72148900	2.18574700
C	-0.62413100	5.20337700	3.05257500
H	-0.12614100	6.08448000	3.45531800
H	-1.42740300	5.49659700	2.37477400
H	-1.02373800	4.58013500	3.85683400
H	3.32174600	7.53421800	-3.34681400
H	2.25080700	5.96707400	-1.89477400
C	3.08750800	-0.80065500	-3.36517200
H	3.54052900	-1.67244300	-2.87912700
H	2.19800900	-1.15493600	-3.90075600
H	3.79523500	-0.42556600	-4.10888700
C	-0.76225500	3.11834500	-1.50956500
C	-1.07970300	3.41828900	-2.84833100
C	-1.64313200	2.28301700	-0.82020400
C	-2.28238400	2.97611800	-3.41727400
C	-2.82086000	1.81296800	-1.39936600
H	-1.44936700	2.02862700	0.21299100
C	-3.16224000	2.18081200	-2.69684900
H	-2.50423200	3.24450700	-4.44504900
H	-3.47651700	1.16711800	-0.82127800
H	-4.08107300	1.82725100	-3.15648500
C	-0.14167800	4.18181800	-3.71868800
O	1.06602400	4.14063900	-3.64285700
O	-0.78810300	4.92089100	-4.63551100
C	0.05150100	5.63822900	-5.53994400
H	0.63570400	4.94470400	-6.15074900
H	-0.62420800	6.22121800	-6.16572100
H	0.73016800	6.29483000	-4.99280700
O	2.26255000	5.24618500	0.43767300
C	3.46850500	5.54352300	0.11078700

C	4.26458600	6.19729800	1.23627600
H	3.63701200	6.89135800	1.80091700
H	4.60774700	5.42128000	1.93131400
H	5.13981000	6.71111300	0.83388300
O	4.00929400	5.34582400	-0.98470500

TS44

N	0.10907200	0.24441400	-1.97281400
C	-0.77410200	1.22641600	-1.53712900
C	-1.02070500	2.33881900	-2.33638700
C	-1.34141200	1.20545900	-0.26168600
C	-1.81566800	3.39051000	-1.90211700
C	-2.16471100	2.23754400	0.15645700
C	-2.42226900	3.34833200	-0.64849500
C	-3.27798300	4.45731000	-0.08668100
F	-2.67743200	2.17615300	1.38308800
F	-1.04304000	0.23643800	0.59664600
F	-0.44674600	2.40950200	-3.53765000
F	-1.97616000	4.41976900	-2.72666500
F	-3.55868700	5.39886200	-0.98972600
F	-2.65558800	5.05542300	0.94270100
F	-4.44212700	3.97851900	0.37203100
C	-0.10049000	-1.11546000	-1.83208700
O	-1.15879200	-1.57670100	-1.45989000
C	1.11217900	-1.98921200	-2.16259700
H	1.11905900	-2.77167100	-1.41013900
H	0.87262400	-2.49719400	-3.09833900
C	2.39350500	-1.19066700	-2.29659600
C	2.78580700	-0.90983500	-3.61003800
C	3.00944300	-0.50649700	-1.17982500
C	3.68455600	0.13567200	-3.85987100
C	3.814448300	0.65450000	-1.49017200
C	4.12599800	0.93722500	-2.84278900
H	3.99790900	0.34056400	-4.87873800
H	4.74137800	1.80106500	-3.06092300
C	3.99927100	-1.46726800	0.93440800
C	3.51613000	-2.81854900	1.52796100
C	2.73172200	-0.80717300	0.33297800
C	2.35528800	-3.16895900	0.59679000
C	2.74545400	-2.52424600	2.83328600
H	4.30383200	-3.56358600	1.64235900
C	1.64361900	-1.81189700	0.77304600
H	2.58167400	0.14469800	0.83911800
H	1.75884600	-4.01843100	0.95000900
H	2.70623100	-3.36531700	-0.41731300
H	2.43810200	-3.47021500	3.29367100
H	3.33005100	-1.98005000	3.57970800
C	1.52133500	-1.72372200	2.31495800
H	0.66949200	-1.69506900	0.30922700
H	0.57911200	-2.17395400	2.64141400
H	1.52962000	-0.68549700	2.65965200
H	0.94528200	0.55616700	-2.45040300
Pd	5.13258200	-1.58818900	-0.77226500
Pd	5.23476100	1.23075100	-0.22544900
I	6.70849400	-1.75036200	-3.06944700
C	8.28283000	1.94077900	0.44535900
C	6.74660900	2.72422300	1.97495600
C	8.53609700	1.35274000	-0.81523400
C	9.36712100	2.34843500	1.25344000
C	7.76163700	3.16431700	2.87912400
C	9.82258500	1.16725700	-1.24122100
C	10.68776600	2.14506300	0.77018600
C	9.07520300	2.93793500	2.52737600
C	7.33645500	3.83705100	4.16959000
C	4.99524500	3.23389500	3.51624400
H	9.97518500	0.70017900	-2.20894000
H	11.51608600	2.46548900	1.39080500
C	5.88296100	4.31487600	4.11143500
H	7.45352300	3.12935500	5.00223800
H	5.53156700	4.57858900	5.11431500
C	6.03703600	-4.34472300	-0.13552700
C	7.55030200	-2.84523700	0.75490500

C	6.71207100	-5.46403200	0.43262200
C	8.23089000	-3.86931300	1.44403600
C	8.04746500	-1.52782300	0.80854200
C	4.30646800	-5.73595900	-1.05736900
C	6.22830000	-6.85406600	0.07760400
C	7.77729100	-5.21521200	1.27121900
C	9.34251000	-3.51756300	2.25863100
H	7.53732900	-0.76621100	0.23121700
C	9.14235600	-1.23332100	1.56806700
C	5.35870300	-6.82474300	-1.17763700
H	7.08298500	-7.51672100	-0.08925600
H	9.84055500	-4.30328900	2.81375000
H	9.50482100	-0.21142600	1.57816600
H	4.87105700	-7.79300000	-1.32875000
N	6.98874600	2.09038900	0.85093900
N	6.41635500	-3.10026000	0.04212100
H	5.07328500	2.30532100	4.09761300
H	5.80207900	5.21189500	3.48513000
H	7.99109700	4.68659500	4.38815700
O	5.45172200	2.93856500	2.19338100
H	7.69673300	1.04617200	-1.43626700
O	4.94385900	-4.46288800	-0.89582600
H	5.97298300	-6.61729800	-2.06241100
H	5.65632500	-7.28068400	0.91308800
C	3.49445700	2.39471600	-0.65474200
C	2.16753900	2.39096700	-0.19244200
C	4.05298300	3.67363500	-0.91925200
C	1.43852200	3.55654800	0.00985100
H	1.66258700	1.45426800	0.00054700
C	3.32696300	4.84507500	-0.67153000
C	2.01608800	4.79863200	-0.22383700
H	0.41148200	3.48919500	0.35943600
H	1.45699100	5.71457100	-0.06034700
C	2.24270800	-1.66265800	-4.80434400
H	1.18913500	-1.43234000	-5.00592800
H	2.81124900	-1.39673900	-5.69890400
H	2.33322100	-2.74631800	-4.67443600
C	3.53812200	3.61581800	3.35689400
H	3.44473900	4.51079200	2.73296700
H	3.00450500	2.79722500	2.86807600
H	3.08521400	3.80943300	4.33453700
C	10.21429800	3.30697800	3.44194900
H	10.79787900	4.13658700	3.02565400
H	9.87154000	3.59996800	4.43497100
H	10.89714000	2.45963500	3.56565800
C	10.93783900	1.56222800	-0.45392500
C	12.34865000	1.34418600	-1.00802500
C	13.43874200	1.77868800	-0.01927900
H	14.42524400	1.59796200	-0.45946200
H	13.37342500	2.84790100	0.21291100
H	13.38661600	1.21462400	0.91916800
C	12.50789500	2.17017500	-2.29963800
H	11.78051300	1.87344800	-3.06178200
H	12.36836800	3.23828400	-2.09911900
H	13.51012300	2.02770200	-2.72067400
C	12.54979100	-0.14981300	-1.32818400
H	13.55747300	-0.31609900	-1.72653900
H	12.43007700	-0.76159900	-0.42868900
H	11.83413000	-0.50992900	-2.07330300
C	8.49007600	-6.33122000	1.98864300
H	8.00092500	-7.29591500	1.85056000
H	9.52496300	-6.42145300	1.63905100
H	8.52557500	-6.13235600	3.06500000
C	9.79681300	-2.22198900	2.35076300
C	10.94707200	-1.78815200	3.26328000
C	11.54949900	-2.96174000	4.04535800
H	12.36002100	-2.60184600	4.68846300
H	10.80555400	-3.44441600	4.68942300
H	11.96996700	-3.71902400	3.37407300
C	12.06124800	-1.14094800	2.42023200
H	12.88349700	-0.80858800	3.06574700
H	12.46425200	-1.85710700	1.69557000
H	11.69456100	-0.27059800	1.86650000

C	10.40895200	-0.75313200	4.27195900
H	9.97471300	0.11624000	3.76550500
H	9.63174100	-1.19517900	4.90595900
H	11.21689700	-0.39796300	4.92301900
C	4.65407100	-0.66048400	2.02129200
O	4.22588600	0.35942100	2.52576400
O	5.74185400	-1.28721900	2.50347100
C	6.42416800	-0.64228000	3.56773300
H	5.74157900	-0.43017900	4.39561200
H	7.20627600	-1.33674500	3.87514600
H	6.87836900	0.29112900	3.22093700
C	3.42214700	-5.60185300	-2.28241900
H	2.87633600	-6.53473200	-2.45492200
H	2.69765900	-4.79325500	-2.15043700
H	4.03294900	-5.37291800	-3.16092300
H	3.69215600	-5.90886700	-0.16110500
H	3.81014300	5.80310300	-0.83582400
C	5.45155200	3.88414400	-1.41840800
O	6.11075700	4.76340600	-0.64157600
O	5.94861700	3.40788900	-2.41661100
C	7.44242300	5.06052000	-1.05690200
H	7.84298500	5.72687900	-0.29293900
H	8.03761600	4.14681700	-1.12009900
H	7.44057600	5.55342900	-2.03286900

N2-L2-Ar₃

Ar₃I

C	-2.40832700	1.79162500	-0.28163100
C	-2.79609200	3.12247900	-0.33229100
C	-3.38852900	0.79920000	-0.21500500
C	-4.14173900	3.47952100	-0.31314100
C	-4.74089300	1.14165200	-0.19713300
C	-5.11010800	2.48090000	-0.24403500
H	-4.43618600	4.52249700	-0.35391800
H	-5.49352500	0.36366200	-0.14759900
H	-6.16027100	2.75522300	-0.22966100
C	-2.92154500	-0.61774100	-0.17017100
O	-1.75834900	-0.95072000	-0.16366300
O	-3.93975700	-1.48962900	-0.14074600
C	-3.56332300	-2.86515100	-0.10031100
H	-4.49855100	-3.42413000	-0.10223100
H	-2.95888900	-3.12317200	-0.97334000
H	-2.99012300	-3.07858300	0.80529800
H	-1.36542400	1.49646800	-0.29496500
I	-1.31329300	4.64155400	-0.46071400

Ar₃Pd(I)(L2)₂

Pd	0.53165200	1.15414800	0.16603300
I	-0.77403600	-0.90813200	-0.89440800
C	0.57729900	3.82610800	1.57852300
C	2.22178800	3.69132200	-0.03307000
C	0.37544200	5.21818800	1.35634100
C	2.09850600	5.06204500	-0.34225400
C	3.14164800	2.90071400	-0.75804100
C	-1.00117800	3.81615900	3.39517300
C	-0.73699400	5.93100600	2.09479900
C	1.13592500	5.83107200	0.38389900
C	2.83674800	5.58120900	-1.43706400
H	3.23997800	1.85152200	-0.50301700
C	3.84317300	3.44476600	-1.79989300
C	-1.73433300	4.93987200	2.68686200
H	-0.31907900	6.56333000	2.89066200
C	3.67523900	4.79820800	-2.19443900
H	2.68055000	6.61580400	-1.71258900
H	4.52592800	2.80676000	-2.35416900
H	-2.34408900	4.50610500	1.88695100
C	2.71743800	-0.96764000	0.39593700
C	1.76533800	-0.70866500	2.47328800
C	3.25718100	-2.24767800	0.71878800
C	2.32404600	-1.92243800	2.92904600

C	0.98486300	0.06729500	3.36008200
C	3.54252300	-1.06352800	-1.88805300
C	3.91196900	-3.02882900	-0.39887200
C	3.07866600	-2.71250100	2.00152900
C	2.08071400	-2.32650600	4.26745200
H	0.57046900	1.00304300	2.99959300
C	0.77787900	-0.35704500	4.64498300
C	3.35767700	-2.56273000	-1.74501400
H	5.00329900	-2.89931500	-0.37947400
C	1.32035800	-1.57480600	5.13419200
H	2.50653800	-3.26346000	4.60434100
H	0.17940400	0.26308200	5.30723600
H	2.28803600	-2.79694400	-1.81404300
C	0.91608700	7.27835200	0.03025200
H	1.86090100	7.78480800	-0.18253500
H	0.28448600	7.34924100	-0.86510200
H	0.42563500	7.82955700	0.83385600
C	4.38637200	5.30513500	-3.45067900
C	3.99568400	6.74903200	-3.79143400
H	4.51183900	7.06327100	-4.70514700
H	2.91761700	6.82711300	-3.97049400
H	4.27774200	7.44992700	-2.99697400
C	3.98077900	4.41560500	-4.64331100
H	4.45162300	4.78354800	-5.56283600
H	4.29725800	3.37647700	-4.50393900
H	2.89438300	4.42654500	-4.77346100
C	5.91062200	5.23981200	-3.24213100
H	6.21880000	5.87617700	-2.40485600
H	6.24774200	4.21920700	-3.03099100
H	6.43175600	5.58286100	-4.14377300
C	3.65271700	-4.02955700	2.45391700
H	4.30687900	-4.47764000	1.70530300
H	4.24343900	-3.89668400	3.36631000
H	2.85488700	-4.74541900	2.68281600
C	1.03872300	-1.99315600	6.58058500
C	-0.48258300	-2.13453300	6.78150500
H	-0.70276900	-2.43687800	7.81221200
H	-1.00723000	-1.19249100	6.59150600
H	-0.89489400	-2.89026000	6.10438500
C	1.58717700	-0.91798300	7.53856700
H	2.66788600	-0.79547300	7.40765200
H	1.11654700	0.05619000	7.36975800
H	1.39674100	-1.20282800	8.58009400
C	1.69665700	-3.33278600	6.93793500
H	1.32400800	-4.14813400	6.30783200
H	2.78712400	-3.28723600	6.83838300
H	1.47006500	-3.58767000	7.97899100
N	1.41555500	3.08189400	0.88968200
N	1.96419800	-0.25603100	1.20028900
O	-0.14537900	3.13112800	2.47152800
O	2.93532000	-0.37412400	-0.78397700
H	-1.26685200	6.59490800	1.40564200
H	-2.40508000	5.44313000	3.39072900
H	-0.36177600	4.23119600	4.18833500
H	3.86839200	-3.06787900	-2.57119300
H	3.71592500	-4.09741200	-0.27590300
C	-1.92167000	2.75596300	3.96813700
H	-1.34513700	1.94583700	4.42316600
H	-2.57255400	3.19372400	4.73129500
H	-2.54273700	2.32911200	3.17468600
C	-0.73604500	2.37561800	-0.74410700
C	-0.26855100	3.21305500	-1.75774700
C	-2.01333600	2.60851000	-0.22800700
C	-0.99845700	4.34033200	-2.14695700
C	-2.76814100	3.70362000	-0.65345200
H	-2.41749300	1.93769900	0.52470000
C	-2.25263600	4.59623900	-1.58549000
H	-3.75999600	3.86732400	-0.23914900
H	-2.81672300	5.47135600	-1.88879400
H	0.70155400	3.05014800	-2.21736000
C	-0.36425900	5.26900500	-3.11645800
O	0.61140700	5.02327600	-3.79245400
O	-0.97540000	6.47407700	-3.15047100

C	-0.41050200	7.41413500	-4.05705800
H	-0.34055600	6.99206900	-5.06231000
H	-1.07987100	8.27457200	-4.04645000
H	0.59082900	7.70994600	-3.72869800
C	2.91114200	-0.47113500	-3.13421000
H	3.36800900	-0.90027300	-4.03196700
H	1.83594600	-0.67522400	-3.13704700
H	3.05087400	0.61423900	-3.15195700
H	4.61617400	-0.82708000	-1.85460000

TS35

Pd	1.80062000	3.48786400	0.45817800
N	0.36190800	-0.79359200	-2.61127700
C	-1.02730700	-0.84312800	-2.77178400
C	-1.58315400	-0.71626300	-4.04325000
C	-1.90124600	-0.96640300	-1.69482500
C	-2.95470800	-0.68433500	-4.22167400
C	-3.27727800	-0.90745600	-1.87421800
C	-3.83287400	-0.75537700	-3.14182700
C	-5.31156400	-0.65117200	-3.41883700
F	-4.03496300	-0.96664600	-0.77836400
F	-1.44496200	-1.10394100	-0.45577500
F	-0.79224900	-0.61575600	-5.10703200
F	-3.43574000	-0.57528600	-5.46279400
F	-5.72406000	-1.64268600	-4.22030600
F	-5.59208300	0.50795200	-4.04387600
F	-6.05270600	-0.69246300	-2.31011100
C	1.05532100	-1.77359000	-1.94080400
O	0.54478700	-2.82692300	-1.61384300
C	2.52644900	-1.46507600	-1.65352300
H	2.70497700	-1.86891800	-0.65252100
H	3.11088300	-2.08979200	-2.33519600
C	2.92561100	-0.01021700	-1.74799500
C	3.71741400	0.46124500	-2.80591400
C	2.41986800	0.89288900	-0.79574200
C	3.99532300	1.82689100	-2.86671000
C	2.64852000	2.27045500	-0.90936900
C	3.46612900	2.72462900	-1.94452100
H	4.62066800	2.20525800	-3.67211500
H	3.68050800	3.78000300	-2.06874900
C	0.82043900	1.67909300	0.95637100
C	0.94935600	1.41732500	2.46603700
C	1.55171500	0.45958400	0.33263700
C	2.42380600	0.98126800	2.54209900
C	0.22106700	0.09125100	2.82504500
H	0.65570100	2.25595800	3.09650200
C	2.25160200	-0.19068300	1.56305400
H	0.79779500	-0.24173200	-0.03580600
H	2.72200300	0.64806800	3.54329500
H	3.11909000	1.75248700	2.19926400
H	0.09726800	0.01673700	3.91055800
H	-0.77736500	0.03618300	2.38383200
C	1.17349700	-1.01636900	2.28480500
H	3.16108000	-0.74343200	1.31306400
H	1.61290500	-1.59452300	3.10508600
H	0.67077600	-1.71894700	1.61243300
H	0.80617500	0.09616300	-2.80972400
I	2.59108000	5.99815000	-0.60841900
C	2.85876200	4.87514100	2.93404600
C	0.61321100	5.23286600	3.25561800
C	3.23809400	5.85697200	3.89607300
C	0.86704800	6.19411000	4.25953300
C	-0.72451300	4.88408200	2.96159200
C	5.17058900	4.27941600	2.48665000
C	4.71242400	6.15328100	4.06927000
C	2.22975800	6.51226000	4.56736200
C	-0.23351500	6.81323300	4.90717400
H	-0.90911800	4.10509400	2.23013900
C	-1.75813100	5.50003900	3.61553400
C	5.49776600	5.72049100	2.83167800
H	4.86429100	7.22357800	4.23434600
C	-1.53844400	6.49717900	4.60260100

H	-0.02802300	7.56041300	5.66339900
H	-2.77440800	5.20443400	3.37020400
H	6.57395300	5.81984300	3.00457100
N	1.62281000	4.61075900	2.57766800
O	3.75922000	4.13745900	2.26956600
C	-2.74098500	7.16126300	5.27972300
C	-3.57821600	6.08569800	5.99860500
H	-2.98284900	5.57532700	6.76340700
H	-4.44514000	6.54483900	6.48767900
H	-3.95263300	5.32756200	5.30303600
C	-3.60393100	7.85527800	4.20787400
H	-4.47254400	8.33573800	4.67284400
H	-3.02784000	8.62404700	3.68127400
H	-3.97695300	7.14499600	3.46259200
C	-2.31929000	8.21410500	6.31354300
H	-3.21126300	8.66266900	6.76505700
H	-1.72653300	7.77424000	7.12313100
H	-1.73920200	9.02316300	5.85609400
C	2.51969600	7.54416100	5.62541300
H	3.58620300	7.65642100	5.82070400
H	2.12264900	8.52307500	5.33393500
H	2.04056600	7.26667900	6.57041200
H	5.23591100	6.35626800	1.97641500
H	5.10486500	5.63744200	4.95630300
H	5.43093700	3.63039500	3.33479200
C	5.82674100	3.76923000	1.21788800
H	6.91431000	3.74302500	1.33849800
H	5.47048100	2.76167400	0.98507400
H	5.57242200	4.41912900	0.37494300
C	-0.54007600	1.82670300	0.36919500
O	-0.83770800	1.57539100	-0.78191400
O	-1.46663500	2.24789900	1.25993900
C	-2.80783200	2.26506700	0.77957900
H	-3.11945000	1.25798300	0.49027600
H	-3.41245200	2.62099500	1.61480100
H	-2.90303200	2.93326300	-0.07840800
C	0.54247500	4.70859300	-0.93916300
C	0.34267400	4.03675100	-2.13861000
C	-0.50528900	5.36335000	-0.29391700
C	-0.94917500	3.94618200	-2.64712800
H	1.14753500	3.52820900	-2.65151000
C	-1.78459900	5.29376800	-0.84281400
H	-0.33114400	5.93070500	0.61155600
C	-2.01612600	4.59080600	-2.01770800
H	-2.60093100	5.80340500	-0.33898400
H	-3.01157700	4.52329400	-2.44055800
C	-1.14462700	3.05873000	-3.82804900
O	-0.30961400	2.28140600	-4.23802900
O	-2.35831600	3.22008400	-4.37214200
C	-2.68614400	2.43750800	-5.52023500
H	-3.66892000	2.00051700	-5.34290500
H	-2.72351700	3.10216100	-6.38702200
H	-1.94084300	1.65904000	-5.68100300
C	4.24668300	-0.46092900	-3.87852900
H	4.81175700	0.10254100	-4.62631500
H	4.91482300	-1.22811100	-3.46913100
H	3.43379300	-0.97833200	-4.40177900

TS36

Pd	2.50596300	3.29096300	0.37257000
N	-0.31026300	-0.65950300	-2.04432900
C	-1.67669200	-0.56193800	-1.79419700
C	-2.50956500	0.01850800	-2.74624700
C	-2.23618900	-0.92330000	-0.56747400
C	-3.85810700	0.23574100	-2.50222600
C	-3.58896200	-0.72747100	-0.33483700
C	-4.42784100	-0.15024700	-1.29003600
C	-5.87736800	0.07678900	-0.93139200
F	-4.07901900	-1.07301900	0.85194400
F	-1.47797500	-1.40526500	0.40389900
F	-1.98585700	0.41192000	-3.90825800
F	-4.56989800	0.81751600	-3.46227200

F	-6.43637400	-1.04739800	-0.46550500
F	-6.60674800	0.48698100	-1.97127000
F	-5.98379000	1.00818300	0.03016500
C	0.45753700	-1.77455600	-1.77181500
O	-0.01821900	-2.83337100	-1.42584800
C	1.96668300	-1.56575000	-1.93211000
H	2.40044600	-1.99469600	-1.02608400
H	2.28813400	-2.21779000	-2.74833300
C	2.38183700	-0.12887800	-2.15539500
C	2.65917200	0.33089800	-3.45261900
C	2.32191100	0.78618000	-1.08344300
C	2.89170200	1.69578600	-3.65268800
C	2.45225200	2.15892600	-1.33346100
C	2.76521300	2.60733200	-2.62015500
H	3.12674700	2.05581300	-4.65049800
H	2.88127600	3.66670600	-2.81455100
C	2.07589800	1.48457900	1.37084400
C	3.29130500	1.23478800	2.29553300
C	2.15322300	0.31779000	0.33728300
C	4.33489400	0.70105500	1.30763100
C	3.01309800	-0.03660400	3.14239100
H	3.56950200	2.09204400	2.90016900
C	3.44193500	-0.43885600	0.80590100
H	1.27616000	-0.33184800	0.43787800
H	5.24180900	0.33681100	1.80327000
H	4.61759800	1.41586700	0.52842700
H	3.79057700	-0.12630000	3.90856500
H	2.05349900	-0.00561000	3.66475400
C	3.10538300	-1.18818200	2.10630100
H	3.88380900	-1.06339500	0.02817300
H	3.90208900	-1.89338600	2.36321000
H	2.17343300	-1.75584600	2.02174700
H	0.13764700	0.14252600	-2.46798500
I	4.06129500	5.41640600	-0.74037900
C	3.64585800	4.81183700	2.75534500
C	1.38917600	5.28198000	2.61409200
C	3.88263900	5.86344300	3.69166900
C	1.50224100	6.29241300	3.59696800
C	0.12134700	5.02962100	2.05404100
C	5.97528800	4.15222300	2.77850400
C	5.31403900	6.16986500	4.07369800
C	2.79898200	6.57988800	4.13722800
C	0.34381100	7.01117300	3.97335400
H	0.01592800	4.24533700	1.31799200
C	-0.97922100	5.75498500	2.43800800
C	6.27143600	5.61992400	3.01996300
H	5.45215700	7.25114100	4.16090000
C	-0.89542900	6.77453800	3.41326300
H	0.44340700	7.78982600	4.72236500
H	-1.92733500	5.52344700	1.96636800
H	7.30993900	5.73298800	3.34649800
N	2.47821700	4.54909600	2.21551400
O	4.61517400	3.99416600	2.33439600
C	-2.11236000	7.60003100	3.85209000
C	-3.38442300	7.20849300	3.08588000
H	-3.65841400	6.16174000	3.25851300
H	-4.22143300	7.82829400	3.42492800
H	-3.27214000	7.36407700	2.00713800
C	-1.83808900	9.09365800	3.59298300
H	-2.70261400	9.69651500	3.89511600
H	-0.96948100	9.45195100	4.15514600
H	-1.64729100	9.27508300	2.52984000
C	-2.36445500	7.37402600	5.35489700
H	-3.23570400	7.95081900	5.68685700
H	-2.55607800	6.31531400	5.56197300
H	-1.50666100	7.68546600	5.96046600
C	2.94550900	7.67082300	5.16483300
H	2.74459800	8.65235400	4.71997700
H	2.23015600	7.52817300	5.98112400
H	3.94231500	7.69569400	5.60580100
H	6.15065900	6.16062300	2.07344000
H	5.55246300	5.73722400	5.05540600
H	6.06496500	3.59968800	3.72521000

C	6.84455200	3.51296400	1.71418500
H	7.89702400	3.57549700	2.00903100
H	6.58240300	2.45971300	1.58426400
H	6.70414300	4.02619000	0.75842600
C	2.67382600	-0.60349300	-4.63873500
H	1.70366800	-1.09505600	-4.77858200
H	2.90057100	-0.05701000	-5.55776900
H	3.42763000	-1.39167000	-4.52791700
C	0.79920500	1.52154900	2.16763400
O	-0.19341400	0.85838100	1.94521400
O	0.88890100	2.33555300	3.22795100
C	-0.27717600	2.42184200	4.04143200
H	-0.05502000	3.18544200	4.78659900
H	-1.14095400	2.72000500	3.44280300
H	-0.48267600	1.45999900	4.51903400
C	0.75032200	3.24588900	-0.77594100
C	0.52052800	4.49484800	-1.35196000
C	-0.31718000	2.37192500	-0.57883800
C	-0.78803300	4.89658000	-1.62942700
C	-1.61909700	2.78892400	-0.84768500
H	-0.17014000	1.37982500	-0.17864100
C	-1.86720900	4.05426700	-1.36176400
H	-2.44103200	2.11051400	-0.63850100
H	-2.87876500	4.38358800	-1.56828600
H	1.32675900	5.18809200	-1.56105700
C	-0.97362100	6.26077200	-2.20528900
O	-0.07261500	7.00845700	-2.50429200
O	-2.27230000	6.57481800	-2.35592200
C	-2.52011200	7.86902100	-2.89936200
H	-3.60358800	7.95177000	-2.98249000
H	-2.12567300	8.64365700	-2.23658400
H	-2.05048700	7.97143000	-3.88069200

TS40

Pd	2.35454300	3.09389000	0.80721500
N	-0.29650600	-0.44240000	-2.28107800
C	-1.65459100	-0.50408100	-1.98213000
C	-2.55717800	0.23347600	-2.74765700
C	-2.14212500	-1.18146300	-0.86719500
C	-3.89734800	0.28645200	-2.41563000
C	-3.49805600	-1.15231300	-0.55220800
C	-4.39928600	-0.41383500	-1.31710200
C	-5.87307300	-0.29220400	-1.01130400
F	-3.88455100	-1.82448300	0.52560100
F	-1.31351600	-1.81881800	-0.05483100
F	-2.10437100	0.92937100	-3.79142200
F	-4.71401100	1.02134400	-3.16718700
F	-6.24851500	-1.03016900	0.03428200
F	-6.61187100	-0.67355900	-2.06268300
F	-6.19023400	0.98455300	-0.74038000
C	0.55605300	-1.52939900	-2.30707400
O	0.16829600	-2.67253000	-2.20984800
C	2.04022300	-1.17567100	-2.46048400
H	2.54157000	-1.75462400	-1.68188500
H	2.36942200	-1.60734800	-3.40906300
C	2.33483900	0.30450300	-2.37007000
C	2.52988200	1.06310500	-3.53456000
C	2.22367100	0.94832200	-1.12011000
C	2.63187800	2.45657400	-3.42796400
C	2.14877400	2.34741100	-1.07557600
C	2.41800000	3.10015900	-2.22424000
H	2.82698600	3.04483000	-4.32042600
H	2.42079100	4.18261100	-2.16618500
C	2.16190500	1.12964600	1.42263400
C	3.47904500	0.83763800	2.18139000
C	2.22150900	0.18568200	0.17821100
C	4.45495500	0.58197800	1.02560300
C	3.38863800	-0.57825100	2.80510800
H	3.74359000	1.61302100	2.89576900
C	3.59943000	-0.52437700	0.39779800
H	1.40966000	-0.55000100	0.21076100
H	5.42637100	0.21258500	1.37284800

H	4.61844600	1.45200500	0.38363300
H	4.25418000	-0.73538300	3.45775600
H	2.49458300	-0.72669400	3.41714100
C	3.43575100	-1.51465600	1.56649700
H	4.01135200	-0.96935600	-0.50939300
H	4.29016300	-2.19738500	1.61398100
H	2.53035500	-2.12130100	1.46571800
H	0.07635900	0.46709000	-2.51842400
C	3.66402800	4.61470200	3.23187700
C	1.45282100	5.16622800	2.89853800
C	4.03083800	5.96839500	3.52237800
C	1.69241000	6.52152300	3.21517700
C	0.13036000	4.75645100	2.63852200
C	5.92776100	3.82503700	3.60858600
C	5.49540400	6.27461300	3.75055200
C	3.03938900	6.92029200	3.50513800
C	0.60965000	7.42817000	3.18993100
H	-0.05677500	3.70972000	2.43246000
C	-0.89948900	5.66498000	2.63200900
C	6.37044800	5.19213500	3.12538700
H	5.74889900	7.24136300	3.30619700
C	-0.67878300	7.03769700	2.88164700
H	0.80614900	8.47364000	3.40356900
H	-1.89717300	5.30303500	2.41107300
H	7.42138500	5.34553400	3.39053500
N	2.46535700	4.24143900	2.84212700
O	4.53545000	3.60906600	3.32477000
C	-1.79990800	8.08143100	2.80442900
C	-3.13908000	7.46064500	2.38039500
H	-3.49460200	6.72342500	3.10921500
H	-3.90081900	8.24521300	2.31061100
H	-3.07332800	6.97059800	1.40295500
C	-1.41282500	9.15284200	1.76614200
H	-2.22787200	9.87727000	1.64450700
H	-0.52112000	9.70982900	2.07279000
H	-1.19681900	8.69449900	0.79538300
C	-1.98902700	8.74058400	4.18322500
H	-2.77764100	9.50111800	4.13803300
H	-2.27356100	7.99666800	4.93554200
H	-1.07133600	9.23045800	4.52554400
C	3.32088800	8.37078000	3.79564100
H	3.08858200	8.99013100	2.92164500
H	2.69369100	8.72399200	4.62124000
H	4.35899300	8.55162800	4.07407300
H	6.28417700	5.21014400	2.03406300
H	5.70703400	6.35477200	4.82600100
H	6.03619800	3.76725600	4.70133100
C	6.66703000	2.67988500	2.94286200
H	7.73887100	2.75107900	3.15503500
H	6.30117400	1.71844300	3.31603100
H	6.50303700	2.72750700	1.86301200
C	2.60675100	0.41726900	-4.89698800
H	1.67517000	-0.10352200	-5.14907800
H	2.78294500	1.16864900	-5.67118400
H	3.41821800	-0.31703000	-4.95576700
C	0.96454500	0.88710900	2.30323400
O	0.09086400	0.06929400	2.09469100
O	0.98376500	1.64473600	3.40679300
C	-0.11211500	1.46705100	4.29776500
H	0.02823100	2.21086600	5.08150100
H	-1.06041800	1.63246900	3.77944300
H	-0.10912900	0.45756000	4.71756100
C	0.51895400	3.06935300	-0.24040400
C	0.15409000	4.38282300	-0.54745700
C	-0.48112500	2.10352800	-0.10376500
C	-1.19144200	4.72282500	-0.68211500
C	-1.82339800	2.45819600	-0.21544100
H	-0.24110100	1.06897100	0.09879400
C	-2.19141900	3.76456800	-0.50699600
H	-2.58380700	1.69541100	-0.07440900
H	-3.23517200	4.03830100	-0.60674500
H	0.90210800	5.16044200	-0.65380300
C	-1.51124200	6.14420000	-0.99506700

O	-0.69096300	7.02192700	-1.14495400
O	-2.83604600	6.35366200	-1.10372800
C	-3.22473100	7.67873100	-1.45792900
H	-4.30390300	7.63659200	-1.60308600
H	-2.97693300	8.38048900	-0.65759900
H	-2.72312200	7.99238500	-2.37638800
O	2.90400700	5.07998900	0.07998600
C	4.18284400	5.05066600	0.10691800
C	4.88707700	6.34606000	-0.24835100
H	4.40331200	6.82454000	-1.10359700
H	4.80232300	7.03298100	0.60227300
H	5.94343600	6.16779400	-0.45926000
O	4.83282700	4.04473600	0.44790300

TS67

Pd	0.71850300	4.35222700	0.20573900
N	-0.44866100	6.08140000	-0.56876100
C	-1.73906400	6.14131900	-0.31211900
C	0.02364600	6.66064600	-1.72377500
C	-2.68974100	6.77355600	-1.17004200
C	-0.85415900	7.19503100	-2.69023100
C	-2.24772600	7.24632100	-2.38514500
N	-0.31199000	0.07056000	-2.97099300
C	-1.31868900	-0.00677000	-3.93870600
C	-1.11555400	0.52647000	-5.20687300
C	-2.55816000	-0.57051800	-3.65730500
C	-2.12307500	0.51427900	-6.15276700
C	-3.57137500	-0.58662600	-4.60929400
C	-3.37310500	-0.03431100	-5.87408300
C	-4.43512900	0.04836800	-6.94429400
F	-4.73693000	-1.11747500	-4.25332800
F	-2.80870900	-1.05239400	-2.44765800
F	0.05404100	1.09549500	-5.50208100
F	-1.88201100	1.04595600	-7.35086500
F	-5.58365100	-0.52247100	-6.58107200
F	-4.02552400	-0.54370300	-8.07367900
F	-4.69946700	1.33424900	-7.23966300
C	0.28385000	-1.06380000	-2.46888900
O	-0.06629500	-2.18041200	-2.78927200
C	1.39878700	-0.82500600	-1.45279800
H	0.97760100	-1.12909500	-0.48921400
H	2.17915000	-1.55426100	-1.69025100
C	1.93467800	0.58140300	-1.37199500
C	2.80412000	1.10572300	-2.34942800
C	1.53673900	1.42019200	-0.33682700
C	3.32184000	2.39435100	-2.18001500
C	1.94689900	2.75288700	-0.27208700
C	2.93317800	3.23046000	-1.13285400
H	4.04021400	2.76838500	-2.90477500
H	3.35753400	4.22234600	-1.02820600
C	1.18450500	2.51433400	1.63418000
C	2.41441400	2.31770000	2.55146800
C	0.94188400	1.12166600	0.99680500
C	3.16364100	1.12968700	1.92733800
C	1.87601200	1.60857100	3.82705200
H	2.96593700	3.23731900	2.73827700
C	1.91281500	0.23565700	1.83198200
H	-0.09561100	0.77989700	1.02360400
H	3.91018200	0.72399100	2.61715100
H	3.65227000	1.34003200	0.97570000
H	2.70339800	1.51353400	4.53679000
H	1.08223600	2.15224200	4.34099700
C	1.42482000	0.21800900	3.29533900
H	2.06320400	-0.75559700	1.39874400
H	1.89671500	-0.59816700	3.85044200
H	0.34062700	0.08196600	3.36163600
H	0.06551800	0.98486900	-2.74891100
I	2.62508700	6.00318600	1.49450700
C	-0.33114300	7.62996100	-3.93480600
C	1.00762900	7.55251800	-4.23529600
C	1.87383300	7.07231400	-3.22028300
C	1.40756500	6.64459300	-2.00624800

C	1.58502700	7.93380100	-5.59949700
H	-1.02457000	8.01104500	-4.67324200
C	-3.20272300	7.80989100	-3.40379800
H	-3.13680000	7.24072600	-4.33768900
H	-4.24006700	7.77733600	-3.07164000
H	-2.95506300	8.85126400	-3.63736900
C	-4.14305700	6.86342400	-0.75257600
C	-4.34019000	6.42787800	0.69359700
H	-4.01520500	7.21109500	1.38929700
C	-3.51378400	5.18310400	0.95564400
H	-4.50772000	7.88709900	-0.88864300
O	-2.11536100	5.51737800	0.81772200
H	-4.74914400	6.22284600	-1.40680300
H	-5.39727000	6.22594500	0.89322900
H	-3.73255700	4.42325100	0.19295400
C	-3.71571900	4.59597500	2.33542800
H	-4.73856100	4.21397000	2.41538600
H	-3.01448700	3.77802100	2.51399200
H	-3.57638900	5.36162100	3.10651600
C	0.50061600	8.40724300	-6.57603100
H	0.95846000	8.65838200	-7.53874000
H	-0.24437700	7.62395500	-6.75750200
H	-0.01395200	9.30355000	-6.21079800
C	2.61416200	9.06668800	-5.42665900
H	3.04948900	9.33286200	-6.39682100
H	2.14428600	9.96158700	-5.00386400
H	3.43502500	8.77408600	-4.76389600
C	2.26903800	6.69270300	-6.20660400
H	3.10326000	6.34771800	-5.58661100
H	1.55574700	5.86807100	-6.29786300
H	2.66981600	6.93031600	-7.19928100
C	0.00577700	3.10366500	2.39262400
O	0.37734300	4.12977100	3.14561100
O	-1.10661000	2.60824300	2.40555800
C	-0.61973100	4.84791500	3.86283700
H	-0.06856800	5.49068600	4.54737100
H	-1.19653600	5.45304900	3.16156000
H	-1.27760300	4.16511600	4.40668500
H	2.94376000	7.03198800	-3.40176500
H	2.09288200	6.30444400	-1.23897000
C	3.19217800	0.28891700	-3.55530700
H	3.62052800	-0.67991000	-3.27389000
H	2.32005100	0.08878100	-4.18877000
H	3.92963000	0.81665700	-4.16545300
C	-0.57335400	3.40763200	-1.04776400
C	-0.37616400	3.67352300	-2.40256400
C	-1.72210200	2.72795700	-0.65304200
C	-1.37310900	3.38543300	-3.33705400
C	-2.69526300	2.38500100	-1.59804300
H	-1.87931900	2.48920600	0.39433100
C	-2.54701100	2.74314500	-2.93195100
H	-3.58580600	1.85089800	-1.27836200
H	-3.32008600	2.51758500	-3.65868500
H	0.51973700	4.17222600	-2.75947200
C	-1.14528400	3.84220200	-4.73661400
O	-2.18822600	3.57428700	-5.53959000
O	-0.14681500	4.41022400	-5.11887000
C	-2.05087300	4.01424100	-6.89031800
H	-2.93159700	3.63768000	-7.40750700
H	-2.01218700	5.10637900	-6.93048700
H	-1.14162800	3.60585500	-7.33419600

TS69

Pd	0.80080200	4.38399200	0.13456200
N	-0.47723500	6.15509900	-0.40781800
C	-1.78040600	6.05589500	-0.25287300
C	0.00692500	6.71182200	-1.56622900
C	-2.73056400	6.44096600	-1.24602800
C	-0.83935800	6.99765100	-2.65606100
C	-2.24876100	6.83960300	-2.47355200
N	-0.39420600	0.17061100	-3.04815900
C	-1.43579500	0.13495800	-3.97829400

C	-1.26017200	0.68078500	-5.24595500
C	-2.68575100	-0.38282200	-3.65768900
C	-2.30446400	0.73181700	-6.14949600
C	-3.73427700	-0.34176700	-4.57025500
C	-3.56417900	0.22785300	-5.83128500
C	-4.66234800	0.37243400	-6.85721400
F	-4.90607600	-0.83139700	-4.17722600
F	-2.91370800	-0.86604600	-2.44425000
F	-0.07993500	1.20593200	-5.57743200
F	-2.08944500	1.27894600	-7.34600300
F	-5.82038000	-0.15140300	-6.45503600
F	-4.32523700	-0.22151600	-8.00937600
F	-4.88001400	1.67297300	-7.12601700
C	0.15889800	-0.98150600	-2.53613400
O	-0.25781600	-2.08573100	-2.81741400
C	1.32015300	-0.77408700	-1.56545100
H	0.93276000	-1.08046800	-0.58862600
H	2.07469500	-1.51713700	-1.84129200
C	1.88940100	0.62017700	-1.49449100
C	2.73528600	1.13091800	-2.49944000
C	1.54053100	1.46588400	-0.44535700
C	3.27923500	2.41273300	-2.35239100
C	1.98843600	2.78623900	-0.39667000
C	2.94847500	3.25201500	-1.28979300
H	3.97889600	2.77213900	-3.10242800
H	3.40688400	4.22535600	-1.17137400
C	1.26901600	2.56006000	1.54717000
C	2.52142700	2.32830800	2.42119600
C	0.97213400	1.17984300	0.90490800
C	3.21780600	1.12493800	1.77067500
C	1.99711000	1.62943300	3.70868300
H	3.12282100	3.21922700	2.57742200
C	1.94239000	0.26388900	1.70813100
H	-0.07273800	0.86368100	0.95724100
H	3.97366500	0.69694000	2.43642100
H	3.68510200	1.33708300	0.80937600
H	2.83968100	1.50917700	4.39656100
H	1.23006000	2.19025600	4.24508600
C	1.49608700	0.25255500	3.18470200
H	2.05295300	-0.72926100	1.26730900
H	1.96328400	-0.57751400	3.72312600
H	0.41110100	0.14233000	3.28210600
H	0.04382600	1.06548800	-2.86025900
C	-0.25631200	7.34693100	-3.89928300
C	1.10556900	7.43520200	-4.07011300
C	1.92368000	7.24679100	-2.92518000
C	1.40106600	6.89680700	-1.70776300
C	1.75985300	7.68501700	-5.43036900
H	-0.91306100	7.49758600	-4.74617700
C	-3.17093600	7.06920300	-3.64047900
H	-2.99660200	6.29837500	-4.40143300
H	-4.22339100	7.01630800	-3.36234300
H	-2.99242600	8.04321500	-4.10702500
C	-4.20892800	6.32228100	-0.94673500
C	-4.45660500	6.13160200	0.54554400
H	-4.28110400	7.06694600	1.09175100
C	-3.51423100	5.06868100	1.07814700
H	-4.73752800	7.21390300	-1.29923300
O	-2.15280800	5.51198500	0.91646000
H	-4.62357200	5.46693300	-1.49695900
H	-5.49367200	5.83224500	0.72711800
H	-3.62580700	4.15374400	0.48341900
C	-3.70052500	4.74814600	2.54592700
H	-4.70888100	4.35410300	2.70785900
H	-2.97187500	3.99684600	2.85842400
H	-3.57782900	5.65004000	3.15558800
C	0.72676300	7.75476000	-6.56285100
H	1.23900700	7.91509800	-7.51771500
H	0.16628200	6.81609300	-6.63572800
H	0.02112000	8.58266400	-6.42598200
C	2.54570100	9.00854100	-5.39180000
H	3.03614900	9.18607300	-6.35603500
H	1.87842600	9.85288500	-5.18539700

H	3.32249400	8.99734500	-4.62004900
C	2.71627800	6.51505100	-5.73780500
H	3.52519900	6.44621400	-5.00274500
H	2.16976700	5.56686600	-5.73592900
H	3.17648000	6.65467400	-6.72322200
C	0.14116100	3.20426600	2.33237300
O	0.58310300	4.21682200	3.07612000
O	-0.99848500	2.77663200	2.37242700
C	-0.38454100	4.99009900	3.77696400
H	0.19164800	5.67871200	4.39326000
H	-0.99557400	5.54097600	3.05960300
H	-1.01659000	4.35089600	4.39953200
H	3.00002000	7.36373800	-3.01212200
H	2.02722400	6.73568200	-0.83540600
C	3.07589000	0.30579700	-3.71466600
H	3.51261700	-0.66228600	-3.44330100
H	2.18172300	0.10373600	-4.31594100
H	3.79211300	0.82850100	-4.35368900
C	-0.51066700	3.47175900	-1.09756900
C	-0.33520400	3.76015600	-2.45274800
C	-1.66832600	2.80708600	-0.69850100
C	-1.35908100	3.51802400	-3.37214700
C	-2.67441500	2.52036200	-1.62618800
H	-1.80471900	2.54673500	0.34713800
C	-2.54607700	2.90940600	-2.95355200
H	-3.57260200	2.00269000	-1.30045600
H	-3.34074500	2.72300100	-3.66811100
H	0.56977600	4.23806300	-2.81727800
C	-1.14361200	3.96660900	-4.77538800
O	-2.25838900	3.85686200	-5.52100900
O	-0.10167500	4.40190500	-5.21212700
C	-2.13573400	4.27459900	-6.88054500
H	-3.05821900	3.95875900	-7.36480900
H	-2.02363300	5.36151600	-6.93211500
H	-1.27310800	3.80056000	-7.35046300
O	2.04418100	5.75661800	1.18382400
C	3.29196700	5.62142700	1.47382500
C	3.82819800	6.73608700	2.36683100
H	3.61467800	7.71283400	1.92180200
H	3.31580000	6.70188700	3.33424400
H	4.90303500	6.62177800	2.51893600
O	4.03132100	4.70518500	1.10657400

TS44

N	-0.90033700	-1.55829900	-3.14153000
C	-2.23348400	-1.19733700	-3.34815200
C	-3.23983400	-2.16086100	-3.29689500
C	-2.59877900	0.11249300	-3.64670300
C	-4.56251800	-1.82703600	-3.52147300
C	-3.93451500	0.45358500	-3.84127800
C	-4.93996600	-0.50909200	-3.78437200
C	-6.40537500	-0.22132700	-4.01584500
F	-4.19933300	1.72503000	-4.11735300
F	-1.67438000	1.05121900	-3.78887000
F	-2.90929600	-3.43000600	-3.03873800
F	-5.48204200	-2.78780200	-3.46772500
F	-7.13834300	-0.62411400	-2.96802500
F	-6.85001700	-0.88334500	-5.09501700
F	-6.65395700	1.07476100	-4.20641900
C	-0.09038000	-0.92834900	-2.20173400
O	-0.48633300	0.00105700	-1.53488900
C	1.29293800	-1.54343000	-2.07141600
H	1.23266400	-2.22373300	-1.23256500
H	1.51968000	-2.16289500	-2.94535800
C	2.37614300	-0.49498100	-1.91209300
C	2.73076600	0.13042400	-3.10923000
C	2.99571900	-0.12397400	-0.66244800
C	3.71189600	1.12486200	-3.10805100
C	3.92106100	0.98202700	-0.68690700
C	4.27896300	1.54051300	-1.93661200
H	4.02973500	1.56638900	-4.04756500
H	5.02800800	2.32316500	-1.97274900

C	3.81306700	-1.50919100	1.26893100
C	3.18066900	-2.85627800	1.71477100
C	2.62320500	-0.65708700	0.75697100
C	2.04602700	-3.01276600	0.70797700
C	2.37391400	-2.61795800	3.01126000
H	3.89789400	-3.67585400	1.78157800
C	1.43796900	-1.61965200	0.98541100
H	2.46158000	0.23130900	1.36679500
H	1.36205500	-3.83553400	0.95035700
H	2.45111900	-3.15630500	-0.29265000
H	1.99322800	-3.57666200	3.38190600
H	2.95472700	-2.16527500	3.81830900
C	1.21729900	-1.70439800	2.51677000
H	0.52682800	-1.33411300	0.45916800
H	0.23984500	-2.14761000	2.73229800
H	1.24261500	-0.71514800	2.98312000
H	-0.60448400	-2.45271000	-3.50389000
Pd	4.86638200	-1.54857400	-0.49918500
Pd	5.49001900	1.27187900	0.53023000
I	6.21879500	-1.58033500	-2.94973100
C	8.62283800	1.52546000	0.67615900
C	7.60160200	2.05693100	2.67479500
C	8.50334100	1.10800200	-0.66943400
C	9.90995700	1.68089800	1.23673700
C	8.84988300	2.29530900	3.32851900
C	9.61647300	0.79269400	-1.39818600
C	11.04317900	1.37552400	0.43615500
C	10.00551900	2.07820000	2.60859600
C	8.84069300	2.77227100	4.76729200
C	6.39082000	2.30753500	4.72552100
H	9.47301900	0.42320400	-2.40875400
H	12.02685800	1.49051500	0.87473800
C	7.46108800	3.28569800	5.17823500
H	9.13792600	1.94902700	5.43178400
H	7.41044800	3.41888200	6.26361200
C	5.55844400	-4.46292200	-0.18952800
C	7.26264300	-3.15997000	0.66038000
C	6.18140100	-5.67088600	0.24535200
C	7.91494500	-4.28313600	1.20882300
C	7.87690600	-1.89477700	0.75810200
C	3.65566400	-5.65849900	-1.04328400
C	5.56071400	-6.99398600	-0.14890600
C	7.33018900	-5.57073000	0.99903600
C	9.13255400	-4.08951000	1.91832200
H	7.38600200	-1.04884700	0.29148000
C	9.06544100	-1.75246400	1.41302900
C	4.59639900	-6.81814200	-1.31782800
H	6.34259100	-7.70587400	-0.42980600
H	9.61266000	-4.95522000	2.35814500
H	9.51747000	-0.76905000	1.45477700
H	4.01813600	-7.73359200	-1.47836000
N	7.48751000	1.69149500	1.41860500
N	6.04897100	-3.26714000	0.04389900
H	6.60272100	1.31202900	5.14327100
H	7.26073000	4.25943200	4.71442800
H	9.58149800	3.56648600	4.90389900
O	6.42659700	2.19311600	3.29907900
H	7.51251500	0.98870100	-1.10427800
O	4.40780900	-4.45057600	-0.87499200
H	5.14934700	-6.60600400	-2.24111400
H	5.02740300	-7.43167500	0.70628900
C	3.79803600	2.48980100	0.63278900
C	3.16029500	2.43143700	1.88337400
C	3.74079200	3.71104800	-0.05098100
C	2.47957100	3.53197600	2.40387300
H	3.24550300	1.54158200	2.49224600
C	3.07217800	4.81570600	0.47409500
C	2.42284200	4.72928000	1.70771500
H	2.00295100	3.44528000	3.37672700
H	1.89299400	5.58678900	2.10645600
C	2.11690200	-0.24882000	-4.43565200
H	1.02723700	-0.13559100	-4.44511200
H	2.51712500	0.38749600	-5.22865600

H	2.35521100	-1.28573100	-4.70519600
C	4.97308200	2.71175000	5.07260900
H	4.72868800	3.67141200	4.60666400
H	4.27792900	1.95648600	4.70017400
H	4.86258200	2.80110500	6.15823800
C	11.36783900	2.22417000	3.23509800
H	11.94682400	3.00907000	2.73562200
H	11.31576800	2.46367700	4.29740600
H	11.93101900	1.28921200	3.13704400
C	10.92353000	0.90774300	-0.85369600
C	12.12145700	0.48200500	-1.70555100
C	13.45571100	0.65567700	-0.96799800
H	14.27707700	0.33562700	-1.61815300
H	13.63743200	1.70220200	-0.69720600
H	13.49974000	0.04674700	-0.05727300
C	12.16267600	1.32888600	-2.99169200
H	11.24805200	1.21583700	-3.58167200
H	12.28302700	2.39194800	-2.75551600
H	13.00557300	1.02013100	-3.62109500
C	11.95949900	-1.00728500	-2.07113500
H	12.80904400	-1.34166200	-2.67822700
H	11.91672600	-1.62524300	-1.16762400
H	11.04474500	-1.19199900	-2.64264600
C	7.99933300	-6.78835800	1.58066600
H	7.40605100	-7.69412700	1.45224100
H	8.97832300	-6.95471600	1.11637800
H	8.16622800	-6.65417200	2.65442900
C	9.71200000	-2.84834400	2.04293300
C	11.00318400	-2.58364400	2.82115000
C	11.57236500	-3.85603700	3.46082500
H	12.48810100	-3.61605300	4.01220200
H	10.86566400	-4.30387000	4.16897200
H	11.82944600	-4.60709600	2.70555200
C	12.06318900	-2.00009000	1.86724800
H	12.98833400	-1.77972400	2.41424400
H	12.30097200	-2.71307300	1.06999300
H	11.71886600	-1.07377800	1.39617900
C	10.70779900	-1.56509900	3.94113700
H	10.30326600	-0.62838300	3.54223100
H	9.97683800	-1.96900800	4.65142000
H	11.62553400	-1.32984100	4.49376400
C	4.61082700	-0.98175500	2.42541000
O	4.28826000	-0.09555000	3.19393800
O	5.69086800	-1.74795800	2.65132700
C	6.50650400	-1.39824800	3.75788700
H	5.91908700	-1.35829600	4.67964800
H	7.26991800	-2.17514900	3.81302600
H	6.98051500	-0.42863300	3.58558100
H	4.20541500	3.84366000	-1.01910500
C	3.07775100	6.06421100	-0.33479700
O	3.63621600	6.19769800	-1.40175700
O	2.38368300	7.05881200	0.25011400
C	2.33993300	8.27885400	-0.48099800
H	1.73317300	8.95815800	0.11804700
H	3.34570800	8.68494500	-0.61857800
H	1.88488600	8.12475500	-1.46288200
C	2.67990500	-5.39053100	-2.17355800
H	2.06621400	-6.27841200	-2.35566300
H	2.01893300	-4.55630200	-1.92475000
H	3.22651000	-5.13733000	-3.08701200
H	3.10947700	-5.83668700	-0.10478400