

Supplementary Information

Overlooked Potential of N, N-Bidentate Directing-Groups in NiCatalyzed C-H Functionalization of Benzamides

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Computational details

The calculations were conducted in the framework of density functional theory (DFT) using the M06 functional¹ with the Gaussian 09 package.² The LANL2DZ basis set³ was chosen for Ni, Ag, P and S atoms whereas the 6-31g(G) basis set was employed for other atoms. An extra polarization functional was added for all atoms with $\xi_p(\text{H}) = 0.11$, $\xi_d(\text{O}) = 0.8$, $\xi_d(\text{N}) = 0.8$, $\xi_f(\text{P}) = 0.387$, $\xi_d(\text{C}) = 0.8$, $\xi_d(\text{F}) = 0.8$, $\xi_f(\text{S}) = 0.503$, $\xi_f(\text{Ag}) = 1.611$ and $\xi_f(\text{Ni}) = 3.130$.⁴ Frequency calculations at the same level of theory were carried out to identify all stationary points as energy minima or transition states. Intrinsic reaction coordinate (IRC) analyses⁵ were performed to confirm the connection of each transition state indeed with its forward and backward minima. To further refine the calculated energies, single-point free energies were evaluated using the solvation model density (SMD)⁶ with a larger combined basis set, in which the SDD⁷ (ECP) basis set is used for Ni, Ag, P and S, and the 6-311++G(d, p) basis set for all the remaining atoms. Chlorobenzene was used as the solvent with the UAKS atomic radii, in accordance with the experimental conditions.

To confirm the reliability of the M06 functional with the basis sets for describing the present system, we have performed single-point energy calculations in chlorobenzene for the key stationary points, **IM5** and **TS5-6** in Fig.1, **IM7**, **TS7-8**, **IM12** and **TS12-13** in Fig.2 by using B3LYP-D3 and wB97X-D functionals, respectively. The calculated results are collected in Table S1. It can be seen that for the three steps, **IM5** \rightarrow **TS5-6**, **IM7** \rightarrow **TS7-8**, **IM12** \rightarrow **TS12-13**, all the functionals give comparable barriers and consistent trends, demonstrating that the employment of the M06-computed method is suitable for the present study.

References

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Table S1 Calculated free-energy barriers (kcal mol⁻¹) using M06, B3LYP-D3 and wB97X-D functionals to refine energies of the critical steps involved in Figs. 1-2.

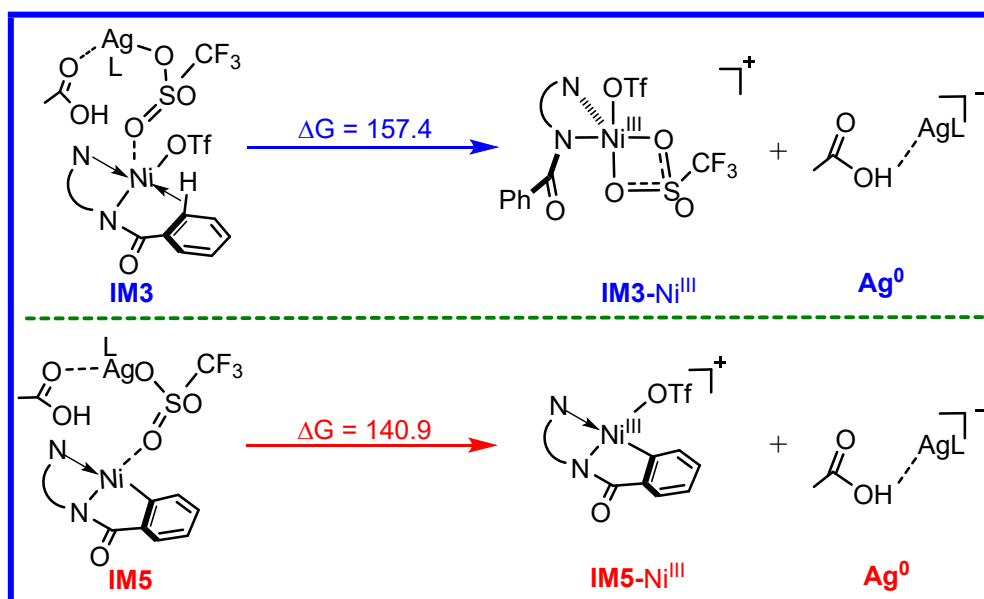
	IM5→TS5-6	IM7→TS7-8	IM12→TS12-13	IM3→TS5-6
M06	31.7	6.3	33.0	37.6
B3LYP-D3	34.2	8.2	34.5	45.1
wB97X-D	33.3	7.7	35.6	43.7

6-311++G(d, p) for C, H, O, N and F atoms, SDD+f for P, S, Ni and Ag.

Table S2 Various structures resulting from the different coordination of Ni(OTf)₂ or AgOAc species. The relative free energies are given in kcal mol⁻¹.

Ni(OTf) ₂			
(0.0)	IM1 (-25.6)	M (-17.2)	N (-4.1)
Q (-9.0)	S (-25.2)	T (-5.2)	W (-15.2)

Scheme S1 The direct redox process from **IM3** and **IM5**, respectively. The relative free energies are given in kcal mol⁻¹.



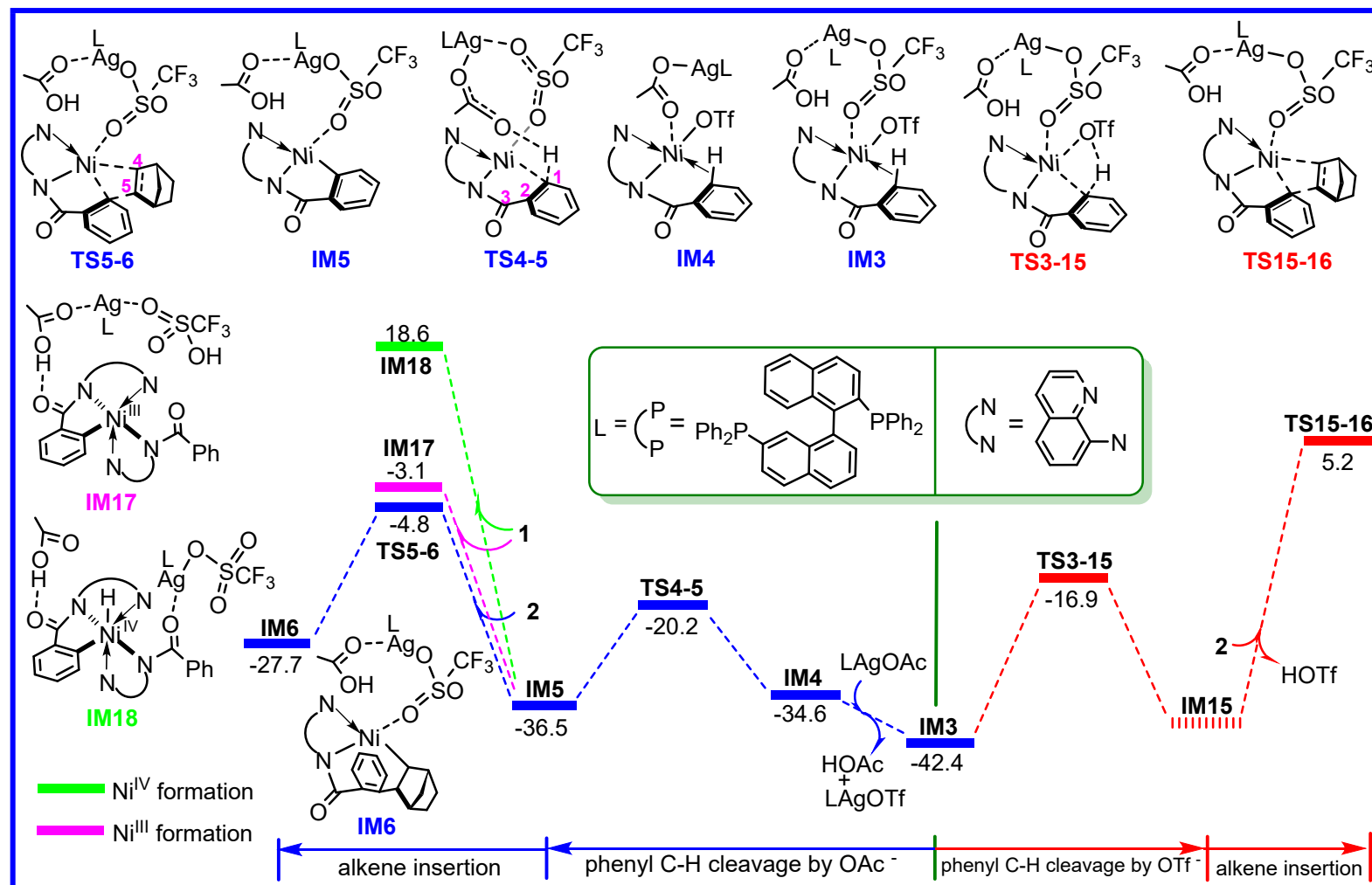


Fig. S1 Gibbs free energy profiles in chlorobenzene solvent for the possible pathways from **IM3**. The free energies are given in kcal mol⁻¹.

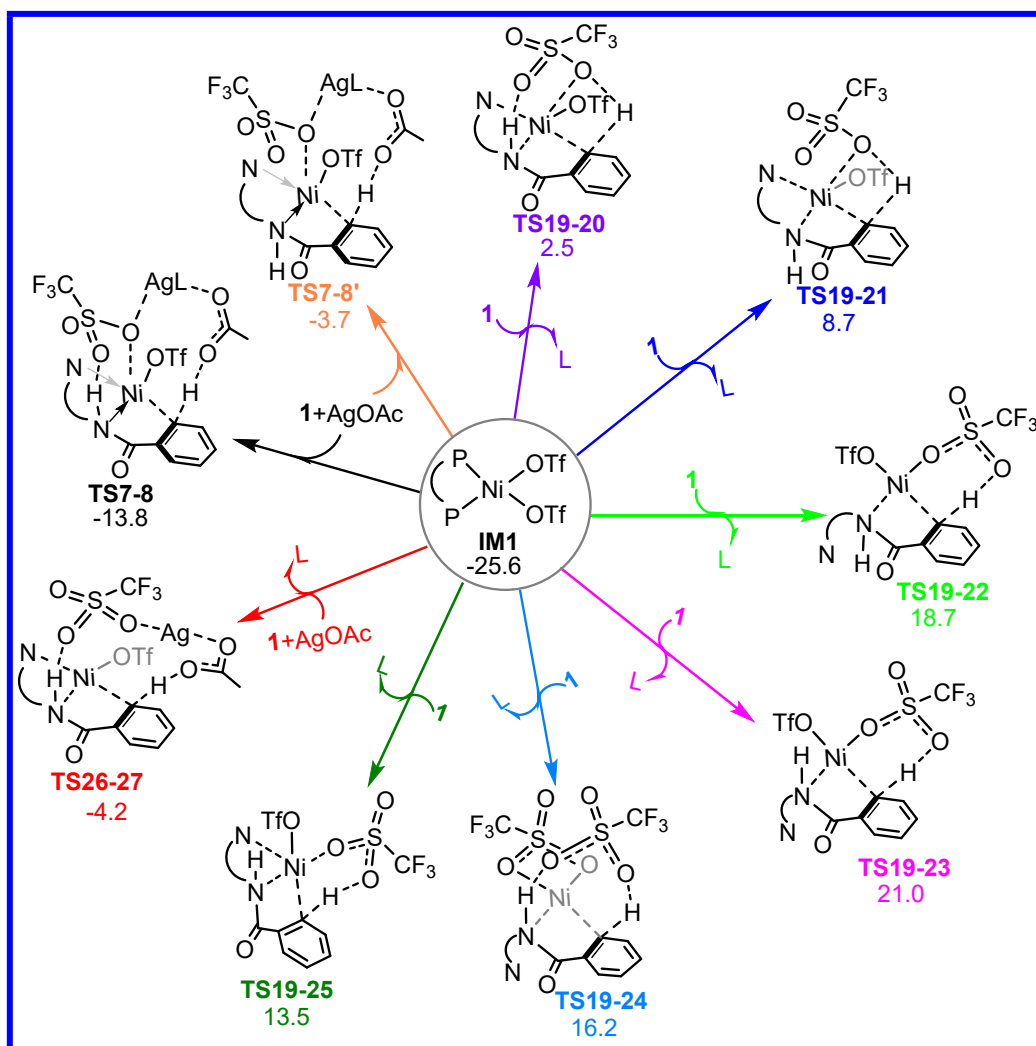


Fig. S2 Schematic structures for the possible C-H activation transition states from **IM1**. The free energies are given in kcal mol⁻¹. $L = \text{P} \curvearrowright \text{P}$

Starting from **IM1**, the reaction undergoes a series of possible phenyl C-H activation transition states, including the involvement of LAgOAc (**TS7-8**, **TS7-8'**), AgOAc (**TS26-27**), no Ag salt (**TS19-20**, **TS19-21**, **TS19-22**, **TS19-23**, **TS19-24**, **TS19-25**), respectively. It is found that the LAgOAc-included TSs are more stable than those AgOAc- and no-Ag salt-included ones. These facts suggest that AgOAc and L ligand are important for promoting the reaction.

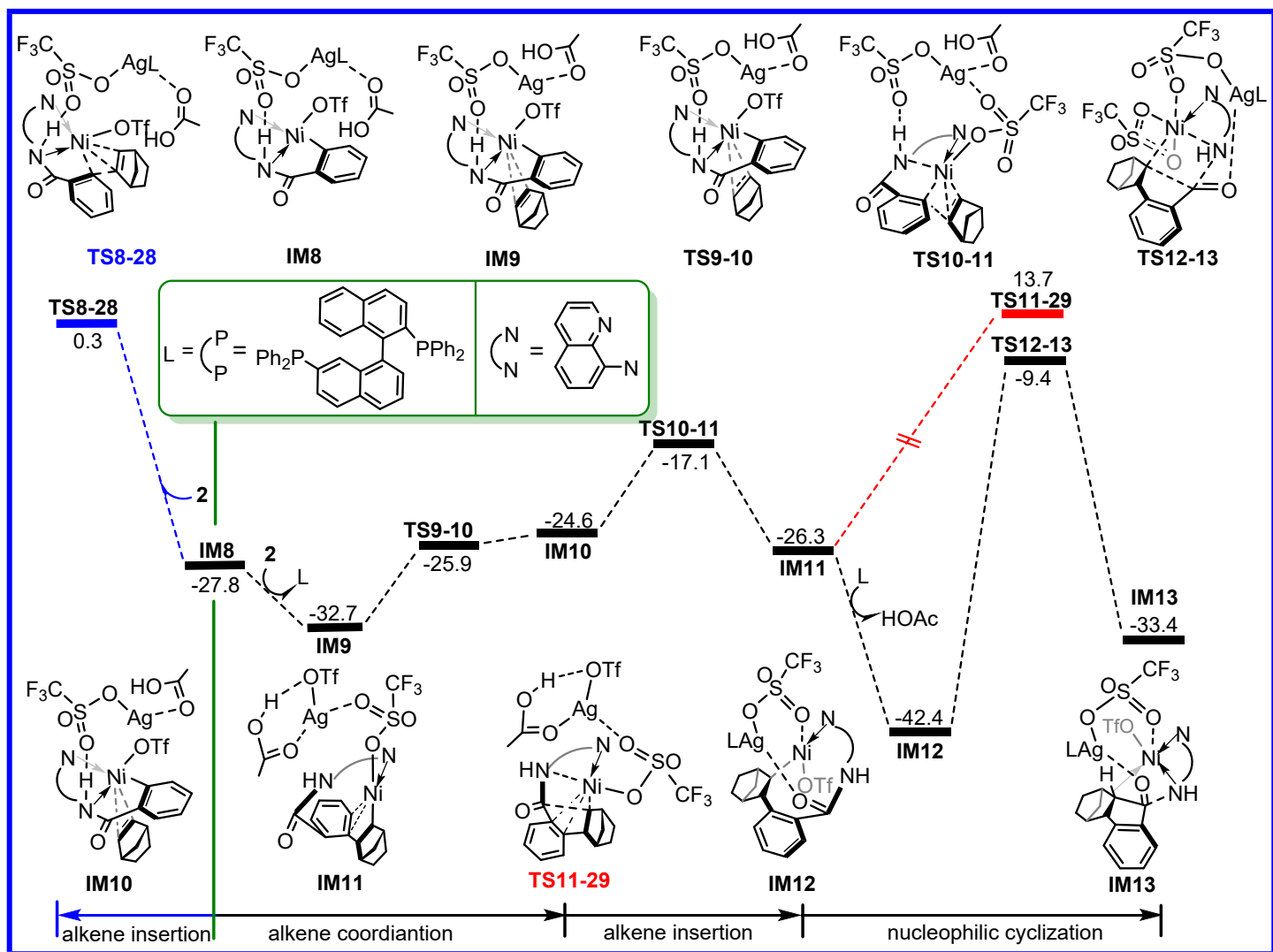


Fig. S3 Gibbs free energy profiles in chlorobenzene solvent along the possible pathways from **IM8** with LAgOAc and AgOAc , respectively. The free energies are given in kcal mol^{-1} .

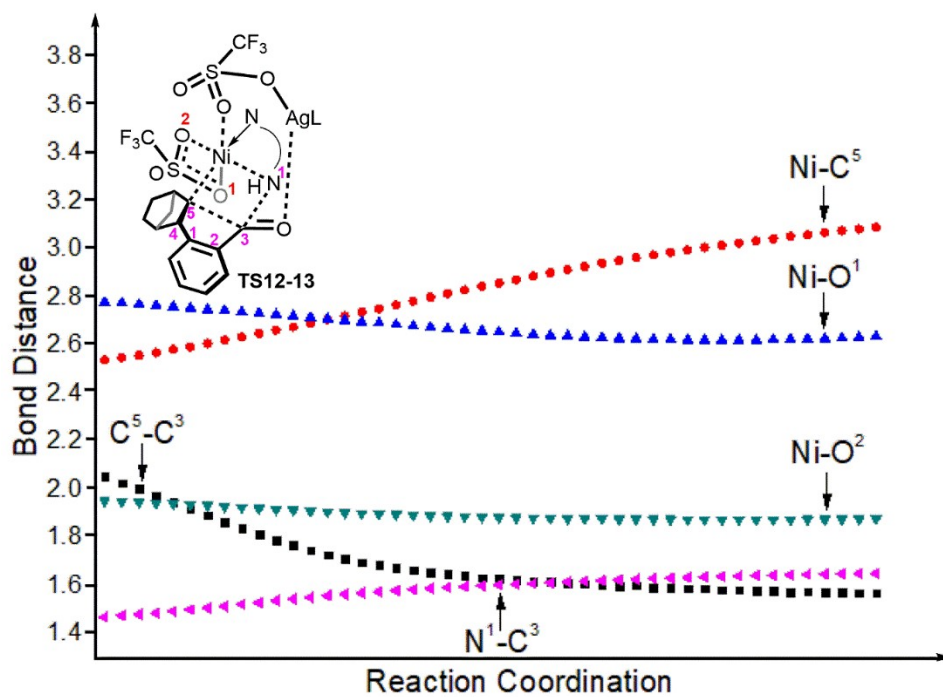


Fig. S4 Diagram of the key bond length scans for the concerted transition state TS12-13 along the IRC pathway. The bond distances are given in Å.

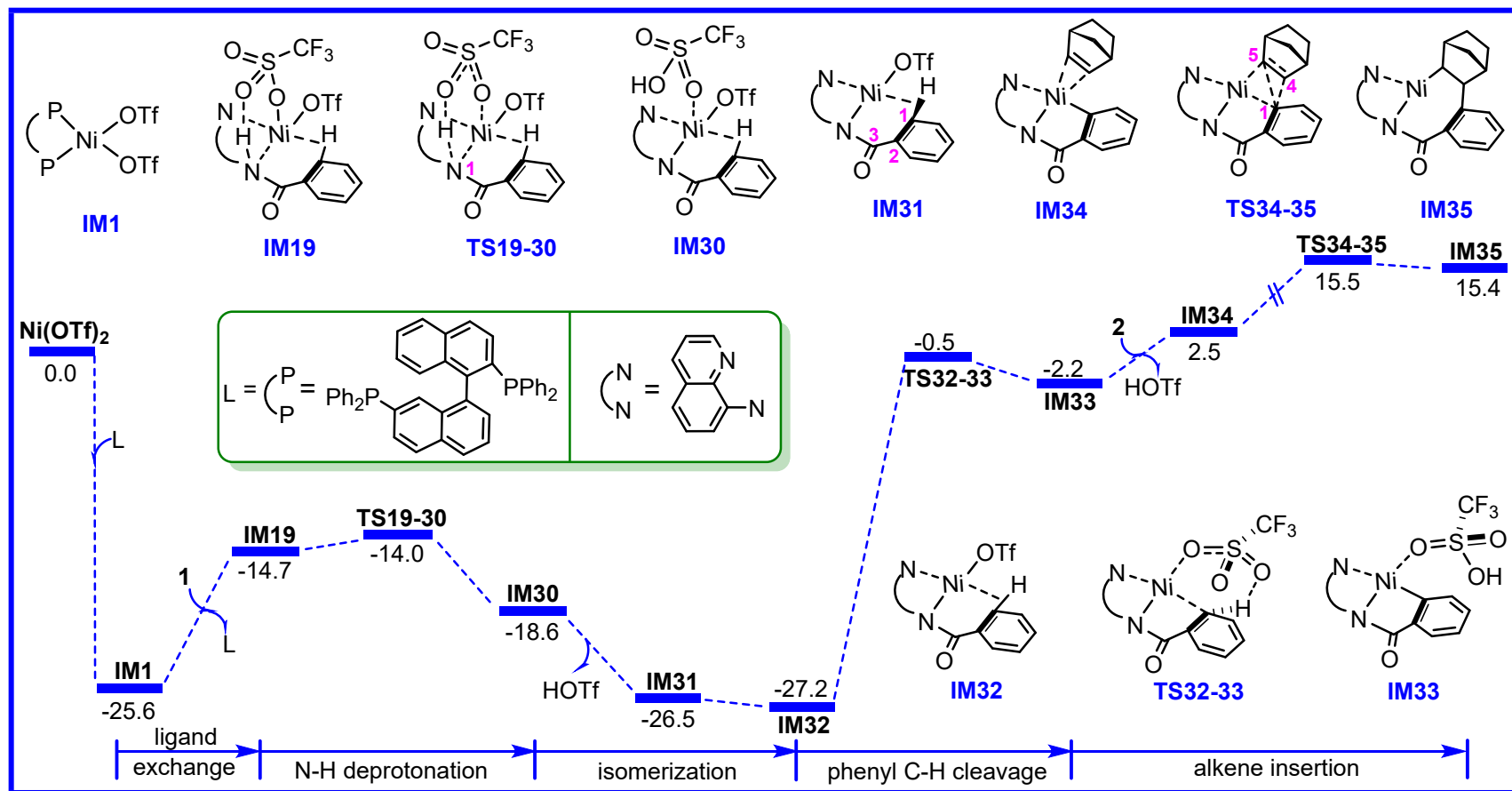


Fig. S5 Gibbs free energy profile in chlorobenzene solvent leading to alkene insertion intermediate **IM35** from **IM1** without participation of AgOAc and L ligand according to the commonly reported route. The free energies are given in kcal mol⁻¹.

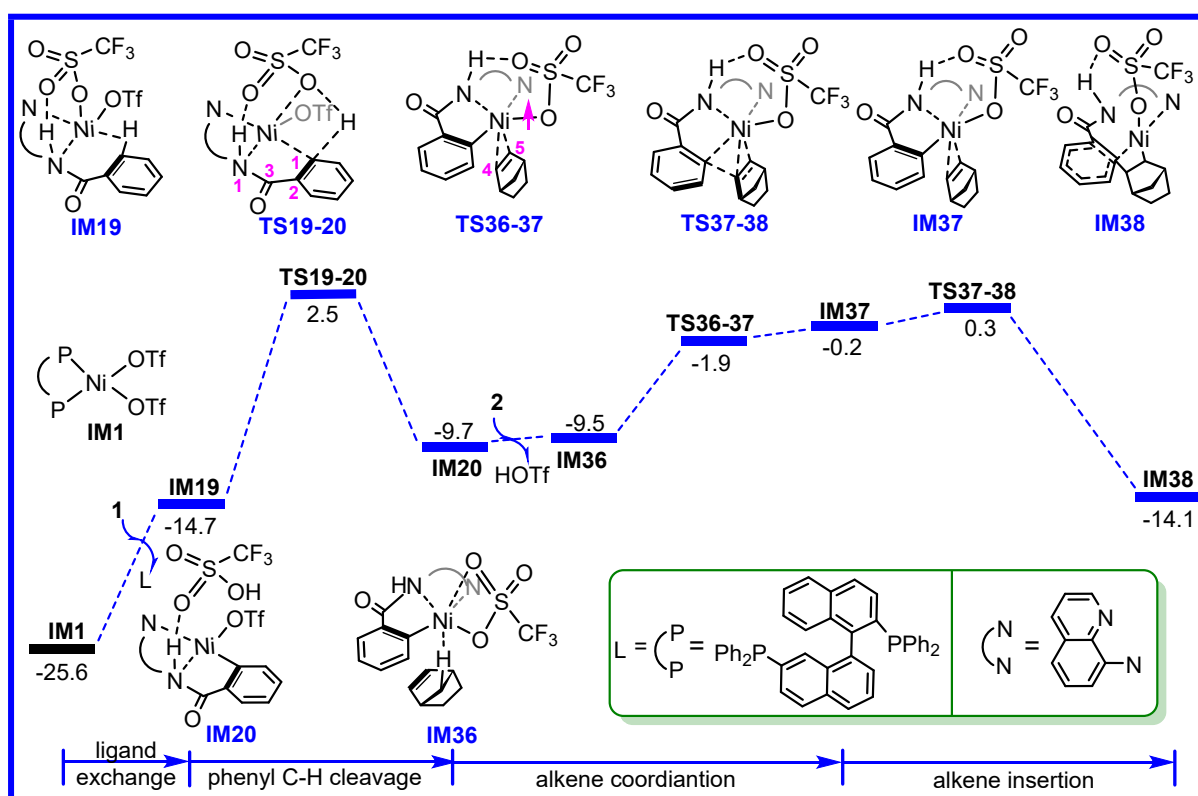


Fig. S6 Gibbs free energy profiles in chlorobenzene solvent along other possible pathway leading to alkene insertion intermediate **IM38** from **IM1** without participation of AgOAc and L ligand. The free energies are given in kcal mol⁻¹.

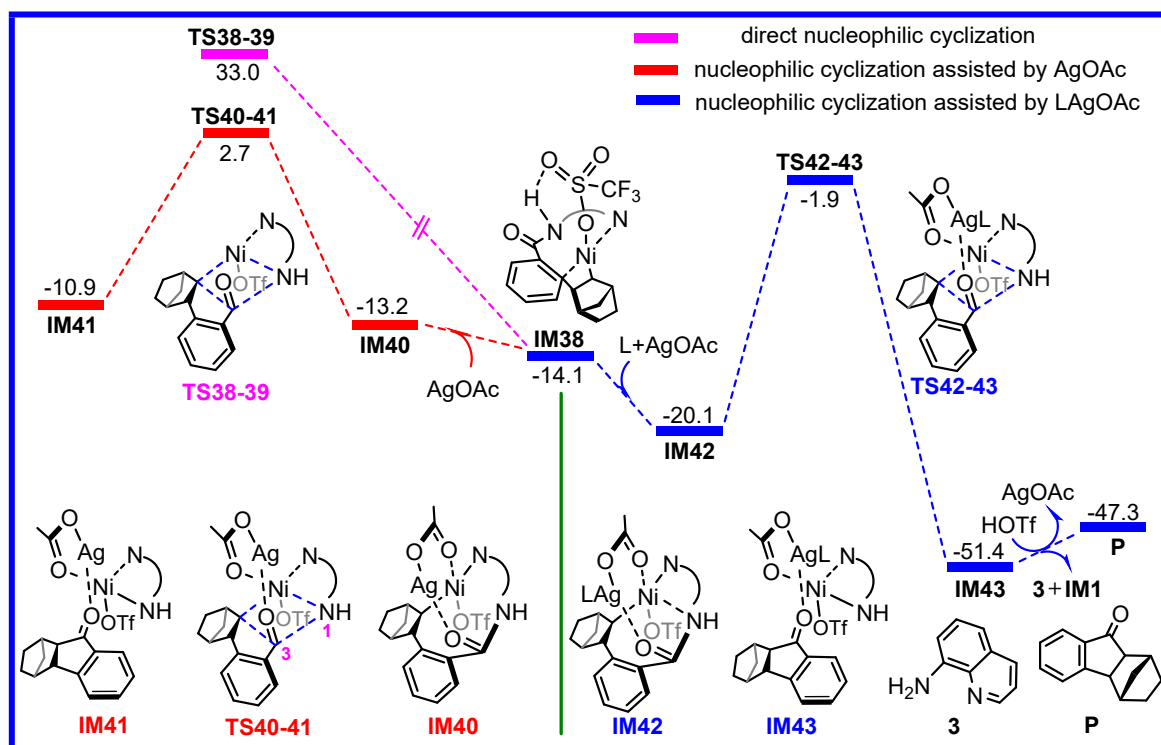
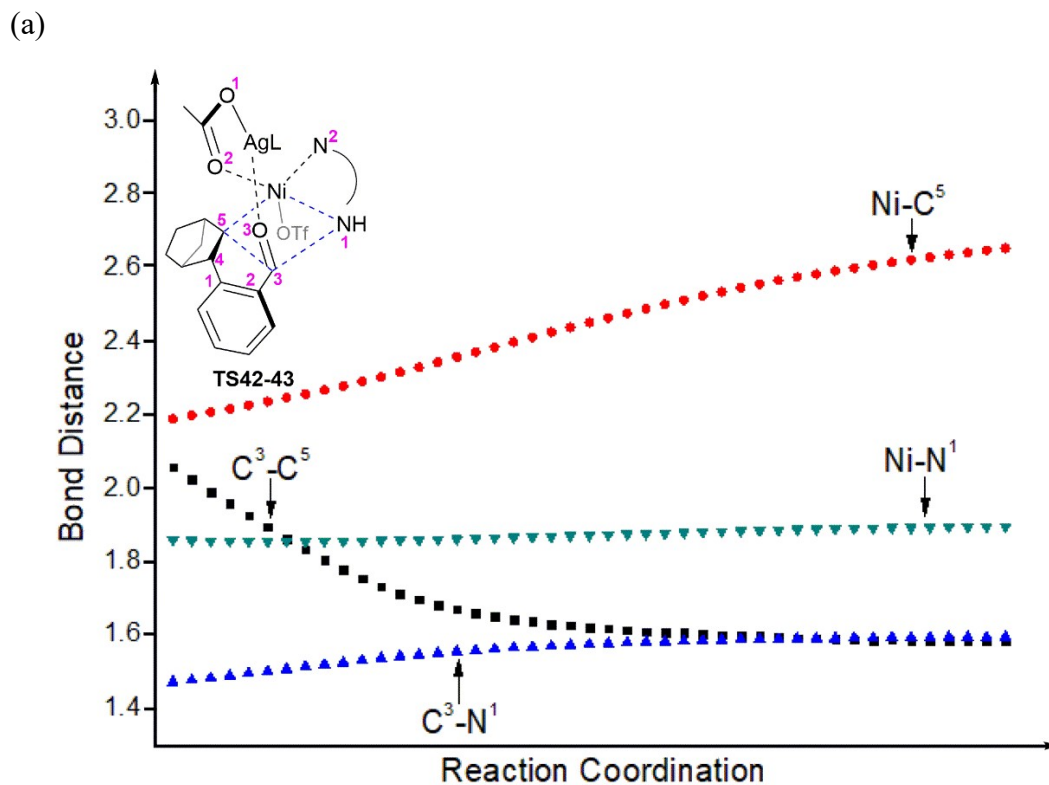


Fig. S7 Gibbs free energy profiles in chlorobenzene solvent along the possible nucleophilic cyclization pathways from **IM38**. The free energies are given in kcal mol⁻¹.



(b)

Atoms	NPA charges	Atoms	NPA charges	Atoms	NPA charges
C ⁵	-0.402	N ²	-0.449	C ²	-0.083
C ³	0.623	C ⁴	-0.253	C ¹	-0.006
Ni	0.497	O ¹	-0.783	Ag	0.641
N ¹	-0.661	O ²	-0.659	O ³	-0.768

Fig. S8 Diagram of the key bond length scans along the IRC pathway(a) and the calculated NPA charges of the key atoms (b) for **TS42-43**. The bond distances and the charges are given in Å and *e*, respectively.

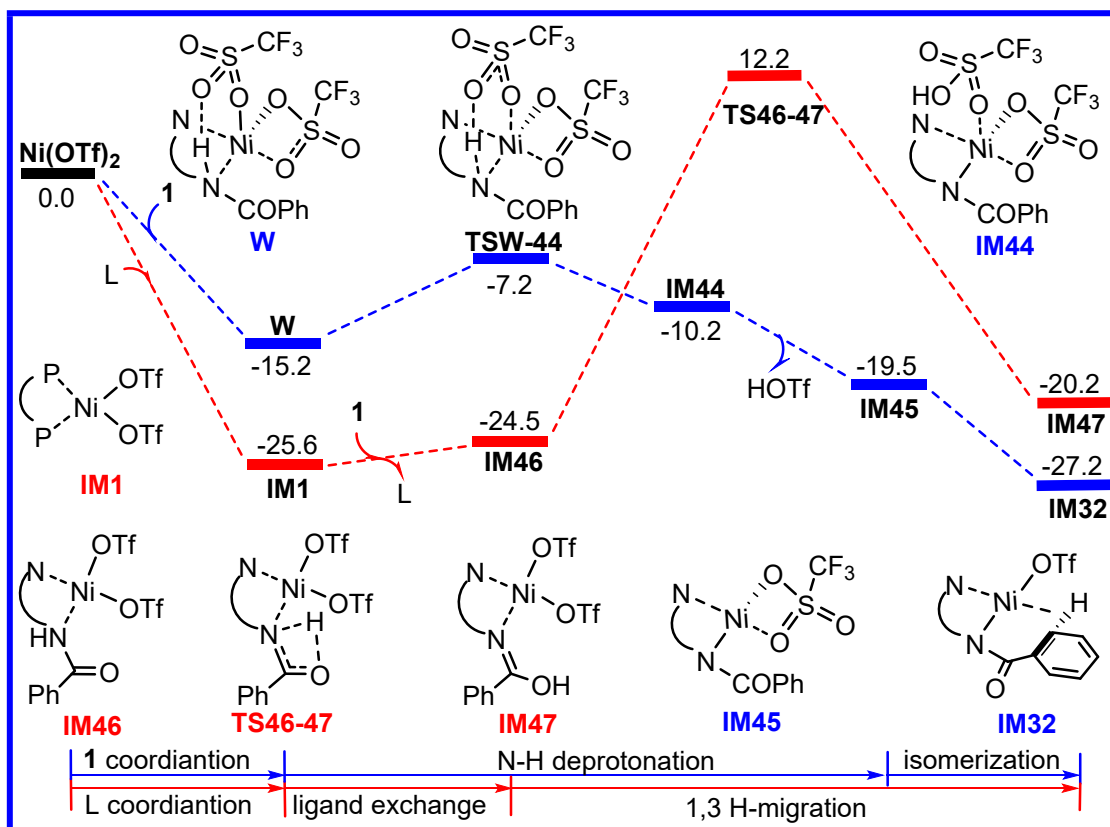


Fig. S9 Gibbs free energy profile in chlorobenzene solvent along other possible pathways for the N-H deprotonation process from the starting materials without participation of AgOAc. The free energies are given in kcal mol⁻¹.

Table S3 Calculated Gibbs free energies in the gas-phase using M06 functional, single-point HF energies in chlorobenzene solvent using M06 functional, and imaginary frequencies for all structures in the present work. The relative energies and the imaginary frequencies are given in Hartree and cm^{-1} , respectively.

Structure	Gibbs Free Energy (M06 gas-phase optimized calculation)	Solvation HF Energy (M06 single- point calculation)	Imaginary Frequency
Ni(OTf) ₂	-1315.379155	-2093.4015886	
IM1	-3023.062200	-4471.220214	
IM2	-4198.378260	-5648.0582201	
TS2-3	-4198.377750	-5648.0542266	-345.61
IM3	-4198.400925	-5648.083872	
IM4	-3624.771442	-4686.245708	
TS4-5	-3624.754360	-4686.218637	-1495.83
IM5	-3624.798028	-4686.257028	
TS5-6	-3897.269692	-4958.811442	-133.74
IM6	-3897.315028	-4958.85194	
IM7	-4198.369668	-5648.04975	
TS7-8	-4198.370137	-5648.039188	-626.48
TS7-8'	-4198.348164	-5648.024563	-722.06
IM8	-4198.405687	-5648.071137	
IM9	-2763.260235	-3542.901694	
TS9-10	-2763.249501	-3542.890643	-23.62
IM10	-2763.249511	-3542.888957	
TS10-11	-2763.249335	-3542.880626	-145.18
IM11	-2763.276542	-3542.902879	
IM12	-4241.971132	-5691.629237	
TS12-13	-4241.896686	-5691.574066	-227.39
IM13	-4241.937165	-5691.611082	
TS13-14	-4241.936556	-5691.609856	-142.46
IM14	-4241.987888	-5691.6588846	
TS3-15	-4198.371865	-5648.041896	-971.65
TS15-16	-3897.170395	-4958.722348	-341.18
IM17	-4425.856679	-5487.554589	
IM18	-4425.804375	-5487.513252	
IM19	-2116.5025101	-2894.784158	
TS19-20	-2116.481377	-2894.753324	-1420.25
IM20	-2116.507431	-2894.777457	
TS19-21	-2116.461270	-2894.74258	-1418.03
TS19-22	-2116.453115	-2894.736361	-1322.09
TS19-23	-2116.459557	-2894.728555	-1439.71
TS19-24	-2116.453869	-2894.72534	-1298.75
TS19-25	-2116.445532	-2894.723446	-1366.49

TS26-27	-2490.686247	-3270.247362	-1580.32
TS8-28	-4470.879227	-5920.62809	-201.68
TS11-29	-2763.193008	-3542.831075	-338.23
P	-616.691021	-616.8810902	
M	-2081.827446	-2753.247417	
N	-1587.908111	-2366.022244	
Q	-646.689458	-648.0814653	
S	-2116.518899	-2894.803326	
T	-1175.273521	-1176.819869	
W	-2116.511059	-2894.787691	
TS19-30	-2116.5015174	-2894.779914	-756.80
IM30	-2116.5116529	-2894.789595	
IM31	-1542.8997612	-1932.980766	
IM32	-1542.899078	-1932.980793	
TS32-33	-1542.867015	-1932.934426	-763.44
IM33	-1542.873121	-1932.731648	
IM34	-1241.765601	-1243.72342	
TS34-35	-1241.747504	-1243.703915	-130.85
IM35	-1241.748324	-1243.703881	
IM36	-1815.401192	-2205.565054	
TS36-37	-1815.395584	-2205.552251	-39.71
IM37	-1815.397821	-2205.551267	
TS37-38	-1815.394935	-2205.549086	-166.16
IM38	-1815.425414	-2205.576878	
TS38-39	-1815.335192	-2205.49881	-371.15
IM40	-2189.629057	-2581.06098	
TS40-41	-2189.580679	-2581.032372	-200.72
IM41	-2189.601029	-2581.055215	
IM42	-3897.292401	-4958.843843	
TS42-43	-3897.261071	-4958.811788	-222.31
IM43	-3897.338214	-4958.889704	
TSW-44	-2116.503840	-2894.770915	-50.81
IM44	-2116.511255	-2894.778233	
IM45	-1542.897792	-1932.965359	
IM46	-2116.518882	-2894.803351	
TS46-47	-2116.460268	-2894.74172	-1795.91
IM47	-2116.524536	-2894.797266	

Table S4 Calculated Gibbs free energies in the gas-phase using M06 functional, single-point HF energies in chlorobenzene solvent using B3LYP-D3 and wB97X-D functionals for the structures in Table S1. The relative energies are given in Hartree.

Structure	B3LYP-D3	wB97X-D
IM5	-4688.7841585	-4687.439577
TS5-6	-4961.568822	-4960.128304
IM7	-5650.849102	-5649.300514
TS7-8	-5650.835505	-5649.28784
IM12	-5694.520924	-5692.910025
TS12-13	-5694.463908	-5692.965293

Cartesian coordinates for all the stationary points involved in the reaction.

Ni(OTf)₂

S	-2.37146300	-0.86546500	-0.00052700
O	-1.35741500	-0.55487300	1.19222300
O	-3.18767200	-2.12411300	0.00475500
C	-3.58817000	0.62276700	0.00058900
O	-1.35866100	-0.56300900	-1.19584200
S	2.37131500	0.86537400	-0.00051700
O	1.35874800	0.56225500	-1.19586600
O	3.18713500	2.12425800	0.00448700
C	3.58834800	-0.62249700	0.00068200
O	1.35730800	0.55496800	1.19222600
Ni	-0.00003700	-0.00018600	-0.00321100
F	4.27921400	-0.55994500	1.11004700
F	4.36068200	-0.49795500	-1.04831100
F	2.87979300	-1.72136300	-0.05704500
F	-4.27848600	0.56068300	1.11030100
F	-2.87939100	1.72143700	-0.05779000
F	-4.36105600	0.49815900	-1.04796500

IM1

S	-2.37146300	-0.86546500	-0.00052700
O	-1.35741500	-0.55487300	1.19222300
O	-3.18767200	-2.12411300	0.00475500
C	-3.58817000	0.62276700	0.00058900
O	-1.35866100	-0.56300900	-1.19584200
S	2.37131500	0.86537400	-0.00051700
O	1.35874800	0.56225500	-1.19586600
O	3.18713500	2.12425800	0.00448700
C	3.58834800	-0.62249700	0.00068200
O	1.35730800	0.55496800	1.19222600
Ni	-0.00003700	-0.00018600	-0.00321100
F	4.27921400	-0.55994500	1.11004700
F	4.36068200	-0.49795500	-1.04831100
F	2.87979300	-1.72136300	-0.05704500
F	-4.27848600	0.56068300	1.11030100
F	-2.87939100	1.72143700	-0.05779000
F	-4.36105600	0.49815900	-1.04796500

IM2

S	-6.86955500	1.02368400	0.49406800
O	-5.40265900	1.34759900	-0.06614400
O	-7.96503600	1.43708600	-0.46932200
C	-6.96962200	2.27666600	1.93146000

O	-6.89596900	-0.35381800	1.15216100
Ni	-4.32326200	-0.18196900	-0.16877700
F	-8.20822500	2.31005800	2.37400500
F	-6.60451200	3.46351300	1.49812800
F	-6.15939300	1.88130300	2.89922000
C	-5.92599900	-0.21290600	-2.81999200
C	-5.42176000	-2.09478400	-1.36621200
C	-6.77715300	-2.42566100	-1.31393400
C	-7.68952000	-1.65198500	-2.01188400
C	-7.27061400	-0.53421100	-2.74349200
H	-5.58503800	0.64818600	-3.39036200
H	-7.09310500	-3.25314600	-0.68285500
H	-8.75026100	-1.88615500	-1.95254400
H	-8.00961900	0.09525100	-3.23266100
C	-4.47633800	-2.77258400	-0.45409300
O	-4.61974200	-3.83785200	0.08336700
N	-3.38978200	-1.85179200	-0.15163700
H	-2.66311000	-1.83549200	-0.95899200
C	-2.67913400	-2.03576000	1.07867200
C	-2.64794500	-0.88575700	1.88209100
C	-1.99364800	-3.16679700	1.44117800
C	-1.84876800	-0.84623000	3.04343800
C	-1.24641000	-3.15545400	2.63847100
H	-2.02309300	-4.04906700	0.80589600
C	-3.31829100	1.32605400	2.12658400
C	-1.79039800	0.38725800	3.73356600
C	-1.16000000	-2.02397800	3.41519300
H	-0.70225900	-4.05195300	2.92954400
C	-2.50683000	1.46297000	3.27250500
H	-3.88441000	2.15946000	1.71809500
H	-1.16381800	0.46724700	4.62212100
H	-0.54219600	-2.01613900	4.31358400
H	-2.46265700	2.42780200	3.76958000
N	-3.39242600	0.18465400	1.47013200
C	-4.98152700	-0.99345300	-2.14026200
S	-1.88107200	1.94227700	-0.88976100
O	-0.71551800	1.31154200	-0.08364200
O	-2.78997500	0.90635400	-1.58698100
C	-1.08477300	2.84294000	-2.37198900
O	-2.57635300	3.06143600	-0.11883800
H	-3.92149700	-0.85128500	-2.36171400
F	-0.61186300	1.96979700	-3.23579800
F	-0.11236900	3.62422300	-1.93684300
F	-2.02093200	3.57372500	-2.94549500

C	-1.47103900	-1.33989500	-4.26118200
H	-0.60301100	-1.38495500	-4.92844900
H	-1.94969200	-0.36390800	-4.42006600
H	-2.18212900	-2.13453400	-4.50852900
C	-1.02012800	-1.41613800	-2.81714700
O	-1.65820300	-2.18593700	-2.03649100
O	-0.04533400	-0.69326300	-2.51024400
Ag	0.70849700	-0.50182400	-0.39358100
C	3.42837800	1.29853700	-0.73143600
C	3.77940000	0.00413400	-1.10085700
C	3.41422800	-0.51087300	-2.38091400
C	2.70904400	0.32897300	-3.29026800
C	2.38533400	1.64635300	-2.89581800
C	2.71676400	2.11169400	-1.65061000
H	4.25062600	-2.49204800	-2.08717800
C	3.71114700	-1.84101200	-2.77520600
C	2.32108500	-0.18452400	-4.54937100
H	1.83805500	2.28126900	-3.59120200
H	2.41721600	3.11433100	-1.34908300
C	2.61497900	-1.47661000	-4.90051200
C	3.31359700	-2.31223300	-4.00111500
H	1.75959200	0.46522400	-5.22186300
H	2.30364300	-1.86634800	-5.86859600
H	3.54075600	-3.33874600	-4.28440500
C	8.84885100	-0.40064000	-0.44992700
C	8.29969000	-1.18493800	0.53168000
C	6.89677900	-1.34549800	0.62841000
C	6.04872000	-0.68257400	-0.30530200
C	8.01371100	0.25455400	-1.37988200
H	6.96180200	-2.62151400	2.37302400
H	9.92907100	-0.28133000	-0.51589600
H	8.93275700	-1.69876100	1.25555700
C	6.31188700	-2.13394400	1.64588900
C	4.62736700	-0.81662400	-0.19003200
H	8.45412000	0.87970100	-2.15461300
C	4.09473200	-1.64114200	0.78880200
C	4.95407000	-2.28059500	1.72128500
H	4.52334400	-2.87722100	2.52486700
P	3.90456900	1.90505300	0.97844800
P	2.26817200	-1.91192000	0.92215600
C	6.65051500	0.11581000	-1.31244200
H	6.01536600	0.62898400	-2.03267100
C	2.01296900	-3.61430600	0.24962700
C	0.80186400	-3.86428800	-0.40521900

C	2.97948700	-4.62499700	0.30248800
C	0.55475800	-5.10437700	-0.98509300
H	0.04085400	-3.08566400	-0.50018900
C	2.72882900	-5.86454900	-0.27711500
H	3.94291500	-4.43891100	0.77837300
C	1.51705200	-6.10633700	-0.92044100
H	-0.38904000	-5.26604800	-1.50477200
H	3.48960500	-6.64240800	-0.23457300
H	1.33126500	-7.07475200	-1.38248500
C	2.09120400	-2.06243100	2.75482300
C	2.09938700	-0.87242100	3.48993100
C	1.99007100	-3.28255300	3.42526600
C	2.01296500	-0.90493700	4.87751000
H	2.18759300	0.08547500	2.97230500
C	1.89497600	-3.31226500	4.81489700
H	1.98275900	-4.21519000	2.85877800
C	1.90742000	-2.12540000	5.54255900
H	2.03143800	0.02650100	5.44157200
H	1.81567700	-4.26841800	5.33031700
H	1.83890000	-2.15161300	6.62882100
C	2.78689200	3.37356400	1.14311300
C	1.40958800	3.12063400	1.16921300
C	3.23320200	4.68618600	1.31127800
C	0.49417600	4.15801100	1.29890900
H	1.02469900	2.10715100	1.04150200
C	2.31731600	5.72315800	1.47629700
H	4.30047500	4.90593700	1.30647000
C	0.95066800	5.46501200	1.45782000
H	-0.57345900	3.93727900	1.25449700
H	2.67921400	6.74268100	1.60475800
H	0.23847700	6.28206200	1.56362000
C	5.54836300	2.68105500	0.59142900
C	6.62739300	2.35960100	1.41723700
C	5.76496100	3.51894500	-0.50914000
C	7.89973900	2.85901300	1.15062400
H	6.46959100	1.69077200	2.26491800
C	7.03144700	4.02737900	-0.77038100
H	4.93306200	3.77171500	-1.16785800
C	8.10173500	3.69644700	0.05914700
H	8.73489900	2.58889400	1.79537700
H	7.18675700	4.68225900	-1.62673400
H	9.09512700	4.09145800	-0.14928900

TS2-3

S	-6.84722400	0.94748000	0.47172700
O	-5.38507600	1.29493700	-0.08076900
O	-7.94966200	1.37192800	-0.47881600
C	-6.96198800	2.16701200	1.93520200
O	-6.86199900	-0.44357500	1.10119600
Ni	-4.28088700	-0.22404500	-0.18718600
F	-8.19591000	2.16014400	2.39198400
F	-6.63184500	3.37250500	1.52423500
F	-6.13100900	1.77321000	2.88637400
C	-5.96689100	-0.28642100	-2.75229800
C	-5.32936300	-2.17797900	-1.36346900
C	-6.66292200	-2.58199100	-1.29443600
C	-7.63128800	-1.83932600	-1.95083100
C	-7.29118500	-0.67938600	-2.65642000
H	-5.68482200	0.60853100	-3.30289800
H	-6.92129400	-3.44347100	-0.68286800
H	-8.67610600	-2.13387000	-1.87706800
H	-8.07264300	-0.07657700	-3.11184200
C	-4.33349900	-2.82776500	-0.48060400
O	-4.41608000	-3.92308500	0.01191400
N	-3.29980200	-1.86506300	-0.16307300
H	-2.54719700	-1.84333200	-1.02208200
C	-2.59989900	-2.02341700	1.07424500
C	-2.57844300	-0.85636600	1.85681400
C	-1.93919100	-3.15242200	1.49150200
C	-1.80256000	-0.78885500	3.03273200
C	-1.22813400	-3.11608800	2.71062200
H	-1.96904200	-4.05649700	0.88889000
C	-3.29240000	1.34625400	2.06401900
C	-1.75726100	0.46137300	3.69336200
C	-1.14008700	-1.96415500	3.45638900
H	-0.71484800	-4.01529300	3.04623700
C	-2.48281200	1.51988100	3.20579400
H	-3.88885300	2.15332300	1.64548000
H	-1.14043900	0.56632300	4.58612700
H	-0.54988200	-1.94117000	4.37271700
H	-2.45482100	2.49455900	3.68471300
N	-3.33805900	0.19396500	1.42464900
C	-4.96602900	-1.03403800	-2.11626700
S	-1.87721100	1.99978600	-0.91284900
O	-0.73300800	1.38294800	-0.05996600
O	-2.77247200	0.95433800	-1.60845500
C	-1.01417100	2.83983000	-2.39236000
O	-2.56995800	3.14773700	-0.18511100

H	-3.91963900	-0.84582800	-2.36910200
F	-0.54563200	1.92484200	-3.21777300
F	-0.02870100	3.60022900	-1.94942500
F	-1.90592900	3.58409000	-3.01601800
C	-1.41434000	-1.12588600	-4.29649000
H	-0.52103000	-0.89255600	-4.88514800
H	-2.08389100	-0.25480700	-4.33925200
H	-1.94464100	-1.98602600	-4.71765800
C	-1.06027800	-1.35403900	-2.84489400
O	-1.84738000	-2.11750200	-2.19046700
O	-0.04845900	-0.77726000	-2.40239700
Ag	0.68429200	-0.40211500	-0.27497300
C	3.39887500	1.31929400	-0.73129200
C	3.73886700	0.01948800	-1.09593300
C	3.37798200	-0.49403600	-2.37784000
C	2.70734100	0.35836300	-3.30094000
C	2.42020100	1.68762100	-2.92124000
C	2.72555200	2.14630100	-1.66685000
H	4.16037400	-2.49389500	-2.06536800
C	3.64472600	-1.83310900	-2.76221100
C	2.32528400	-0.15001000	-4.56359300
H	1.91536600	2.33805400	-3.63425600
H	2.44379500	3.15923900	-1.38182800
C	2.58374900	-1.45312600	-4.90232400
C	3.24724200	-2.30187400	-3.98939600
H	1.80083800	0.51465000	-5.25165400
H	2.27454500	-1.83950100	-5.87234800
H	3.44878500	-3.33602900	-4.26396000
C	8.81155000	-0.41991300	-0.50918400
C	8.27037100	-1.21642100	0.46714700
C	6.86801400	-1.36332200	0.58486600
C	6.01082500	-0.67643600	-0.32286100
C	7.96756600	0.26160700	-1.41129600
H	6.95119200	-2.66610000	2.30848300
H	9.89173500	-0.31068800	-0.59118600
H	8.90972900	-1.74954300	1.17132200
C	6.29356900	-2.16039800	1.60086400
C	4.59037200	-0.80347500	-0.18898400
H	8.40129300	0.89834400	-2.18042500
C	4.06769200	-1.63186800	0.79183300
C	4.93579200	-2.29050700	1.70189800
H	4.51427300	-2.88910800	2.50883800
P	3.85012100	1.91264500	0.98974300
P	2.24114300	-1.88300000	0.95337900

C	6.60406300	0.13603900	-1.32286700
H	5.96315900	0.67170100	-2.02136200
C	1.94904200	-3.56444400	0.24789300
C	0.76143700	-3.75932100	-0.46507400
C	2.86793700	-4.61665100	0.33823300
C	0.48428800	-4.98639600	-1.05882500
H	0.04473600	-2.94450500	-0.58953700
C	2.58861100	-5.84312800	-0.25489800
H	3.81637600	-4.47386000	0.85689700
C	1.39630000	-6.03070700	-0.95109600
H	-0.44225500	-5.10571900	-1.61919900
H	3.31129500	-6.65427600	-0.18131900
H	1.18645600	-6.99043000	-1.42069000
C	2.09305800	-2.05329500	2.78599100
C	2.10319600	-0.87126400	3.53477200
C	2.01332900	-3.28166400	3.44295800
C	2.03748300	-0.92266900	4.92305600
H	2.17393600	0.09446200	3.02787600
C	1.93797000	-3.33013300	4.83294900
H	2.00441000	-4.20694500	2.86488900
C	1.95052000	-2.15182000	5.57446300
H	2.05660000	0.00175200	5.49852000
H	1.87395300	-4.29288800	5.33789600
H	1.89682800	-2.19103600	6.66122600
C	2.76705900	3.40976000	1.12376600
C	1.39032100	3.16892200	1.20810100
C	3.22427500	4.72818900	1.18120200
C	0.48274300	4.21843200	1.28253500
H	0.99962300	2.15014600	1.17039600
C	2.31772700	5.78006400	1.29559200
H	4.29212800	4.93927900	1.12920200
C	0.94943300	5.53011600	1.33138700
H	-0.58664800	4.00229700	1.27426000
H	2.68663200	6.80419000	1.33974500
H	0.24474500	6.35804500	1.39309500
C	5.52991400	2.62874200	0.64582900
C	6.56752500	2.27888900	1.51249700
C	5.81385300	3.44599200	-0.45458200
C	7.86432200	2.73352100	1.28838800
H	6.35549500	1.62459000	2.35989700
C	7.10521400	3.91078500	-0.67346600
H	5.01633000	3.71420300	-1.14908000
C	8.13290500	3.55245200	0.19737800
H	8.66646700	2.44117100	1.96456200

H	7.31357500	4.55002400	-1.53045900
H	9.14608300	3.91108400	0.02071100

IM3

S	6.92451200	-1.19856700	0.68979900
O	5.42844300	-1.40053600	0.17028300
O	7.94209900	-1.97516600	-0.12341800
C	6.82066600	-2.10859700	2.36113100
O	7.17585800	0.26306800	1.05254200
Ni	4.58029900	0.25513900	-0.18079200
F	8.02399900	-2.16750000	2.89365000
F	6.34625200	-3.32309900	2.17210500
F	6.01133200	-1.43372400	3.16238400
C	6.61987500	-0.13556800	-2.43665800
C	5.77339300	2.00300800	-1.63181000
C	7.07579300	2.49297300	-1.57473000
C	8.13230500	1.67142200	-1.93884100
C	7.91149200	0.35345000	-2.35196000
H	6.43236800	-1.15820200	-2.75748500
H	7.23870800	3.50594900	-1.21234400
H	9.15168500	2.04752400	-1.87154800
H	8.75359900	-0.29288200	-2.58685300
C	4.65767200	2.80378600	-1.04488900
O	4.59072600	4.02072700	-1.04919800
N	3.78693400	1.92328000	-0.43941900
H	2.56182700	1.66585600	-1.94221700
C	2.88609600	2.28875100	0.55804800
C	2.65096300	1.24111800	1.48254100
C	2.22723400	3.49247500	0.72619100
C	1.73267000	1.37833600	2.54322400
C	1.33915900	3.64569200	1.81449800
H	2.41844800	4.31013400	0.03687400
C	3.19573500	-0.93918300	2.08732100
C	1.54773600	0.24837300	3.37602200
C	1.09178400	2.62921800	2.70807300
H	0.84022600	4.60597700	1.94593600
C	2.25578800	-0.90351700	3.13693200
H	3.77590200	-1.82796500	1.85207100
H	0.83743200	0.31121000	4.20135900
H	0.41689400	2.77503100	3.54896700
H	2.11871400	-1.79052300	3.74982300
N	3.39304800	0.10715800	1.30825900
C	5.53319800	0.67955000	-2.07821700
S	1.89189900	-1.97009400	-0.81468800

O	0.72176900	-1.32468000	-0.01258100
O	2.71343500	-0.97600400	-1.64524400
C	1.00792400	-2.97734500	-2.16636700
O	2.63039400	-3.01560000	0.00761200
H	4.52309500	0.35572800	-2.35939600
F	0.39979400	-2.13869600	-2.99869800
F	0.11571100	-3.78879900	-1.63182400
F	1.90798800	-3.67276200	-2.82979300
C	0.82783600	0.59172700	-4.39124700
H	-0.24981800	0.47706200	-4.53312900
H	1.32072500	-0.38177200	-4.50473200
H	1.24999600	1.26835400	-5.14126600
C	1.10957900	1.09113200	-3.01333700
O	2.33950400	1.56272600	-2.89832800
O	0.30385800	1.07878500	-2.09690200
Ag	-0.71683900	0.37606700	0.00660700
C	-3.38167500	-1.24332700	-0.74400700
C	-3.92221300	0.01324500	-1.00020500
C	-3.73003900	0.64560700	-2.26355700
C	-3.00791000	-0.04419500	-3.27944100
C	-2.45559100	-1.31187500	-2.98645700
C	-2.61364400	-1.88500400	-1.74903700
H	-4.80905000	2.46306900	-1.78372700
C	-4.25054200	1.93332100	-2.55460700
C	-2.86090800	0.56051000	-4.55184700
H	-1.88941300	-1.82626300	-3.76215900
H	-2.16271200	-2.85312600	-1.52882200
C	-3.36500700	1.81201000	-4.79941900
C	-4.05737800	2.50892800	-3.78475400
H	-2.34007500	0.00648200	-5.33426300
H	-3.23856500	2.26886000	-5.77950600
H	-4.45252400	3.50363300	-3.98423300
C	-8.94807800	-0.07607800	0.08056300
C	-8.38377500	0.70760000	1.05376300
C	-6.99502300	0.98234300	1.04535800
C	-6.17891600	0.43330700	0.01425100
C	-8.14512300	-0.61330200	-0.94894700
H	-7.01994000	2.20608800	2.82712000
H	-10.01662400	-0.28404700	0.09619200
H	-8.99351100	1.13470400	1.85021200
C	-6.39365300	1.78853600	2.03839200
C	-4.77058600	0.67953500	0.02585800
H	-8.59743600	-1.23881100	-1.71661700
C	-4.22224400	1.50013600	0.99856700

C	-5.04972900	2.04729900	2.01357600
H	-4.61077900	2.67199700	2.79004600
P	-3.72694300	-2.02656000	0.92620100
P	-2.41864500	1.91766800	0.96659500
C	-6.79713000	-0.36259700	-0.98430000
H	-6.18659600	-0.78205100	-1.78210200
C	-2.36361800	3.50244200	0.03184900
C	-1.22916100	3.76327000	-0.74086000
C	-3.42393500	4.41558100	0.03044100
C	-1.15279000	4.92406300	-1.50395900
H	-0.40873400	3.04440000	-0.76417000
C	-3.34785900	5.57004000	-0.74009800
H	-4.32037300	4.21154700	0.61780500
C	-2.21325500	5.82389100	-1.50811100
H	-0.26504800	5.11674900	-2.10404300
H	-4.17935400	6.27285700	-0.74435200
H	-2.15962800	6.72624500	-2.11503000
C	-2.14030400	2.35996200	2.73244400
C	-2.04302700	1.30118400	3.64115900
C	-2.05720300	3.67395200	3.19336700
C	-1.86627500	1.55718100	4.99609800
H	-2.11110100	0.27002300	3.28507600
C	-1.86962000	3.92690500	4.55034300
H	-2.12769400	4.50398800	2.48986900
C	-1.77375600	2.87107500	5.45212300
H	-1.79880800	0.72843400	5.69940200
H	-1.79858300	4.95436200	4.90323300
H	-1.62749700	3.07093300	6.51212100
C	-2.51382900	-3.42581700	0.95061600
C	-1.21718600	-3.09329000	1.35617400
C	-2.80098400	-4.76071100	0.64892500
C	-0.21545200	-4.05361900	1.42344700
H	-0.97375200	-2.05798200	1.60547700
C	-1.80644300	-5.73017700	0.74401900
H	-3.80745100	-5.04943400	0.34743200
C	-0.51424400	-5.37940300	1.12503600
H	0.80049100	-3.75476000	1.67936000
H	-2.04390500	-6.76773300	0.51211200
H	0.26414100	-6.13840600	1.18272800
C	-5.33470400	-2.87245100	0.53164400
C	-6.33961200	-2.82655200	1.50066800
C	-5.59575100	-3.52057600	-0.68124200
C	-7.57827200	-3.41772600	1.26839200
H	-6.15163200	-2.30246700	2.43907600

C	-6.82870000	-4.12016600	-0.91150600
H	-4.82827000	-3.55054900	-1.45630100
C	-7.82228500	-4.06856400	0.06366700
H	-8.35540100	-3.36478100	2.02943300
H	-7.01673300	-4.62646700	-1.85746600
H	-8.78995300	-4.53423900	-0.11835000

IM4

S	2.46285200	1.15027600	-2.13500500
O	2.63215100	2.48782300	-1.44206200
O	1.08119300	0.46764000	-2.10985800
C	2.71284100	1.47956200	-3.98900000
O	3.63590300	0.10810100	-1.94406700
Ni	4.22490300	-0.59285300	-0.28297300
C	8.10105900	1.64265400	-0.38956000
C	6.49045400	0.35997900	0.84387800
C	5.44654300	1.12280400	0.27681100
C	5.75355700	2.12952300	-0.65342000
C	7.07448600	2.37965100	-0.98912200
H	9.13731600	1.85603700	-0.64877300
H	4.43947700	1.13783400	0.74943500
H	4.93845300	2.71183600	-1.08022800
H	7.31708400	3.16086400	-1.70698100
C	6.15375600	-0.83702700	1.67018400
O	6.85533900	-1.26942400	2.57457200
N	5.00177400	-1.38135400	1.19213300
C	4.43704100	-2.57784200	1.59401900
C	3.38512200	-2.98248700	0.73686300
C	4.74196500	-3.35942200	2.69501200
C	2.60514100	-4.12786700	1.00247300
C	3.96734400	-4.51032700	2.95618000
H	5.55806200	-3.06507400	3.34821600
C	2.17971200	-2.47043700	-1.18180700
C	1.56730900	-4.41579700	0.08888900
C	2.91861400	-4.89225200	2.15087900
H	4.21202200	-5.10714300	3.83358700
C	1.35496600	-3.59540900	-0.99278500
H	2.02184300	-1.78898600	-2.01468800
H	0.93901000	-5.29147700	0.25653400
H	2.33052700	-5.78081100	2.37680300
H	0.56501200	-3.78986900	-1.71743500
N	3.16452700	-2.18378200	-0.34926100
C	7.81575200	0.63281400	0.52034300
H	8.60121900	0.03312900	0.97670500

F	2.63864800	0.33390200	-4.63811900
F	3.89273700	2.03193000	-4.17125800
F	1.76065200	2.29219800	-4.40325400
C	2.68506500	-0.39998800	3.33695500
H	2.12775200	0.23004000	4.04598000
H	2.61403900	-1.43603400	3.68793900
H	3.73068700	-0.07002200	3.33235900
C	2.04234500	-0.24372100	1.97541800
O	2.43093800	0.69101000	1.21862500
O	1.10462700	-1.03771900	1.68786500
Ag	0.03691300	0.23935500	0.08562300
C	-2.73340600	-1.31832600	0.15740500
C	-3.10567200	-0.39765200	1.13157900
C	-2.63387400	-0.53306200	2.47022500
C	-1.70262200	-1.56690700	2.77622100
C	-1.33606800	-2.48342400	1.76577800
C	-1.84749400	-2.37340900	0.49884400
H	-3.77023500	1.11966500	3.29276100
C	-3.02132200	0.35752900	3.50429400
C	-1.12574900	-1.61856900	4.06711700
H	-0.59310700	-3.24636700	1.99906200
H	-1.53846900	-3.07839700	-0.27398300
C	-1.48116800	-0.71017800	5.03056100
C	-2.45674000	0.27269700	4.75133700
H	-0.37799100	-2.38645000	4.26556200
H	-1.02244100	-0.75088400	6.01722500
H	-2.74826600	0.98140700	5.52521800
C	-8.16412800	0.33594500	0.53186800
C	-7.57554500	1.49508600	0.09543500
C	-6.17276000	1.67126700	0.17923900
C	-5.36946800	0.62070100	0.71154800
C	-7.37376400	-0.69629800	1.08385400
H	-6.15934200	3.66119100	-0.66418300
H	-9.24340400	0.21031900	0.46087600
H	-8.17665200	2.30338500	-0.32197600
C	-5.54359100	2.85977700	-0.25477300
C	-3.95057300	0.76992100	0.74681300
H	-7.84794500	-1.61293000	1.43027500
C	-3.36887400	1.96778400	0.34606400
C	-4.18479400	3.01056800	-0.15924500
H	-3.71970200	3.93638300	-0.49583000
P	-3.38565000	-1.05497800	-1.57470600
P	-1.52653100	2.17404000	0.43116200
C	-6.01218900	-0.55798500	1.17120300

H	-5.40503100	-1.35982800	1.58875900
C	-1.24714400	2.84636900	2.12748400
C	0.01744900	2.66969600	2.69840800
C	-2.23997600	3.51953800	2.84513700
C	0.27683000	3.16108100	3.97490900
H	0.81123800	2.16008000	2.14337900
C	-1.97552800	4.00651700	4.12078200
H	-3.23122900	3.65478900	2.40887900
C	-0.71755200	3.82326000	4.68839100
H	1.26463600	3.02189000	4.41199800
H	-2.75583700	4.52849000	4.67306200
H	-0.51156300	4.20126600	5.68878800
C	-1.17798600	3.61166800	-0.66745100
C	-0.80057700	3.34504800	-1.98709000
C	-1.26584700	4.93731900	-0.23263100
C	-0.54322600	4.39214500	-2.86585500
H	-0.67795400	2.31173700	-2.31795600
C	-0.99970800	5.98114600	-1.11176200
H	-1.53546000	5.15422500	0.80148700
C	-0.64446200	5.70932700	-2.42977200
H	-0.24968600	4.17746000	-3.89176400
H	-1.06533300	7.01094300	-0.76407800
H	-0.43344600	6.52750800	-3.11664100
C	-2.21895300	-2.09646500	-2.57843500
C	-1.08390100	-1.42952800	-3.05395900
C	-2.41238700	-3.43214000	-2.94301500
C	-0.15337400	-2.07802600	-3.85921700
H	-0.92357400	-0.37987400	-2.80396000
C	-1.48646400	-4.08223700	-3.75659500
H	-3.29969000	-3.96665000	-2.60262200
C	-0.35617000	-3.40944100	-4.21569700
H	0.71913400	-1.52885500	-4.21396000
H	-1.65449700	-5.12078100	-4.03944400
H	0.36003500	-3.92022000	-4.85784400
C	-4.92026300	-2.10202900	-1.50062500
C	-6.04494300	-1.62506300	-2.17865200
C	-5.02702500	-3.28957400	-0.76781000
C	-7.24835700	-2.32333100	-2.13741200
H	-5.97992500	-0.67874300	-2.71806200
C	-6.22650200	-3.99181400	-0.72973400
H	-4.16656000	-3.65696400	-0.20570500
C	-7.33939500	-3.50888800	-1.41571000
H	-8.11938400	-1.93464700	-2.66309500
H	-6.29605200	-4.91583000	-0.15707000

H	-8.28039200	-4.05625200	-1.38104800
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TS4-5

S	2.43058900	0.43085500	-2.50137200
O	2.60009700	1.92637200	-2.32380900
O	1.08569500	-0.20808700	-2.08920300
C	2.41703200	0.12034400	-4.37932300
O	3.65210000	-0.46440400	-2.07621100
Ni	4.01525800	-0.84895300	-0.22719900
C	7.73180900	1.91841800	0.30911900
C	6.08654300	0.38100700	1.11639400
C	5.20182100	0.73833200	0.07706600
C	5.62836000	1.68911400	-0.86191400
C	6.88297800	2.27821300	-0.73893500
H	8.71170600	2.38686600	0.39428500
H	3.94699800	0.98799700	0.46481100
H	4.95118400	1.99435100	-1.65924500
H	7.20558800	3.02773900	-1.46032800
C	5.62053700	-0.68934900	2.03990100
O	6.14355300	-0.95619900	3.11470100
N	4.52803400	-1.30978400	1.49123700
C	3.85894900	-2.38365200	2.04173700
C	2.92950500	-2.96966100	1.14066600
C	3.96917000	-2.91684700	3.31730700
C	2.11772000	-4.06379100	1.51636900
C	3.15249600	-4.00489300	3.69069900
H	4.69173900	-2.49348100	4.00796900
C	2.03851500	-2.91043100	-1.00323800
C	1.22638700	-4.56074000	0.53917000
C	2.24242500	-4.57441800	2.82987900
H	3.25698400	-4.40481700	4.69839800
C	1.18133300	-3.98735500	-0.70845500
H	2.02968300	-2.43374900	-1.98021100
H	0.57447500	-5.39818600	0.79207000
H	1.62510400	-5.41880000	3.13471400
H	0.49536400	-4.33952900	-1.47740100
N	2.88118900	-2.42034800	-0.11064700
C	7.33745500	0.96653200	1.24581200
H	7.98583600	0.66020200	2.06570300
F	2.56443100	-1.17220400	-4.60494400
F	3.38811600	0.79557500	-4.94824200
F	1.24495700	0.51914900	-4.84271300
C	3.21757900	1.12950800	3.19879900
H	2.64348500	1.81571500	3.83579100

H	3.42030000	0.22675100	3.78697300
H	4.16053700	1.61156300	2.92013000
C	2.36520900	0.78948600	2.00626200
O	2.69776000	1.24826200	0.84179100
O	1.32982800	0.12661200	2.17500600
Ag	0.25824900	0.34068600	0.08713900
C	-2.51742400	-1.16674300	0.37777400
C	-2.78187900	-0.11148100	1.24515200
C	-2.19932500	-0.08404300	2.54670100
C	-1.31847600	-1.13467800	2.93828100
C	-1.03139800	-2.16920200	2.01919400
C	-1.61003200	-2.18509600	0.77402100
H	-3.10860600	1.78185100	3.16556200
C	-2.43670500	0.97581200	3.45777600
C	-0.71719000	-1.09390200	4.21757200
H	-0.31786700	-2.94248200	2.31100100
H	-1.37275000	-2.98752100	0.07387500
C	-0.96106900	-0.05200400	5.07366200
C	-1.82419200	0.99638100	4.68507500
H	-0.03474500	-1.89794900	4.49423500
H	-0.48237000	-0.02263100	6.05094200
H	-2.00668100	1.82693100	5.36537600
C	-7.86891900	0.67121600	1.35215900
C	-7.35731400	1.71223800	0.62114400
C	-5.96040700	1.84935500	0.43524800
C	-5.08103700	0.88592300	1.01070300
C	-7.00072800	-0.27922200	1.93274000
H	-6.09130600	3.64478800	-0.76055900
H	-8.94473500	0.57514100	1.48973700
H	-8.01676900	2.45558300	0.17237900
C	-5.41430300	2.91567300	-0.31439800
C	-3.67375200	0.99748700	0.78967300
H	-7.41302100	-1.10441500	2.51078100
C	-3.17146900	2.08488200	0.08385200
C	-4.05981500	3.03730900	-0.47393200
H	-3.65730200	3.86697900	-1.05396000
P	-3.37363500	-1.15811200	-1.28461000
P	-1.34414900	2.28637700	-0.12502000
C	-5.64320600	-0.17544900	1.76635200
H	-4.97934500	-0.91716700	2.20809200
C	-0.90061000	3.47679200	1.21283500
C	0.46444700	3.64462200	1.47394000
C	-1.83955100	4.14946300	1.99717400
C	0.87942200	4.46548700	2.51583400

H	1.20611900	3.12019700	0.86567800
C	-1.41885000	4.96406400	3.04516100
H	-2.90511500	4.02871300	1.79706800
C	-0.06174900	5.11748300	3.30940900
H	1.94396900	4.58857000	2.71165300
H	-2.15695300	5.47934000	3.65823500
H	0.26405300	5.74872700	4.13478900
C	-1.13305100	3.26427900	-1.67046000
C	-0.76856000	2.57965100	-2.83393900
C	-1.28419800	4.65421600	-1.71059100
C	-0.58349300	3.27362400	-4.02526400
H	-0.58651800	1.50301100	-2.80326400
C	-1.10134800	5.34402900	-2.90368600
H	-1.53459600	5.19983500	-0.79941600
C	-0.75521800	4.65316500	-4.06220400
H	-0.28243900	2.73092700	-4.91971400
H	-1.21865400	6.42629900	-2.92677600
H	-0.60225400	5.19592700	-4.99371200
C	-2.38064300	-2.41607300	-2.21820800
C	-1.25417300	-1.90834000	-2.87412900
C	-2.69546300	-3.76878200	-2.37340300
C	-0.45009500	-2.72900100	-3.65531000
H	-0.99596900	-0.85294600	-2.77810100
C	-1.89901200	-4.59063200	-3.16820600
H	-3.57842200	-4.18110400	-1.88467400
C	-0.77594800	-4.07441200	-3.81155500
H	0.42317100	-2.30095900	-4.14578500
H	-2.16258800	-5.64038000	-3.29165600
H	-0.16111700	-4.71808500	-4.43942400
C	-4.92100400	-2.08685900	-0.83617700
C	-6.11329100	-1.64157800	-1.41256400
C	-4.96670900	-3.15121900	0.07196300
C	-7.32564600	-2.24777800	-1.09630600
H	-6.08885300	-0.79322700	-2.09816700
C	-6.17534600	-3.76535900	0.38102000
H	-4.04834800	-3.49308700	0.55267300
C	-7.35718400	-3.31255800	-0.20225100
H	-8.24844200	-1.88158600	-1.54400100
H	-6.19739100	-4.59559000	1.08579100
H	-8.30456200	-3.78909800	0.04601200
IM5			
S	-0.82881500	2.59731900	-2.05490400
O	-2.39486200	2.47455600	-2.17063000

O	-0.19476500	1.25051000	-1.69615200
C	-0.28280300	2.86901900	-3.85788500
O	-0.34907300	3.84342600	-1.32137700
Ni	-3.21996000	1.34162000	-0.83442300
C	-3.61921300	-2.77629000	-3.08546900
C	-4.03619300	-1.25451200	-1.28242800
C	-3.18940100	-0.28184200	-1.84556200
C	-2.53763500	-0.60050500	-3.04203700
C	-2.74802600	-1.84271100	-3.64748100
H	-3.77777900	-3.73669900	-3.57530300
H	-4.52268500	-3.01204800	1.16484600
H	-1.85200000	0.10560400	-3.50523800
H	-2.22058100	-2.08288700	-4.57086400
C	-4.60540500	-0.89140900	0.03305000
O	-5.35013400	-1.62620400	0.69906400
N	-4.17164100	0.34126600	0.39986100
C	-4.36814300	0.92924400	1.63360700
C	-3.89667700	2.27154500	1.69291900
C	-4.91278800	0.37019300	2.78056000
C	-3.98103100	3.03206000	2.88315900
C	-4.98870000	1.13120700	3.96450600
H	-5.27965500	-0.64949500	2.75002200
C	-2.88257000	4.00566800	0.53166700
C	-3.47191500	4.35043100	2.83471900
C	-4.54028100	2.43063000	4.03438500
H	-5.42131400	0.66604300	4.84935900
C	-2.92990300	4.83452100	1.67011000
H	-2.43854600	4.35167200	-0.39976200
H	-3.51280700	4.96784000	3.73239700
H	-4.60815700	3.00491900	4.95737500
H	-2.52791300	5.84233600	1.60757000
N	-3.34209200	2.76736600	0.54539900
C	-4.26962300	-2.48375000	-1.88938600
H	-4.94692200	-3.19579900	-1.41606700
F	1.03418900	2.97041800	-3.85886700
F	-0.82567600	3.97320500	-4.32126800
F	-0.64538000	1.83549500	-4.59272900
C	-2.74033500	-3.28478200	1.77293100
O	-3.96263100	-3.74268800	1.55137500
O	-2.35743000	-2.17374700	1.44092200
Ag	-1.21246500	-0.51019000	-0.20863100
C	1.62031200	1.05226000	1.03193200
C	1.73649800	-0.19803300	1.62082000
C	0.79893900	-0.62870100	2.61733400

C	-0.33196300	0.18342600	2.91513400
C	-0.49138200	1.40296400	2.20941500
C	0.46137200	1.83379800	1.32566700
H	1.81009900	-2.48516800	3.10433600
C	0.95382700	-1.84782800	3.32490600
C	-1.25739100	-0.23342400	3.89935400
H	-1.37555100	2.01344500	2.40560400
H	0.31118900	2.78426400	0.81069600
C	-1.06052500	-1.40374100	4.58929500
C	0.05850200	-2.21182600	4.30142200
H	-2.12587400	0.39742000	4.10002600
H	-1.76889900	-1.71328900	5.35672700
H	0.20816400	-3.14137200	4.84996900
C	6.47598600	-1.50268500	3.20519300
C	6.23546400	-2.27233500	2.09471100
C	5.00373200	-2.18341400	1.40437300
C	4.01475400	-1.26906200	1.86580400
C	5.49465200	-0.60086100	3.66786400
H	5.50342100	-3.64805400	-0.10778000
H	7.42545100	-1.58560600	3.73178700
H	6.98832700	-2.97014200	1.72653600
C	4.73078900	-2.97214200	0.26041200
C	2.76996000	-1.17190100	1.17334900
H	5.69303600	0.00553100	4.55009700
C	2.50987600	-2.01010300	0.09863300
C	3.52047800	-2.88933300	-0.37318900
H	3.32265700	-3.50017300	-1.25467600
P	2.64653400	1.77081600	-0.36631200
P	0.83430600	-2.04591700	-0.69902200
C	4.29634400	-0.48152300	3.00895000
H	3.54050000	0.22156000	3.35877600
C	0.23518200	-3.77134100	-0.41915400
C	-1.05630800	-4.03765600	-0.89237100
C	0.95385600	-4.79410300	0.20148000
C	-1.60625000	-5.30715600	-0.77622600
H	-1.63765200	-3.24517000	-1.37145600
C	0.39851600	-6.06745700	0.32180100
H	1.95452700	-4.60641800	0.59026500
C	-0.87529100	-6.32869100	-0.17116700
H	-2.61491200	-5.48933500	-1.14655600
H	0.96917500	-6.85880600	0.80563400
H	-1.30486100	-7.32477000	-0.07492500
C	1.24331200	-2.07695000	-2.50601300
C	1.48317100	-0.85128100	-3.13985000

C	1.29103000	-3.25518500	-3.25584600
C	1.77573500	-0.81270500	-4.49914500
H	1.41278600	0.08005000	-2.57494100
C	1.57712100	-3.20938600	-4.61772900
H	1.09686500	-4.21604600	-2.77805800
C	1.82000400	-1.98968600	-5.24148200
H	1.95495500	0.14895100	-4.97832100
H	1.60796100	-4.13368100	-5.19293700
H	2.04023100	-1.95612900	-6.30740700
C	2.84060400	3.49310200	0.30195200
C	3.05402700	3.78637200	1.65426200
C	2.75925000	4.54686500	-0.61126500
C	3.20982900	5.10016900	2.07878400
H	3.07820300	2.97577100	2.38532500
C	2.91688100	5.86409300	-0.18759100
H	2.54544300	4.33053600	-1.65861400
C	3.14655400	6.14146300	1.15529400
H	3.37629000	5.31407100	3.13386100
H	2.84641000	6.67617800	-0.90955100
H	3.26515100	7.17193900	1.48739600
C	4.39213100	1.13603400	-0.24138500
C	4.79380800	0.29371900	-1.28459900
C	5.34189800	1.51902900	0.71118200
C	6.10170600	-0.17619700	-1.36214600
H	4.06737100	0.00036500	-2.04588800
C	6.64792300	1.04988700	0.63652400
H	5.06400800	2.19611800	1.51830800
C	7.03034300	0.20026200	-0.39872900
H	6.39287400	-0.83368700	-2.18039000
H	7.37233400	1.34743400	1.39412600
H	8.05621500	-0.16192200	-0.45551600
C	-1.89677400	-4.27595600	2.51168100
H	-2.14514000	-5.29791700	2.20811300
H	-2.09858000	-4.17716900	3.58642200
H	-0.83860600	-4.06558000	2.33397900

TS5-6

S	-1.61337900	-2.94294200	0.81702100
O	-3.02824100	-3.51015000	0.96521400
O	-1.53080000	-1.39149800	0.96759600
C	-0.82913100	-3.54798800	2.45553000
O	-0.78303000	-3.52263500	-0.32499700
Ni	-3.51917600	-0.41614100	0.01819800
C	-2.41081800	3.02681900	3.03701700

C	-3.32375500	2.17756400	0.97388200
C	-3.55829200	0.89893500	1.55330400
C	-3.04000200	0.69691400	2.84104400
C	-2.45847900	1.73877700	3.56089700
H	-1.98814300	3.84507600	3.61990800
H	-2.45893300	4.48193400	-1.36570800
H	-3.09533500	-0.28672600	3.30291800
H	-2.04780400	1.53784800	4.55016200
C	-3.32520400	2.29956600	-0.50941000
O	-3.65727500	3.32729900	-1.11793100
N	-2.85236300	1.13905200	-1.04840400
C	-2.87887600	0.87614300	-2.41875400
C	-3.10190200	-0.49768700	-2.72936500
C	-2.68492700	1.76975000	-3.45776300
C	-3.05254600	-0.95414800	-4.06969700
C	-2.67430700	1.31548500	-4.79163600
H	-2.52960800	2.81893600	-3.23200000
C	-3.55232600	-2.63606800	-1.93476600
C	-3.22594600	-2.33931400	-4.29222100
C	-2.83140200	-0.01479900	-5.10373200
H	-2.52292700	2.04237500	-5.58909700
C	-3.45924900	-3.17615100	-3.23206200
H	-3.75035300	-3.26669800	-1.06788000
H	-3.17057900	-2.72281500	-5.31126500
H	-2.80008700	-0.36131500	-6.13618300
H	-3.58467400	-4.24692100	-3.36789200
N	-3.37733200	-1.34814800	-1.68868900
C	-2.83151100	3.23649500	1.72538700
H	-2.70694600	4.20436000	1.23418500
F	0.40615100	-3.10632100	2.62115900
F	-0.82400900	-4.86778500	2.46140700
F	-1.58049400	-3.09600600	3.45219800
C	0.57201900	5.27750900	-2.06858500
H	0.46888900	6.28580000	-1.65597200
H	1.51337000	4.81845300	-1.75018700
H	0.58509900	5.35608900	-3.16398000
C	-0.58528700	4.41391400	-1.66956800
O	-1.70592000	5.11396000	-1.53635800
O	-0.52314500	3.20637900	-1.51863900
Ag	-0.59743200	0.74320500	-0.22673200
C	-5.28274000	-1.04569200	0.41308900
C	-5.18742800	0.12959600	1.29361000
C	-5.66160500	-0.42675200	2.64048500
C	-5.71548700	-2.21179200	1.27406900

H	-5.42324400	0.20539500	3.50319200
H	-5.78784400	-0.93107200	-0.55362100
H	-5.69820900	1.03447800	0.94906600
H	-5.47427400	-3.20441500	0.88177100
C	-7.21338300	-1.95482900	1.55459100
H	-7.79293200	-1.79751300	0.63500600
H	-7.65662900	-2.81347000	2.07842900
C	-5.10396100	-1.85451100	2.62687400
H	-4.01316900	-1.94346900	2.61739600
H	-5.50652100	-2.46388200	3.44822600
C	-7.17180600	-0.70014500	2.46290300
H	-7.69966600	0.16201300	2.03266600
H	-7.62635100	-0.89925500	3.44253400
C	1.91564000	-1.00305800	-1.34712900
C	2.63735800	0.17779100	-1.42887700
C	2.34447500	1.14713800	-2.43996200
C	1.25070500	0.92808100	-3.32309400
C	0.44992500	-0.22544700	-3.13824900
C	0.76893500	-1.16147300	-2.18699600
H	3.94692000	2.51690000	-1.92725800
C	3.11288000	2.32771700	-2.60246100
C	0.97650600	1.86770800	-4.34279900
H	-0.41966000	-0.36825800	-3.78256900
H	0.14037400	-2.04683800	-2.06130000
C	1.76052800	2.98336300	-4.49753000
C	2.83653800	3.21362600	-3.61487400
H	0.12975700	1.67768300	-5.00368900
H	1.55300600	3.69471700	-5.29607800
H	3.45008200	4.10605400	-3.73427900
C	7.78960600	-0.09318900	-1.06117700
C	7.35578000	0.38194900	0.15126800
C	5.97960700	0.60259500	0.39207700
C	5.03900800	0.30681000	-0.63439600
C	6.85947000	-0.38211400	-2.08196200
H	6.23357400	1.29293900	2.42571300
H	8.85221400	-0.25200400	-1.23766000
H	8.06519000	0.60080700	0.94999000
C	5.51083200	1.09640700	1.63300400
C	3.64871900	0.51729500	-0.39301100
H	7.21046100	-0.76057400	-3.04052600
C	3.23133900	1.06437000	0.81126400
C	4.17748800	1.32785900	1.83553400
H	3.83362900	1.72017200	2.79283700
P	2.09088200	-2.36444400	-0.07669100

P	1.47380600	1.61352100	1.04914500
C	5.51587800	-0.19549500	-1.87012700
H	4.79582200	-0.42893100	-2.65438200
C	1.66665100	3.45277800	1.03132900
C	0.50454800	4.19783600	1.24992200
C	2.87393300	4.12511400	0.83447500
C	0.54708500	5.58387000	1.31566000
H	-0.44210800	3.67340200	1.37234400
C	2.91579700	5.51802500	0.88830200
H	3.79190900	3.56724700	0.65195000
C	1.75965000	6.24865100	1.13885700
H	-0.37200600	6.14432700	1.48771100
H	3.86419200	6.03176600	0.73826500
H	1.79964800	7.33582200	1.18610500
C	1.15412600	1.26464100	2.83626000
C	0.60734600	0.01373900	3.14022400
C	1.41209400	2.17089200	3.86884600
C	0.35338300	-0.33942600	4.46189500
H	0.35628700	-0.68224900	2.33803800
C	1.14225800	1.82041000	5.18867100
H	1.81856700	3.15733500	3.64154600
C	0.62005000	0.56409400	5.48708500
H	-0.06989700	-1.31836800	4.68145100
H	1.34419100	2.53210700	5.98797000
H	0.41437400	0.29212600	6.52145100
C	2.17858600	-3.82688100	-1.21882100
C	2.70899100	-3.78225900	-2.51194100
C	1.73806000	-5.05270100	-0.71299600
C	2.80501900	-4.93898200	-3.27911500
H	3.04788600	-2.83032000	-2.92564000
C	1.84188600	-6.21092300	-1.47550000
H	1.28380600	-5.09200100	0.27683300
C	2.37503000	-6.15658900	-2.75959800
H	3.21803700	-4.88860100	-4.28595600
H	1.49148000	-7.15839100	-1.06888700
H	2.44951300	-7.06277600	-3.35928800
C	3.84154200	-2.40459600	0.56540300
C	4.00029600	-2.07575500	1.91589000
C	4.94801500	-2.89801900	-0.13493400
C	5.23528400	-2.20809600	2.54502100
H	3.14025500	-1.71506800	2.48483700
C	6.18185100	-3.03035200	0.49018900
H	4.84245200	-3.19090400	-1.17944400
C	6.32906800	-2.68498400	1.83170800

H	5.33753100	-1.94394900	3.59701600
H	7.03513400	-3.40518100	-0.07422100
H	7.29601200	-2.79664200	2.32108500

IM6

S	-1.64824400	-2.59457600	0.46290300
O	-3.13788200	-2.76628300	0.01571500
O	-1.31633100	-1.18137000	0.99193000
C	-1.57077900	-3.63521000	2.05428500
O	-0.63898000	-3.23912100	-0.48274800
Ni	-3.84822300	-1.06880900	-0.69078400
C	-2.14493600	1.55894900	3.02252000
C	-3.80434800	1.26598500	1.27112600
C	-4.44176200	0.26103800	2.01637600
C	-3.88315000	-0.08874600	3.24764500
C	-2.74069700	0.53112700	3.74140800
H	-1.26703100	2.07010400	3.42095700
H	-3.11032600	3.85287000	-0.95215600
H	-4.35450100	-0.86660400	3.84547400
H	-2.32730800	0.22432600	4.70171000
C	-4.17393400	1.71305400	-0.11607100
O	-4.30491600	2.93572800	-0.33091800
N	-4.16580700	0.75269000	-1.05959700
C	-3.98306700	1.06413800	-2.40185200
C	-3.22095600	0.09495000	-3.12760800
C	-4.43361300	2.18386300	-3.08362700
C	-2.96314300	0.25771300	-4.51268800
C	-4.14206300	2.35479300	-4.45231200
H	-5.01700300	2.92795000	-2.55232100
C	-2.13735800	-1.95569800	-3.07736100
C	-2.27890300	-0.79084400	-5.16906400
C	-3.42708000	1.42299100	-5.16573900
H	-4.51584900	3.24622100	-4.95444000
C	-1.88114300	-1.89930100	-4.46177600
H	-1.80406800	-2.80448800	-2.47799800
H	-2.08692200	-0.70846000	-6.23966100
H	-3.23367500	1.54976100	-6.23069100
H	-1.36132200	-2.72463800	-4.94282700
N	-2.77131200	-0.99176500	-2.43114000
C	-2.68956700	1.92583300	1.79655200
H	-2.27010500	2.74931700	1.21715200
F	-0.31013000	-3.68987300	2.44876500
F	-2.01817800	-4.84580400	1.80310100
F	-2.29841200	-3.05967300	2.98902800

C	-0.05832000	4.24918100	-1.91318800
H	0.01091600	5.26030200	-1.49999400
H	0.82006200	3.65910300	-1.62987100
H	-0.07338400	4.32037400	-3.00848400
C	-1.30658800	3.56573500	-1.45786500
O	-2.30479900	4.38950500	-1.23501300
O	-1.40913700	2.34838000	-1.32764000
Ag	-0.35400900	0.69244300	-0.00458300
C	-5.53081600	-1.18784100	0.20472500
C	-5.72408400	-0.35176100	1.49731100
C	-6.39776400	-1.37172200	2.43105700
C	-5.98024700	-2.60012000	0.59751100
H	-6.41480900	-1.07149100	3.48688600
H	-6.15958100	-0.79613000	-0.61167800
H	-6.41569300	0.48622100	1.30183500
H	-5.56593600	-3.40146800	-0.02595000
C	-7.51754600	-2.57960200	0.64870300
H	-7.96205600	-2.19433400	-0.27892300
H	-7.91350900	-3.59450500	0.80463900
C	-5.64434300	-2.66378200	2.08785900
H	-4.56764200	-2.61695200	2.28076900
H	-6.06473500	-3.54932300	2.58767300
C	-7.80018000	-1.67693600	1.87696300
H	-8.34271400	-0.75759700	1.61470900
H	-8.40383600	-2.20387100	2.62855200
C	2.24044300	-0.74434400	-1.18012400
C	2.92818700	0.45676800	-1.26761100
C	2.63840900	1.38871200	-2.31868000
C	1.58034200	1.11030800	-3.23009200
C	0.81518800	-0.06433900	-3.04242300
C	1.13924600	-0.96602200	-2.06402400
H	4.18031400	2.82762800	-1.80771700
C	3.37136600	2.59042600	-2.49752500
C	1.30809000	2.00802600	-4.28752700
H	-0.03094300	-0.25422200	-3.70372800
H	0.54246300	-1.87271300	-1.94697000
C	2.06052200	3.14446100	-4.45464200
C	3.09665300	3.43824500	-3.54418400
H	0.48611100	1.77318500	-4.96568800
H	1.85355600	3.82509200	-5.27904100
H	3.68507000	4.34554100	-3.67122400
C	8.07990200	0.44381700	-0.83509300
C	7.61091300	0.95462400	0.34934300
C	6.22318200	1.11712100	0.56896100

C	5.30734900	0.72538700	-0.44807100
C	7.17504200	0.06232700	-1.84798600
H	6.42722800	1.94263400	2.55748500
H	9.15067000	0.32967500	-0.99571700
H	8.30064900	1.24906500	1.14085800
C	5.72099300	1.65438600	1.77821600
C	3.90441100	0.86604300	-0.22169600
H	7.55337200	-0.34306700	-2.78486300
C	3.44974200	1.42597500	0.96332000
C	4.37544100	1.80856300	1.96895600
H	4.00616800	2.22484300	2.90600600
P	2.39128000	-2.05634700	0.14857000
P	1.64476300	1.75721700	1.24104500
C	5.82194100	0.19302200	-1.65587200
H	5.12371300	-0.11352500	-2.43444100
C	1.56826200	3.60405700	1.19837200
C	0.34270100	4.20968800	1.50407100
C	2.63169100	4.40550700	0.77805800
C	0.18479900	5.58559200	1.40009900
H	-0.49931800	3.59675600	1.82850400
C	2.47083800	5.78511900	0.66905100
H	3.59262500	3.95382700	0.53272100
C	1.25172800	6.37750700	0.97945500
H	-0.77863500	6.03569600	1.63318800
H	3.30809800	6.39862000	0.33988000
H	1.12924700	7.45561300	0.89062100
C	1.40810900	1.33894800	3.02372200
C	0.97077500	0.04181800	3.31902400
C	1.60473800	2.25212400	4.06375600
C	0.76164000	-0.34039200	4.63994100
H	0.76496800	-0.66911500	2.51432700
C	1.37483700	1.87030400	5.38220400
H	1.91905500	3.27275300	3.84124400
C	0.95810000	0.57357100	5.67146900
H	0.41629200	-1.35013000	4.85634000
H	1.51963200	2.59009700	6.18625800
H	0.77671400	0.27844000	6.70372200
C	2.48365000	-3.56910100	-0.92389100
C	3.03459000	-3.59192100	-2.20916800
C	2.01436200	-4.76293700	-0.37079000
C	3.12372100	-4.78411600	-2.92017900
H	3.39093800	-2.66544200	-2.66322200
C	2.11056500	-5.95712300	-1.07721000
H	1.54687100	-4.74716800	0.61354300

C	2.66555300	-5.96985500	-2.35277100
H	3.55299300	-4.78691400	-3.92133600
H	1.73734000	-6.87913900	-0.63430600
H	2.73412400	-6.90341700	-2.90930500
C	4.13941400	-2.04019600	0.79337700
C	4.30363800	-1.66412900	2.13057600
C	5.25574800	-2.49781700	0.08564100
C	5.55429900	-1.71762700	2.73949400
H	3.43853200	-1.32470800	2.70444100
C	6.50563100	-2.54953700	0.69045200
H	5.14705200	-2.82415500	-0.94857000
C	6.65834000	-2.15844100	2.01840200
H	5.66196200	-1.41702900	3.78095500
H	7.36661000	-2.89852900	0.12147900
H	7.63844500	-2.20524500	2.49156900

IM7

S	3.76952500	-2.80968000	-0.51410900
O	2.71964500	-1.65782500	-0.11250700
O	3.32645200	-3.65919800	-1.68780100
C	3.60767200	-3.98843700	0.97898800
O	5.18392800	-2.23467300	-0.46880500
Ni	3.56400300	0.01085000	-0.34794900
F	4.49246300	-4.95086600	0.83221100
F	2.38971200	-4.48432500	0.98601000
F	3.84087600	-3.33473700	2.10250800
C	2.37519500	-0.72734200	-3.12893600
C	4.48912200	0.39104700	-2.67212400
C	5.14471700	-0.47168500	-3.54743100
C	4.41380700	-1.44951500	-4.20724900
C	3.03859700	-1.58204500	-3.99531000
H	1.29246900	-0.80088800	-3.00800100
H	6.22152300	-0.38149800	-3.67109200
H	4.92216700	-2.13526800	-4.88209000
H	2.48114300	-2.36641500	-4.50286000
C	5.30074000	1.31414000	-1.85329800
O	6.42653600	1.67439900	-2.07092500
N	4.59709400	1.60513600	-0.61602000
H	3.79794600	2.33522800	-0.66372100
C	5.37556300	1.91384700	0.55773400
C	4.97704100	1.17325500	1.68066100
C	6.30985500	2.90906700	0.67421900
C	5.50116400	1.45733000	2.95900900
C	6.88062000	3.16458900	1.94223400

H	6.59619800	3.49753900	-0.19257600
C	3.51937900	-0.42775400	2.51462900
C	4.96955100	0.72729400	4.04315900
C	6.48464500	2.46849300	3.05826500
H	7.63003700	3.94770400	2.03127100
C	3.97455100	-0.19442600	3.82444800
H	2.74169600	-1.15501200	2.29399400
H	5.34344500	0.91772200	5.04860300
H	6.91073200	2.69524500	4.03454100
H	3.52853700	-0.75104700	4.64461200
N	4.03220400	0.20860600	1.48147300
C	3.09162700	0.27105200	-2.44145400
S	1.93063200	2.90140200	1.11603800
O	2.65425100	3.29711800	-0.20203800
O	1.12252300	1.58272800	1.02686800
C	0.60983700	4.27004200	1.22565700
O	2.78530300	3.03965800	2.37432400
H	2.48900200	1.09528000	-2.01009200
F	-0.34606000	4.01679900	0.35810500
F	1.17011300	5.43022800	0.96269800
F	0.11588600	4.28630500	2.45331700
C	0.79743300	2.44206000	-4.51962800
H	-0.03056400	2.77927800	-5.15514700
H	1.40969300	1.76685200	-5.13278100
H	1.40373600	3.29909200	-4.20939800
C	0.24627300	1.67515900	-3.33117600
O	0.65546500	2.03650500	-2.17698000
O	-0.54908300	0.74065400	-3.54390300
Ag	-0.38840100	0.63932600	-0.71459400
C	-3.44480500	0.99950100	0.57334200
C	-3.42470600	-0.24213200	1.20002200
C	-2.87323800	-0.38766300	2.50671300
C	-2.24155100	0.73168400	3.12113200
C	-2.20903100	1.96198100	2.42880500
C	-2.81223700	2.10098700	1.20398500
H	-3.41043100	-2.47322800	2.75926600
C	-2.93215300	-1.61124300	3.22376800
C	-1.67154900	0.58531800	4.40941500
H	-1.71020100	2.80819300	2.89736300
H	-2.79313300	3.06575700	0.69701900
C	-1.75284200	-0.60763800	5.08074600
C	-2.39760400	-1.71361500	4.48262700
H	-1.17918200	1.44781600	4.85938700
H	-1.32357700	-0.70648300	6.07684500

H	-2.46270600	-2.65730000	5.02229200
C	-7.95860500	-2.70225300	0.83349300
C	-7.10812100	-3.37058500	-0.00906700
C	-5.75217700	-2.97950600	-0.12840800
C	-5.27862100	-1.86770700	0.62649600
C	-7.48588700	-1.61514300	1.60115200
H	-5.21351800	-4.51977600	-1.54605500
H	-8.99917900	-3.01146300	0.91840400
H	-7.45780600	-4.21861200	-0.59857500
C	-4.85008200	-3.66777800	-0.97064700
C	-3.92182800	-1.45036300	0.48465200
H	-8.16486300	-1.09239800	2.27276000
C	-3.05496900	-2.16968900	-0.32775700
C	-3.53773600	-3.28431300	-1.05910600
H	-2.86007800	-3.83591500	-1.70917700
P	-4.26996600	1.13340500	-1.10768200
P	-1.25434500	-1.69803900	-0.40755400
C	-6.18020500	-1.20852600	1.50080600
H	-5.82157700	-0.36642100	2.09031600
C	-0.57327800	-2.61529400	1.04667800
C	0.28101500	-1.94580000	1.92624100
C	-0.97611600	-3.92156100	1.34544700
C	0.70546400	-2.57087500	3.09633700
H	0.59006800	-0.91961500	1.70788700
C	-0.53991400	-4.54669500	2.50807000
H	-1.65514800	-4.44680500	0.67245100
C	0.29331300	-3.86600700	3.39217300
H	1.33275400	-2.02637800	3.80337300
H	-0.86289100	-5.56232800	2.73119900
H	0.61835100	-4.34523900	4.31464300
C	-0.69713300	-2.61195600	-1.90407700
C	-1.19531900	-2.15530200	-3.13332600
C	0.20962500	-3.66948300	-1.87644600
C	-0.80126600	-2.77125400	-4.31345100
H	-1.86962500	-1.29916400	-3.16595900
C	0.60710700	-4.28000500	-3.06430000
H	0.61532900	-4.02562900	-0.93166900
C	0.09651200	-3.83888000	-4.27956700
H	-1.18970400	-2.40615300	-5.26257700
H	1.32909500	-5.09345600	-3.02981400
H	0.40302700	-4.32212200	-5.20709600
C	-6.04244400	1.29549300	-0.56442500
C	-7.00682400	0.67333200	-1.36109000
C	-6.45550200	1.96755900	0.59208900

C	-8.35495600	0.72624900	-1.01920400
H	-6.69024600	0.12326800	-2.24849200
C	-7.80277800	2.02942300	0.93101000
H	-5.71172000	2.43263500	1.24190100
C	-8.75466100	1.40912300	0.12459800
H	-9.09386900	0.22938400	-1.64625200
H	-8.11126400	2.56053500	1.83086300
H	-9.80913900	1.45275500	0.39413500
C	-3.81828800	2.87780000	-1.54177500
C	-2.59796200	3.01249800	-2.21124000
C	-4.53229800	4.02684600	-1.19138800
C	-2.06490600	4.27241100	-2.46579000
H	-2.06610300	2.11802300	-2.54378800
C	-4.01161900	5.28650700	-1.47232400
H	-5.49665900	3.94053100	-0.69170000
C	-2.77035400	5.41164300	-2.09162100
H	-1.08983400	4.35770100	-2.94407000
H	-4.57516700	6.17681200	-1.19527200
H	-2.35713500	6.39976400	-2.28944100

TS7-8

S	3.95081200	3.00322800	0.31153500
O	2.92159900	1.78716200	0.10710700
O	3.67837100	3.81795500	1.56427100
C	3.38671400	4.15087600	-1.09934800
O	5.37028000	2.56863600	-0.03155200
Ni	3.80315200	0.12590200	0.30875100
F	4.16460000	5.21185100	-1.10607400
F	2.13821800	4.50475700	-0.87719400
F	3.48192200	3.52049600	-2.25689300
C	3.60713200	1.31706400	3.17238500
C	5.18283500	-0.42445600	2.61180900
C	5.97941700	-0.07950300	3.69919500
C	5.57983800	0.96763200	4.52282500
C	4.40005900	1.66454200	4.25991800
H	2.66263800	1.82438700	2.98423300
H	6.91047800	-0.61635600	3.87086300
H	6.19599400	1.24865800	5.37508100
H	4.09757700	2.48802500	4.90507000
C	5.64416100	-1.44610100	1.66430700
O	6.65996100	-2.08805600	1.73567300
N	4.73498400	-1.54688800	0.51410900
H	3.88372800	-2.15721800	0.68860100
C	5.29480500	-1.97517800	-0.75079500

C	4.80370800	-1.23823500	-1.84195200
C	6.11567000	-3.05385700	-0.95599500
C	5.13905300	-1.59832900	-3.16496700
C	6.49004400	-3.39233200	-2.27649800
H	6.46940600	-3.64134500	-0.11528900
C	3.38233700	0.45113300	-2.55133300
C	4.53098100	-0.86175400	-4.20174400
C	6.01537400	-2.69070100	-3.35594500
H	7.15168400	-4.24181000	-2.42997900
C	3.64618100	0.14359500	-3.89722500
H	2.69783300	1.24589400	-2.26482300
H	4.75740500	-1.11314000	-5.23749800
H	6.28858600	-2.97635500	-4.37082100
H	3.14832700	0.71127200	-4.67893400
N	3.96127000	-0.20150300	-1.56241300
C	3.98589500	0.26630200	2.33010200
S	1.79770200	-2.89644200	-1.04991900
O	2.46176900	-3.03724700	0.34505300
O	0.92512200	-1.62827700	-1.22423500
C	0.51855800	-4.31000500	-1.04654800
O	2.71138300	-3.19513100	-2.23378600
H	2.93721500	-0.27648200	1.98008000
F	-0.43625100	-4.04985800	-0.17331900
F	1.12093200	-5.43756100	-0.73265000
F	-0.00229200	-4.40327200	-2.25860600
C	2.05078400	-2.31429600	3.56769600
H	2.51947800	-1.55073800	4.20215300
H	2.84762100	-2.84839300	3.03107200
H	1.51376200	-3.03552500	4.18933800
C	1.12550000	-1.68854400	2.55296700
O	0.00033000	-2.18289900	2.35341800
O	1.54131400	-0.66125100	1.91253500
Ag	-0.57714200	-0.82098700	0.46463000
C	-3.70099900	-0.94844800	-0.46609000
C	-3.65572100	0.30619000	-1.06639100
C	-3.12615000	0.46136100	-2.38065000
C	-2.52533800	-0.65975100	-3.02482100
C	-2.49935200	-1.90126500	-2.35116800
C	-3.09781600	-2.05150700	-1.12403300
H	-3.61698100	2.56368700	-2.58373200
C	-3.16214400	1.70130700	-3.07044000
C	-1.96875400	-0.50028300	-4.31729600
H	-2.01096000	-2.74751300	-2.83355500
H	-3.08888400	-3.02708800	-0.63718300

C	-2.02999900	0.70828900	-4.96225000
C	-2.63986700	1.81694100	-4.33315100
H	-1.50063300	-1.36374800	-4.79046700
H	-1.60956500	0.81829600	-5.96084300
H	-2.68716900	2.77322200	-4.85188500
C	-8.03566400	2.96977900	-0.32528100
C	-7.11112800	3.53546400	0.51449400
C	-5.77129700	3.07647100	0.53175600
C	-5.39339300	2.00379800	-0.32795700
C	-7.65836000	1.91976200	-1.19207500
H	-5.08861600	4.47736900	2.02934500
H	-9.06281800	3.33105300	-0.33047200
H	-7.38898800	4.35367500	1.17951300
C	-4.79534500	3.65728000	1.37313100
C	-4.05643000	1.51226100	-0.28583900
H	-8.39790400	1.47173800	-1.85404000
C	-3.11262800	2.13695600	0.52086700
C	-3.49878000	3.21325900	1.35702400
H	-2.75710500	3.67940300	2.00498500
P	-4.47650000	-1.08687100	1.23772700
P	-1.34618700	1.56349900	0.45769600
C	-6.37043100	1.44947800	-1.19340800
H	-6.08290700	0.63442200	-1.85629900
C	-0.68520300	2.54092900	-0.96027500
C	0.12318900	1.89282900	-1.89668600
C	-1.03627800	3.87994200	-1.16250900
C	0.55889300	2.57676000	-3.02837600
H	0.38080300	0.83868100	-1.75682600
C	-0.57986000	4.56386100	-2.28253600
H	-1.67840200	4.38754400	-0.44145300
C	0.21556400	3.91046500	-3.22030100
H	1.15703600	2.05761600	-3.77737600
H	-0.85235600	5.60790800	-2.42879000
H	0.56043000	4.44098200	-4.10688400
C	-0.60344700	2.31660400	1.96409300
C	-1.01593300	1.80154700	3.20094900
C	0.38646800	3.29679100	1.92285400
C	-0.46863200	2.29261400	4.37833400
H	-1.76989600	1.01008800	3.23479800
C	0.94178600	3.78104800	3.10688500
H	0.75231700	3.67187300	0.96739000
C	0.50801800	3.28836900	4.33243100
H	-0.80162400	1.89466600	5.33566000
H	1.73768100	4.52177900	3.05042400

H	0.93890600	3.66987000	5.25757400
C	-6.27215500	-1.13455000	0.75823200
C	-7.18017600	-0.50047700	1.60958300
C	-6.75294800	-1.75141200	-0.40267700
C	-8.54062400	-0.48859600	1.31595200
H	-6.81005000	0.00332600	2.50369400
C	-8.11206000	-1.74502300	-0.69566000
H	-6.05238900	-2.23036200	-1.08933300
C	-9.00805300	-1.11363400	0.16481500
H	-9.23604800	0.01452600	1.98627500
H	-8.47439400	-2.23147100	-1.60057500
H	-10.07225200	-1.10565100	-0.06725200
C	-4.12187100	-2.86529000	1.61859000
C	-2.87587100	-3.10526300	2.20560400
C	-4.95046400	-3.95072600	1.32168700
C	-2.43492500	-4.40346600	2.43787700
H	-2.22156200	-2.27434600	2.47024400
C	-4.52244900	-5.24916200	1.58227200
H	-5.93378500	-3.78642200	0.88236700
C	-3.26042100	-5.47900400	2.12554600
H	-1.44159800	-4.55371400	2.85705400
H	-5.17624500	-6.08872200	1.34863600
H	-2.92528700	-6.49863400	2.31114000

IM8

S	-4.12918000	-3.05838900	0.63318900
O	-3.20689300	-1.77901000	0.36747900
O	-3.83587100	-3.71708100	1.97340000
C	-3.39987000	-4.29755400	-0.61684400
O	-5.55954200	-2.82316700	0.17429000
Ni	-4.17165500	-0.13626700	0.31313700
F	-4.05250700	-5.43489300	-0.49295800
F	-2.12027900	-4.48246500	-0.35272800
F	-3.54841400	-3.83813100	-1.84802400
C	-4.08422800	-0.81821000	3.23669500
C	-5.39875600	1.03646700	2.48833500
C	-5.85555900	1.28424600	3.78475900
C	-5.39621800	0.48406600	4.82014500
C	-4.51677800	-0.56329800	4.53921400
H	-3.42545200	-1.66577900	3.05409700
H	-6.56615500	2.09240300	3.95492400
H	-5.73031100	0.65976100	5.84105000
H	-4.16972300	-1.20471800	5.34965200
C	-5.88778600	1.82481400	1.35772900

O	-6.84998200	2.54930300	1.31224600
N	-5.01812500	1.59166800	0.19821700
H	-4.11070100	2.10640000	0.32820100
C	-5.49097600	1.85827800	-1.13973700
C	-4.92262200	0.99549300	-2.10005000
C	-6.30278800	2.89093400	-1.53335300
C	-5.15098900	1.20417600	-3.47773100
C	-6.57453800	3.06923800	-2.91005100
H	-6.72577100	3.56410000	-0.79524400
C	-3.47571700	-0.76475200	-2.49659800
C	-4.46905700	0.35382000	-4.37331400
C	-6.00824700	2.26028300	-3.86255000
H	-7.22736000	3.88598700	-3.21068400
C	-3.62384200	-0.61377400	-3.88735000
H	-2.82500700	-1.52179700	-2.06187400
H	-4.61123300	0.48634300	-5.44569400
H	-6.19964600	2.42688500	-4.92201300
H	-3.07555000	-1.27011200	-4.55913000
N	-4.11971500	-0.00308700	-1.63639200
C	-4.50952600	-0.00934200	2.17820000
S	-1.77985300	2.57233300	-1.18155000
O	-2.41764100	2.68624900	0.22709100
O	-0.83922400	1.35209300	-1.35944300
C	-0.54055600	4.02109300	-1.20884800
O	-2.72141000	2.83364500	-2.34922600
H	-2.30576900	0.08866900	1.95498600
F	0.43527200	3.77583900	-0.34307000
F	-1.15120100	5.13954300	-0.88443800
F	-0.02845100	4.12090900	-2.42293300
C	-1.98038500	1.97461100	3.48575000
H	-2.28669100	1.17183200	4.16877100
H	-2.88578600	2.34769400	2.98893300
H	-1.51148800	2.78937800	4.04123200
C	-1.02988200	1.45655200	2.45605100
O	0.05472000	1.96917900	2.22528800
O	-1.38311900	0.37338200	1.77776700
Ag	0.89878500	0.92224500	0.19916800
C	3.82196900	0.87583400	-0.58238000
C	3.74780600	-0.42286700	-1.07612700
C	3.15473000	-0.68338400	-2.34586700
C	2.52602500	0.38387200	-3.05230100
C	2.53889700	1.67977400	-2.48812200
C	3.19211100	1.92672400	-1.30237500
H	3.62163000	-2.79969500	-2.38924300

C	3.13600200	-1.98106600	-2.91937800
C	1.88712900	0.11623600	-4.28768200
H	2.02496700	2.48635600	-3.01171800
H	3.21382800	2.94019800	-0.90010400
C	1.88545200	-1.14980600	-4.81415100
C	2.52011500	-2.20646200	-4.12390100
H	1.39657800	0.93930300	-4.80733700
H	1.39389300	-1.34520800	-5.76595300
H	2.50486900	-3.21154700	-4.54297400
C	8.14851000	-2.95941700	-0.09973700
C	7.23198500	-3.45202700	0.79406700
C	5.88520300	-3.01485100	0.76556000
C	5.49590000	-2.03701000	-0.19620400
C	7.75690200	-2.01154100	-1.07102900
H	5.21965800	-4.26806500	2.39583600
H	9.18060100	-3.30490500	-0.06928800
H	7.52313800	-4.19350100	1.53850100
C	4.91573100	-3.52106200	1.66198500
C	4.15517200	-1.55788400	-0.19821100
H	8.48826600	-1.63413400	-1.78340800
C	3.21898400	-2.10426800	0.67251800
C	3.61462900	-3.09241000	1.60671700
H	2.87673400	-3.49585100	2.30041000
P	4.64939000	1.13334900	1.08223600
P	1.46537500	-1.51184100	0.58933300
C	6.46323600	-1.55942500	-1.11632700
H	6.16058500	-0.82387700	-1.86081100
C	0.71835200	-2.62115000	-0.67585300
C	-0.14383400	-2.06165000	-1.62208000
C	1.06040500	-3.97467100	-0.76268300
C	-0.62849200	-2.84932800	-2.66311800
H	-0.41629700	-1.00342300	-1.56428900
C	0.55335400	-4.75981000	-1.79076000
H	1.74074200	-4.41227700	-0.03056700
C	-0.28710900	-4.19450500	-2.74633500
H	-1.26908900	-2.40349800	-3.42381500
H	0.81872000	-5.81416100	-1.84908900
H	-0.67557800	-4.80562200	-3.55998600
C	0.71342100	-1.98150400	2.19650000
C	1.18492700	-1.31552200	3.33566200
C	-0.42323900	-2.78507600	2.28851500
C	0.53059400	-1.46084000	4.55130300
H	2.06176200	-0.66690100	3.26274300
C	-1.08036000	-2.92568700	3.50991400

H	-0.82616600	-3.28548700	1.40850300
C	-0.60914800	-2.26111500	4.63703900
H	0.90417300	-0.94164000	5.43279600
H	-1.97602100	-3.54413500	3.55360300
H	-1.12531500	-2.36990200	5.59023400
C	6.41976700	1.27152200	0.53838800
C	7.38565900	0.71181200	1.37811500
C	6.82916900	1.87115600	-0.65838700
C	8.73510600	0.76196400	1.04066000
H	7.06992100	0.21103100	2.29458300
C	8.17709600	1.92442600	-0.99617600
H	6.08365000	2.28973000	-1.33691600
C	9.13196500	1.37255600	-0.14443100
H	9.47663100	0.31786100	1.70306900
H	8.48455800	2.39628100	-1.92850100
H	10.18717200	1.41245300	-0.41100600
C	4.17364100	2.89254500	1.41604000
C	2.93615700	3.05960200	2.04693200
C	4.91260700	4.02579100	1.06772300
C	2.41857000	4.32944900	2.27854900
H	2.35635100	2.18739600	2.35533000
C	4.40618000	5.29763400	1.32147700
H	5.88802800	3.91658800	0.59447600
C	3.15587200	5.45233500	1.91464500
H	1.43851600	4.42904300	2.74250600
H	4.99094200	6.17470800	1.04681100
H	2.75950400	6.44983700	2.09848800

IM9

S	0.92489000	-2.04722300	1.96797100
O	0.15829600	-0.88978600	1.16811600
O	1.00087800	-3.36520300	1.21674100
C	-0.43137100	-2.28945500	3.28115700
O	2.14734900	-1.51443300	2.69791000
Ni	0.78174900	-0.06110800	-0.41501000
F	-0.08418400	-3.26991800	4.08613200
F	-1.55755900	-2.59131100	2.65855400
F	-0.57284800	-1.16941900	3.95945600
C	-0.61896200	-2.55305600	-1.36131100
C	0.30999600	-1.01264800	-2.95664400
C	-0.03653900	-1.85015600	-4.01423700
C	-0.74128100	-3.01832500	-3.74717300
C	-1.02767700	-3.36314100	-2.42927200
H	-0.71294700	-2.94108200	-0.34527900

H	0.25771300	-1.57976100	-5.02780900
H	-1.04156200	-3.67543500	-4.56081100
H	-1.54202100	-4.29936300	-2.21624900
C	1.14933500	0.16894100	-3.17395600
O	1.82809600	0.43412000	-4.13354100
N	1.09397600	1.02169700	-1.98057700
H	0.17442700	1.52856000	-1.97672400
C	2.10581800	2.01868600	-1.72215700
C	2.35268900	2.21218100	-0.34444800
C	2.73949400	2.80115400	-2.65506100
C	3.23063800	3.23002700	0.08997000
C	3.65232500	3.79086800	-2.22194000
H	2.54314400	2.65370400	-3.71200400
C	1.85879900	1.56498800	1.82530300
C	3.38547200	3.38821900	1.48629100
C	3.88801400	4.01290900	-0.88789300
H	4.15938200	4.39628400	-2.97014900
C	2.69351600	2.57365800	2.34729900
H	1.31699600	0.87770200	2.47212100
H	4.05324100	4.16296300	1.86269200
H	4.57790700	4.79173500	-0.56499700
H	2.78838800	2.67785900	3.42459500
N	1.71029600	1.38276900	0.52843100
C	0.02952500	-1.33040500	-1.61124600
S	-2.15132400	2.28640500	-0.73455800
O	-3.15379500	1.34130600	-1.46449900
O	-1.74519200	1.70861300	0.63500100
C	-3.17542400	3.83706000	-0.33971200
O	-1.01112500	2.79210900	-1.62983000
H	-4.49918000	0.82993900	-0.52913400
F	-4.21207600	3.46210300	0.38167600
F	-3.57461800	4.38100500	-1.46642900
F	-2.42412100	4.67622700	0.33785500
C	-6.37793000	-0.99079100	1.36591400
H	-6.19993600	-1.93802400	1.87855000
H	-7.21903800	-1.08922200	0.67044800
H	-6.65041600	-0.21650000	2.09227900
C	-5.15266500	-0.56709800	0.62006800
O	-5.32103700	0.56179600	-0.02936000
O	-4.11610200	-1.22287900	0.62980700
Ag	-2.01614900	-0.70635000	-0.18321100
C	3.80464900	-0.99708500	-1.53615700
C	3.72157200	-1.41872500	-0.26449400
C	3.87374200	-2.92402400	-0.27932800

C	4.00466200	-2.21805600	-2.40669600
H	3.50997300	-3.45180700	0.60691000
H	3.88415900	0.03166900	-1.88894500
H	3.69854500	-0.81382900	0.64130600
H	3.76979500	-2.09684400	-3.47046600
C	5.45271100	-2.70518300	-2.11431200
H	6.19161900	-1.90760200	-2.26210600
H	5.71989900	-3.53070300	-2.78844800
C	3.20249200	-3.26173300	-1.61667700
H	2.12092300	-3.07386700	-1.60832200
H	3.39571000	-4.29331200	-1.94649600
C	5.36290400	-3.18624500	-0.64424200
H	6.04998700	-2.65285600	0.02426500
H	5.58965800	-4.25797100	-0.56204500

TS9-10

S	0.71272000	-1.51396300	2.33268900
O	0.49028200	-0.39275700	1.25517600
O	-0.30230300	-2.65595000	2.12641400
C	0.13857500	-0.61830800	3.90887400
O	2.17492000	-1.87299900	2.57358200
Ni	1.63729700	-0.25214600	-0.47035200
F	0.28675900	-1.43374200	4.93263700
F	-1.12047800	-0.27694400	3.77032500
F	0.89444900	0.45012100	4.07038000
C	-0.33353200	-2.36177300	-1.27476900
C	0.00797900	-0.45508600	-2.69182900
C	-0.96158500	-0.90908600	-3.58569200
C	-1.65949300	-2.07349900	-3.29711700
C	-1.34283000	-2.79408900	-2.14577600
H	-0.06666400	-2.99467200	-0.42577400
H	-1.17281400	-0.32483600	-4.48074600
H	-2.44162300	-2.42719200	-3.96615300
H	-1.87939800	-3.71496900	-1.91613900
C	0.72987500	0.80908700	-2.92261600
O	1.03706000	1.30144900	-3.98451900
N	1.11616600	1.35483200	-1.65511900
H	0.29543700	1.56250100	-1.04365100
C	2.07778100	2.39843500	-1.50432500
C	2.84973800	2.29137600	-0.32063000
C	2.23078800	3.48382900	-2.33194400
C	3.71512000	3.34568000	0.05955200
C	3.14769000	4.50173600	-1.98527700
H	1.63903800	3.55264900	-3.23965800

C	3.35590300	1.06599100	1.58340400
C	4.38530000	3.21523000	1.29672600
C	3.85598200	4.45239000	-0.81032600
H	3.26367900	5.35282500	-2.65305700
C	4.18766600	2.09563600	2.06597100
H	3.21717200	0.13408900	2.13717600
H	5.04941200	4.01362900	1.62758600
H	4.53219600	5.25951000	-0.53066100
H	4.67803800	1.97545400	3.02833300
N	2.72736800	1.15224100	0.42612400
C	0.34855800	-1.16455200	-1.52896700
S	-2.03867700	1.70593600	0.17547600
O	-2.22553800	0.93080000	-1.16044400
O	-2.48058900	0.88207700	1.39667400
C	-3.32881200	3.09841900	0.07976800
O	-0.68141200	2.42159700	0.22813900
H	-3.66173600	0.04243900	-1.35675200
F	-4.51368200	2.54537300	-0.09023900
F	-3.04190700	3.87603700	-0.94327200
F	-3.30258800	3.78788400	1.19948700
C	-6.17283600	-1.98793800	-1.16553400
H	-6.30218100	-2.95324000	-0.67190300
H	-6.32687400	-2.08610300	-2.24574300
H	-6.92607900	-1.28192800	-0.79620600
C	-4.80601900	-1.44185400	-0.88802300
O	-4.55896400	-0.34546400	-1.56759000
O	-4.03086100	-1.97851200	-0.10577800
Ag	-1.87195900	-1.37154700	0.60033500
C	3.06455000	-1.54835000	-1.81391800
C	3.81594600	-1.28851000	-0.70613200
C	4.08645400	-2.60086000	-0.01656700
C	2.86056000	-3.04637600	-1.85069000
H	4.37060400	-2.54923900	1.03821300
H	2.97804700	-0.90153600	-2.68768900
H	4.40081800	-0.38688000	-0.54024100
H	2.03970200	-3.40758600	-2.47825900
C	4.26279000	-3.61228900	-2.21867100
H	4.66748000	-3.15486800	-3.13022800
H	4.19228900	-4.69298300	-2.39823000
C	2.82009500	-3.38564400	-0.35662800
H	1.94085600	-3.00538400	0.17353500
H	2.92089900	-4.46145500	-0.16017300
C	5.10876000	-3.30503400	-0.95695600
H	5.98377000	-2.67738700	-1.16866000

H	5.47313600	-4.22639900	-0.48409500
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IM10

S	0.70644400	-1.48621400	2.33572700
O	0.49007900	-0.37494500	1.24753000
O	-0.31588000	-2.62463000	2.14309700
C	0.14487900	-0.57457700	3.90710000
O	2.16609900	-1.85761500	2.57610400
Ni	1.67138100	-0.28878900	-0.47182600
F	0.29966700	-1.38082400	4.93723500
F	-1.11440300	-0.23344800	3.77413300
F	0.90339200	0.49418000	4.05304700
C	-0.32196600	-2.38442200	-1.26243600
C	-0.00555800	-0.45899800	-2.66131200
C	-0.99630300	-0.89834000	-3.53889100
C	-1.69003600	-2.06561700	-3.25188800
C	-1.35231700	-2.80164600	-2.11638200
H	-0.04128500	-3.02593700	-0.42462200
H	-1.22783800	-0.29953600	-4.41916700
H	-2.48793300	-2.40783000	-3.90815400
H	-1.88879700	-3.72230500	-1.88577400
C	0.70902900	0.81176500	-2.88638600
O	1.00766900	1.31143200	-3.94763700
N	1.10011800	1.34838000	-1.61955900
H	0.28735000	1.53550000	-0.99259900
C	2.05569800	2.39557900	-1.46564800
C	2.85186100	2.27304300	-0.29946700
C	2.18339500	3.49751900	-2.27558500
C	3.71358200	3.32947000	0.08404300
C	3.09758400	4.51733900	-1.92835100
H	1.57276900	3.57762500	-3.16982000
C	3.40480700	1.02105700	1.57449800
C	4.40682200	3.18536500	1.30690500
C	3.82797000	4.45311400	-0.76771600
H	3.19307400	5.38165000	-2.58225000
C	4.23304800	2.05176800	2.06092800
H	3.28004700	0.08101100	2.11782500
H	5.06831200	3.98523400	1.63949800
H	4.50137700	5.26160600	-0.48523600
H	4.73967000	1.92123600	3.01347600
N	2.75653000	1.11896000	0.42898100
C	0.36081500	-1.18818400	-1.51881400
S	-2.05936700	1.70387500	0.19480000
O	-2.24023100	0.93765700	-1.14758800

O	-2.51162300	0.87012900	1.40550700
C	-3.34525600	3.10058500	0.10196200
O	-0.70177300	2.41682600	0.26223900
H	-3.68052400	0.05193700	-1.33459000
F	-4.53149400	2.55339700	-0.07687400
F	-3.05098700	3.88405300	-0.91455500
F	-3.32157200	3.78270500	1.22634200
C	-6.19131900	-1.97773200	-1.12899800
H	-6.31305800	-2.95035500	-0.64792900
H	-6.36337100	-2.05906900	-2.20783200
H	-6.93800600	-1.27752400	-0.73600000
C	-4.82005400	-1.43603500	-0.86487200
O	-4.57998900	-0.33448700	-1.53877900
O	-4.03596200	-1.98012400	-0.09698300
Ag	-1.87205800	-1.37554700	0.59887600
C	3.01414500	-1.59403900	-1.84609100
C	3.78844600	-1.28036500	-0.76481700
C	4.09665500	-2.56413000	-0.03638200
C	2.83470200	-3.09499300	-1.82271800
H	4.40615700	-2.47161600	1.00850400
H	2.90624300	-0.98568400	-2.74450700
H	4.38036600	-0.37349100	-0.66296100
H	2.00635400	-3.49280100	-2.41714600
C	4.23836800	-3.64768200	-2.20564000
H	4.61284700	-3.21489900	-3.14183800
H	4.18284600	-4.73483900	-2.34701300
C	2.83632700	-3.38141100	-0.31759200
H	1.96295100	-2.99864400	0.22034500
H	2.96146500	-4.44764400	-0.08647100
C	5.10854100	-3.28281300	-0.97620600
H	5.96684100	-2.64797700	-1.23069400
H	5.50050600	-4.18091300	-0.48124900

TS10-11

S	0.46298100	-1.83195800	1.70406800
O	0.22795900	-0.55700000	0.80588600
O	-0.23840500	-3.04398500	1.06549700
C	-0.51817500	-1.41610000	3.28823500
O	1.90645300	-1.99080800	2.17492500
Ni	1.88051800	0.36647700	0.10935800
F	-0.30992800	-2.38903100	4.15229200
F	-1.78679000	-1.30594100	3.00855700
F	-0.04196100	-0.28162200	3.76575900
C	1.22570300	-1.60685400	-2.03082400

C	0.72598700	0.73457600	-2.36075900
C	-0.03817900	0.42829000	-3.48112300
C	-0.20659500	-0.90005600	-3.85938900
C	0.40376900	-1.91603000	-3.12190500
H	1.73091500	-2.40813900	-1.48693800
H	-0.53000100	1.23251200	-4.02746800
H	-0.82325300	-1.14993300	-4.72095000
H	0.25960900	-2.95786400	-3.40848800
C	0.91261800	2.13765600	-1.86324900
O	1.48513600	3.01371500	-2.48456800
N	0.49991200	2.26110100	-0.54899800
H	-0.24130400	1.64253100	-0.20559200
C	0.90564300	3.26104900	0.35770600
C	1.54057500	2.83285800	1.56087400
C	0.66975700	4.59872100	0.14639500
C	1.79856500	3.79056500	2.57836500
C	0.99740800	5.55230000	1.13103300
H	0.20095600	4.90140200	-0.78652700
C	2.42797200	1.12741000	2.87229500
C	2.34302900	3.32885400	3.79760200
C	1.51894200	5.15543600	2.33605800
H	0.79557300	6.60434500	0.94145200
C	2.63023500	1.99856600	3.95879200
H	2.69064300	0.07012400	2.93761300
H	2.52662600	4.04574500	4.59790700
H	1.73092400	5.87983200	3.12181600
H	3.03657700	1.60887800	4.88822000
N	1.92015900	1.52304900	1.71932700
C	1.39068500	-0.27604100	-1.64286500
S	-2.69515900	0.67063400	0.17668000
O	-2.14759800	0.69765500	-1.28835700
O	-3.07313300	-0.76299000	0.58694500
C	-4.36936700	1.56381300	0.03706500
O	-1.86624600	1.53162100	1.12716200
H	-3.09354200	-0.18069300	-2.39214200
F	-5.11442700	0.92255100	-0.84260800
F	-4.16011800	2.80052300	-0.36700100
F	-4.95640200	1.56467500	1.21544300
C	-4.73860000	-2.45388400	-4.00607200
H	-4.56799900	-3.52312700	-4.14730600
H	-4.73316200	-1.93189400	-4.96898500
H	-5.72862000	-2.29839300	-3.56069300
C	-3.69788500	-1.87737100	-3.09652900
O	-3.74904400	-0.56613700	-3.04436100

O	-2.90263900	-2.57841000	-2.48153400
Ag	-1.35668900	-1.96495000	-0.82939400
C	3.43193000	0.30325500	-1.43740800
C	3.70323300	1.03434900	-0.25891100
C	4.76306600	0.24557300	0.48621100
C	4.31959800	-0.91914000	-1.38665200
H	4.87395800	0.47599000	1.55186300
H	3.25849800	0.80989600	-2.38528600
H	3.68795600	2.12772500	-0.24238300
H	4.03462700	-1.74457000	-2.04711100
C	5.73630200	-0.34257400	-1.65218000
H	5.76697600	0.28763200	-2.55055800
H	6.44488000	-1.16579900	-1.80868800
C	4.40312900	-1.20016500	0.11575500
H	3.46860900	-1.55950500	0.56686100
H	5.20887200	-1.90486500	0.36274000
C	6.05184700	0.44033600	-0.35217700
H	6.27343800	1.49975500	-0.53435800
H	6.91331100	0.00979800	0.17548500

IM11

S	0.52317200	-2.84511400	0.95367400
O	0.42068300	-1.27834200	0.82837100
O	-0.70330500	-3.49526100	0.27265900
C	0.23050300	-3.08225200	2.82025900
O	1.89147400	-3.45105300	0.68719700
Ni	1.71180900	-0.02457400	-0.12473400
F	0.32040300	-4.36535900	3.09313400
F	-0.95235200	-2.62203100	3.14185700
F	1.17501500	-2.41720600	3.46644300
C	2.05515700	-2.17862700	-2.08805200
C	1.12689300	0.02165400	-2.48622000
C	-0.08862300	-0.56774400	-2.84373600
C	-0.22713800	-1.95262800	-2.83316700
C	0.84156700	-2.75614100	-2.43762100
H	2.86991900	-2.81816200	-1.75705900
H	-0.92793200	0.06526300	-3.13367000
H	-1.17776300	-2.40173400	-3.12155000
H	0.72064000	-3.83511200	-2.37293000
C	1.25618200	1.52159100	-2.42004100
O	2.07712600	2.16622900	-3.04027500
N	0.38824100	2.06373500	-1.49115000
H	-0.24616700	1.40979700	-1.02670300
C	0.78159800	3.10768600	-0.62973500

C	1.10387700	2.76571400	0.71721400
C	0.80921300	4.42003800	-1.03539600
C	1.25824000	3.81904500	1.65787400
C	1.08063900	5.45254200	-0.11603900
H	0.57838600	4.64142500	-2.07489100
C	1.35563300	1.17426100	2.39112900
C	1.39845700	3.47450200	3.02019700
C	1.25850000	5.16140900	1.21230900
H	1.09360400	6.48484100	-0.45882400
C	1.40150000	2.15705800	3.39410900
H	1.42379100	0.11727200	2.64500200
H	1.49026500	4.26971400	3.75980500
H	1.39705000	5.95351600	1.94746700
H	1.47118200	1.85531600	4.43530800
N	1.25112700	1.45412900	1.10165500
C	2.23978300	-0.78508700	-2.11427000
S	-2.40639800	1.05300000	1.19120600
O	-1.98768000	0.95563000	-0.32966200
O	-2.47785000	-0.35443300	1.79962700
C	-4.23918800	1.54488000	1.02468800
O	-1.72655400	2.17068700	1.96026700
H	-3.09134200	1.00198300	-1.61466400
F	-4.85178500	0.58241900	0.35239800
F	-4.32964600	2.67997200	0.36087600
F	-4.77142300	1.67017900	2.21966300
C	-5.08860600	-0.37924300	-3.73241300
H	-5.21807700	-1.41919400	-4.03868600
H	-4.81809200	0.24367800	-4.59193900
H	-6.03612600	0.00886100	-3.33975300
C	-4.03970700	-0.27852800	-2.67055700
O	-3.73636500	0.96924400	-2.37618100
O	-3.53167000	-1.26131400	-2.14423700
Ag	-1.94500600	-1.56692500	-0.38834700
C	3.59009600	-0.10343200	-1.84107400
C	3.36750000	0.77441300	-0.60371100
C	4.39503500	0.29343000	0.40489900
C	4.73986100	-1.01678100	-1.39141600
H	4.19075900	0.58409000	1.44396400
H	3.85533500	0.48476700	-2.73087400
H	3.32171000	1.85894100	-0.75844300
H	4.85941400	-1.92609700	-1.99359400
C	6.00381700	-0.13965700	-1.35036700
H	6.14110300	0.42793800	-2.28011100
H	6.89511000	-0.76609200	-1.21674900

C	4.46657300	-1.21144400	0.10569400
H	3.54418000	-1.76596200	0.33260600
H	5.29810100	-1.70792300	0.62537100
C	5.76934300	0.76977700	-0.11764100
H	5.76585400	1.83861600	-0.36849300
H	6.54073000	0.61510600	0.64969600

IM12

S	-0.82394300	10.13157000	1.04445100
O	-0.05167600	9.17445800	2.04355400
O	-0.29585600	11.55750500	0.99406000
C	-2.46264000	10.26874300	1.99581200
O	-1.17907200	9.44175900	-0.28043400
Ni	1.55793600	8.32054700	1.51669800
F	-3.28389500	11.03797600	1.31021200
F	-2.21920200	10.80262100	3.17473900
F	-2.98386800	9.06906100	2.14325300
C	-2.41352600	6.08505000	2.07711700
C	-0.83828800	6.15514300	0.29320100
C	-1.89200800	6.24194100	-0.61891200
C	-3.21123700	6.22003900	-0.19244000
C	-3.46460300	6.14877100	1.16931900
H	-2.65749200	6.06873100	3.13561600
H	-1.66391900	6.33534800	-1.68076800
H	-4.02464700	6.27939600	-0.91270800
H	-4.48919600	6.15757000	1.53890700
C	0.52933000	6.23156700	-0.29711400
O	1.34999000	5.30774400	-0.26020700
N	0.74391000	7.41370200	-0.93009800
H	0.03558900	8.14693900	-0.76085400
C	1.90369700	7.82580900	-1.61256300
C	2.45104900	9.08738600	-1.25195300
C	2.43946800	7.12080400	-2.66637800
C	3.40321200	9.69031800	-2.11163400
C	3.47196000	7.67789600	-3.44742300
H	2.02067100	6.14675400	-2.91283500
C	2.46192000	10.90731300	0.16872400
C	3.81288500	11.00884000	-1.80305200
C	3.90811100	8.95756600	-3.20981600
H	3.89468700	7.10110400	-4.26921900
C	3.31653600	11.63152900	-0.68946800
H	2.10402800	11.34707400	1.09842300
H	4.52227500	11.51025600	-2.46226300
H	4.66147500	9.41855600	-3.84840000

H	3.59823000	12.64852200	-0.42933800
N	2.05280100	9.67977800	-0.08588600
C	-1.07262800	6.07504700	1.67960700
S	4.56691800	7.65616700	2.06640200
O	5.56655200	6.59753800	1.57524000
O	3.30137700	7.54172700	1.10933300
C	5.35641700	9.30180400	1.53003700
O	4.29929800	7.81403700	3.54789300
F	4.62057000	10.29905700	1.97765100
F	5.41332100	9.33160400	0.21098400
F	6.56764500	9.37138100	2.03633400
C	0.05351500	5.89476300	2.68744200
C	1.21560200	6.94312900	2.81647900
C	1.06581800	7.50538900	4.24084400
C	-0.41855200	5.82967100	4.15576800
H	1.46474900	8.51878100	4.36728800
H	0.52108300	4.93341000	2.42072500
H	2.16276300	6.38913100	2.74044800
H	-1.34880900	5.26814500	4.29958100
C	0.72341300	5.26791100	5.02023300
H	1.19893600	4.40253800	4.53326700
H	0.34097800	4.91937500	5.98992500
C	-0.42444100	7.31342400	4.54136100
H	-1.07596900	7.93437900	3.91352000
H	-0.66799800	7.48237500	5.60062400
C	1.69015300	6.46497700	5.18298500
H	2.72951200	6.22944400	4.91881000
H	1.68998700	6.83573300	6.21939200
C	4.87605000	3.13902600	-1.47211600
C	4.39050400	2.00708300	-0.81432700
C	3.10293500	1.48632800	-1.13966000
C	2.28307600	2.17798500	-2.07955600
C	2.78452000	3.34461100	-2.69405100
C	4.04625000	3.80580200	-2.41044500
H	3.21465300	-0.24291600	0.16400600
C	2.59565000	0.29892100	-0.54956500
C	0.98957700	1.68145200	-2.37284900
H	2.15226900	3.86816700	-3.41342700
H	4.42288800	4.70035800	-2.90832300
C	0.52655900	0.53665600	-1.77829500
C	1.34366400	-0.16373400	-0.86291400
H	0.37231700	2.22956700	-3.08504200
H	-0.46897500	0.16252300	-2.01084800
H	0.97169100	-1.07340300	-0.39426300

C	7.77942400	-1.90144600	-0.58062200
C	7.74575400	-1.36676800	0.68115600
C	6.87861500	-0.29074200	0.98964300
C	6.05074100	0.25644800	-0.03446600
C	6.93960700	-1.38171500	-1.58936700
H	7.44152200	-0.17392900	3.07257300
H	8.44585800	-2.73223000	-0.80651000
H	8.37847100	-1.76684900	1.47389300
C	6.80095000	0.24312200	2.29494300
C	5.19046900	1.35458400	0.26906500
H	6.96484500	-1.81349200	-2.58874900
C	5.09170200	1.80317900	1.58213800
C	5.91664000	1.24695700	2.58968300
H	5.84752600	1.62942600	3.60739800
P	6.59176700	3.76580600	-1.04980300
P	3.82855500	3.08778300	2.01695200
C	6.10058200	-0.32977300	-1.32442900
H	5.45644200	0.06673600	-2.10772000
C	2.28720700	2.09082600	2.18633500
C	1.11544800	2.56177700	1.59018000
C	2.26393600	0.88076400	2.89045300
C	-0.07597000	1.85452100	1.73338900
H	1.13049100	3.47450000	0.99053000
C	1.07520900	0.17360700	3.02430800
H	3.18201700	0.48942600	3.33238500
C	-0.09812300	0.66577500	2.45366400
H	-0.98372500	2.23929000	1.27010700
H	1.06247600	-0.76422800	3.57766100
H	-1.02963500	0.11292600	2.56656100
C	4.27075800	3.59327100	3.73207400
C	5.34147300	4.48608700	3.86330600
C	3.56857800	3.19211300	4.87088000
C	5.69500300	4.97575000	5.11446100
H	5.87805400	4.82951300	2.97810700
C	3.92487900	3.68886100	6.12153100
H	2.72680200	2.50611000	4.78563200
C	4.98468000	4.58108400	6.24497900
H	6.51239000	5.68939900	5.19858300
H	3.35854000	3.38495300	7.00077200
H	5.25050900	4.97936900	7.22273300
C	6.75631700	5.27758300	-2.13453500
C	6.56196800	6.52227900	-1.51956600
C	7.15515700	5.24970900	-3.47597000
C	6.77411300	7.70165900	-2.22940700

H	6.27588400	6.57416200	-0.46654900
C	7.36048700	6.42927800	-4.18395100
H	7.33817900	4.29884000	-3.97312200
C	7.17890000	7.65873600	-3.55894500
H	6.63477500	8.66072200	-1.73313600
H	7.68262700	6.38461900	-5.22358300
H	7.36256900	8.58315400	-4.10632500
Ag	3.59684300	5.09703900	0.49355300
C	7.60957600	2.53391900	-2.00330300
C	8.82711000	2.14145000	-1.44317500
C	7.22974200	1.99318100	-3.23728500
C	9.65708000	1.24188900	-2.10714400
H	9.11916000	2.53805100	-0.46976100
C	8.06295700	1.10623700	-3.90879300
H	6.26438500	2.26199800	-3.67131200
C	9.27876400	0.72901300	-3.34331500
H	10.59970700	0.93844500	-1.65433100
H	7.75811200	0.69862200	-4.87202500
H	9.92852400	0.02781600	-3.86509200

TS12-13

S	0.60922900	10.98519100	2.20503700
O	1.86690600	10.01573900	2.29307600
O	0.93052900	12.30762900	1.52371700
C	0.35972900	11.42460300	4.04160100
O	-0.63542200	10.20065200	1.77466800
Ni	1.50300100	8.59740700	0.99637100
F	-0.70520500	12.19307500	4.14397800
F	1.42735200	12.06484400	4.46660400
F	0.18717100	10.31873800	4.73640600
C	-2.58227500	4.83906300	1.65064900
C	-0.89395400	5.89417900	0.31641700
C	-1.73899100	5.89905000	-0.79000800
C	-3.02495600	5.38213800	-0.66483900
C	-3.43879800	4.84596500	0.55269900
H	-2.91740900	4.41911300	2.59880300
H	-1.39866500	6.29897500	-1.74786400
H	-3.70276400	5.39246100	-1.51668700
H	-4.44327600	4.43680100	0.64980400
C	0.55549500	6.27017600	0.24490800
O	1.37418300	5.37160300	-0.09124800
N	0.75788300	7.58988000	-0.37417600
H	-0.13840900	8.08975800	-0.44656600
C	1.55061000	7.74070900	-1.56756100

C	2.28093800	8.94280900	-1.59514200
C	1.59711900	6.87042700	-2.62654700
C	2.99584000	9.32471500	-2.74966000
C	2.34434100	7.22910500	-3.77199300
H	1.07662400	5.91679500	-2.56963100
C	2.95808700	10.80918500	-0.40414700
C	3.69723800	10.55096000	-2.68389100
C	3.00620800	8.43168500	-3.84722400
H	2.38458600	6.53785800	-4.61180200
C	3.67863200	11.28235700	-1.52257300
H	2.92379300	11.36141800	0.53197200
H	4.25851900	10.89409000	-3.55330500
H	3.57581200	8.69513800	-4.73774300
H	4.21373500	12.22431700	-1.43961300
N	2.27693500	9.68035300	-0.44746700
C	-1.30303600	5.37830200	1.53698200
S	4.71231200	7.64248300	2.24203700
O	5.86580000	6.64934900	2.04402600
O	3.71170000	7.54912700	1.02978200
C	5.53913200	9.33597600	1.97343300
O	4.06057100	7.73331600	3.61067200
F	4.65291500	10.29863200	2.12560700
F	6.03990600	9.38457700	0.74797400
F	6.50976500	9.47419200	2.85262500
C	-0.27120700	5.45609500	2.62134000
C	0.84938000	6.49556500	2.26896200
C	0.77710400	7.42594900	3.50292900
C	-0.84293100	5.94677900	3.96384100
H	1.28925700	8.38285800	3.42715800
H	0.18696200	4.45664900	2.74149700
H	1.84977800	6.05099200	2.18011900
H	-1.84838200	5.55802800	4.17078500
C	0.18443000	5.64544900	5.05387400
H	0.49088500	4.58920500	5.05418300
H	-0.22963100	5.86690300	6.04780700
C	-0.71933100	7.46267300	3.81326400
H	-1.31921000	7.88669000	2.99526900
H	-0.95006200	8.00241900	4.74146300
C	1.33680700	6.60648600	4.69074600
H	2.27328200	6.09577600	4.43032100
H	1.57683600	7.29255700	5.51568600
C	4.91710000	3.12406600	-1.41004900
C	4.46012500	1.96892700	-0.77744700
C	3.22881900	1.37066000	-1.17758300

C	2.42072900	2.01904400	-2.15738000
C	2.87781500	3.22624700	-2.72778200
C	4.09599400	3.75467500	-2.38178700
H	3.38583000	-0.36555900	0.10958000
C	2.77217600	0.14241700	-0.63321000
C	1.18647600	1.43748500	-2.53615600
H	2.25236100	3.72337500	-3.47171900
H	4.43804400	4.67555600	-2.85585200
C	0.77029700	0.25370500	-1.98467700
C	1.57674600	-0.40128200	-1.02742700
H	0.57702800	1.95082000	-3.28055600
H	-0.17950100	-0.18665200	-2.28357700
H	1.24200100	-1.34190200	-0.59289900
C	8.21909000	-1.55509500	-0.32754400
C	8.04288000	-1.04204000	0.93154600
C	7.03867400	-0.07679200	1.18764100
C	6.21994800	0.37908400	0.11291800
C	7.38933500	-1.12810200	-1.38752700
H	7.44860400	0.08720200	3.30280400
H	8.99278800	-2.29851800	-0.51249200
H	8.66785300	-1.37317900	1.76139800
C	6.82016500	0.43937300	2.48425000
C	5.23673700	1.38267300	0.35832800
H	7.52894400	-1.54318900	-2.38442400
C	5.01960400	1.83128400	1.65774400
C	5.82496300	1.35221900	2.71833700
H	5.65687100	1.72753100	3.72720000
P	6.60193000	3.79934500	-0.92430400
P	3.67632600	3.06863000	1.97542700
C	6.41678200	-0.18548400	-1.17327300
H	5.78312400	0.14349800	-1.99559500
C	2.15737000	2.02211900	1.96146600
C	1.02059800	2.47614200	1.29003200
C	2.12154700	0.79193600	2.62929400
C	-0.14679300	1.71442300	1.30297900
H	1.04847000	3.42303300	0.74461200
C	0.95472900	0.03768100	2.64232400
H	3.01266500	0.42526200	3.14227400
C	-0.18188700	0.50094100	1.98046700
H	-1.02807700	2.08217100	0.77719100
H	0.93124200	-0.91532300	3.16900400
H	-1.09573200	-0.09172900	1.99235200
C	3.87240200	3.55140900	3.74255300
C	4.91287700	4.44037900	4.03782900

C	2.99360000	3.16066500	4.75651100
C	5.07535400	4.92292100	5.33043800
H	5.57333700	4.79813100	3.24591800
C	3.16237500	3.64781600	6.04983900
H	2.16490100	2.48715900	4.53932000
C	4.20074400	4.52725400	6.33857900
H	5.86967100	5.63827000	5.53475100
H	2.46570900	3.34740000	6.83157400
H	4.31840100	4.91856500	7.34779500
C	6.58782500	5.38225100	-1.89541500
C	6.03762500	6.48507000	-1.23175800
C	7.01598700	5.53462500	-3.21644200
C	5.84999400	7.69276800	-1.89529400
H	5.79436800	6.41560900	-0.16872400
C	6.86321200	6.75497700	-3.86932300
H	7.47308300	4.69791000	-3.74354500
C	6.26566600	7.82913700	-3.21627000
H	5.39852800	8.52799500	-1.36110900
H	7.21126800	6.86405400	-4.89594200
H	6.14603100	8.78225000	-3.73283200
Ag	3.61956500	5.16533500	0.55771700
C	7.68169100	2.70727700	-1.97306400
C	8.91172300	2.32500600	-1.43286000
C	7.32699200	2.23832100	-3.24338200
C	9.77722400	1.50320600	-2.14931700
H	9.18259400	2.66304300	-0.43158900
C	8.19345800	1.42435800	-3.96422100
H	6.35574500	2.50338600	-3.66586300
C	9.42081400	1.05613500	-3.41717500
H	10.72973000	1.20717500	-1.71238500
H	7.90796600	1.06986300	-4.95398300
H	10.09727100	0.41385800	-3.97948600

IM13

S	1.05349800	11.21112000	2.71735200
O	2.17754100	10.10035400	2.46898400
O	1.51811400	12.58710800	2.26838000
C	1.05179400	11.25617200	4.62124100
O	-0.32131500	10.69448900	2.30171400
Ni	1.63591700	8.81131200	1.21620900
F	0.17299000	12.15442100	5.01266700
F	2.25341600	11.57282000	5.04217000
F	0.70688500	10.06322400	5.06947700
C	-2.81999400	4.86057100	1.31103300

C	-0.84255900	5.69362400	0.20446300
C	-1.52404200	5.75428400	-1.00803000
C	-2.86236400	5.37671400	-1.05188900
C	-3.50590100	4.92661500	0.10255100
H	-3.32173800	4.50941700	2.21382300
H	-1.02049400	6.09406900	-1.91433900
H	-3.41057300	5.42769200	-1.99147500
H	-4.55223500	4.62826000	0.05563500
C	0.63541500	5.94692600	0.46922500
O	1.43316900	5.17625200	-0.20424700
N	0.89016600	7.55772800	-0.00590200
H	-0.05708900	7.94952900	-0.09090300
C	1.53823400	7.75385000	-1.28138000
C	2.13903200	9.02076800	-1.41986500
C	1.58446600	6.87874300	-2.34500000
C	2.71434300	9.44345900	-2.63961800
C	2.19203000	7.27830900	-3.55755100
H	1.18153000	5.87783800	-2.22761800
C	2.69252600	11.01892700	-0.35473200
C	3.27952700	10.73694200	-2.66957600
C	2.72567000	8.53183700	-3.72010200
H	2.22532000	6.56642500	-4.38068000
C	3.26332500	11.51837500	-1.54065900
H	2.67581800	11.61228700	0.55821300
H	3.73332100	11.09748100	-3.59308800
H	3.18440000	8.83067700	-4.66209700
H	3.69317900	12.51597200	-1.53307900
N	2.15153100	9.81295000	-0.30598700
C	-1.48394300	5.25124100	1.35622000
S	4.74035700	7.55095900	2.25708800
O	5.81789700	6.47010700	2.11837300
O	3.72947200	7.48602000	1.05519700
C	5.69542900	9.16724400	1.91139700
O	4.07860900	7.75337300	3.61222600
F	4.84758400	10.15423800	1.68949500
F	6.45628900	8.99549700	0.84368600
F	6.44906800	9.44644100	2.95434500
C	-0.58191000	5.27761000	2.55533500
C	0.75987500	5.88388900	2.02803700
C	0.86383500	7.15161400	2.87713600
C	-1.03375200	6.27132700	3.64513500
H	1.70667000	7.84269700	2.62605300
H	-0.44719700	4.26531800	2.97202200
H	1.62215100	5.23317500	2.23812600

H	-2.10074700	6.18925200	3.88929800
C	-0.08814100	6.12191300	4.84191500
H	0.03283100	5.07109900	5.14214500
H	-0.46702600	6.67355500	5.71253400
C	-0.58637600	7.61487400	3.05307600
H	-1.11029600	7.87745100	2.12450100
H	-0.68375800	8.45926300	3.74524500
C	1.23125800	6.73608500	4.31879900
H	2.08484100	6.04618100	4.32942800
H	1.53240900	7.62240400	4.89027700
C	4.89294600	3.04716400	-1.38367000
C	4.49453000	1.88040600	-0.73210400
C	3.27591100	1.23563500	-1.09911900
C	2.41831400	1.85234000	-2.05738400
C	2.81105600	3.07723500	-2.63688200
C	4.02003600	3.64758000	-2.32938800
H	3.52633300	-0.48928100	0.18944200
C	2.87789000	-0.00723400	-0.54123600
C	1.19706500	1.22516300	-2.40399100
H	2.14125900	3.55485500	-3.35387600
H	4.30888500	4.58380900	-2.80893100
C	0.84039700	0.02662600	-1.84311400
C	1.69465200	-0.59612900	-0.90614500
H	0.54917800	1.71663000	-3.13035400
H	-0.09962700	-0.44944700	-2.11746400
H	1.40586000	-1.54758200	-0.46216800
C	8.39664200	-1.48854100	-0.31934800
C	8.21335500	-0.98244700	0.94173200
C	7.17457300	-0.05756700	1.20855700
C	6.32757300	0.36477500	0.14201400
C	7.53908300	-1.09612900	-1.37056900
H	7.59535500	0.11980700	3.32070500
H	9.19755300	-2.20052700	-0.51223900
H	8.85970800	-1.28852300	1.76484200
C	6.94755500	0.44926800	2.50776500
C	5.31115400	1.33206800	0.39537500
H	7.68432100	-1.50594600	-2.36884400
C	5.09145700	1.77578600	1.69690500
C	5.92144500	1.32497200	2.75063200
H	5.74755000	1.69491700	3.76073900
P	6.56560000	3.78529400	-0.95008300
P	3.72753000	2.99038000	2.00171000
C	6.53171400	-0.19343100	-1.14582400
H	5.87542600	0.10874600	-1.96064600

C	2.22014700	1.92478400	2.01133500
C	1.08335700	2.33458000	1.31154100
C	2.19226500	0.73053700	2.74162300
C	-0.07378000	1.55810800	1.35290100
H	1.10721000	3.25221000	0.71554900
C	1.03466900	-0.03635800	2.78418000
H	3.08211500	0.40538900	3.28405100
C	-0.10113500	0.37963300	2.09042400
H	-0.95422100	1.88297500	0.79864000
H	1.01740100	-0.96151800	3.35862800
H	-1.00817800	-0.22270300	2.12365400
C	3.87368200	3.51572600	3.76241900
C	4.96447700	4.32546200	4.10119700
C	2.86375600	3.29798700	4.70558100
C	5.04898900	4.89608800	5.36480600
H	5.72519600	4.55526900	3.35528900
C	2.95730800	3.86810900	5.97265800
H	1.99464200	2.69141200	4.45145600
C	4.04690300	4.66703300	6.30376800
H	5.88849800	5.54713700	5.60095400
H	2.16510200	3.69394400	6.70004700
H	4.10791100	5.12534800	7.28947500
C	6.45573700	5.37357800	-1.90791600
C	5.90540200	6.45143800	-1.20561700
C	6.80553700	5.55158500	-3.24857600
C	5.63781200	7.65917300	-1.84326700
H	5.72224800	6.35705500	-0.13329700
C	6.57262600	6.77128600	-3.87874300
H	7.26173100	4.73573700	-3.80856300
C	5.97461800	7.81951600	-3.18346400
H	5.19081500	8.47479900	-1.27245300
H	6.85774800	6.90129700	-4.92222300
H	5.79104200	8.77054400	-3.68453600
Ag	3.60389800	5.05841900	0.52532600
C	7.65315500	2.73950500	-2.03712700
C	8.91139400	2.40138900	-1.53306700
C	7.27787100	2.25600200	-3.29595200
C	9.78397300	1.60932400	-2.27377200
H	9.19899100	2.74940600	-0.53988700
C	8.15118000	1.47156400	-4.04121500
H	6.28505000	2.48406100	-3.68883400
C	9.40636400	1.14767600	-3.53025700
H	10.75861400	1.34747400	-1.86465600
H	7.84925600	1.10496300	-5.02164500

H	10.08797600	0.52826900	-4.11172000
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S	1.12057300	11.23798300	2.80365800
O	2.11599800	10.02195700	2.53144200
O	1.71623100	12.56890700	2.36825300
C	1.15658000	11.25692500	4.70776600
O	-0.30955800	10.88514600	2.40750300
Ni	1.53782800	8.83041000	1.19210200
F	0.38445100	12.23730500	5.12756800
F	2.39170900	11.43931300	5.11141000
F	0.69503000	10.10084200	5.15238100
C	-2.98275800	5.09702600	1.32779400
C	-0.91898900	5.62322000	0.19421200
C	-1.56822500	5.63249000	-1.03682700
C	-2.93666600	5.38971600	-1.07601400
C	-3.63917100	5.12196200	0.10174600
H	-3.53128900	4.87926600	2.24498600
H	-1.01389900	5.83338700	-1.95430400
H	-3.46480700	5.40404700	-2.02811500
H	-4.71006600	4.92913100	0.05729400
C	0.55437300	5.77500800	0.47585400
O	1.36956500	5.10073000	-0.22261300
N	0.83151500	7.60664200	-0.04414100
H	-0.13198000	7.94140400	-0.16669900
C	1.51066200	7.79835600	-1.29012600
C	2.13219000	9.05841200	-1.41548600
C	1.58834000	6.91861100	-2.34925700
C	2.75261800	9.47325300	-2.61387400
C	2.23783200	7.31022500	-3.54326400
H	1.17328000	5.92007900	-2.24816200
C	2.65429500	11.05343200	-0.33154100
C	3.32642300	10.76344600	-2.62474100
C	2.78791200	8.55866100	-3.69234800
H	2.29075200	6.59747000	-4.36491000
C	3.27268800	11.54561800	-1.49725700
H	2.61265100	11.65135300	0.57893200
H	3.81612800	11.12129700	-3.53091500
H	3.27672800	8.85052500	-4.62124400
H	3.70896000	12.54031100	-1.47482900
N	2.10239800	9.85177000	-0.30110000
C	-1.61391700	5.35159600	1.36871300
S	4.76572800	7.54609300	2.22819000
O	5.86916100	6.48890500	2.11787800

O	3.75314200	7.42745800	1.02837300
C	5.67925800	9.18397900	1.83961900
O	4.09923100	7.75940200	3.57864600
F	4.81537300	10.10965700	1.46436700
F	6.54099400	8.97024800	0.86073700
F	6.31952900	9.57777300	2.91996000
C	-0.71836200	5.36540200	2.57567700
C	0.67900800	5.79527800	2.02308500
C	0.91722700	7.10665200	2.77621500
C	-1.05753100	6.46078400	3.60355600
H	1.83419800	7.64275100	2.42662200
H	-0.68718200	4.37071700	3.05032100
H	1.47063600	5.07447200	2.28097600
H	-2.12446800	6.50237600	3.85809500
C	-0.11628500	6.30040500	4.80342800
H	-0.08020600	5.26136100	5.16160800
H	-0.44327300	6.92864300	5.64274300
C	-0.48978600	7.71502700	2.92579200
H	-1.00659800	7.96733300	1.99044800
H	-0.50494400	8.60297700	3.56718300
C	1.24552600	6.77628400	4.24430200
H	2.04755500	6.03022500	4.31654100
H	1.60758200	7.68269000	4.74399300
C	4.90909500	3.07396400	-1.39269000
C	4.50964500	1.90562600	-0.74452900
C	3.29262300	1.26030800	-1.11564200
C	2.43495200	1.88021000	-2.07173100
C	2.82759900	3.10736800	-2.64686100
C	4.03661600	3.67666300	-2.33709000
H	3.54761200	-0.47227400	0.16175100
C	2.89776500	0.01277600	-0.56573600
C	1.21486200	1.25242500	-2.42166000
H	2.15802000	3.58749200	-3.36242500
H	4.32714700	4.61368900	-2.81400700
C	0.86128000	0.04911200	-1.86876700
C	1.71716800	-0.57799500	-0.93614000
H	0.56644900	1.74616300	-3.14603100
H	-0.07701100	-0.42798300	-2.14726700
H	1.43156600	-1.53383200	-0.49962600
C	8.43129300	-1.43989600	-0.32573400
C	8.24211500	-0.93563800	0.93523200
C	7.19538800	-0.01935600	1.20061000
C	6.34800100	0.39754700	0.13227600
C	7.57238400	-1.05427800	-1.37836300

H	7.60958800	0.15946400	3.31399000
H	9.23801400	-2.14560400	-0.51743400
H	8.88936700	-1.23712700	1.75928700
C	6.96038500	0.48342100	2.50001500
C	5.32329700	1.35628600	0.38416600
H	7.72215100	-1.46327300	-2.37626500
C	5.09351200	1.79236100	1.68629300
C	5.92436400	1.34763400	2.74199400
H	5.74381600	1.71363400	3.75235000
P	6.58328300	3.81060200	-0.96094600
P	3.70522900	2.97809100	1.99379400
C	6.55840200	-0.15862300	-1.15538700
H	5.90139800	0.13903500	-1.97129400
C	2.22231300	1.87772900	2.02152700
C	1.06899200	2.25191800	1.32951800
C	2.22815600	0.69068400	2.76387400
C	-0.07145600	1.45360800	1.39298300
H	1.06921500	3.15523700	0.71534100
C	1.08843000	-0.10143300	2.82581100
H	3.12998300	0.39064900	3.30068100
C	-0.06504100	0.28299300	2.14331300
H	-0.96430700	1.75340700	0.84486300
H	1.09842000	-1.02112400	3.40903100
H	-0.95838200	-0.33809700	2.19423000
C	3.85134100	3.51499600	3.75122400
C	4.93351500	4.34037900	4.07953700
C	2.84852600	3.28970700	4.70034800
C	5.01733700	4.91871700	5.33971500
H	5.68711000	4.57915400	3.32875900
C	2.94192600	3.86761000	5.96395500
H	1.98473200	2.67268800	4.45364400
C	4.02350500	4.68132300	6.28532600
H	5.84829100	5.58410400	5.56588000
H	2.15561400	3.68802400	6.69623300
H	4.08372900	5.14560100	7.26824900
C	6.47769400	5.40049500	-1.91555600
C	5.92665800	6.47569700	-1.21053000
C	6.83827900	5.58522600	-3.25239600
C	5.67197500	7.69011100	-1.83990800
H	5.73029300	6.37124300	-0.14250500
C	6.61879100	6.81169400	-3.87438700
H	7.29417100	4.77102800	-3.81500100
C	6.02316100	7.85877900	-3.17545900
H	5.22264200	8.50414900	-1.26819700

H	6.91333700	6.94822000	-4.91440500
H	5.85164300	8.81518100	-3.67041900
Ag	3.57261700	5.06585900	0.55594800
C	7.66859700	2.76732300	-2.05245800
C	8.92986800	2.43270700	-1.55370900
C	7.29140900	2.28750300	-3.31209600
C	9.80337400	1.64713600	-2.30022800
H	9.21952400	2.77894300	-0.56051200
C	8.16534900	1.50901200	-4.06285500
H	6.29714700	2.51477400	-3.70183500
C	9.42352500	1.18835800	-3.55709000
H	10.78069400	1.38840700	-1.89553100
H	7.86204300	1.14533600	-5.04394500
H	10.10592800	0.57427000	-4.14324700

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S	2.59114600	10.94458600	2.97301300
O	3.71574200	10.37830000	1.98777500
O	2.43339700	12.44908600	2.79138000
C	3.39204900	10.78315800	4.72711800
O	1.35327600	10.05653400	2.98900300
Ni	3.04020900	9.37945000	0.50172600
F	2.96059700	11.81089300	5.43334200
F	4.70093800	10.83299800	4.62567000
F	3.00425300	9.66727400	5.29884100
C	-2.88429500	4.58324800	1.24957300
C	-0.77554700	5.06682900	0.19357400
C	-1.31098700	4.87016400	-1.07886400
C	-2.65179400	4.53017500	-1.17596400
C	-3.42797900	4.39232400	-0.01718100
H	-3.50051300	4.46614700	2.14093100
H	-0.67929700	4.99089800	-1.95816500
H	-3.10968000	4.37441400	-2.15103600
H	-4.48028700	4.12758500	-0.11298200
C	0.60416600	5.39168900	0.55582900
O	1.55120600	5.47389300	-0.23011000
N	2.31700600	8.39248000	-0.86903700
H	2.42918500	7.38411500	-0.93686700
C	2.04947500	9.08592200	-1.99125900
C	2.14681500	10.49773000	-1.81918700
C	1.69248900	8.62207800	-3.25910100
C	1.84925700	11.41360500	-2.85072700
C	1.39432600	9.53539800	-4.28484200
H	1.63601000	7.54890500	-3.44112300

C	2.72688700	12.17532700	-0.31520800
C	2.00836300	12.78166300	-2.53415600
C	1.45648700	10.90370800	-4.11001500
H	1.10801500	9.13964400	-5.25937300
C	2.44186600	13.15481600	-1.28481800
H	3.04653300	12.44502200	0.68898000
H	1.78900100	13.53202200	-3.29432800
H	1.23321100	11.59170500	-4.92360000
H	2.56936000	14.20154800	-1.02094100
N	2.57739700	10.88606300	-0.58241000
C	-1.53792600	4.91840200	1.35611100
S	4.83958000	7.63647000	2.35082100
O	5.45184700	6.23238300	2.14020800
O	3.74061500	7.73755800	1.20149000
C	6.29970700	8.82565400	1.80509900
O	4.41011800	8.02068600	3.74875200
F	6.46974600	9.74703900	2.71448800
F	6.02524400	9.35882400	0.63141100
F	7.37834700	8.07892100	1.70298100
C	-0.71978400	5.14818100	2.59727900
C	0.68098000	5.53701300	2.05139700
C	0.85732400	6.99895900	2.53829100
C	-1.12262900	6.38744900	3.42116800
H	1.58114100	7.57679900	1.95805200
H	-0.69845200	4.23774000	3.21825500
H	1.50086300	4.90735900	2.43413100
H	-2.19317600	6.41813200	3.66432400
C	-0.18723000	6.45403200	4.64213400
H	-0.11103900	5.48146400	5.15201900
H	-0.56619600	7.17677700	5.37634100
C	-0.57919800	7.52585500	2.55173300
H	-1.04479200	7.59263100	1.55870600
H	-0.63441000	8.51172600	3.02904200
C	1.16425100	6.92138700	4.03685500
H	2.00060200	6.24185800	4.25923300
H	1.44889800	7.91745400	4.39505000
C	4.63140100	2.69582700	-1.29724100
C	4.36484000	1.53327400	-0.57640900
C	3.26803600	0.69673900	-0.94875600
C	2.41063000	1.09717700	-2.01532500
C	2.66135300	2.32346900	-2.66894400
C	3.74065600	3.09615600	-2.32556900
H	3.63020300	-0.84234600	0.53449600
C	2.98736100	-0.52609600	-0.28591100

C	1.32068500	0.27131200	-2.38250200
H	1.98732700	2.64290800	-3.46477200
H	3.91842800	4.03281700	-2.85235900
C	1.07659400	-0.90393100	-1.72022000
C	1.91995500	-1.30221900	-0.65975400
H	0.67889000	0.59389600	-3.20301500
H	0.23581800	-1.53270500	-2.00863800
H	1.71934400	-2.23357900	-0.13238900
C	8.48063400	-1.50764500	0.17112600
C	8.20649200	-0.95606600	1.39582000
C	7.10389500	-0.08462800	1.56796800
C	6.28171200	0.23277500	0.44706200
C	7.65167500	-1.21882900	-0.93454000
H	7.41208300	0.20906100	3.68635900
H	9.33173400	-2.17549400	0.04925000
H	8.83002800	-1.18116200	2.26143000
C	6.79007100	0.46823700	2.82916000
C	5.19932500	1.14991000	0.60629000
H	7.86958200	-1.66347800	-1.90428900
C	4.91431100	1.66036900	1.87025800
C	5.71590400	1.30461500	2.98112200
H	5.48025100	1.71139100	3.96336500
P	6.14494800	3.70106800	-0.83463600
P	3.51810900	2.86123800	2.05842300
C	6.57975400	-0.37409200	-0.79968900
H	5.94651700	-0.15458400	-1.65753600
C	2.01515000	1.80365600	1.93599000
C	1.03444500	2.10679700	0.99087700
C	1.84105800	0.70009200	2.77870200
C	-0.12080400	1.33429900	0.90450500
H	1.18901300	2.93496300	0.29681200
C	0.68519700	-0.06642900	2.69641500
H	2.61405300	0.44677800	3.50639400
C	-0.29824500	0.25401100	1.76191300
H	-0.87615100	1.57945400	0.15836500
H	0.55190800	-0.91971000	3.35961700
H	-1.20285100	-0.34878800	1.69736200
C	3.53633700	3.40986200	3.82080100
C	4.62756600	4.18391700	4.23929000
C	2.44108000	3.25997000	4.67755000
C	4.62994900	4.77557500	5.49581600
H	5.46225500	4.36270200	3.56146800
C	2.44904500	3.85609300	5.93627100
H	1.56972500	2.68620300	4.36315500

C	3.54041100	4.61282300	6.34758900
H	5.47513600	5.39208100	5.79506400
H	1.58870500	3.73444000	6.59303900
H	3.53646600	5.09042300	7.32565000
C	5.96571000	5.18066900	-1.94527900
C	5.57095400	6.36979100	-1.32132100
C	6.13453300	5.18129800	-3.33465800
C	5.27273200	7.51017800	-2.06619100
H	5.53792100	6.41807800	-0.23081500
C	5.85435300	6.32225200	-4.07824500
H	6.48145300	4.28184500	-3.84276600
C	5.40194900	7.48176000	-3.44933700
H	4.93724700	8.41338700	-1.55711800
H	5.98266300	6.30473000	-5.15979900
H	5.16010700	8.36667200	-4.03609600
Ag	3.72301000	5.07187500	0.80514800
C	7.45438200	2.70611900	-1.70175000
C	8.70546100	2.62806800	-1.08488800
C	7.25400600	2.03147600	-2.91141800
C	9.74183900	1.90780200	-1.67182800
H	8.86120100	3.12832200	-0.12807000
C	8.29112200	1.31970300	-3.50364400
H	6.26965700	2.04335000	-3.38330200
C	9.53717200	1.25787900	-2.88459000
H	10.71017500	1.85079900	-1.17717800
H	8.12391900	0.80334500	-4.44820200
H	10.34767000	0.69530000	-3.34570600

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H	-2.07863800	1.50738100	1.42703100
S	-1.73189800	-2.40643700	0.75143500
O	-0.44844300	-1.88847900	0.02140900
O	-2.55898100	-1.28917100	1.39968700
C	-0.99609200	-3.35732300	2.22886700
O	-2.44213800	-3.48010200	-0.06272000
F	-0.52301200	-2.49611500	3.11574300
F	-0.01911400	-4.13457000	1.79761200
F	-1.94045200	-4.08725100	2.78572000
C	-1.52492900	0.33748600	4.33175400
H	-0.61815200	0.01577800	4.84946500
H	-2.22754200	-0.50336000	4.26558000
H	-2.02453600	1.14623800	4.87504300
C	-1.20669200	0.75379000	2.93429600
O	-2.20984400	1.43548800	2.39289200

O	-0.16807900	0.49735000	2.35247800
Ag	0.52523800	0.08248800	0.02713800
C	3.34662700	-1.33688000	0.54455900
C	3.55710500	-0.08428100	1.11585000
C	3.15086700	0.17978900	2.45963500
C	2.56217900	-0.86803300	3.22439500
C	2.38508800	-2.13434500	2.62612500
C	2.74000300	-2.35727900	1.32224100
H	3.74102500	2.26810200	2.48632800
C	3.30344300	1.45418500	3.06426000
C	2.15710300	-0.61393400	4.55578100
H	1.92239100	-2.93116500	3.20681000
H	2.53504100	-3.32885800	0.87328000
C	2.31560000	0.62959300	5.11216000
C	2.88978000	1.67376800	4.35400700
H	1.70429100	-1.42943000	5.12194800
H	1.99821400	0.81750900	6.13693200
H	3.00754700	2.66045200	4.79900100
C	8.55225000	1.03148300	0.89216700
C	7.94813600	1.94969900	0.07233600
C	6.54334300	1.95115500	-0.09967600
C	5.75062000	0.98807100	0.58896000
C	7.77169000	0.07730200	1.57873700
H	6.51615300	3.61743700	-1.47838600
H	9.63387300	1.03605700	1.01646700
H	8.53762500	2.69484100	-0.46239000
C	5.90633800	2.88352600	-0.95102300
C	4.33116900	0.96578700	0.39218600
H	8.25599100	-0.65485600	2.22259400
C	3.74447600	1.90923700	-0.43736800
C	4.54916200	2.86313200	-1.11599900
H	4.07764200	3.58019900	-1.78719200
P	3.86745100	-1.61006500	-1.23822700
P	1.92022900	1.95490200	-0.71861000
C	6.40754300	0.05823100	1.43592400
H	5.81731900	-0.68724100	1.96597300
C	1.30836000	3.41930900	0.20652700
C	-0.08046800	3.52348100	0.33134100
C	2.12354200	4.39233600	0.78728900
C	-0.66134000	4.58184100	1.01818000
H	-0.71935100	2.76803300	-0.13428300
C	1.54485600	5.44618600	1.49045400
H	3.20825100	4.32576800	0.69604800
C	0.16044200	5.54130700	1.60619600

H	-1.74883200	4.64494700	1.09122400
H	2.18280000	6.19977900	1.94965900
H	-0.28246600	6.36863300	2.15813800
C	1.85144800	2.44249300	-2.49473000
C	2.07935700	1.43926500	-3.44189700
C	1.65734000	3.75941900	-2.91400100
C	2.12690300	1.75652100	-4.79501400
H	2.23968800	0.40884900	-3.11304700
C	1.70598300	4.07317400	-4.26975300
H	1.46823100	4.54129000	-2.17695600
C	1.94164800	3.07413800	-5.21019400
H	2.31342400	0.97304500	-5.52815800
H	1.55769300	5.10285800	-4.59189100
H	1.98089000	3.32198200	-6.26969100
C	3.01960200	-3.22377600	-1.57718700
C	1.62414700	-3.17290200	-1.67229900
C	3.65688900	-4.45913700	-1.71354700
C	0.87189000	-4.33280100	-1.81331200
H	1.09913600	-2.22088800	-1.57874300
C	2.90752800	-5.61760000	-1.90492800
H	4.74305300	-4.52428600	-1.65934000
C	1.51749600	-5.56116400	-1.93507300
H	-0.21668600	-4.26883200	-1.81001200
H	3.41609200	-6.57508400	-2.01123700
H	0.93650700	-6.47470600	-2.05125000
C	5.63655900	-2.10677900	-0.96470600
C	6.61340500	-1.47892500	-1.74035100
C	6.03585800	-3.02651700	0.01249500
C	7.96292000	-1.76327000	-1.54908300
H	6.30905900	-0.74377200	-2.48746500
C	7.38150300	-3.32235000	0.19502000
H	5.28435900	-3.50684700	0.64110500
C	8.34687300	-2.68959500	-0.58577100
H	8.71517200	-1.25668800	-2.15181500
H	7.68025700	-4.04431300	0.95398300
H	9.40178900	-2.91591800	-0.43643600
S	-6.51526400	-1.62523600	-0.59166400
O	-7.36298800	-2.76621700	-0.09038300
O	-7.05657200	-0.15688200	-0.29233900
C	-6.54138100	-1.69043600	-2.50198200
O	-4.98893100	-1.64794900	-0.24250500
Ni	-4.24690200	0.16465200	-0.06504000
C	-5.73721700	1.78617100	4.05748100
C	-5.07247400	2.07974000	1.77637500

C	-5.31614300	0.72122800	1.49771600
C	-5.70899500	-0.10752300	2.55661600
C	-5.92082400	0.42321700	3.82669300
H	-5.91497100	2.19471400	5.05164700
H	-6.18170000	0.36096300	0.43692600
H	-5.86758100	-1.17321500	2.38206600
H	-6.23622400	-0.22645800	4.64197000
C	-4.34288400	2.84884300	0.73474500
O	-4.15139200	4.06168700	0.76143000
N	-3.82533500	1.96994900	-0.18340000
C	-3.06725700	2.31553200	-1.28955000
C	-2.60388400	1.17968700	-2.01057800
C	-2.71392200	3.57542100	-1.75072800
C	-1.74675200	1.30268700	-3.12627300
C	-1.88164800	3.69433700	-2.88333200
H	-3.07094700	4.45395000	-1.22312100
C	-2.65239500	-1.14037300	-2.16812200
C	-1.29732300	0.09856900	-3.71956200
C	-1.39142500	2.60024400	-3.55812500
H	-1.60430200	4.69353900	-3.21890000
C	-1.74046800	-1.11081100	-3.24249500
H	-3.04574700	-2.07614800	-1.76885300
H	-0.60277300	0.15091500	-4.55872600
H	-0.72720800	2.71374500	-4.41383900
H	-1.40909000	-2.04945100	-3.67961600
N	-3.04836000	-0.03343400	-1.56648400
C	-5.30012800	2.62095000	3.03260000
H	-5.08307700	3.67488900	3.20184000
F	-5.93635200	-2.79737500	-2.86868500
F	-7.78958400	-1.68251800	-2.90529600
F	-5.89560000	-0.64245800	-2.96421500

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Ni	-4.35879900	0.12900300	-0.66687900
C	-5.78195400	-2.23468600	0.76972600
C	-5.33613300	-0.14351500	1.93581100
C	-5.75219600	-0.73259300	3.12004300
C	-6.15519800	-2.06943700	3.14384400
C	-6.13056300	-2.83094500	1.97578000
H	-5.77184500	-2.80605700	-0.15371700
H	-5.72587600	-0.13445000	4.03015300
H	-6.46939500	-2.52281300	4.08342400
H	-6.41489300	-3.88228200	1.99974400
C	-4.72490000	1.23658000	1.98368500

O	-4.54493300	1.91397500	2.99895600
N	-4.26753000	1.50206100	0.73217700
H	-1.89786800	-0.62040000	1.10428700
C	-3.45008700	2.52504100	0.34191400
C	-2.59457800	2.22651600	-0.79698800
C	-3.37413500	3.81464300	0.86377000
C	-1.78027800	3.22983600	-1.39035300
C	-2.56746300	4.79860500	0.25744800
H	-3.97676100	4.05449500	1.73590000
C	-1.78945800	0.59772000	-2.25992700
C	-0.98680700	2.84458800	-2.49347000
C	-1.79297600	4.53798600	-0.85078700
H	-2.57008300	5.80319100	0.68083500
C	-0.96596100	1.53152300	-2.91450600
H	-1.82587800	-0.44732800	-2.56839700
H	-0.38558900	3.59943400	-3.00181300
H	-1.17689000	5.31059600	-1.31058700
H	-0.35963100	1.21858000	-3.76334200
N	-2.59151500	0.94130800	-1.26594600
C	-5.42499500	-0.88647600	0.72416900
S	-2.17392100	-2.94598100	-0.29170200
O	-1.24116000	-1.69911100	-0.26228700
O	-3.64063400	-2.55199400	0.09145000
C	-1.69250800	-3.92142000	1.27860400
O	-2.00612600	-3.92961600	-1.43389300
F	-1.65036000	-3.10553200	2.31355500
F	-0.49706000	-4.46944600	1.10346300
F	-2.58375500	-4.86651300	1.47219400
C	-1.43394000	1.31402000	3.60401000
H	-0.58622000	1.95963500	3.85048600
H	-1.62156900	0.60790600	4.42230900
H	-2.36230600	1.89110700	3.47056100
C	-1.15640000	0.56713200	2.34535600
O	-2.12832700	-0.24753200	1.99114900
O	-0.13315500	0.69830600	1.68121100
Ag	0.55826000	0.05906200	-0.54882200
C	2.94358500	-1.38516800	0.26228900
C	3.36483600	-0.32193000	1.05800100
C	2.85305400	-0.15299500	2.37598300
C	1.92585000	-1.10781900	2.88665200
C	1.51972800	-2.17754200	2.06132900
C	1.98878500	-2.30082800	0.77798400
H	3.92248200	1.68107100	2.81574700
C	3.21333200	0.94653900	3.19516700

C	1.39919100	-0.93596900	4.18882200
H	0.81273000	-2.90829200	2.44479000
H	1.62271900	-3.11284200	0.14813800
C	1.75211400	0.14953500	4.94899800
C	2.66344500	1.10314500	4.44204400
H	0.68858200	-1.67442500	4.56285000
H	1.32781200	0.28284800	5.94298300
H	2.93677700	1.96511900	5.04868500
C	8.49988800	-0.31308800	0.89965100
C	8.11387000	0.77649800	0.16170200
C	6.74546900	1.11621000	0.03485600
C	5.76350100	0.30955900	0.67965800
C	7.53090100	-1.10656100	1.55099500
H	7.08055100	2.85268400	-1.20789800
H	9.55478000	-0.56724600	0.98919400
H	8.85320600	1.40091100	-0.34052600
C	6.32567900	2.23357000	-0.72234900
C	4.37993200	0.62029100	0.50826400
H	7.84408900	-1.96864800	2.13713900
C	4.00471700	1.73109400	-0.23348000
C	4.99641800	2.53908000	-0.84567600
H	4.69397900	3.40783200	-1.42914300
P	3.69907600	-1.54802900	-1.44792900
P	2.20867300	2.13599200	-0.44115600
C	6.19738700	-0.80290400	1.44578200
H	5.45572100	-1.42468000	1.94498400
C	1.89031900	3.31396500	0.94620800
C	0.57696200	3.53978000	1.36441100
C	2.93326400	4.01716600	1.56026400
C	0.31312700	4.43671900	2.39537000
H	-0.25173700	3.01132600	0.89512100
C	2.66777300	4.90469300	2.59677100
H	3.96214700	3.86394700	1.23311400
C	1.35704900	5.11027300	3.02041800
H	-0.71800500	4.59439600	2.71104300
H	3.48785000	5.44049600	3.07238000
H	1.14975500	5.80244500	3.83507100
C	2.23398700	3.23756600	-1.92297200
C	2.48166800	2.64899400	-3.16902100
C	1.94690500	4.60184600	-1.85691900
C	2.43854900	3.41196300	-4.32902800
H	2.71853000	1.58332000	-3.22560100
C	1.89577000	5.36406500	-3.02290400
H	1.75102800	5.07221400	-0.89325100

C	2.13712900	4.77189000	-4.25804600
H	2.63708300	2.94517800	-5.29244400
H	1.66640000	6.42691800	-2.96198000
H	2.09348300	5.36830000	-5.16769800
C	2.40998700	-2.60739700	-2.24569900
C	1.36885700	-1.91018400	-2.87481400
C	2.37199100	-4.00235300	-2.23785800
C	0.28538200	-2.58706500	-3.42336300
H	1.42805400	-0.81891200	-2.95942200
C	1.29408600	-4.67985800	-2.80203400
H	3.18684100	-4.56499700	-1.78178500
C	0.24321400	-3.97619900	-3.38007300
H	-0.52055000	-2.03092000	-3.89954500
H	1.26989300	-5.76813700	-2.77875500
H	-0.61172700	-4.50681500	-3.79152800
C	5.09545500	-2.70937400	-1.06173000
C	6.30923100	-2.45925800	-1.70790800
C	5.03056200	-3.74850000	-0.12607600
C	7.43105300	-3.23814400	-1.44095300
H	6.37731600	-1.62704700	-2.41017000
C	6.14835300	-4.53295200	0.13569200
H	4.10378400	-3.93543900	0.41839400
C	7.34977600	-4.27951300	-0.52268600
H	8.37170900	-3.02606700	-1.94694300
H	6.08407100	-5.34125200	0.86281600
H	8.22586200	-4.89119000	-0.31204700
C	-6.57851200	-0.05296600	-0.36833000
C	-5.95164500	0.67939100	-1.44059000
C	-6.54618700	0.14843400	-2.72995400
C	-7.63759400	-0.92880900	-1.08173500
H	-5.95764900	0.29561000	-3.64167100
H	-7.05452800	0.63389800	0.34315000
H	-6.02784000	1.77406700	-1.35138900
H	-8.05780200	-1.75976200	-0.50324400
C	-8.69413400	0.04448400	-1.64166200
H	-9.06727400	0.73098000	-0.86906100
H	-9.55866600	-0.51624700	-2.02126500
C	-6.87272800	-1.29938500	-2.35739600
H	-5.96991000	-1.89556600	-2.16323600
H	-7.48278100	-1.81384200	-3.11289800
C	-7.95463300	0.77118500	-2.79859100
H	-7.93828000	1.86310300	-2.68339100
H	-8.41948600	0.55213500	-3.77055200

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S	-3.76705500	-2.93397900	0.58753000
O	-2.74559000	-1.72567900	0.30803500
O	-3.50921300	-3.64522400	1.90435800
C	-3.24263100	-4.21677500	-0.72327400
O	-5.19300300	-2.52731900	0.20622700
Ni	-3.82703800	-0.14182500	0.23281200
F	-4.08781400	-5.22307600	-0.66317900
F	-2.02496400	-4.62939300	-0.45028200
F	-3.28595900	-3.67325100	-1.92615200
C	-3.80299200	-0.88377900	3.26772500
C	-5.13908500	0.95717600	2.46847300
C	-5.88091500	0.95942200	3.64203000
C	-5.59128100	0.01164700	4.62340100
C	-4.56947400	-0.91455800	4.42867700
H	-2.94881800	-1.54738300	3.14669400
H	-6.68687000	1.68046800	3.77171900
H	-6.17195200	-0.00426300	5.54398800
H	-4.35340600	-1.65657200	5.19665700
C	-5.52154400	1.81333000	1.32801100
O	-5.89429000	2.95317000	1.32514700
N	-5.42787800	0.99000700	0.12344200
H	-6.03151100	0.16656300	0.26219500
C	-5.59062000	1.51149400	-1.20991200
C	-4.79749100	0.83283000	-2.15261000
C	-6.42844200	2.52305800	-1.59978400
C	-4.88573500	1.14801300	-3.52375000
C	-6.50433400	2.85706100	-2.97131000
H	-7.01339200	3.06572200	-0.86348900
C	-3.09669100	-0.70446100	-2.51122200
C	-4.01831800	0.45891400	-4.39706300
C	-5.76939400	2.18053600	-3.91287100
H	-7.16107900	3.66868500	-3.27599300
C	-3.12808600	-0.45754200	-3.89503300
H	-2.40173200	-1.40573200	-2.05610200
H	-4.04642900	0.68546700	-5.46207300
H	-5.83161300	2.45073000	-4.96581900
H	-2.42221600	-0.97141800	-4.54225800
N	-3.91475600	-0.09369800	-1.67634800
C	-4.07454900	0.05168100	2.26240300
S	-1.91838500	2.44768300	-1.30897400
O	-2.78266200	2.33868900	-0.03701900
O	-0.86717600	1.30877600	-1.45304100
C	-0.84251300	3.99775400	-1.02872400

O	-2.66556800	2.76565800	-2.60127100
H	-2.97302700	0.42620200	1.85243500
F	-0.04744400	3.82165600	0.00825200
F	-1.63101500	5.03470000	-0.81866800
F	-0.11277100	4.20478700	-2.11236100
C	-2.09134400	2.43963700	3.45189900
H	-2.64323400	1.73343200	4.08605300
H	-2.82217800	2.98438600	2.83789300
H	-1.55560600	3.16211400	4.07381300
C	-1.13392400	1.72367200	2.53192400
O	-0.01260200	2.21442000	2.30943200
O	-1.51994000	0.63485900	1.97559900
Ag	0.45756100	0.70497800	0.44347700
C	3.59304700	0.98208800	-0.57551200
C	3.60783600	-0.32156000	-1.06149900
C	3.03250000	-0.62649500	-2.32996800
C	2.32750100	0.39235000	-3.03423600
C	2.24083700	1.68320000	-2.46797800
C	2.88018700	1.98000000	-1.28966200
H	3.63289800	-2.71239500	-2.37189000
C	3.11291100	-1.92001800	-2.90931400
C	1.71513000	0.08251900	-4.27444500
H	1.65389500	2.44182400	-2.98462900
H	2.81505300	2.99006500	-0.88338100
C	1.82406800	-1.17274200	-4.81489700
C	2.53535600	-2.18121800	-4.12588100
H	1.16450600	0.87109800	-4.78871900
H	1.36347900	-1.39788100	-5.77588600
H	2.61035200	-3.17863800	-4.55564000
C	8.16793600	-2.66578400	-0.30721900
C	7.31977400	-3.19323700	0.63250200
C	5.95714400	-2.80642800	0.67735400
C	5.47669500	-1.84660800	-0.25979300
C	7.68802800	-1.72897500	-1.24919600
H	5.43496600	-4.07769100	2.34554300
H	9.21299800	-2.96940100	-0.33166300
H	7.67686500	-3.92262800	1.35858800
C	5.06054300	-3.34850100	1.62622600
C	4.11746100	-1.42391700	-0.19353800
H	8.36764500	-1.30990700	-1.98978800
C	3.25311800	-2.01259200	0.72379000
C	3.74131400	-2.97685800	1.63850900
H	3.05950800	-3.40936400	2.36979900
P	4.43133100	1.31273000	1.06882300

P	1.45595300	-1.55721500	0.68043100
C	6.37661500	-1.33020700	-1.22618300
H	6.01092300	-0.60167000	-1.94863300
C	0.82222700	-2.75463900	-0.57188200
C	0.06384900	-2.25825300	-1.63396100
C	1.19172400	-4.10336700	-0.55866600
C	-0.30386000	-3.10183200	-2.67870600
H	-0.20520100	-1.19709200	-1.65763000
C	0.80918800	-4.94462400	-1.59610100
H	1.79689400	-4.49269000	0.26111800
C	0.06424800	-4.44228500	-2.66068000
H	-0.86399000	-2.70418500	-3.52487300
H	1.09983500	-5.99387100	-1.57913300
H	-0.22190600	-5.09758300	-3.48239100
C	0.79154600	-2.09772700	2.30642600
C	1.30192400	-1.47104500	3.45161100
C	-0.32709000	-2.92032600	2.41516200
C	0.71626800	-1.69433500	4.68965300
H	2.15472700	-0.79287000	3.36755100
C	-0.91764300	-3.13707200	3.65852100
H	-0.76862500	-3.37552300	1.52909400
C	-0.39682600	-2.52828800	4.79465600
H	1.12124600	-1.20629900	5.57483600
H	-1.80193000	-3.77058300	3.71444600
H	-0.86099000	-2.69518800	5.76620300
C	6.20097400	1.40896900	0.50881200
C	7.17131300	0.88604400	1.36572000
C	6.60340500	1.95725300	-0.71453900
C	8.51832700	0.91279600	1.01448600
H	6.86118700	0.43853200	2.31104000
C	7.94878800	1.98888600	-1.06609100
H	5.85236300	2.35383600	-1.39989000
C	8.90723900	1.46528300	-0.20100100
H	9.26340300	0.49419100	1.68972000
H	8.25130100	2.42057300	-2.01962600
H	9.96061500	1.48653800	-0.47880200
C	3.99777000	3.09335800	1.33070200
C	2.76482200	3.30830700	1.95215200
C	4.76994500	4.19444200	0.95176600
C	2.28602200	4.59787200	2.15342100
H	2.15346600	2.46422000	2.27525200
C	4.30070000	5.48638900	1.17650300
H	5.74169600	4.04841100	0.48162600
C	3.05629200	5.69057800	1.76684700

H	1.30415500	4.72463200	2.60869900
H	4.91072400	6.33997900	0.88228600
H	2.69023700	6.70344000	1.92815900

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S	-3.37440700	3.10270300	-1.51011300
O	-3.54684900	1.67595000	-0.86354300
O	-2.43086500	3.08164000	-2.70914900
C	-2.37016700	3.96878700	-0.12846500
O	-4.65990700	3.90860500	-1.60431500
Ni	-4.84602900	-0.22765900	0.03086600
F	-1.83596400	5.08680500	-0.57439500
F	-1.41668700	3.13203800	0.25686300
F	-3.16345900	4.22720800	0.89653000
C	-5.69222000	-0.30974000	-2.76574400
C	-5.85376600	-2.33657100	-1.45218300
C	-5.97566000	-3.09403600	-2.61454400
C	-5.91439700	-2.46969600	-3.85256200
C	-5.75644300	-1.08588400	-3.92190600
H	-5.59310600	0.76146100	-2.85311000
H	-6.09299000	-4.17367100	-2.53190800
H	-5.98046800	-3.05777100	-4.77053000
H	-5.68202600	-0.59766200	-4.89480800
C	-5.85257000	-2.95381700	-0.09491600
O	-6.72495600	-3.66541400	0.35937500
N	-4.76644900	-2.46155200	0.62399400
H	-3.86609100	-2.37884800	0.11070100
C	-4.61110400	-2.43109900	2.02424100
C	-3.93212000	-1.27909800	2.51237100
C	-4.96833000	-3.43495800	2.88854300
C	-3.44863700	-1.26934400	3.84548100
C	-4.59457100	-3.35849100	4.24765500
H	-5.50723500	-4.30256600	2.50478800
C	-2.94662200	0.78340300	2.06867200
C	-2.60930700	-0.20469200	4.21737900
C	-3.81479000	-2.33137200	4.70882800
H	-4.88213000	-4.16573500	4.91981000
C	-2.31895000	0.79796900	3.32606500
H	-2.82612600	1.59985400	1.36159300
H	-2.17506500	-0.19954300	5.22458000
H	-3.45355800	-2.31330800	5.73582000
H	-1.63386700	1.60224300	3.57912000
N	-3.73086400	-0.20161900	1.67076400
C	-5.72663000	-0.92736300	-1.50665400

S	-1.21993200	-2.61434700	0.72938900
O	-2.16949300	-2.15007900	-0.40944500
O	-0.24091700	-1.51953500	1.23099100
C	-0.08174800	-3.86507000	-0.13560100
O	-1.87868200	-3.42382300	1.83957000
H	-2.01223900	0.94892200	-1.02892500
F	0.68575600	-3.21827000	-1.00113800
F	-0.81001400	-4.76041800	-0.76447500
F	0.67961100	-4.45837400	0.76553200
C	-2.13046700	-0.28643000	-3.08605000
H	-2.41301900	0.72923400	-3.41227800
H	-2.98792800	-0.70695100	-2.54011500
H	-1.89725200	-0.91844400	-3.95382200
C	-0.96110900	-0.21046500	-2.15958200
O	0.09378900	-0.81216000	-2.32616200
O	-1.09036500	0.58538300	-1.10950100
Ag	1.25558900	-0.41066700	-0.18896000
C	4.27207200	-1.11090400	0.40601300
C	4.33189300	-0.00669600	1.24960400
C	3.65868000	-0.00193300	2.50353000
C	2.82528400	-1.10146700	2.83838500
C	2.73851500	-2.19998500	1.95077800
C	3.45521400	-2.21396800	0.77859500
H	4.37784300	1.93706900	3.15183100
C	3.73653500	1.09109900	3.40051200
C	2.06023700	-1.05952500	4.02742100
H	2.07503400	-3.02542700	2.20511600
H	3.36323800	-3.06394400	0.09810000
C	2.14652200	0.02064000	4.87546500
C	3.00787700	1.09982800	4.56203500
H	1.39182700	-1.88864700	4.24855900
H	1.56607500	0.04732200	5.79495200
H	3.07832200	1.94209800	5.24062800
C	9.13857300	1.87440500	1.24430700
C	8.39697200	2.76355800	0.51371300
C	7.00089500	2.58912800	0.35347500
C	6.37304600	1.45881000	0.96578300
C	8.51321800	0.77248400	1.86846000
H	6.69040500	4.35259300	-0.85935300
H	10.21111700	2.01877900	1.35211500
H	8.86766500	3.62184300	0.03288700
C	6.21054900	3.48746400	-0.40145900
C	4.97889700	1.23992500	0.75226600
H	9.10792900	0.06768000	2.44537800

C	4.23054100	2.14461100	0.01220900
C	4.86448800	3.28124800	-0.55352800
H	4.27676000	3.97392200	-1.15320800
P	5.14043600	-0.99050400	-1.24201300
P	2.42637100	1.82149800	-0.28520800
C	7.16154900	0.56757000	1.73662700
H	6.68817700	-0.28494400	2.20976200
C	1.59067500	3.05992900	0.79649500
C	0.97381200	2.60359800	1.96521500
C	1.58003100	4.43064400	0.50964800
C	0.37761900	3.50908000	2.84275000
H	0.95119000	1.53449000	2.19719500
C	0.96448100	5.32897800	1.36876000
H	2.02877300	4.79670200	-0.41450600
C	0.36878600	4.86786500	2.54227100
H	-0.08165800	3.15230800	3.76080500
H	0.94484400	6.38801900	1.12958500
H	-0.10967000	5.57262400	3.21798400
C	2.13055200	2.39646100	-2.00340800
C	3.08352800	2.14896500	-3.00986000
C	0.85383500	2.85504400	-2.35701800
C	2.76925300	2.40196800	-4.34599900
H	4.07453200	1.76636300	-2.75023300
C	0.53775100	3.08456400	-3.69002300
H	0.07896900	2.99292100	-1.59339300
C	1.49867900	2.87136900	-4.68334000
H	3.51616300	2.22519900	-5.11795600
H	-0.46531100	3.43293400	-3.93792500
H	1.26156900	3.05841500	-5.73383700
C	6.81319100	-1.62898000	-0.75970200
C	7.92498100	-0.96577200	-1.29180500
C	7.01803200	-2.65894200	0.16338700
C	9.21385600	-1.34263700	-0.93165400
H	7.77113700	-0.13251200	-1.97937700
C	8.30485400	-3.03321200	0.52312100
H	6.16188000	-3.16706400	0.60669100
C	9.40557200	-2.38362800	-0.02123700
H	10.07030600	-0.81420100	-1.34229500
H	8.45428000	-3.84479600	1.24135000
H	10.41506900	-2.67488400	0.27091300
C	4.35674100	-2.38850900	-2.16502300
C	3.12789700	-2.08668200	-2.77685400
C	4.88522900	-3.67339500	-2.30189700
C	2.44388100	-3.06185000	-3.48828500

H	2.71156200	-1.08013800	-2.70708800
C	4.20476200	-4.63872500	-3.02895300
H	5.84665100	-3.91546900	-1.84789200
C	2.97645800	-4.34143100	-3.61806600
H	1.47664200	-2.81201600	-3.92396200
H	4.62550400	-5.64114800	-3.13218300
H	2.44029400	-5.10184000	-4.17704900
C	-7.02074200	-0.11881500	-0.05923000
C	-6.34737100	0.61985300	0.96588400
C	-6.68753000	2.06892000	0.72868600
C	-7.82766500	0.90473800	-0.83409600
H	-5.98794900	2.80815400	1.14221000
H	-7.45923600	-1.09821100	0.15291100
H	-6.27030800	0.22568600	1.98123700
H	-8.19652900	0.57681300	-1.80447300
C	-8.92864100	1.34209300	0.17163600
H	-9.46225600	0.48449200	0.60852200
H	-9.67274900	1.95014300	-0.35737900
C	-6.90719100	2.12098100	-0.78161300
H	-5.97582200	2.02018300	-1.34613500
H	-7.39652200	3.04845700	-1.10962600
C	-8.15790600	2.17779400	1.22440900
H	-8.28388200	1.79871400	2.24873200
H	-8.47753300	3.22655100	1.22361700

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S	-4.16229100	1.30394700	1.04490500
O	-4.11011300	2.14967900	2.30551100
O	-4.22600200	2.04707700	-0.31268900
C	-5.80384700	0.34024900	1.10517800
O	-3.10693500	0.13280400	1.02008600
Ni	-1.40531500	0.44914200	0.08170100
F	-5.91936800	-0.38363200	0.01138500
F	-6.78703100	1.20800900	1.18249400
F	-5.78869200	-0.43572800	2.16631500
C	-2.75325200	-2.80527600	-0.76488700
C	-1.35306900	-0.96355000	-1.45024100
C	-2.45272300	-0.36065800	-2.10034400
C	-3.69899800	-0.97839400	-2.05942800
C	-3.83486300	-2.19913500	-1.41053700
H	-2.89945000	-3.74782200	-0.23973800
H	-2.32319100	0.57605600	-2.64484000
H	-4.55945200	-0.49678400	-2.51846900
H	-4.80915200	-2.68550500	-1.38300400

C	0.05239000	-0.42898200	-1.60208900
O	0.92541800	-0.87838200	-2.31952500
N	0.01467300	1.02907200	-1.24669800
H	-0.12553700	1.59250700	-2.09721900
C	1.07834300	1.57212800	-0.45378900
C	0.74841200	1.88340300	0.88212700
C	2.32907700	1.85910000	-0.93803800
C	1.68250400	2.54062500	1.71221100
C	3.27656200	2.49424800	-0.10470600
H	2.57312500	1.60493000	-1.96772600
C	-0.86838300	1.86947000	2.56398500
C	1.26200700	2.87762200	3.01892100
C	2.96032900	2.84123200	1.18499500
H	4.26054200	2.72822500	-0.50478300
C	-0.00286700	2.55107600	3.43915200
H	-1.88090200	1.59719700	2.86075200
H	1.94932000	3.41179000	3.67376300
H	3.67722800	3.36429000	1.81572600
H	-0.35904100	2.81653500	4.43022300
N	-0.50140200	1.54613700	1.33633300
C	-1.50893900	-2.19760400	-0.76696900
C	-0.28343700	-2.66782700	-0.02532800
C	0.50928800	-1.40775700	0.36294200
C	0.49158600	-1.42027100	1.88994000
C	-0.58006000	-3.31579500	1.34123900
H	0.69977100	-0.45961200	2.37731100
H	0.28571300	-3.35441700	-0.67319400
H	1.52653300	-1.33680600	-0.03850200
H	-1.36929400	-4.07844100	1.31814300
C	0.75260300	-3.82822500	1.90695100
H	1.31113500	-4.42127100	1.16990500
H	0.57712200	-4.47405900	2.77757700
C	-0.84066700	-2.09319900	2.23147400
H	-1.72735800	-1.50908800	1.95031900
H	-0.91993200	-2.36127900	3.29481900
C	1.48608700	-2.52563000	2.31353300
H	2.46327700	-2.41159800	1.82656400
H	1.65542700	-2.48639600	3.40015900
S	-0.19207200	5.25867900	0.16210200
O	0.03326300	4.39775800	-1.12917000
O	-1.37514300	4.65367600	0.95874500
C	-0.93255000	6.85294300	-0.56646200
O	1.05194900	5.66273200	0.92729200
H	-0.49172500	4.71869300	-2.68103300

F	-2.03618100	6.52428300	-1.22094600
F	-0.06485100	7.38555500	-1.40335200
F	-1.21429100	7.69404400	0.40143500
C	-2.05132700	3.70433400	-5.31261100
H	-2.54311000	2.75635200	-5.53935000
H	-1.23218700	3.88822800	-6.01624400
H	-2.76575500	4.52795000	-5.43014300
C	-1.53173600	3.69956000	-3.91056600
O	-0.84259300	4.77783300	-3.61748700
O	-1.73829800	2.78026500	-3.12018500
Ag	-2.17256500	3.09126700	-0.68864300

P

C	-3.58666300	-0.13742100	0.31616000
C	-1.38229800	0.65316100	-0.13692400
C	-0.93594100	-0.64418200	-0.38502000
C	-1.82509900	-1.70911500	-0.27655000
C	-3.14677600	-1.44389700	0.07103800
H	-4.62644800	0.03731300	0.58715400
H	-1.49622300	-2.73183200	-0.46404800
H	-3.85438800	-2.26788500	0.15438400
C	-2.70125900	0.92626200	0.21613000
H	-3.00625000	1.95473100	0.40542300
C	0.52891700	-0.67727200	-0.73078500
C	0.97109400	0.81180500	-0.68262300
C	2.06251800	0.82783900	0.40225000
C	1.42679200	-1.33287800	0.34010000
H	2.24629900	1.83297300	0.79942100
H	0.68908200	-1.14987400	-1.71184600
H	1.34999800	1.20331600	-1.63709400
H	1.05042200	-2.30218600	0.69226200
C	2.85846000	-1.37107800	-0.21455200
H	2.89625800	-1.79392400	-1.22785800
H	3.50133300	-1.99527000	0.42026300
C	1.53985500	-0.22250400	1.39082300
H	0.58416300	0.04305400	1.86209000
H	2.26474200	-0.45941200	2.18172700
C	3.29816800	0.11737800	-0.16547900
H	3.58513900	0.51114600	-1.14966800
H	4.16011000	0.25256500	0.50169400
C	-0.26516400	1.60713500	-0.27667300
O	-0.29998300	2.80423700	-0.07766000

M

C	-1.26849900	-0.49835200	-0.93778400
C	-0.22143100	0.33356600	-1.33773400
C	0.60532400	-0.02400500	-2.44656400
C	0.38609700	-1.26652000	-3.10748300
C	-0.69489100	-2.07586300	-2.69672300
C	-1.50466200	-1.69811700	-1.65866000
H	1.85115100	1.75365400	-2.40415100
C	1.67266000	0.79774000	-2.89478800
C	1.25475800	-1.66174900	-4.15217900
H	-0.86407200	-3.02390700	-3.20824700
H	-2.32166000	-2.35031800	-1.35474800
C	2.28730300	-0.85253800	-4.55183800
C	2.48947000	0.39410700	-3.92041000
H	1.08390000	-2.62703800	-4.62861300
H	2.95071800	-1.16666600	-5.35598800
H	3.30968000	1.03543000	-4.23997000
C	-1.38868900	5.28501300	-2.18053800
C	-0.72834300	5.26646300	-0.97838000
C	-0.23287400	4.05375200	-0.44246100
C	-0.44929900	2.83598000	-1.14935800
C	-1.59125300	4.08352300	-2.89188400
H	0.64914400	4.95754800	1.31252800
H	-1.75260500	6.22547900	-2.59112400
H	-0.55914700	6.18804300	-0.42069000
C	0.49901500	4.02539600	0.76692400
C	0.06403100	1.61086600	-0.61905200
H	-2.10961100	4.10418100	-3.84919100
C	0.85103500	1.63988500	0.52574700
C	1.04404900	2.85677500	1.22828200
H	1.63551200	2.85955700	2.14340200
P	-2.09873300	-0.23148200	0.72436600
P	1.75831100	0.10923600	1.04640800
C	-1.14478700	2.88933100	-2.38412700
H	-1.31029700	1.96454200	-2.93475700
C	3.26728400	0.15018000	-0.00410300
C	3.62534700	-1.01565000	-0.68678700
C	4.01764800	1.31822300	-0.18553100
C	4.73489400	-1.01532600	-1.52790600
H	3.02029800	-1.92119200	-0.59019300
C	5.12629500	1.31165400	-1.02255600
H	3.72455500	2.23905000	0.32170200
C	5.48642600	0.14273300	-1.69157100
H	4.99953100	-1.92398000	-2.06541900
H	5.70877300	2.22159900	-1.15855200

H	6.35290200	0.14087700	-2.35139500
C	2.29124800	0.49802700	2.76371400
C	1.29025400	0.49932700	3.74366100
C	3.61369400	0.74471100	3.13199200
C	1.60898300	0.76315000	5.06904400
H	0.25590500	0.28975900	3.45969500
C	3.93032300	0.99700100	4.46508100
H	4.40143400	0.73280400	2.37939100
C	2.93149600	1.01131600	5.43173100
H	0.82467900	0.76500300	5.82403000
H	4.96560500	1.18296100	4.74631900
H	3.18277000	1.20910400	6.47241900
C	-2.89951100	1.42632700	0.54797200
C	-2.76862300	2.31703300	1.61599100
C	-3.61421900	1.82788700	-0.58542300
C	-3.34336400	3.58336000	1.55910400
H	-2.19829200	2.01507700	2.49587200
C	-4.19123800	3.09081700	-0.64317600
H	-3.70764200	1.14375800	-1.43099000
C	-4.05637000	3.96983300	0.42926300
H	-3.22945500	4.27016400	2.39656000
H	-4.73668700	3.39752800	-1.53483900
H	-4.50260700	4.96195700	0.37822000
C	-3.54727600	-1.39441000	0.68577100
C	-3.28458600	-2.75402300	0.91365500
C	-4.87589300	-0.97883800	0.55802200
C	-4.32717900	-3.67310300	0.96458600
H	-2.25956200	-3.11552600	1.03306000
C	-5.91655500	-1.90058100	0.63001100
H	-5.10906700	0.07437800	0.41103100
C	-5.64596500	-3.25031700	0.82547500
H	-4.10028900	-4.72585500	1.12745100
H	-6.94561300	-1.55732300	0.53074000
H	-6.46152100	-3.97026700	0.87806900
C	0.24583000	-4.47632000	-0.26002400
O	-0.32082800	-4.01986500	0.79446100
O	1.18401600	-3.91058300	-0.85135000
Ag	0.66370100	-2.05071300	0.85765900
C	-0.33459200	-5.76367200	-0.80237600
H	-1.36874000	-5.57625700	-1.12397400
H	0.24752400	-6.13715200	-1.64971400
H	-0.38050100	-6.52370900	-0.01408100

N

S	-2.22216600	-1.43724700	-0.74402700
O	-1.61387600	-0.04800100	-1.17558000
O	-3.21487000	-2.15473800	-1.61366600
C	-3.03945100	-1.12705200	0.96708300
O	-0.85507800	-2.18258400	-0.36555900
S	0.77203900	1.97997700	0.41176900
O	-0.04332300	1.22020300	1.45593000
O	2.07730200	2.65442900	0.77647800
C	-0.37285800	3.34132000	-0.28127900
O	0.93124600	1.04412700	-0.89858900
Ni	0.19481400	-0.60807500	-0.58260300
F	0.24650100	3.94134500	-1.27176600
F	-0.61884600	4.19131600	0.69244200
F	-1.48428000	2.78162900	-0.69500100
F	-2.11557100	-0.69337500	1.78231400
F	-3.98674200	-0.23888300	0.79908600
F	-3.53141900	-2.27263000	1.37520700
C	1.72754500	-1.33010300	0.67125500
C	1.88693900	-2.03157800	-0.50976400
C	3.27953900	-1.76471900	-0.99989700
C	3.03110900	-0.61422200	0.92190100
H	3.48016500	-1.98933000	-2.05067100
H	1.00777100	-1.56675700	1.45784300
H	1.27855200	-2.87515200	-0.83207600
H	2.99985900	0.22849300	1.61761500
C	3.97316800	-1.78610600	1.33631200
H	3.56054500	-2.38851900	2.15490600
H	4.92969400	-1.37516700	1.68170700
C	3.54967800	-0.34512100	-0.49609200
H	2.99572600	0.43138400	-1.02711300
H	4.62021900	-0.10378800	-0.50079100
C	4.13822300	-2.58410800	0.01964400
H	3.81282600	-3.62861700	0.10270500
H	5.18054300	-2.59210100	-0.32272400
Q			
C	1.55197500	-0.68909300	-0.81031200
C	1.55237600	0.68564500	-0.81508400
C	2.31768800	1.12797700	0.41157300
C	2.31728200	-1.12366300	0.41907900
H	2.15082400	2.15742000	0.74034300
H	1.37743700	-1.32739600	-1.67600300
H	1.37790300	1.31845400	-1.68478900
H	2.14996500	-2.15083000	0.75466900
C	3.79796700	-0.77367700	0.08955500

H	4.12307800	-1.20704800	-0.86407800
H	4.45679000	-1.17162000	0.87180500
C	1.98950100	0.00547900	1.40357800
H	0.94396100	0.00684000	1.74514100
H	2.65042500	0.00828400	2.28070700
C	3.79827100	0.77519700	0.08439800
H	4.12359000	1.20213200	-0.87206500
H	4.45721700	1.17808300	0.86401200
C	-4.63712700	0.00896600	0.55245000
H	-5.03171000	-1.00346100	0.67198800
H	-5.17717100	0.52278600	-0.25154100
H	-4.80722500	0.58548500	1.46907100
C	-3.16330800	-0.00902200	0.23367000
O	-2.57223900	1.10217400	0.10199800
O	-2.57331400	-1.11893800	0.10730600
Ag	-0.61230700	-0.00067800	-0.32206700
S			
S	1.15848800	2.14954100	0.54366300
O	0.27930200	1.83589900	1.74820200
O	2.64663500	2.38250500	0.67887900
C	0.45847000	3.76971800	-0.18227200
O	0.76411300	1.16745800	-0.68189400
S	2.82161100	-1.63876400	0.00062600
O	1.81202800	-0.73732600	0.88503100
O	3.36986700	-2.77518500	0.84544300
C	4.26861900	-0.43434500	-0.31794900
O	2.19112900	-1.92517000	-1.36283400
Ni	0.24166900	-0.49961700	-0.08459700
F	5.23056600	-1.13259800	-0.89017000
F	4.67120700	0.04209300	0.83279000
F	3.85323700	0.51090300	-1.11959600
F	-0.82614700	3.60556900	-0.43747300
F	0.61664400	4.72329200	0.71227300
F	1.11022400	4.06642800	-1.28402100
C	-4.54685700	2.74082600	0.67870600
C	-2.80889000	1.30331600	-0.18134000
C	-2.57963000	0.80687200	1.10516200
C	-3.33266900	1.27856800	2.17137100
C	-4.31965000	2.23598500	1.95807400
H	-5.31109100	3.49828600	0.51700800
H	-1.77756300	0.09517300	1.29342900
H	-3.13380100	0.90968800	3.17497800
H	-4.90850100	2.60154800	2.79759900

C	-2.04929500	0.88204900	-1.36700900
O	-2.02231900	1.46050400	-2.42257800
N	-1.31045600	-0.39720000	-1.28079000
H	-0.81735900	-0.45245400	-2.18187100
C	-2.13418000	-1.57454300	-1.08101300
C	-1.63594800	-2.50099800	-0.14800900
C	-3.31211700	-1.81738600	-1.74092100
C	-2.33712000	-3.69778300	0.11907000
C	-4.02222500	-3.00962800	-1.47726400
H	-3.69325200	-1.09682700	-2.46396900
C	0.03434600	-3.01026400	1.38116600
C	-1.77049200	-4.57105500	1.07693000
C	-3.54829600	-3.93053100	-0.57382100
H	-4.95520000	-3.19564400	-2.00412000
C	-0.59760900	-4.22893300	1.70088700
H	0.96923400	-2.70583100	1.84916600
H	-2.27621200	-5.50770700	1.30939200
H	-4.10029500	-4.84833700	-0.37597300
H	-0.13746300	-4.87974600	2.43867600
N	-0.47080500	-2.17941500	0.48631900
C	-3.78871200	2.28315700	-0.38632900
H	-3.93206600	2.67419700	-1.39176600
T			
C	-4.26825900	2.23588100	-0.26985400
C	-2.15456400	1.41101900	0.55134100
C	-1.94382300	0.74394000	-0.65813600
C	-2.90271800	0.81107500	-1.66169600
C	-4.05763200	1.56503100	-1.47372200
H	-5.17671100	2.81650700	-0.11946200
H	-1.06299300	0.12343300	-0.82107800
H	-2.73997900	0.25707500	-2.58452100
H	-4.80478300	1.62323900	-2.26397800
C	-1.23305700	1.27077400	1.70512200
O	-1.60698800	1.33269100	2.86008500
N	0.11242200	0.96064800	1.43880700
H	0.58918900	0.71436100	2.30481200
C	0.94243500	1.55353400	0.46683900
C	2.12702100	0.85637600	0.08313000
C	0.68566800	2.79135900	-0.08306200
C	3.04627600	1.48317100	-0.80277500
C	1.57097700	3.37521200	-1.00973500
H	-0.21095500	3.33079000	0.21517700
C	3.47936000	-1.01499900	0.25827400

C	4.23989300	0.79018600	-1.10402700
C	2.74192800	2.74916300	-1.35171600
H	1.32848300	4.35005700	-1.42725600
C	4.47199600	-0.44630500	-0.55951700
H	3.60911700	-2.01977600	0.66090700
H	4.96391500	1.25350600	-1.77408100
H	3.44853500	3.20914900	-2.04116200
H	5.38197300	-1.00190700	-0.76987100
N	2.35084000	-0.40120000	0.56962800
C	-3.32828800	2.14518600	0.74683300
H	-3.48937900	2.62689800	1.70967000
C	-2.69323100	-3.35565800	-1.49031500
H	-2.61367200	-3.41270000	-2.58005800
H	-3.55719900	-2.72582900	-1.23848800
H	-2.87512100	-4.34782100	-1.06534300
C	-1.45209600	-2.72974800	-0.89456100
O	-1.23504800	-2.97899000	0.33963100
O	-0.74004000	-1.98371500	-1.60012700
Ag	0.48919300	-1.68264200	0.64307300
W			
S	0.48993900	3.00786400	0.79060900
O	-0.31805300	2.31114600	-0.39916800
O	0.01941500	4.34303700	1.29757400
C	2.33937800	3.22704500	0.14115100
O	0.48837100	1.77178400	1.79928000
S	2.43161800	-0.66203000	-1.28800100
O	3.56240500	-0.09578800	-2.12368400
C	3.12568000	-2.25411200	-0.50474900
O	2.03606700	0.15405500	-0.03035000
Ni	-0.23429700	0.61711400	0.43699200
C	-5.77279300	1.25988800	-0.97976700
C	-3.45073100	0.60017800	-0.89056100
C	-3.54393200	0.47808800	0.49977500
C	-4.74367900	0.74913900	1.14331000
C	-5.85947000	1.13274100	0.40457600
H	-6.64336600	1.56604700	-1.55626300
H	-2.67146000	0.20147900	1.09063500
H	-4.80628100	0.66698800	2.22648200
H	-6.79999500	1.34104400	0.91177900
C	-2.20765900	0.36073000	-1.65619600
O	-2.03006200	0.72602900	-2.78978400
N	-1.13353500	-0.36846100	-0.98563900
C	-1.42859600	-1.69879300	-0.50366600

C	-0.86060200	-2.01084400	0.74263500
C	-2.10790600	-2.65889400	-1.20725800
C	-0.93965200	-3.31415000	1.27696700
C	-2.22918900	-3.95911200	-0.66486300
H	-2.52769300	-2.42872200	-2.18554500
C	0.39999000	-1.22719200	2.53087600
C	-0.28232300	-3.53437100	2.50902000
C	-1.65377400	-4.28791300	0.53926000
H	-2.77049000	-4.71477600	-1.22942100
C	0.38957400	-2.50463500	3.12410500
H	0.91938000	-0.37883400	2.97467500
H	-0.30835600	-4.52726400	2.95689800
H	-1.73412500	-5.29890000	0.93587600
H	0.91244700	-2.65544200	4.06431000
N	-0.22311100	-0.99800300	1.39233000
C	-4.57207300	1.00196000	-1.62407700
H	-4.47598300	1.10838700	-2.70255400
F	4.18462600	-1.96160900	0.22580900
F	3.45285500	-3.11324300	-1.44894100
F	2.19510900	-2.79814700	0.27770400
F	2.40160600	2.76902500	-1.07067600
F	2.56557100	4.51844100	0.17305700
F	3.12326400	2.59513900	0.96549500
O	1.19347300	-1.19895000	-2.04742200
H	-0.31582800	-0.46277100	-1.64803400

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S	-3.09389300	-0.24699200	-0.71431000
O	-1.57196300	-0.31870800	-1.22185800
O	-3.91762600	-1.42529000	-1.19264700
C	-3.70329900	1.25093100	-1.72544900
O	-3.13557500	0.19539100	0.74618400
Ni	-0.36456400	-0.23796200	0.20417300
F	-5.00023700	1.37902600	-1.55550900
F	-3.42078700	1.05351400	-2.99608600
F	-3.07895300	2.33233800	-1.29147500
C	-1.55473300	-3.08853000	0.33431400
C	-0.84712100	-1.75793400	2.24350100
C	-2.02365600	-2.08707900	2.91091900
C	-2.95248000	-2.91250600	2.29127000
C	-2.73478600	-3.39073100	0.99734700
H	-1.36755400	-3.46089200	-0.67051600
H	-2.21437700	-1.64839500	3.88793100
H	-3.88071400	-3.15473100	2.80468900

H	-3.49840800	-3.98393200	0.50070000
C	0.00553500	-0.68923200	2.80900900
O	-0.01686400	-0.26856300	3.93467700
N	0.78759000	-0.08032700	1.74643100
H	1.63170000	-0.68092900	1.43890900
C	1.23922100	1.28094400	1.89929800
C	0.95384100	2.08286100	0.77993200
C	1.98897800	1.77382700	2.93484300
C	1.49407000	3.38040100	0.66476600
C	2.47526900	3.09957200	2.85842300
H	2.21755700	1.14888000	3.79352300
C	-0.00867000	2.17693400	-1.33491700
C	1.25238900	4.06525700	-0.54695600
C	2.25254100	3.87963600	1.74997300
H	3.06245000	3.49011500	3.68627600
C	0.52533200	3.46197200	-1.54410800
H	-0.60512100	1.65883100	-2.08396400
H	1.66385300	5.06469800	-0.68453900
H	2.66516900	4.88549700	1.68599200
H	0.34987700	3.95791700	-2.49449100
N	0.17855000	1.53421000	-0.20007900
C	-0.58978200	-2.28038800	0.94919500
S	2.71684700	-0.75983900	-0.81517300
O	1.31880200	-1.09019000	-1.38389000
O	3.21057900	0.66846300	-1.01028900
C	3.90345400	-1.86900400	-1.80429500
O	2.86118900	-1.31528000	0.64021800
H	0.41027000	-2.25529300	0.49794500
F	3.88119600	-1.48672500	-3.06475900
F	3.49973700	-3.11924800	-1.70334600
F	5.11881200	-1.74278300	-1.31478000

TS19-30

S	-3.13417700	-0.25850300	-0.68136600
O	-1.62139200	-0.26313500	-1.21720600
O	-3.93848200	-1.43057100	-1.20695100
C	-3.79559100	1.27444600	-1.60132800
O	-3.16147600	0.10791800	0.80032700
Ni	-0.38946500	-0.23007800	0.19498700
F	-5.09254300	1.36127800	-1.40546700
F	-3.52960600	1.15303900	-2.88519400
F	-3.19002200	2.34561900	-1.11901000
C	-1.54834600	-3.08866800	0.20073100
C	-0.74155000	-1.87388800	2.14989800

C	-1.87855300	-2.25393900	2.85714200
C	-2.83643500	-3.04513500	2.23710400
C	-2.68718700	-3.44338200	0.90657700
H	-1.41526500	-3.39622200	-0.83418900
H	-2.01482100	-1.88415100	3.87101800
H	-3.73373400	-3.32674800	2.78452500
H	-3.47229800	-4.01404700	0.41709600
C	0.15018900	-0.84571500	2.73966600
O	0.22542300	-0.55284300	3.90586200
N	0.81799800	-0.13730400	1.68370800
H	1.73367600	-0.70991000	1.23235100
C	1.25579400	1.21209200	1.90302400
C	0.94438200	2.06483200	0.82810700
C	2.01361700	1.67098600	2.95039200
C	1.46201400	3.37525000	0.76439000
C	2.48131900	3.00563100	2.92554700
H	2.25703700	1.01260600	3.77887300
C	-0.08160400	2.25041600	-1.25209800
C	1.17629200	4.11535600	-0.40417300
C	2.23269800	3.83452400	1.85867000
H	3.07480200	3.36566400	3.76294000
C	0.42703800	3.55277800	-1.40921300
H	-0.69449100	1.76230400	-2.00808200
H	1.56751600	5.12753400	-0.50213900
H	2.62826400	4.84893100	1.83737000
H	0.21224500	4.09634000	-2.32489200
N	0.15183100	1.55236500	-0.15862300
C	-0.55719600	-2.30788600	0.81156100
S	2.70595700	-0.65925700	-0.93746800
O	1.33717500	-1.01006600	-1.54314100
O	3.21174100	0.76609300	-1.09300800
C	3.95356600	-1.77974800	-1.83883200
O	2.79864000	-1.21640500	0.54361600
H	0.41725000	-2.24666100	0.31121300
F	3.97850300	-1.42217900	-3.10539800
F	3.55634900	-3.02926500	-1.72565000
F	5.14085400	-1.62297300	-1.29694100

IM30

S	-3.18216900	-0.13040600	-0.86911800
O	-1.64162700	-0.08896900	-1.30396800
O	-3.99141300	-1.10912600	-1.69495500
C	-3.73177500	1.60792100	-1.42603300
O	-3.29352800	-0.10951000	0.65292500

Ni	-0.51995600	-0.26961500	0.20171700
F	-5.03045100	1.72192800	-1.25397400
F	-3.42042400	1.77782800	-2.69593700
F	-3.09810200	2.50369100	-0.68798500
C	-1.77221800	-3.04604700	-0.23421400
C	-0.86042300	-2.20699500	1.86636700
C	-1.99104700	-2.66820900	2.53554100
C	-2.99826200	-3.30223400	1.82298000
C	-2.90253300	-3.47506300	0.43808400
H	-1.67834000	-3.18592000	-1.30907500
H	-2.07392800	-2.49043100	3.60565100
H	-3.89048500	-3.64356800	2.34469300
H	-3.72031700	-3.93320200	-0.11279000
C	0.10716800	-1.33385100	2.59429200
O	0.34358000	-1.39695100	3.78501100
N	0.59456400	-0.39450200	1.69934500
H	2.07018800	-1.05320000	0.87784400
C	1.13016700	0.84036100	2.10261000
C	0.92211400	1.85020500	1.13510300
C	1.85152700	1.13798600	3.23934100
C	1.49656300	3.13153800	1.26148500
C	2.39171000	2.43564200	3.39173800
H	1.99840000	0.37545000	3.99874900
C	-0.02386600	2.35201200	-0.93096800
C	1.27497200	4.03201100	0.19665100
C	2.24046500	3.40911500	2.43282400
H	2.95818000	2.65727000	4.29423700
C	0.53478500	3.64225700	-0.89464700
H	-0.61829000	1.99370200	-1.76925700
H	1.70408900	5.03238300	0.24864100
H	2.68286400	4.39591800	2.56084100
H	0.36731100	4.31444400	-1.73155800
N	0.14718500	1.50333100	0.06525100
C	-0.73718400	-2.40550700	0.46826100
S	2.77339000	-0.46419900	-1.10528100
O	1.48109700	-0.82312400	-1.81533100
O	3.21495200	0.96973800	-0.92001200
C	4.19331200	-1.41483700	-1.96470900
O	2.86822400	-1.30782900	0.32489100
H	0.23128600	-2.29651200	-0.03637200
F	4.31171700	-0.92403400	-3.17549300
F	3.86771700	-2.68261000	-2.00514500
F	5.28875500	-1.22534600	-1.27237500

IM31

S	2.47385400	-0.64855700	0.07310700
O	1.33858900	-0.73569100	-1.05404300
O	3.84723500	-0.36823900	-0.50259100
C	2.50692000	-2.46809200	0.63409700
O	1.94961800	0.13196800	1.27422800
Ni	-0.11974900	0.38765900	-0.62528700
F	3.46957800	-2.63123700	1.51377900
F	2.70891000	-3.24076800	-0.41566100
F	1.33908700	-2.75786300	1.18224000
C	2.19953100	2.28670700	-1.30492200
C	0.20113900	2.88105700	-0.03576700
C	0.99831500	3.51177800	0.91539800
C	2.37612800	3.51781700	0.75753600
C	2.98095600	2.89346200	-0.33953500
H	2.66029900	1.80906300	-2.16730200
H	0.51939800	3.97001400	1.77842100
H	3.00006300	3.99504300	1.51116200
H	4.06447700	2.87369300	-0.42813000
C	-1.26276000	2.69483300	0.20744400
O	-1.98826600	3.50559200	0.75960700
N	-1.58128000	1.43907400	-0.22035500
C	-2.74820600	0.75108000	0.05667200
C	-2.59976300	-0.64390600	-0.13786400
C	-3.97532400	1.23686800	0.47048100
C	-3.67153800	-1.54509700	0.03817100
C	-5.04498700	0.33496400	0.66297600
H	-4.09933100	2.30137000	0.64408000
C	-1.12184300	-2.34152100	-0.73476600
C	-3.39772600	-2.90896900	-0.20639800
C	-4.91840100	-1.01885400	0.45103800
H	-6.00308800	0.73585400	0.98942800
C	-2.13915600	-3.30306500	-0.59683000
H	-0.10782400	-2.59493500	-1.03632800
H	-4.19469700	-3.64217100	-0.08274900
H	-5.75859000	-1.69444300	0.60306800
H	-1.91107900	-4.34668000	-0.79613700
N	-1.34994900	-1.06203100	-0.49974300
C	0.80022300	2.26492500	-1.16152400
H	0.18364300	2.01219400	-2.03456700

IM32

S	2.72748700	-0.04493100	-0.34894200
O	3.93723300	0.76805300	0.06840100

O	2.11212400	0.15042500	-1.73193300
C	3.26395400	-1.87292700	-0.28759700
O	1.58736300	-0.05909300	0.77310400
Ni	-0.12851400	0.42000100	0.15258100
C	0.02176300	4.76055400	1.09107800
C	-0.97852700	2.95943800	-0.13997700
C	0.30692000	2.45395200	-0.43719100
C	1.44609100	3.10897400	0.06143800
C	1.29740500	4.25028500	0.83340100
H	-0.08252900	5.66619400	1.68672700
H	0.44767000	1.75152200	-1.28023200
H	2.44092500	2.73120900	-0.17516900
H	2.17517400	4.75885300	1.22602500
C	-2.18175200	2.14594100	-0.48436100
O	-3.29282000	2.60992000	-0.68763900
N	-1.83415600	0.82638400	-0.43062600
C	-2.72973300	-0.22890500	-0.40129400
C	-2.14923500	-1.40823800	0.12416600
C	-4.05691800	-0.26160900	-0.79180200
C	-2.87697700	-2.61120500	0.25300700
C	-4.78259900	-1.46735200	-0.67746400
H	-4.52296100	0.64062300	-1.17492700
C	-0.23786300	-2.33276600	1.08273800
C	-2.19616800	-3.70439300	0.83260300
C	-4.22521200	-2.62064100	-0.17511600
H	-5.82295400	-1.47333300	-0.99792500
C	-0.89397700	-3.56526600	1.25165200
H	0.79308300	-2.17298400	1.39049400
H	-2.71871700	-4.65342200	0.95200700
H	-4.80631900	-3.53738900	-0.08915500
H	-0.35760200	-4.39068700	1.71175700
N	-0.84898500	-1.29880100	0.53195000
C	-1.11522200	4.12021400	0.61215800
H	-2.11597600	4.48931800	0.82833400
F	2.27268200	-2.60914400	-0.75745100
F	3.50894300	-2.20498200	0.96546300
F	4.33925400	-2.03641900	-1.02317800

TS32-33

S	2.35202400	-1.49982200	0.04705100
O	3.71770000	-1.97120500	-0.37891300
O	2.30042200	-0.37294600	1.17532700
C	1.45649600	-2.95614600	0.90627900
O	1.35277400	-1.07956700	-1.09058700

Ni	0.13869700	0.32688900	-0.50016300
C	2.72132400	4.25000300	-0.46841000
C	0.85905900	2.90266900	0.21300500
C	1.50275000	1.72797000	-0.22569600
C	2.75442400	1.86531200	-0.84417400
C	3.36204100	3.11417600	-0.95718800
H	3.20223200	5.22313500	-0.55653800
H	1.79826500	0.59596800	0.64404100
H	3.28552700	0.98528300	-1.21318700
H	4.34156600	3.20136100	-1.42466800
C	-0.56392500	2.77345600	0.62855300
O	-1.22126700	3.66029400	1.15449000
N	-1.02508400	1.53578700	0.25603700
C	-2.33715800	1.11478600	0.33608500
C	-2.54093000	-0.16405000	-0.24876800
C	-3.43263700	1.76356700	0.88721600
C	-3.81466800	-0.77776900	-0.29247400
C	-4.69985900	1.14496900	0.85161100
H	-3.29707000	2.74205200	1.33670900
C	-1.52958200	-1.94317500	-1.35364800
C	-3.88863000	-2.04047800	-0.92058400
C	-4.90828900	-0.09026900	0.28143100
H	-5.54112900	1.67536600	1.29526300
C	-2.75892700	-2.61840500	-1.45114600
H	-0.60627500	-2.36689300	-1.74722800
H	-4.85245800	-2.54623900	-0.98092800
H	-5.89740500	-0.54515600	0.26042600
H	-2.79795800	-3.58755600	-1.94160500
N	-1.42984000	-0.75987500	-0.77373300
C	1.45852700	4.14852900	0.11051000
H	0.91058700	5.02497500	0.45420200
F	0.32904600	-2.50498300	1.40189200
F	1.22400800	-3.86786900	-0.01182000
F	2.23423100	-3.42413900	1.84892500

IM33

S	2.50136700	-1.35685600	-0.07035500
O	3.87214600	-1.74742100	-0.54588000
O	2.53339100	-0.26270000	1.16252400
C	1.73791200	-2.81882100	0.91746900
O	1.42914100	-0.94399100	-1.11179400
Ni	0.06554100	0.37528300	-0.55912500
C	2.53131300	4.36165900	-0.16996100
C	0.58842200	2.99316300	0.14073200

C	1.22842500	1.87965400	-0.42932200
C	2.53343100	2.05021400	-0.90177200
C	3.17977500	3.28537500	-0.76550100
H	3.04393500	5.31701100	-0.06877200
H	2.16796500	0.60545800	0.80177500
H	3.06307300	1.23644400	-1.40456600
H	4.19694800	3.40321900	-1.13792300
C	-0.83777200	2.78740300	0.49893500
O	-1.56306400	3.62779400	1.01178800
N	-1.20702700	1.51237800	0.12888700
C	-2.47126500	0.97839900	0.24902200
C	-2.56160400	-0.36581900	-0.21593100
C	-3.62543100	1.57364200	0.74144800
C	-3.78280600	-1.08341800	-0.19963000
C	-4.83411400	0.84977500	0.76673600
H	-3.57972100	2.59545000	1.10103200
C	-1.41536700	-2.14631400	-1.16669700
C	-3.75498100	-2.39885700	-0.71208000
C	-4.93458400	-0.44530400	0.31231700
H	-5.71988100	1.34642200	1.16054300
C	-2.58283400	-2.92799500	-1.19888500
H	-0.46377700	-2.52782400	-1.53763900
H	-4.67521200	-2.98340100	-0.71946800
H	-5.88084500	-0.98376300	0.33453000
H	-2.54267600	-3.93531700	-1.60560200
N	-1.40412100	-0.91536700	-0.68678300
C	1.21932200	4.22009200	0.27926200
H	0.66898300	5.04912700	0.72347000
F	0.59664500	-2.41274500	1.40778300
F	1.56297100	-3.80288000	0.06831000
F	2.58063100	-3.14511600	1.86047500

IM34

Ni	0.26630800	-0.07281500	-0.03353800
C	2.76435900	3.94016900	-0.55194800
C	0.85678800	2.64866500	0.12194900
C	1.44607500	1.45121800	-0.30405400
C	2.67778200	1.54614400	-0.94995300
C	3.32713500	2.77857800	-1.07110800
H	3.28692200	4.89152100	-0.63871100
H	3.15767800	0.67611200	-1.39160400
H	4.28964800	2.82344100	-1.58131500
C	-0.57629800	2.56426300	0.46664500
O	-1.26586800	3.49320500	0.86629700

N	-1.01315700	1.28983500	0.17703300
C	-2.33168900	0.90767800	0.20066200
C	-2.52757300	-0.47249000	-0.08212500
C	-3.45832800	1.69335300	0.42702500
C	-3.82816800	-1.03000000	-0.19232100
C	-4.74285900	1.12558400	0.34608100
H	-3.32460300	2.74349600	0.66210200
C	-1.52049100	-2.48777300	-0.59489700
C	-3.91262200	-2.39254400	-0.54728300
C	-4.94711800	-0.19999100	0.03695200
H	-5.60146500	1.77077100	0.52760800
C	-2.76554900	-3.11558300	-0.76524800
H	-0.60046800	-3.05119300	-0.73144400
H	-4.89491600	-2.85360000	-0.65352700
H	-5.94888000	-0.61985800	-0.04227200
H	-2.79934900	-4.16354700	-1.05236800
N	-1.39283000	-1.21510400	-0.25620000
C	1.50412500	3.87578800	0.02965100
H	0.97890200	4.76548700	0.37738300
C	1.20580400	-1.86146800	0.67716300
C	2.08357300	-0.84255900	0.96879400
C	3.38224800	-1.18336000	0.27850400
C	1.95168700	-2.84269100	-0.20510200
H	4.09658700	-0.36656600	0.15518000
H	0.38679800	-2.16810600	1.32732600
H	2.03415600	-0.19157700	1.83981200
H	1.34774500	-3.53847500	-0.79838600
C	2.95846500	-3.53420300	0.75114800
H	2.46536000	-3.95985800	1.63414700
H	3.47110000	-4.35556900	0.23296500
C	2.88312800	-1.90795800	-0.97761100
H	2.34419100	-1.25809900	-1.67937600
H	3.68294300	-2.44234800	-1.50806300
C	3.93610100	-2.38581000	1.09534100
H	3.98308700	-2.16651200	2.16915400
H	4.95732100	-2.61551900	0.76464800

TS34-35

Ni	0.12767800	-0.24779300	-0.28758000
C	2.87731000	3.54315400	-0.90516600
C	1.19330100	2.23752100	0.23947800
C	1.73839200	1.01751200	-0.26349400
C	2.75434800	1.15355500	-1.22003600
C	3.30956300	2.39105400	-1.54497500

H	3.33778900	4.50534000	-1.12272000
H	3.17565700	0.27757800	-1.70329100
H	4.10578500	2.43769700	-2.28654200
C	-0.23045200	2.31030500	0.71257600
O	-0.68201900	3.20706400	1.41581000
N	-0.91255800	1.30144400	0.10002400
C	-2.25561000	1.05599000	0.21649300
C	-2.60506500	-0.27504600	-0.16497900
C	-3.27525200	1.90600200	0.62407400
C	-3.95178800	-0.71511900	-0.18262200
C	-4.61066300	1.45906500	0.61517500
H	-3.02133100	2.91048800	0.94875100
C	-1.82199000	-2.35355800	-0.85729600
C	-4.18554800	-2.04368200	-0.59979600
C	-4.96262000	0.18937700	0.21458300
H	-5.38888500	2.15211200	0.93246600
C	-3.13158500	-2.85646800	-0.94294300
H	-0.95801300	-2.97611800	-1.08397800
H	-5.21045200	-2.41310900	-0.64079100
H	-6.00279200	-0.13301900	0.20237300
H	-3.28945200	-3.88305800	-1.26377200
N	-1.56704000	-1.10853500	-0.48943800
C	1.79270000	3.45792100	-0.03628200
H	1.32415900	4.34848100	0.38231000
C	1.09218100	-1.64621900	0.53698400
C	1.99461600	-0.47831900	0.74060200
C	3.36128300	-1.08012100	0.38765800
C	1.94820500	-2.79015200	0.03609400
H	4.15278600	-0.34477300	0.20989800
H	0.40396200	-1.90225200	1.35405500
H	1.95062900	0.00611200	1.72174300
H	1.40805300	-3.58640300	-0.49225800
C	2.75320300	-3.27430900	1.25923000
H	2.10696400	-3.51423700	2.11351500
H	3.32673800	-4.17988800	1.01542100
C	3.02965100	-2.05654000	-0.75152300
H	2.63797900	-1.59118700	-1.66368800
H	3.88433700	-2.69582000	-1.01326800
C	3.68827300	-2.06975200	1.52857400
H	3.53480900	-1.61780300	2.51751800
H	4.74491000	-2.36184500	1.46944600

IM35

Ni	0.10217700	-0.25913700	-0.37218800
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C	2.74034800	3.52084500	-1.10851200
C	1.22902800	2.17757100	0.22930800
C	1.85887300	0.96608200	-0.20186500
C	2.83417500	1.11702300	-1.20399800
C	3.25994100	2.36050400	-1.66196300
H	3.09807000	4.49806700	-1.42822200
H	3.33485400	0.24483400	-1.61052100
H	4.02851300	2.41069400	-2.43149500
C	-0.17190000	2.23085400	0.79151100
O	-0.56194100	3.07835000	1.58626000
N	-0.89761200	1.28977700	0.13264200
C	-2.23758400	1.04464800	0.28195200
C	-2.61304500	-0.25544800	-0.17755900
C	-3.23239200	1.87195500	0.78445900
C	-3.96416300	-0.68166300	-0.17626500
C	-4.57242200	1.43866400	0.79219600
H	-2.95488000	2.84851700	1.17043300
C	-1.87869700	-2.29387300	-1.03118900
C	-4.22859400	-1.97671500	-0.67380700
C	-4.95052400	0.20272900	0.31666900
H	-5.33181000	2.11449500	1.18352200
C	-3.19710700	-2.77572400	-1.10573000
H	-1.02979500	-2.90977800	-1.32278500
H	-5.25884000	-2.33198200	-0.70374000
H	-5.99397200	-0.10926900	0.31781500
H	-3.37792000	-3.77687800	-1.48877700
N	-1.59717400	-1.07779800	-0.59322500
C	1.70879600	3.41473900	-0.18147800
H	1.19244100	4.29678200	0.19577000
C	1.09786100	-1.61239900	0.43575900
C	2.00491200	-0.40230800	0.72057700
C	3.39098500	-1.05335200	0.51739300
C	2.00829700	-2.76066800	0.05182700
H	4.20303300	-0.32593700	0.39931000
H	0.40581000	-1.87409300	1.25163000
H	1.87959700	-0.01061800	1.73848500
H	1.52126000	-3.56595700	-0.51342100
C	2.68357300	-3.22714200	1.35658300
H	1.95306700	-3.43993500	2.14796300
H	3.26495200	-4.14519300	1.18982400
C	3.16381100	-2.04478400	-0.63678400
H	2.86242900	-1.59760100	-1.59073000
H	4.03674500	-2.69111500	-0.80510500
C	3.60498400	-2.02739800	1.69208000

H	3.37077300	-1.56122200	2.65832100
H	4.65880500	-2.33347800	1.72999700

TS19-20

S	-2.89432700	-1.07256800	-0.54524800
O	-1.44448300	-0.67931300	-1.12245000
O	-3.30023300	-2.48127100	-0.92616900
C	-3.97100300	0.08562500	-1.61669200
O	-3.06149600	-0.56608000	0.88267900
Ni	-0.29635100	-0.05822900	0.21414400
F	-5.23073700	-0.26972400	-1.50315700
F	-3.58251100	0.00299100	-2.87435100
F	-3.80868300	1.32540800	-1.18476900
C	-0.71638100	-3.03306000	0.83486000
C	-0.06592100	-1.42526700	2.51363900
C	-0.58934900	-2.23160600	3.51868300
C	-1.16278200	-3.45040800	3.17348000
C	-1.22271500	-3.85175200	1.83940100
H	-0.77679200	-3.33824600	-0.20910600
H	-0.56973100	-1.88328300	4.54972000
H	-1.58146200	-4.08914800	3.94886000
H	-1.68775500	-4.80060500	1.57955100
C	0.40879800	-0.07184000	2.83696400
O	0.40622800	0.48068900	3.90482900
N	0.85177300	0.60539800	1.60694700
H	1.78926500	0.23937100	1.29180000
C	0.90606400	2.04634200	1.57369600
C	0.28295500	2.60522900	0.44107400
C	1.55704100	2.84809400	2.47533900
C	0.34817300	3.99461500	0.19615200
C	1.59408200	4.24415900	2.25450500
H	2.03751900	2.41196300	3.34643400
C	-0.89909500	2.20708800	-1.51674200
C	-0.25586600	4.46263000	-0.99292500
C	1.01594900	4.80688300	1.14274800
H	2.10708100	4.87531600	2.97651900
C	-0.86231500	3.57563400	-1.84784300
H	-1.37836400	1.46881400	-2.15686500
H	-0.22481400	5.52729800	-1.22270700
H	1.06875200	5.88135700	0.97233300
H	-1.31966700	3.90835600	-2.77533000
N	-0.36152000	1.74832200	-0.40460700
C	-0.12431100	-1.80575100	1.15325300
S	2.65703800	-0.68717600	-1.00599500

O	1.76627200	-1.95856700	-0.67777200
O	2.07643100	0.23498900	-2.06322600
C	4.19928900	-1.51479300	-1.75630800
O	3.16266000	-0.03908800	0.30196500
H	0.85306600	-1.69489300	0.23675600
F	3.83717300	-2.16706600	-2.83626500
F	4.70706400	-2.33317500	-0.86518400
F	5.06068000	-0.56708300	-2.05505800

IM20

S	-2.74236900	1.37532900	0.19507100
O	-1.56604900	0.37069800	-0.29003000
O	-3.96749400	0.59693400	0.63039100
C	-3.19752300	2.12300100	-1.50257600
O	-2.16914400	2.51982400	1.00521800
Ni	0.12592100	0.46545900	0.57102000
F	-4.27952400	2.85402600	-1.36375700
F	-3.40896000	1.14473900	-2.35956300
F	-2.19261600	2.87365400	-1.91856300
C	-1.66074600	-0.59144800	2.72202400
C	0.57743700	0.08184000	3.24954500
C	0.37043700	-0.15003600	4.61339700
C	-0.86242900	-0.62576000	5.02380000
C	-1.86464500	-0.85166700	4.07570700
H	-2.48314900	-0.75778200	2.02715600
H	1.17785200	0.04313100	5.31877900
H	-1.05342800	-0.82556300	6.07644700
H	-2.83255100	-1.23084100	4.40221200
C	1.86071900	0.55392900	2.74827600
O	2.77811500	1.07353000	3.32846000
N	1.90387300	0.29449200	1.28649800
H	1.91505100	-0.72658300	1.12134300
C	2.87587700	0.94891900	0.44738300
C	2.36970800	1.33710600	-0.81374100
C	4.19588300	1.16005600	0.75975600
C	3.22678700	1.91789200	-1.77665100
C	5.04354700	1.77522000	-0.18949500
H	4.57872900	0.86382400	1.73116100
C	0.55092600	1.40898900	-2.24100400
C	2.65960100	2.23749900	-3.03107600
C	4.58040500	2.13768800	-1.42982900
H	6.08498900	1.94827500	0.07279700
C	1.33436000	1.97278900	-3.26736700
H	-0.50234000	1.18420400	-2.39116200

H	3.28878600	2.68515100	-3.80004900
H	5.24587600	2.59465000	-2.16132400
H	0.87493300	2.19299400	-4.22696800
N	1.04307400	1.11982600	-1.05329200
C	-0.42636400	-0.11121800	2.28556600
S	0.14026200	-2.42754000	-1.05803200
O	-1.33087200	-2.27857800	-0.32587400
O	0.14777100	-1.73996900	-2.40651400
C	0.02598400	-4.31169900	-1.33914700
O	1.28714500	-2.24177500	-0.07440100
H	-1.59348100	-1.30313000	-0.31791300
F	-0.99455600	-4.55066800	-2.12340700
F	-0.12100900	-4.88822500	-0.17385100
F	1.15027300	-4.68351700	-1.90658300

IM36

S	2.81517500	-1.45248600	0.15687300
O	2.93882800	-2.60354600	1.14469900
O	2.57571100	-1.74252500	-1.32155200
C	4.47806500	-0.52712700	0.23657500
O	1.83119300	-0.32134100	0.70519200
Ni	0.37132100	-0.05847300	-0.47970300
F	5.45467500	-1.38393800	0.02758800
F	4.60374700	0.02808600	1.42486200
F	4.48366400	0.40298800	-0.69890300
C	1.85265000	2.49186000	-0.28347200
C	-0.22212800	2.41925600	-1.48452700
C	-0.21832900	3.80943300	-1.65519100
C	0.84643800	4.53475500	-1.15125100
C	1.87393800	3.87188900	-0.46953000
H	2.64365500	2.00877200	0.28604900
H	-1.05119400	4.29024100	-2.16801200
H	0.88319000	5.61567700	-1.27297100
H	2.70302100	4.45212400	-0.06449800
C	-1.35231000	1.61482500	-1.92127100
O	-2.44449500	1.95681100	-2.29373400
N	-0.97310000	0.16600800	-1.84189600
H	-0.36939600	-0.03284800	-2.64917100
C	-2.01508200	-0.82745600	-1.71479600
C	-1.75957800	-1.81673600	-0.73620000
C	-3.17551900	-0.85865700	-2.44802400
C	-2.71633900	-2.82819500	-0.48650200
C	-4.13055900	-1.87001500	-2.19748000
H	-3.36695400	-0.09590300	-3.19618200

C	-0.33037800	-2.63129400	0.89412900
C	-2.40926800	-3.77336700	0.51954800
C	-3.91319200	-2.83011100	-1.24057700
H	-5.05037600	-1.87842100	-2.77814600
C	-1.22516400	-3.67646500	1.20443700
H	0.62105800	-2.53228400	1.41889200
H	-3.12277600	-4.56795700	0.73698800
H	-4.65517100	-3.60500400	-1.05090400
H	-0.95942700	-4.38624000	1.98289300
N	-0.58370100	-1.73932600	-0.04604600
C	0.80084400	1.73796200	-0.80336000
C	-2.51225300	2.07704700	1.00090300
C	-2.92078200	0.80493300	1.09669100
C	-2.35984700	0.24932000	2.38818800
C	-1.66941500	2.37586300	2.21921800
H	-2.32345500	-0.84429100	2.47234400
H	-2.83359700	2.81553300	0.26898900
H	-3.65376800	0.30219500	0.46562300
H	-0.99491800	3.23610600	2.13902600
C	-2.66732800	2.42995800	3.41189700
H	-3.48861900	3.13394200	3.22984000
H	-2.15157300	2.75306200	4.32625000
C	-1.02642100	1.00539300	2.47081800
H	-0.29982900	0.71814400	1.69724900
H	-0.54742100	0.92774700	3.45793400
C	-3.14558800	0.95979600	3.52767100
H	-4.23061200	0.85226900	3.40623400
H	-2.87741900	0.53074600	4.50276500

TS36-37

S	-1.59071100	-2.09179600	-0.51483200
O	-1.13041200	-3.19793000	-1.44990500
O	-1.16908500	-2.16219100	0.96189400
C	-3.48962200	-2.18019800	-0.45451100
O	-1.38386400	-0.64213400	-1.13182800
Ni	-0.01520900	0.21885100	0.01150500
F	-3.84517100	-3.33037600	0.07930700
F	-3.96365700	-2.08148300	-1.67991200
F	-3.93097800	-1.18293500	0.28425100
C	-2.47940700	1.74055800	0.56295100
C	-0.78415000	1.58799900	2.26341400
C	-1.50259000	2.44444400	3.10294900
C	-2.72582800	2.93238500	2.67102300
C	-3.20951700	2.57405300	1.40846400

H	-2.86754900	1.48034700	-0.42180400
H	-1.08961400	2.71163400	4.07530500
H	-3.31166500	3.58966000	3.31098900
H	-4.17457000	2.95873200	1.07824200
C	0.54177500	1.07342500	2.63045800
O	1.33290600	1.52938600	3.42315500
N	0.83644300	-0.08060400	1.80839300
H	0.10166900	-0.81077900	1.87615500
C	2.13882200	-0.64831800	1.66015200
C	2.39010500	-1.18226400	0.36990600
C	3.09038400	-0.74627400	2.64615800
C	3.59165800	-1.88542900	0.11655500
C	4.31139100	-1.40308400	2.37316800
H	2.89541700	-0.31600900	3.62402900
C	1.62024100	-1.53146800	-1.78850500
C	3.75020400	-2.44597400	-1.17242300
C	4.55299100	-1.97865100	1.15017600
H	5.05810400	-1.47170300	3.16139800
C	2.76450700	-2.28730300	-2.11316100
H	0.82168300	-1.37097700	-2.51256400
H	4.65670200	-3.00655000	-1.40023900
H	5.48484100	-2.50899100	0.95682500
H	2.85150700	-2.72337400	-3.10454400
N	1.44877400	-0.98194100	-0.60250100
C	-1.24895100	1.24262300	0.98260400
C	0.62628500	2.80335600	-0.65643900
C	1.60155000	2.00396800	-1.13268600
C	1.42488700	1.93283600	-2.63327900
C	-0.19970600	3.25828000	-1.83457700
H	1.91907400	1.09688100	-3.14216400
H	0.55653800	3.22436800	0.34433500
H	2.48559700	1.66864400	-0.59134600
H	-1.20025200	3.63730300	-1.60246400
C	0.71735000	4.25491700	-2.60086900
H	1.10059600	5.04779300	-1.94686700
H	0.15654600	4.73947600	-3.41107000
C	-0.10251300	2.03386500	-2.75382800
H	-0.63862900	1.15526700	-2.36950000
H	-0.43412600	2.24528300	-3.78057600
C	1.83519800	3.33861600	-3.15945300
H	2.83744400	3.62969800	-2.82148200
H	1.84291300	3.34393500	-4.25755200

IM37

S	-1.88336798	-1.83956602	-0.43174088
O	-1.50389403	-3.07707906	-1.22538083
O	-1.59121193	-1.81039395	1.07450811
C	-3.77321998	-1.67802198	-0.54985282
O	-1.45606597	-0.48733206	-1.14395596
Ni	0.02467807	0.50407794	-0.39199305
F	-4.32678998	-2.76574495	-0.05654675
F	-4.10387202	-1.53398604	-1.81691682
F	-4.14703493	-0.62260294	0.14160214
C	-2.35662288	2.17576201	-0.04757106
C	-0.92666383	1.78470608	1.86399391
C	-1.76829079	2.56393913	2.66132790
C	-2.91470079	3.12302013	2.11380491
C	-3.20966284	2.91984607	0.76518993
H	-2.58262492	2.03247196	-1.10436505
H	-1.51264275	2.70931618	3.71065689
H	-3.58204976	3.71797417	2.73456290
H	-4.11309685	3.35490807	0.33844994
C	0.31707618	1.18081508	2.42025590
O	1.10123521	1.74894210	3.15850485
N	0.52800613	-0.09193095	1.90476296
H	-0.29815389	-0.63702295	1.61195801
C	1.75285312	-0.77276798	1.85367395
C	2.06432507	-1.41065305	0.61679797
C	2.63489415	-0.85722495	2.90736293
C	3.20440705	-2.25156808	0.53831298
C	3.80958713	-1.62908098	2.79154193
H	2.39855119	-0.33162390	3.82838791
C	1.48034798	-1.88013914	-1.57615698
C	3.40953299	-2.96033114	-0.66811699
C	4.07622408	-2.34105304	1.64863196
H	4.48824516	-1.68653195	3.64011091
C	2.52998396	-2.80939717	-1.70859797
H	0.80050596	-1.68830117	-2.40591097
H	4.26516298	-3.63099416	-0.74737699
H	4.95625006	-2.97926106	1.57704096
H	2.64221492	-3.36247122	-2.63708695
N	1.27154003	-1.18104709	-0.47770201
C	-1.21420288	1.60933201	0.50241593
C	0.77250010	2.50959491	-0.83563618
C	1.78678509	1.62422590	-0.51627817
C	2.50060004	1.32226382	-1.82090717
C	0.82659606	2.73882583	-2.32618619
H	3.12871802	0.42403481	-1.83064915

H	0.35475414	3.24788395	-0.15673420
H	2.27755512	1.57348994	0.45762982
H	-0.08446795	3.13450083	-2.78620618
C	2.09532207	3.61883680	-2.50776227
H	2.08169411	4.50570383	-1.86172932
H	2.15964404	3.97127875	-3.54542129
C	1.34933701	1.39364880	-2.83514314
H	0.60530800	0.58946282	-2.75026308
H	1.70671698	1.44411974	-3.87280715
C	3.24821606	2.63896979	-2.16769026
H	3.87487209	2.98633482	-1.33696730
H	3.90634303	2.48106273	-3.03216928

TS37-38

S	-1.77435400	-1.86602100	-0.51531400
O	-1.34863200	-2.98871400	-1.44687100
O	-1.43454000	-1.99015600	0.97728200
C	-3.67468100	-1.82031700	-0.56327300
O	-1.45239700	-0.42172500	-1.06531000
Ni	0.14381300	0.51171500	-0.38193700
F	-4.14281400	-2.98449300	-0.16254100
F	-4.05922600	-1.57800200	-1.80046500
F	-4.09532300	-0.86395200	0.23812800
C	-2.17835100	2.28354700	0.15280400
C	-0.78803100	1.55350800	1.99133000
C	-1.74632700	1.98953300	2.89938600
C	-2.93449400	2.54839700	2.43703500
C	-3.15108800	2.68171000	1.06788100
H	-2.35318900	2.39262400	-0.91793900
H	-1.55960400	1.87480800	3.96690300
H	-3.69242700	2.87849700	3.14485500
H	-4.08727200	3.10435500	0.70528400
C	0.50941600	0.94170500	2.43069700
O	1.36698100	1.53027100	3.06373500
N	0.65678000	-0.33239900	1.91964300
H	-0.18674900	-0.82326600	1.58486200
C	1.86718500	-1.01218200	1.70492900
C	2.12482700	-1.47615400	0.37940200
C	2.77224500	-1.27796500	2.70685600
C	3.22635400	-2.34332300	0.15278000
C	3.91264400	-2.06640700	2.45252200
H	2.57426100	-0.88844500	3.70210400
C	1.49464400	-1.60353100	-1.85568100
C	3.38173300	-2.88219300	-1.14495400

C	4.11764700	-2.62253600	1.21469800
H	4.60992400	-2.26753000	3.26314700
C	2.50174500	-2.54413600	-2.13956200
H	0.80673000	-1.26344300	-2.62986200
H	4.20444500	-3.57164700	-1.33417700
H	4.96675200	-3.27908500	1.02784300
H	2.58003500	-2.96179700	-3.13937300
N	1.32706600	-1.06967300	-0.66060400
C	-0.99402900	1.71286100	0.60671600
C	0.71716100	2.59282000	-0.23147600
C	1.71953100	1.65802100	-0.59925000
C	1.96747900	1.87491400	-2.08186500
C	0.37454200	3.35344300	-1.49470800
H	2.46247400	1.05077700	-2.60881300
H	0.77328000	3.12504800	0.71682400
H	2.53064900	1.38115100	0.07914300
H	-0.57783800	3.89309400	-1.48003400
C	1.61762800	4.24634800	-1.74013200
H	1.89609800	4.81994500	-0.84658800
H	1.40439100	4.97061800	-2.53661000
C	0.57102800	2.28633100	-2.57711700
H	-0.17902400	1.48163300	-2.54251000
H	0.59417000	2.71337300	-3.58906100
C	2.70740200	3.23171900	-2.17153600
H	3.59698800	3.25988200	-1.52959000
H	3.03961700	3.41615900	-3.20211400

IM38

S	-2.40440500	-0.99327200	-0.56430000
O	-2.31816700	-1.92104300	-1.76623900
O	-2.12521000	-1.58115100	0.82657700
C	-4.21585200	-0.42211400	-0.48052600
O	-1.68744300	0.39259500	-0.76521900
Ni	0.23250200	0.52657300	-0.32550400
F	-4.99329900	-1.47823900	-0.35362700
F	-4.51130700	0.22668900	-1.58789300
F	-4.36777600	0.37449000	0.56233100
C	-0.65008600	3.30498400	0.35470200
C	-0.07456500	1.47129400	1.82398600
C	-1.37390000	1.49822500	2.33930200
C	-2.29110900	2.43151600	1.88317500
C	-1.93274200	3.32638600	0.87729900
H	-0.38365900	4.01065500	-0.42983500
H	-1.66231200	0.77171300	3.09820300

H	-3.29983400	2.44183300	2.29097800
H	-2.65997800	4.03993100	0.49524000
C	0.88987600	0.40317500	2.27421700
O	1.99786300	0.62664200	2.71865500
N	0.40130000	-0.87251100	2.03236900
H	-0.54237300	-0.94796300	1.62850800
C	1.26953300	-1.89055700	1.57869700
C	1.35362100	-2.14663800	0.17504100
C	2.00121700	-2.65344100	2.45686300
C	2.07725300	-3.29070600	-0.26168100
C	2.78617700	-3.73297900	2.00622700
H	1.93114000	-2.41867900	3.51654600
C	0.74103400	-1.65731700	-2.01973500
C	2.05524500	-3.60872500	-1.63810400
C	2.79549400	-4.06791800	0.67696200
H	3.35054000	-4.32210500	2.72576000
C	1.36124000	-2.81702500	-2.51400400
H	0.21514900	-0.97931700	-2.69093200
H	2.58992100	-4.49435200	-1.98124900
H	3.35368100	-4.93272000	0.31966500
H	1.29867600	-3.04780800	-3.57354500
N	0.76019000	-1.31277800	-0.74255200
C	0.32240900	2.40107400	0.81934900
C	1.78629700	2.44234800	0.35540500
C	2.05852400	1.07421000	-0.28259500
C	2.50749900	1.38688000	-1.70055800
C	2.10382300	3.40741300	-0.79718500
H	2.44983200	0.54166600	-2.39955600
H	2.41735900	2.63406000	1.23487800
H	2.70934500	0.39276100	0.27831600
H	1.69234500	4.41734700	-0.67640700
C	3.63231700	3.39746000	-0.97294700
H	4.15355900	3.55133700	-0.01913000
H	3.94224100	4.20598100	-1.64789300
C	1.66128300	2.62175200	-2.04099300
H	0.58120200	2.41423300	-2.08824100
H	1.96599100	3.10555400	-2.97968100
C	3.91592600	2.00803300	-1.59703300
H	4.58967500	1.39333200	-0.98609500
H	4.36950700	2.10109000	-2.59401500
IM40			
S	1.93909500	2.34221000	0.08529500
O	1.01112000	2.72724100	1.24634200

O	3.41506600	2.65302400	0.19509400
C	1.31716900	3.42427800	-1.41589900
O	1.70057600	0.86313100	-0.41569700
Ni	0.04282000	-0.00673200	-0.77945000
F	0.97568800	2.62760500	-2.42221000
F	2.28553800	4.22253700	-1.79830900
F	0.26661400	4.13409400	-1.04982000
C	4.00020700	-1.02026600	1.26821600
C	1.82511500	-0.67319500	2.17183800
C	2.37206100	0.15064900	3.15809000
C	3.74024400	0.36744700	3.22407100
C	4.55086100	-0.22230700	2.26560800
H	4.67295400	-1.42716700	0.51895400
H	1.70764900	0.62145800	3.88213300
H	4.16041500	1.00404500	3.99928000
H	5.62526500	-0.04789900	2.27527200
C	0.35264300	-0.79590800	2.13370800
O	-0.22952100	-1.89887300	2.11053800
N	-0.30333500	0.39482800	2.11154300
H	0.25771600	1.23702900	1.89709500
C	-1.70132200	0.53600700	1.98138500
C	-2.24424100	1.16954600	0.81970800
C	-2.54263500	0.10467600	2.98612300
C	-3.64310500	1.43447200	0.79253800
C	-3.93365600	0.31336000	2.91410000
H	-2.10129700	-0.38148400	3.85431500
C	-1.97489500	2.09982600	-1.27666800
C	-4.16420600	2.11700400	-0.33025900
C	-4.47047600	0.99167600	1.85021400
H	-4.56987800	-0.03776400	3.72334700
C	-3.32885800	2.47777500	-1.35258600
H	-1.30547700	2.30292000	-2.11167300
H	-5.23007600	2.34171300	-0.36335300
H	-5.53979400	1.19305800	1.79633600
H	-3.69082700	3.01253000	-2.22698100
N	-1.44308100	1.46290600	-0.25052300
C	2.63116900	-1.28181500	1.18599000
C	2.05500200	-2.19445500	0.10691400
C	1.01283200	-1.65161700	-0.93541900
C	1.73588800	-1.71357400	-2.29080100
C	3.11503300	-2.75630200	-0.86567100
H	1.37851900	-0.97777100	-3.02210900
H	1.56746900	-3.01938800	0.65091300
H	0.15102600	-2.34143500	-0.94815400

H	4.04428200	-3.06744500	-0.37460700
C	2.49824900	-3.89978200	-1.69580600
H	1.90210200	-4.57850300	-1.06893600
H	3.28918600	-4.50397600	-2.15919000
C	3.21218000	-1.62353300	-1.89582600
H	3.48002300	-0.65210100	-1.46353900
H	3.88888600	-1.85394600	-2.73136400
C	1.64697800	-3.16934300	-2.76476000
H	0.61013800	-3.53001500	-2.81906200
H	2.08662500	-3.28044900	-3.76715500
C	-3.09429800	-1.13928600	-3.45447800
H	-4.01319300	-1.73032000	-3.47233900
H	-2.40833900	-1.48129400	-4.23720400
H	-3.32881800	-0.08894900	-3.66934200
C	-2.41183800	-1.22431600	-2.11137500
O	-3.01774300	-1.83074600	-1.18591300
O	-1.28370200	-0.66191300	-2.03857200
Ag	-1.84016300	-1.99155300	0.60840600

TS40-41

S	-0.94475600	2.64135900	-1.62950200
O	-0.10390700	2.81038300	-0.33092600
O	-0.66128400	3.65085500	-2.72358200
C	-2.70632000	3.02676800	-1.01536200
O	-1.09384000	1.16109000	-2.04715000
Ni	-0.10919200	-0.60610500	-0.53847700
F	-3.56995600	2.88213600	-2.00279600
F	-2.77108200	4.25313100	-0.53780500
F	-3.01034900	2.16279300	-0.04507300
C	4.51254500	1.81171100	1.51238900
C	2.23722200	1.07671700	1.69828700
C	1.97950000	2.03701100	2.66959000
C	3.00592200	2.88680600	3.06838000
C	4.27250800	2.75979900	2.50303200
H	5.49882600	1.74067900	1.05428800
H	0.98421900	2.14445100	3.10032100
H	2.81755700	3.65248600	3.81853700
H	5.07549800	3.42308900	2.82022600
C	1.29337000	-0.02019600	1.30937200
O	1.38102400	-1.10359000	1.99795800
N	-0.05615100	0.45413100	0.98807200
H	-0.07132000	1.44084800	0.60607100
C	-1.19601400	0.13710000	1.80735300
C	-2.25719000	-0.45471800	1.09502200

C	-1.35441500	0.43526600	3.13623900
C	-3.52963300	-0.62818000	1.67769800
C	-2.60629500	0.20135700	3.75328300
H	-0.52938200	0.85138700	3.71064100
C	-2.94515800	-1.28416600	-0.95528900
C	-4.54746600	-1.13246500	0.83503900
C	-3.67674400	-0.28953800	3.04398300
H	-2.72273100	0.44243100	4.80761000
C	-4.26280900	-1.43411200	-0.47522100
H	-2.66540600	-1.53194900	-1.97821600
H	-5.55190300	-1.27020000	1.23429900
H	-4.64393300	-0.43141600	3.52435400
H	-5.03191700	-1.80353700	-1.14801900
N	-1.97979300	-0.83501600	-0.18323300
C	3.48000900	0.97784700	1.09545400
C	3.52995500	-0.00874700	-0.03275300
C	2.07118100	-0.41078300	-0.48234900
C	1.98253000	0.25229900	-1.89630800
C	4.11284100	0.62536700	-1.30785700
H	0.98154600	0.48705800	-2.27189300
H	4.09169000	-0.90920700	0.26387700
H	2.03926300	-1.51301600	-0.54738300
H	5.04298100	1.17396700	-1.11287200
C	4.24065500	-0.45059800	-2.39309300
H	4.71051800	-1.36608600	-2.00572000
H	4.86499800	-0.09476400	-3.22297300
C	2.92157000	1.45321400	-1.78969300
H	2.57768000	2.21459100	-1.07763600
H	3.08493800	1.93079600	-2.76519000
C	2.77450200	-0.66769900	-2.84019500
H	2.44351400	-1.71275400	-2.77992100
H	2.62068800	-0.33947400	-3.87767600
C	-0.34386900	-3.89227200	-3.16518800
H	-0.56671300	-4.94774900	-2.99060600
H	0.59545300	-3.80746900	-3.72600200
H	-1.12263800	-3.43043300	-3.78227200
C	-0.20211500	-3.14200900	-1.86505100
O	-0.17525600	-3.81485300	-0.79958500
O	-0.11506000	-1.88155300	-1.97754100
Ag	0.45729900	-2.81753700	1.02678200

IM41

S	-0.91878900	2.73496800	-1.55816100
O	-0.00114000	2.81387900	-0.31121300

O	-0.62176400	3.72067200	-2.67030300
C	-2.61082900	3.24110800	-0.84837100
O	-1.20285000	1.27215800	-1.99491900
Ni	-0.49806800	-0.58333900	-0.77584300
F	-3.53462600	3.15356600	-1.78632700
F	-2.55663200	4.47240700	-0.38279000
F	-2.91866800	2.40953500	0.14461700
C	4.90359900	1.55468900	1.10920500
C	2.62463300	0.81602800	1.47612200
C	2.45525600	1.81067100	2.43616500
C	3.51871100	2.65220400	2.74888400
C	4.74693100	2.51071400	2.10694100
H	5.84608500	1.46932700	0.56686300
H	1.49441400	1.97855100	2.91754700
H	3.38298200	3.43416400	3.49411900
H	5.57384300	3.17047000	2.36454000
C	1.67745300	-0.29142900	1.01675800
O	1.57483900	-1.31306200	1.87279900
N	0.22626000	0.29180700	0.76431400
H	0.24654900	1.29914300	0.46815600
C	-0.71350700	0.12514700	1.84773500
C	-1.99608300	-0.29063400	1.44348300
C	-0.49196900	0.30588000	3.19349200
C	-3.09403700	-0.34328100	2.33271700
C	-1.56727400	0.21431900	4.10744800
H	0.50893600	0.49295700	3.56512600
C	-3.29464900	-1.01458500	-0.35262400
C	-4.34435500	-0.70752700	1.78533200
C	-2.84743100	-0.06529700	3.69581600
H	-1.36402000	0.38266300	5.16290300
C	-4.44993600	-1.01778000	0.45021700
H	-3.31302300	-1.28145000	-1.40740900
H	-5.21892000	-0.73995700	2.43450800
H	-3.67061000	-0.10863900	4.40734900
H	-5.40350000	-1.28736200	0.00499500
N	-2.11843300	-0.68932700	0.14608700
C	3.83413300	0.72709100	0.78698600
C	3.77180100	-0.23910000	-0.35786200
C	2.28891900	-0.72135200	-0.36100800
C	1.77056800	-0.14706900	-1.69571100
C	3.92147000	0.44423700	-1.73007300
H	0.69292700	0.07207500	-1.88853600
H	4.48723300	-1.06763500	-0.24472600
H	2.23842200	-1.82106000	-0.39065900

H	4.80734100	1.08769400	-1.79993200
C	3.83877300	-0.64162700	-2.81521500
H	4.49317800	-1.49464600	-2.58936100
H	4.14488200	-0.24427600	-3.79126800
C	2.57056600	1.15089000	-1.87450900
H	2.35983200	1.90876300	-1.11034000
H	2.41006700	1.60000400	-2.86378200
C	2.33534700	-1.02779100	-2.81684100
H	2.15792100	-2.09678700	-2.62979500
H	1.85496400	-0.77707500	-3.77149000
C	-1.45258600	-3.83601700	-3.13201000
H	-1.71423300	-4.85422500	-2.83322700
H	-0.61080300	-3.87831800	-3.83495400
H	-2.28490800	-3.35592300	-3.65651800
C	-1.03595000	-3.01757100	-1.93875300
O	-0.73462300	-3.61647400	-0.88057000
O	-1.01710600	-1.75451100	-2.14321600
Ag	0.37713500	-2.78689700	0.83534500

IM42

S	6.00570000	-1.03113600	0.17496200
O	5.70944300	-0.00798400	-0.96349700
O	7.10320000	-0.63315000	1.14532100
C	6.71363800	-2.51181200	-0.79206600
O	4.70937200	-1.62732500	0.76340000
Ni	2.46145600	-0.42517900	0.75436400
F	7.03282600	-3.47614600	0.05149100
F	7.78342600	-2.14275900	-1.47168800
F	5.78944200	-2.95767000	-1.63440900
C	3.62172400	4.36504800	-0.99568000
C	2.73692200	2.26500200	-1.65958500
C	2.78593500	2.67918600	-2.99967100
C	3.30281300	3.91670800	-3.34132400
C	3.71611600	4.76620800	-2.31961200
H	3.90317400	5.07808800	-0.22496700
H	2.40178300	2.00571100	-3.76726000
H	3.36344100	4.22144800	-4.38432500
H	4.10145800	5.75767700	-2.55213400
C	2.14652100	0.91464900	-1.51663500
O	1.01278300	0.65898200	-1.88838200
N	3.01662400	-0.11878400	-1.09680200
H	4.03545600	0.14415000	-1.03345400
C	2.87673600	-1.34087900	-1.85310100
C	2.27376300	-2.43479500	-1.21127500

C	3.31386800	-1.44221900	-3.14819100
C	2.09634800	-3.65298400	-1.91045000
C	3.14206600	-2.65521400	-3.85054900
H	3.81102300	-0.59305000	-3.61721100
C	1.34792800	-3.27522100	0.71850000
C	1.47923200	-4.71045000	-1.20283000
C	2.54166900	-3.73596100	-3.25074500
H	3.49945700	-2.72996300	-4.87531300
C	1.10701100	-4.52317300	0.10378900
H	1.07098100	-3.10852800	1.75814900
H	1.31521600	-5.66477200	-1.70331700
H	2.41323900	-4.67307900	-3.79161100
H	0.62501700	-5.30892300	0.68057100
N	1.90185300	-2.26411000	0.08543300
C	3.15730300	3.09579600	-0.61443200
C	2.95341700	2.80628100	0.86494200
C	2.80149800	1.36580200	1.46456400
C	4.06015700	1.18665200	2.34943700
C	4.12864700	3.33580200	1.73105800
H	4.38992300	0.15089600	2.47321300
H	2.03166800	3.36530000	1.11885500
H	1.90403400	1.40217800	2.10201000
H	4.55278400	4.28300700	1.38253900
C	3.69275300	3.39436400	3.20627500
H	2.68312500	3.81874300	3.31585500
H	4.37522100	4.03344800	3.78228300
C	5.06944200	2.13313100	1.70161900
H	5.37042600	1.83656600	0.68644000
H	5.97618000	2.26242500	2.30769200
C	3.77340100	1.91795800	3.66653000
H	2.85003900	1.56444300	4.14629200
H	4.59654300	1.76651600	4.38022100
C	1.01540200	-1.28656900	4.61686300
H	0.15972200	-1.92108600	4.87635200
H	0.91657300	-0.35810900	5.19504400
H	1.95563600	-1.77019200	4.89515300
C	0.98515300	-0.93680500	3.14744700
O	-0.12773400	-0.66698100	2.63660300
O	2.10322200	-0.93668000	2.55468900
C	-2.72741600	-1.26442200	-0.58927700
C	-3.13704500	-0.05618700	-1.15480400
C	-2.58328000	0.38168800	-2.39386600
C	-1.53801600	-0.37722000	-2.99643300
C	-1.09420300	-1.56060700	-2.36573600

C	-1.68493000	-2.00527500	-1.20715900
H	-3.82503500	2.14818600	-2.59071500
C	-3.01308400	1.57326100	-3.03454100
C	-0.93351800	0.09891100	-4.18423500
H	-0.25889800	-2.10724700	-2.81028600
H	-1.35566500	-2.93730600	-0.74381200
C	-1.35287300	1.26720300	-4.76515500
C	-2.41277600	2.00412100	-4.18947600
H	-0.10928400	-0.47659000	-4.60812700
H	-0.87564800	1.62975400	-5.67428200
H	-2.74705900	2.92766400	-4.65964200
C	-8.29096600	0.34008500	-0.90161000
C	-7.80731300	1.15624000	0.08794100
C	-6.41377000	1.34423200	0.25553400
C	-5.50799900	0.65174800	-0.60141200
C	-7.39738500	-0.32284300	-1.77161100
H	-6.59289300	2.72908000	1.90527800
H	-9.36441200	0.20717800	-1.02617000
H	-8.48667400	1.68568700	0.75644300
C	-5.89726400	2.21359200	1.24252600
C	-4.10257100	0.81290000	-0.41465700
H	-7.78753300	-0.96124600	-2.56255400
C	-3.63762100	1.74706400	0.50545400
C	-4.54861100	2.43266600	1.34560600
H	-4.16395000	3.13208300	2.08798500
P	-3.54744400	-1.82051800	0.99809900
P	-1.83017600	2.14892200	0.56146800
C	-6.04233400	-0.17466800	-1.62261800
H	-5.35783100	-0.68877800	-2.29584000
C	-1.69675800	3.50346900	-0.67884700
C	-0.55508100	3.55145700	-1.47950400
C	-2.70359000	4.45981100	-0.85388900
C	-0.41162400	4.55024900	-2.43822700
H	0.20765200	2.77946300	-1.38278800
C	-2.56032700	5.45320600	-1.81503400
H	-3.60787600	4.42055100	-0.24453300
C	-1.41306500	5.50014600	-2.60578200
H	0.48266000	4.56891200	-3.06024200
H	-3.34677000	6.19449600	-1.94914900
H	-1.30483300	6.27934000	-3.35906800
C	-1.60314200	2.97080900	2.19523100
C	-1.54018600	2.13685600	3.31946400
C	-1.43881100	4.34889400	2.34956500
C	-1.32857800	2.68207000	4.57990400

H	-1.62881500	1.05517800	3.20349100
C	-1.21396700	4.88705400	3.61441900
H	-1.47610300	5.00404500	1.47952600
C	-1.16166500	4.05739800	4.72911000
H	-1.28569600	2.02815200	5.44951800
H	-1.07986900	5.96183000	3.72631900
H	-0.98580400	4.48208900	5.71614000
C	-2.61434400	-3.36739500	1.46673500
C	-1.78861800	-3.26114600	2.59148800
C	-2.77204300	-4.62365500	0.86934800
C	-1.12615200	-4.37725400	3.09843200
H	-1.66580200	-2.28848200	3.06676200
C	-2.12120200	-5.74103300	1.38161600
H	-3.43500200	-4.74081100	0.01279200
C	-1.29764900	-5.62140900	2.49959800
H	-0.49177200	-4.27818300	3.97933600
H	-2.26871200	-6.71380100	0.91381500
H	-0.80139800	-6.50008100	2.91036700
Ag	-0.21560500	0.19161600	0.47992700
C	-5.10109300	-2.57108500	0.29932500
C	-6.25121600	-2.47770000	1.08599300
C	-5.18331700	-3.21643300	-0.93992100
C	-7.45418000	-3.02980900	0.65594700
H	-6.20057400	-1.95375200	2.04184200
C	-6.38173000	-3.77681200	-1.36760100
H	-4.30440300	-3.26389700	-1.58635800
C	-7.51941700	-3.68592800	-0.56873900
H	-8.34342500	-2.94473300	1.27877200
H	-6.43096600	-4.28060600	-2.33233400
H	-8.45928100	-4.11990000	-0.90708900

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S	-6.19922100	1.07464300	0.26147500
O	-5.90974300	0.12753800	-0.93780800
O	-7.35349100	0.66671800	1.15758500
C	-6.75118300	2.66791300	-0.62118900
O	-4.90364900	1.55173300	0.96153500
Ni	-2.70851300	0.53011300	0.76956800
F	-7.03370900	3.59820500	0.27132800
F	-7.81084800	2.42952700	-1.37060600
F	-5.75280500	3.08780100	-1.39071000
C	-3.35684500	-4.48226200	-1.69233200
C	-2.82834900	-2.14394000	-1.76003800
C	-2.92197400	-2.14360100	-3.15046300

C	-3.27718800	-3.31494700	-3.80848100
C	-3.50067800	-4.48163100	-3.07544100
H	-3.50371900	-5.40425200	-1.12953200
H	-2.69384400	-1.23628900	-3.71138800
H	-3.37473100	-3.32464500	-4.89282600
H	-3.77945300	-5.39965300	-3.59077500
C	-2.31012700	-0.95477000	-1.00689100
O	-1.07803500	-0.69853200	-1.15249300
N	-3.21016300	0.21366100	-0.99498900
H	-4.23321000	-0.02319000	-1.01002700
C	-2.92960000	1.35636800	-1.80949700
C	-2.29656800	2.43004100	-1.15765300
C	-3.30394700	1.47329400	-3.12444200
C	-1.96783700	3.60920800	-1.86497500
C	-2.99362600	2.65399600	-3.83632100
H	-3.86004300	0.66678500	-3.59976400
C	-1.42162200	3.24275800	0.82084600
C	-1.28962400	4.61995900	-1.14455300
C	-2.32906800	3.69365900	-3.23043600
H	-3.29355900	2.73608600	-4.87885100
C	-1.01101700	4.43452500	0.18608500
H	-1.21861900	3.07748500	1.87706900
H	-0.99752600	5.53638400	-1.65700500
H	-2.08763100	4.59940400	-3.78555500
H	-0.47590100	5.18123800	0.76843200
N	-2.03870800	2.27590400	0.17462100
C	-3.01795500	-3.30284500	-1.02871100
C	-2.78589900	-3.16529600	0.44512100
C	-2.72422500	-1.65909400	0.88494700
C	-3.98186500	-1.55243200	1.80874500
C	-3.95074300	-3.72940500	1.27649800
H	-4.40708100	-0.55471500	1.95899500
H	-1.83549300	-3.66679800	0.70701700
H	-1.78166400	-1.50144000	1.44030900
H	-4.30297300	-4.69998800	0.90398100
C	-3.54685900	-3.73491700	2.75551500
H	-2.54881100	-4.17237900	2.90438300
H	-4.25415300	-4.32754700	3.35075900
C	-4.94511400	-2.57174600	1.20128300
H	-5.26410100	-2.31937200	0.18069100
H	-5.84011000	-2.71333100	1.82166100
C	-3.60540400	-2.23542800	3.13459800
H	-2.65868900	-1.85710600	3.54269200
H	-4.38515700	-2.04061700	3.88441400

C	-1.37538500	0.84086100	4.74758800
H	-0.52108500	1.38545300	5.16381900
H	-1.33790200	-0.18374200	5.14172900
H	-2.31966900	1.29272000	5.06420000
C	-1.27781500	0.77018000	3.24293800
O	-0.13504300	0.72058600	2.73042800
O	-2.38129900	0.74768700	2.62109700
C	2.82651500	1.21847500	-0.59651700
C	3.19798700	-0.00418400	-1.15459000
C	2.53597500	-0.49974300	-2.31594400
C	1.39994600	0.19900900	-2.81911700
C	1.00246300	1.40137500	-2.19406000
C	1.70799600	1.91473300	-1.13016000
H	3.81895600	-2.22368000	-2.59968900
C	2.93815200	-1.69639400	-2.96425800
C	0.66884500	-0.35013400	-3.89913900
H	0.11542700	1.91408400	-2.57107100
H	1.39501500	2.85543700	-0.67094900
C	1.06745000	-1.52171300	-4.48814300
C	2.22743100	-2.18723100	-4.02921000
H	-0.22501500	0.17763400	-4.23637700
H	0.49294500	-1.94494000	-5.31071000
H	2.54688900	-3.10850400	-4.51330400
C	8.35630200	-0.41112700	-1.07850700
C	7.90650900	-1.18164300	-0.03707200
C	6.51932800	-1.36250300	0.18489600
C	5.58884700	-0.70761200	-0.67511400
C	7.43573300	0.21453100	-1.94853800
H	6.74609700	-2.66526800	1.89471700
H	9.42526400	-0.28472100	-1.24274100
H	8.60936800	-1.67802500	0.63259200
C	6.03076300	-2.17887900	1.23085900
C	4.19287900	-0.85185500	-0.43128800
H	7.80017600	0.81966300	-2.77683900
C	3.74941800	-1.72797500	0.55509900
C	4.68412200	-2.37908800	1.39487600
H	4.32064300	-3.03200700	2.18917000
P	3.78910200	1.82125500	0.89064800
P	1.92792000	-2.03762400	0.71289900
C	6.08650300	0.07640600	-1.74717300
H	5.37633400	0.56934600	-2.41070000
C	1.68507400	-3.44301600	-0.45725700
C	0.51500800	-3.46889100	-1.21823100
C	2.63854600	-4.45570000	-0.61981800

C	0.29223200	-4.50308900	-2.12491000
H	-0.19793500	-2.64486700	-1.14215100
C	2.41390900	-5.48390300	-1.52720600
H	3.56519100	-4.43438800	-0.04396000
C	1.23912000	-5.50959100	-2.27796000
H	-0.62202600	-4.50452100	-2.71921100
H	3.15999400	-6.26755400	-1.65218400
H	1.06946600	-6.31535500	-2.99107600
C	1.70711800	-2.78203200	2.38564800
C	1.64590400	-1.89516800	3.46899300
C	1.51073900	-4.14689300	2.60767400
C	1.41211200	-2.37187600	4.75325100
H	1.75471100	-0.82188100	3.30161900
C	1.26498400	-4.61855000	3.89499700
H	1.54166800	-4.84497800	1.77154500
C	1.21779900	-3.73464800	4.96772400
H	1.37154600	-1.67358000	5.58810300
H	1.10794600	-5.68379600	4.05760100
H	1.02292800	-4.10675200	5.97224900
C	2.79316900	3.27950400	1.47625500
C	1.86451200	3.00251300	2.48622800
C	2.97924300	4.60943400	1.08446000
C	1.13017300	4.02357800	3.08166700
H	1.70572700	1.97651800	2.81887100
C	2.25968400	5.63418700	1.69424900
H	3.71291800	4.85382100	0.31681200
C	1.33580000	5.34587900	2.69633800
H	0.41238100	3.78185600	3.86649500
H	2.43264400	6.66661400	1.39251800
H	0.78776500	6.15153400	3.18376100
Ag	0.32460000	-0.01104100	0.59430700
C	5.21281700	2.65082000	0.03222800
C	6.46278200	2.56000700	0.64879700
C	5.10482400	3.33805400	-1.18233100
C	7.58241500	3.15232000	0.07225300
H	6.56057100	1.99351000	1.57636800
C	6.22080000	3.93834500	-1.75516000
H	4.13834100	3.39428000	-1.68787900
C	7.46148200	3.84647300	-1.12666100
H	8.55349900	3.06286800	0.55710300
H	6.12493100	4.47371900	-2.69892200
H	8.33620600	4.31194800	-1.57880100

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S	5.53932300	-1.01993900	1.74622800
O	6.36485400	-0.47396400	0.58681600
O	5.85806700	-0.57533700	3.16073100
C	5.84336900	-2.90173000	1.71522200
O	3.97245400	-0.96207900	1.51117600
Ni	3.09136700	-1.59863900	-0.04151300
F	5.11752300	-3.46577200	2.66071200
F	7.12238200	-3.13743400	1.92777700
F	5.49108000	-3.38129900	0.53389800
C	4.19128900	4.61779700	-2.13874800
C	2.74523600	2.70246400	-1.96728800
C	2.89472800	2.40132500	-3.32023600
C	3.71425300	3.22209800	-4.08037400
C	4.35790500	4.31642700	-3.48855800
H	4.69420500	5.47772000	-1.69616700
H	2.38726500	1.53689400	-3.74844400
H	3.86883600	3.01085400	-5.13767200
H	5.00113500	4.94752100	-4.10086900
C	1.95492300	1.98514400	-0.97212500
O	1.24438500	1.00724700	-1.20562700
N	4.07686000	-0.56939300	-1.21663100
H	5.00919700	-0.25081800	-0.95185600
C	3.82748000	-0.82110500	-2.51377100
C	2.70970900	-1.68358300	-2.73303000
C	4.48747700	-0.34968100	-3.65473200
C	2.23843900	-2.02648500	-4.02164800
C	4.00474900	-0.67084700	-4.93311200
H	5.36391000	0.28766400	-3.54317900
C	1.19702800	-3.08859900	-1.66082800
C	1.17432400	-2.95838000	-4.06658000
C	2.89630400	-1.47225000	-5.14324800
H	4.53610200	-0.26967500	-5.79689100
C	0.66849700	-3.49120500	-2.90261000
H	0.82798900	-3.48386700	-0.71456600
H	0.77907900	-3.26656000	-5.03523600
H	2.56010600	-1.72533900	-6.14735200
H	-0.13880200	-4.22219100	-2.91346100
N	2.18138600	-2.20708900	-1.59318500
C	3.36740500	3.80262100	-1.37017300
C	3.00324600	3.92704800	0.08443600
C	2.09450100	2.69552100	0.35645000
C	2.86902100	1.90825400	1.43315700
C	4.16418000	3.71770300	1.07758700
H	2.58137300	0.85372700	1.50433900

H	2.48885000	4.88392700	0.26864400
H	1.08892900	2.95987700	0.72027300
H	5.05673500	4.30922400	0.83529200
C	3.60807000	3.95154200	2.49190400
H	3.03159400	4.88560100	2.55780900
H	4.42720300	4.02338800	3.21897000
C	4.32784200	2.19431100	1.05963500
H	4.63260800	1.78170600	0.08907500
H	5.03096800	1.83299100	1.82350200
C	2.74055500	2.68830200	2.74608800
H	1.69523100	2.92343500	2.99395700
H	3.14868300	2.08459200	3.56763500
C	1.88394200	-2.89489300	3.48239500
H	1.06707600	-2.77010200	4.20077500
H	2.77751800	-2.39295000	3.88163600
H	2.13724300	-3.95221200	3.35212500
C	1.56970900	-2.23721300	2.16384300
O	0.80412200	-1.24592900	2.17280100
O	2.12927500	-2.74123200	1.13714000
C	-2.84713500	-1.01613000	-0.74195800
C	-3.43974000	0.23710500	-0.87435800
C	-3.10643800	1.07639400	-1.97734800
C	-2.04515700	0.69439600	-2.85199900
C	-1.37902400	-0.52960900	-2.62221300
C	-1.79749600	-1.37773900	-1.62383000
H	-4.58432800	2.60456000	-1.55378900
C	-3.77833100	2.30264700	-2.22203000
C	-1.68103900	1.55415500	-3.91756300
H	-0.52945100	-0.80216100	-3.25264000
H	-1.30548000	-2.34190000	-1.50125000
C	-2.36025400	2.72541400	-4.13514200
C	-3.42567700	3.09608600	-3.28323600
H	-0.85678200	1.25486700	-4.56583100
H	-2.08169400	3.37322300	-4.96478000
H	-3.95649100	4.03026000	-3.46014300
C	-8.49100500	0.24197300	0.36279200
C	-7.83713000	0.77354900	1.44431000
C	-6.43487000	0.97318100	1.41741000
C	-5.70287900	0.59576100	0.25304700
C	-7.77019000	-0.10926900	-0.80065800
H	-6.30805200	1.82049900	3.40119500
H	-9.56944500	0.09572000	0.39411200
H	-8.38607200	1.05869000	2.34219400
C	-5.74332400	1.54345900	2.51044900

C	-4.28922700	0.76371000	0.23473100
H	-8.29624200	-0.52758100	-1.65731800
C	-3.65333700	1.38856000	1.30218200
C	-4.39157900	1.76646800	2.44866400
H	-3.87406700	2.22803800	3.28991400
P	-3.37910100	-2.10791500	0.68159100
P	-1.84005400	1.76194500	1.15035900
C	-6.41128400	0.06299300	-0.85347100
H	-5.85571100	-0.21066900	-1.74944600
C	-1.89345700	3.38441300	0.25957700
C	-1.01352200	3.60709700	-0.80070100
C	-2.80299000	4.38962600	0.60958500
C	-0.99648900	4.82968600	-1.46547200
H	-0.36187200	2.80191700	-1.13314200
C	-2.79920400	5.60434600	-0.06619800
H	-3.52443800	4.21878800	1.41010200
C	-1.88590700	5.83173300	-1.09430700
H	-0.29376500	4.98390600	-2.28399400
H	-3.50992100	6.38045900	0.21359100
H	-1.87990700	6.78851500	-1.61428000
C	-1.33012100	2.19586000	2.87038300
C	-1.07769200	1.11678300	3.72755100
C	-1.11908800	3.49752400	3.33121000
C	-0.63863100	1.33889700	5.02671100
H	-1.20515500	0.09398400	3.36754500
C	-0.67258100	3.71520000	4.63280400
H	-1.29226200	4.34762000	2.67227400
C	-0.43431100	2.63961500	5.48110800
H	-0.43769400	0.49112800	5.67907000
H	-0.50480900	4.73316900	4.98101500
H	-0.07649400	2.81292700	6.49453300
C	-2.30438400	-3.60789100	0.44067800
C	-1.22543900	-3.74081200	1.32119700
C	-2.51227200	-4.60255100	-0.52199100
C	-0.36075300	-4.82994500	1.22854200
H	-1.05555200	-2.97438000	2.08059700
C	-1.65171200	-5.69124600	-0.61317300
H	-3.36289700	-4.53896500	-1.19930100
C	-0.57169600	-5.80510600	0.25993700
H	0.48469300	-4.91208900	1.90850500
H	-1.82964400	-6.46000100	-1.36444800
H	0.10141100	-6.65801800	0.19004400
Ag	-0.08135100	-0.04718600	0.46817500
C	-5.00873800	-2.71461400	0.01952400

C	-6.02385300	-2.94905400	0.94994100
C	-5.27101500	-2.94505200	-1.33606500
C	-7.26728600	-3.42236100	0.54113800
H	-5.83815400	-2.74122100	2.00482900
C	-6.50907800	-3.42617600	-1.74577900
H	-4.50324100	-2.73117200	-2.08199000
C	-7.50887500	-3.66826900	-0.80631500
H	-8.05022400	-3.59392500	1.27836000
H	-6.69742000	-3.60822900	-2.80323500
H	-8.48014400	-4.04127400	-1.12836400

TS26-27

S	3.25819300	-0.72852200	-0.95829300
O	1.73971800	-0.21358900	-1.15006900
O	4.26516200	0.26938300	-1.49110000
C	3.26383100	-2.17451500	-2.21077700
O	3.43474200	-1.36968500	0.41193900
Ni	0.76212300	-0.19438300	0.45227700
F	4.50493100	-2.54787100	-2.42148800
F	2.70629400	-1.77208900	-3.33573800
F	2.56860100	-3.17659300	-1.70220000
C	2.95986600	1.88934100	0.82538200
C	1.79102800	0.90396700	2.69383000
C	2.86396300	1.17148200	3.53779800
C	3.98525400	1.80435800	3.01326600
C	4.03425800	2.15984700	1.66357800
H	2.99676000	2.17669500	-0.22558200
H	2.81714000	0.86375600	4.58081700
H	4.83523100	2.01924000	3.65844800
H	4.92366900	2.64172000	1.26219100
C	0.64342800	0.13103500	3.18551400
O	0.46416100	-0.27360100	4.30278500
N	-0.27045300	-0.21827600	2.07427200
H	-0.96296700	0.52782500	1.83217100
C	-0.99838400	-1.46995300	2.18467000
C	-0.96612600	-2.24195100	1.00958500
C	-1.75409700	-1.87181300	3.25621800
C	-1.71287000	-3.43576100	0.90991100
C	-2.46941600	-3.08834300	3.17749000
H	-1.79905300	-1.26377900	4.15425700
C	-0.26583900	-2.38145800	-1.19913500
C	-1.69897100	-4.10033700	-0.33450200
C	-2.45567900	-3.85243500	2.03714700
H	-3.05699100	-3.40509900	4.03610700

C	-0.99542000	-3.56788500	-1.38703700
H	0.30966800	-1.92628100	-2.00275800
H	-2.26870800	-5.02137400	-0.45224100
H	-3.03259600	-4.77421600	1.97803100
H	-0.99082200	-4.04259000	-2.36396300
N	-0.23001600	-1.75992600	-0.03478000
C	1.81290100	1.25630500	1.32684700
S	-3.09761800	0.06812800	-0.38724300
O	-2.36279600	0.92838800	0.66784900
O	-2.31034800	0.06526600	-1.74538700
C	-4.61500500	1.13472900	-0.80007600
O	-3.61651500	-1.29221600	0.04623100
H	0.78270000	1.89998300	0.88759900
F	-4.18464500	2.30138200	-1.23670400
F	-5.33365800	1.29393600	0.29058000
F	-5.32456600	0.53342700	-1.73052800
C	0.96235100	5.15579100	0.09862400
H	1.18942200	5.70714700	-0.81748400
H	1.86387300	5.09480200	0.72391500
H	0.20367800	5.68367600	0.68695000
C	0.49933100	3.75682500	-0.19529700
O	0.07679300	3.07105100	0.79798300
O	0.58698700	3.31702300	-1.36719700
Ag	-0.64209900	1.50837500	-1.54612400

TSW-44

S	-1.51755800	2.64007900	0.72025200
O	-1.55834800	1.58197800	-0.46670400
O	-2.74871300	3.44274400	1.03898300
C	-0.09788800	3.91111700	0.26028900
O	-0.90831700	1.69757600	1.85136500
S	2.29325100	1.00152400	-1.19813300
O	2.91888700	2.16038900	-1.93440200
C	3.67964700	-0.27569400	-0.92714300
O	1.68668000	1.18648200	0.19639400
Ni	-0.65281900	0.26613200	0.59077400
C	-5.25330000	-1.67223100	-1.63586600
C	-2.89487800	-1.45558000	-1.15904600
C	-3.16954200	-1.55703200	0.20790500
C	-4.47705800	-1.71239700	0.64942200
C	-5.51954700	-1.76369200	-0.27125900
H	-6.06895800	-1.71281300	-2.35516600
H	-2.35877200	-1.51552500	0.93394100
H	-4.68298500	-1.78821000	1.71530400

H	-6.54516300	-1.87500800	0.07660200
C	-1.52480700	-1.30627000	-1.70373300
O	-1.27028500	-1.42783300	-2.88059200
N	-0.44625600	-1.02613300	-0.77761300
C	0.20309600	-2.18222700	-0.27462000
C	0.58150200	-2.09546600	1.08123300
C	0.54464100	-3.31039600	-0.98840200
C	1.31632100	-3.11563700	1.72298100
C	1.26844100	-4.34372700	-0.35248600
H	0.27990800	-3.38550300	-2.04145500
C	0.53606000	-0.76670500	2.99073200
C	1.64695300	-2.89812900	3.08005700
C	1.65542800	-4.26055300	0.96505100
H	1.53512300	-5.22383100	-0.93449800
C	1.26223900	-1.73668000	3.70777600
H	0.22252100	0.17602800	3.43645800
H	2.21149300	-3.65940600	3.61793800
H	2.21829300	-5.06492800	1.43584800
H	1.51242500	-1.54828300	4.74818400
N	0.20267900	-0.95713800	1.72900600
C	-3.94727200	-1.52608200	-2.07845800
H	-3.71281300	-1.45454100	-3.13848900
F	4.57763000	0.24157600	-0.11653300
F	4.22173100	-0.57681000	-2.08391600
F	3.14479800	-1.35519400	-0.37902500
F	0.48071000	3.51511600	-0.83711600
F	-0.68473500	5.07017400	0.09086300
F	0.73040700	3.95030900	1.26955900
O	1.30148800	0.15672500	-2.13821100
H	0.49558500	-0.36916200	-1.52575100

IM44

S	-2.55896000	1.16702500	0.98265900
O	-2.05164100	0.28389400	-0.22922000
O	-4.01254400	1.13910800	1.36938200
C	-2.11898200	3.01406400	0.50882800
O	-1.48018800	0.72544800	2.06781500
S	1.31508800	1.85655700	-1.37485800
O	0.97289600	3.06448900	-2.20382700
C	3.22329600	1.71298800	-1.35937700
O	0.88309400	1.67604800	0.07208400
Ni	-0.59513200	-0.44937000	0.82442300
C	-4.21212000	-2.34869600	-2.13411600
C	-1.98581400	-2.41979000	-1.21469600

C	-2.52043000	-2.66054700	0.05359800
C	-3.89624600	-2.73024700	0.22887700
C	-4.74230800	-2.55494700	-0.86308900
H	-4.87621100	-2.22300300	-2.98737400
H	-1.85220000	-2.79553900	0.90510500
H	-4.31142400	-2.91388300	1.21815400
H	-5.82152500	-2.58736100	-0.72352400
C	-0.52119200	-2.30380800	-1.43463300
O	0.02922400	-2.78248500	-2.41439400
N	0.17698400	-1.58601300	-0.45745700
C	1.49818200	-1.92419300	-0.13197500
C	1.85555200	-1.52466600	1.17954000
C	2.45064800	-2.57850800	-0.89377600
C	3.13057400	-1.77880100	1.73147100
C	3.72619400	-2.83874600	-0.34454700
H	2.20617400	-2.88316400	-1.90573300
C	1.11676700	-0.45219800	3.11413200
C	3.35141600	-1.33099600	3.05296800
C	4.07684600	-2.45743400	0.92926000
H	4.45430200	-3.35749900	-0.96579100
C	2.35544500	-0.67724100	3.74044300
H	0.30520600	0.08252600	3.60469200
H	4.32161800	-1.50766300	3.51721200
H	5.06783400	-2.66456200	1.32998400
H	2.50848900	-0.32150000	4.75565700
N	0.88603000	-0.87428800	1.88477300
C	-2.83573500	-2.29847500	-2.31351100
H	-2.39967100	-2.14099400	-3.29854500
F	3.68828600	2.75129800	-0.70214800
F	3.65576400	1.70955700	-2.59568600
F	3.54608100	0.59790000	-0.74392400
F	-1.60065200	3.00857200	-0.68933800
F	-3.24158600	3.68953700	0.53038500
F	-1.27988600	3.47696300	1.39801200
O	0.94780900	0.48615000	-2.22884000
H	0.58815400	-0.19241600	-1.58578200

IM45

S	-2.15673800	-1.48066500	-0.38546500
O	-1.75194000	-0.04095900	0.11896800
O	-3.40155100	-1.69013800	-1.20141100
C	-2.34356700	-2.52893800	1.20716700
O	-0.75392000	-1.94414600	-0.97319300
Ni	0.12809400	-0.33803700	-0.35410400

C	-3.17484200	3.67437100	0.12897700
C	-0.97646800	2.68772300	0.01217500
C	-1.16644300	2.43797500	-1.34846000
C	-2.35839700	2.79748200	-1.96518700
C	-3.36820400	3.40407800	-1.22393900
H	-3.96131400	4.15892200	0.70530400
H	-0.36933700	1.96605800	-1.92374900
H	-2.50117800	2.60475500	-3.02722400
H	-4.30677500	3.67577900	-1.70471500
C	0.30212700	2.36700000	0.70395100
O	0.75552600	3.12347200	1.55413400
N	0.94800900	1.21541200	0.29096200
C	2.31177400	1.04376600	0.48485800
C	2.80662900	-0.14011200	-0.11906700
C	3.24080900	1.86949000	1.10665500
C	4.17768200	-0.48567000	-0.14122600
C	4.60939300	1.52678000	1.09185800
H	2.90352400	2.77296600	1.60093600
C	2.19963700	-2.06223500	-1.30018200
C	4.51732800	-1.68882200	-0.79684700
C	5.09129900	0.38799200	0.48857100
H	5.30660600	2.20241500	1.58514700
C	3.54177000	-2.46895400	-1.37491400
H	1.38727100	-2.65009700	-1.72343800
H	5.56367400	-1.99142000	-0.83676000
H	6.15260500	0.14554200	0.49303900
H	3.78719600	-3.39726900	-1.88361800
N	1.86247800	-0.93647000	-0.69349600
C	-1.97672100	3.33251000	0.74038000
H	-1.79669200	3.55251700	1.79115500
F	-1.27470300	-2.34361300	1.94640200
F	-3.42211100	-2.13049300	1.83682900
F	-2.44824900	-3.78695200	0.84648100

IM46

S	-1.27239500	-2.13037000	0.50348100
O	-0.34577200	-1.90329800	1.69149000
O	-2.76749800	-2.27836300	0.67483900
C	-0.69055400	-3.76461100	-0.29580000
O	-0.85197500	-1.13787700	-0.70334000
S	-2.73232900	1.77237400	0.04081700
O	-1.75595700	0.81307100	0.90063800
O	-3.18769600	2.94074100	0.89733900
C	-4.26008600	0.65842600	-0.22755800

O	-2.12425800	2.01821800	-1.33997800
Ni	-0.21926900	0.48424800	-0.09120700
F	-5.19579700	1.41509300	-0.76795800
F	-4.65244100	0.20676900	0.93677700
F	-3.93137800	-0.30995500	-1.04116300
F	0.58423500	-3.65919400	-0.61833200
F	-0.85088400	-4.73182800	0.58384900
F	-1.41468500	-3.99872100	-1.36744400
C	4.53029000	-2.76767000	0.87587600
C	2.78044100	-1.39368400	-0.06045100
C	2.54535500	-0.83125400	1.19744300
C	3.30301500	-1.23728200	2.28697900
C	4.29974500	-2.19518200	2.12534300
H	5.30140100	-3.52564500	0.75408700
H	1.73364300	-0.12088700	1.34640600
H	3.10181900	-0.81658800	3.26958400
H	4.89308000	-2.50802700	2.98285800
C	2.01789500	-1.04479700	-1.26886900
O	1.95905400	-1.70716800	-2.27199700
N	1.32552900	0.26272800	-1.27874900
H	0.84124000	0.27469700	-2.18569400
C	2.19081800	1.41835200	-1.14028100
C	1.75336900	2.38813300	-0.22143700
C	3.35701000	1.59859100	-1.84013900
C	2.50847400	3.56237500	-0.00760600
C	4.11759100	2.77062200	-1.63381600
H	3.69053800	0.84296700	-2.55088100
C	0.14873300	3.00413700	1.33799000
C	2.00558600	4.48165800	0.94272400
C	3.70552900	3.73191300	-0.74205600
H	5.03991700	2.90733700	-2.19331500
C	0.83965600	4.20268000	1.60956200
H	-0.78547100	2.75191700	1.83774600
H	2.55383000	5.40311700	1.13617300
H	4.29565600	4.63374900	-0.58553600
H	0.42776100	4.88980700	2.34305600
N	0.59348200	2.13164600	0.45099300
C	3.76638000	-2.37678200	-0.21187000
H	3.91453100	-2.81988500	-1.19485900

TS46-47

S	0.66925600	-2.20855000	-0.68177100
O	-0.28262800	-1.76175900	-1.78729500
O	2.08652300	-2.63995200	-0.98495800

C	-0.14125500	-3.74135100	0.11123200
O	0.52315100	-1.22020000	0.58502100
S	3.13231200	1.12235700	0.10455400
O	1.95553600	0.53602000	-0.83328800
O	3.91561400	2.17339000	-0.66357300
C	4.29416000	-0.38062600	0.30255600
O	2.58112600	1.42766100	1.49498800
Ni	0.34081500	0.56152100	0.08623500
F	5.36419800	0.04370700	0.94844800
F	4.62381900	-0.81517600	-0.88830400
F	3.67909400	-1.29918400	1.00104700
F	-1.37882300	-3.44137400	0.46562500
F	-0.15785800	-4.71347500	-0.77793700
F	0.55633600	-4.10142500	1.16493200
C	-4.87155900	-2.44575100	-0.20232200
C	-3.04610300	-0.95678300	0.28994100
C	-3.02459400	-0.51688600	-1.04015800
C	-3.92747400	-1.04816600	-1.94673300
C	-4.84992900	-2.00356800	-1.52584500
H	-5.59175000	-3.19794800	0.11142300
H	-2.26966500	0.19775600	-1.36321200
H	-3.90226900	-0.73165400	-2.98643200
H	-5.55751300	-2.41847200	-2.24173600
C	-2.09125800	-0.44523900	1.23645700
O	-1.79887200	-0.95257700	2.35346400
N	-1.30644800	0.70352500	1.12151700
H	-1.07141600	0.09170100	2.33065500
C	-1.92737000	1.95908000	0.87790600
C	-1.17962800	2.84866200	0.08043900
C	-3.13934400	2.36274400	1.39082000
C	-1.64930600	4.15334800	-0.18828800
C	-3.61991900	3.66193000	1.12024500
H	-3.72412200	1.68554600	2.01295700
C	0.73071500	3.15156300	-1.20188300
C	-0.83477900	4.96867100	-1.00773800
C	-2.89489200	4.54420700	0.35523800
H	-4.57894000	3.96498400	1.53462400
C	0.34177300	4.47122900	-1.50807500
H	1.65796900	2.72598000	-1.58315900
H	-1.15470400	5.98499500	-1.23579500
H	-3.26932000	5.54674700	0.15391300
H	0.98856700	5.07326400	-2.13998300
N	-0.00717400	2.37204200	-0.43039000
C	-3.96544000	-1.93048100	0.70766800

H	-3.94670200	-2.26916400	1.74183400
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IM47

S	1.79843900	-2.12284200	-0.81243700
O	1.31560200	-1.72182100	-2.19428700
O	3.25836800	-2.19021900	-0.43384200
C	1.12352800	-3.89713400	-0.53476200
O	0.89540400	-1.35998800	0.32242600
S	2.68428800	1.71586600	0.49268100
O	2.08637200	0.77106300	-0.67683400
O	3.29593600	2.96845500	-0.10743800
C	4.13278200	0.66167800	1.15299700
O	1.67684300	1.81336400	1.63641000
Ni	0.32042100	0.33894500	-0.26143700
F	4.77106900	1.39423300	2.04573500
F	4.92795500	0.36430900	0.15533900
F	3.63971600	-0.41196500	1.71575900
F	-0.10751700	-3.95245000	-1.00348200
F	1.89487000	-4.74504300	-1.17538700
F	1.12571900	-4.16015800	0.75703100
C	-5.60851600	-2.26573300	1.34418100
C	-3.63326000	-1.23238000	0.42737300
C	-4.39188900	-0.70430900	-0.62127200
C	-5.75399600	-0.96020600	-0.68211700
C	-6.36470100	-1.72987500	0.30627900
H	-6.08369200	-2.87627000	2.10914600
H	-3.90835400	-0.10797300	-1.39366200
H	-6.34242500	-0.56183100	-1.50596500
H	-7.43518100	-1.92117600	0.25983800
C	-2.17068200	-1.02866700	0.47536700
O	-1.51791700	-2.13114800	0.70220300
N	-1.53991100	0.10448800	0.27939000
H	-0.52336800	-1.95605300	0.68068500
C	-2.17556900	1.36645400	0.32916800
C	-1.47730000	2.37661500	-0.37055500
C	-3.31552800	1.72225600	1.02209400
C	-1.98959800	3.68640200	-0.49436300
C	-3.81393400	3.03907900	0.93831100
H	-3.84413200	0.99168800	1.62854600
C	0.41079300	2.88843400	-1.63055500
C	-1.23852200	4.59669500	-1.27368500
C	-3.19107100	4.00050400	0.17984400
H	-4.71840100	3.28683700	1.48991300
C	-0.06262000	4.19534000	-1.85495900

H	1.36914200	2.54497000	-2.01336500
H	-1.60454900	5.61545500	-1.39767800
H	-3.59418400	5.00948900	0.10926800
H	0.53521900	4.87330900	-2.45702700
N	-0.27509200	2.02329400	-0.90455700
C	-4.23971400	-2.03280600	1.39784700
H	-3.63283000	-2.46382400	2.19161400

TS19-21

S	-2.85313800	-1.38344400	0.47813300
O	-1.72274400	-0.43536200	1.11267600
O	-2.88702000	-2.75361800	1.12802300
C	-4.43620700	-0.49249500	1.05710700
O	-2.84228000	-1.25487200	-1.04925300
Ni	-0.47694200	-0.18101200	-0.28978600
F	-5.47519600	-1.16292100	0.60876400
F	-4.44461600	-0.45205300	2.37026900
F	-4.44043400	0.73123900	0.56273800
C	-2.05893700	2.41510600	-0.15113100
C	-0.62396200	1.99977700	-2.04373700
C	-1.24623000	2.99685700	-2.77997300
C	-2.30386600	3.69080200	-2.19300300
C	-2.70945900	3.40030800	-0.89157400
H	-2.35034100	2.21105200	0.87691100
H	-0.91728500	3.21552500	-3.79469000
H	-2.81382900	4.47113100	-2.75488900
H	-3.53496800	3.95486100	-0.44900500
C	0.47081600	1.18716800	-2.60445100
O	1.28702500	1.49385700	-3.42633400
N	0.38847800	-0.17293900	-2.02268100
H	-0.43569500	-0.61631900	-2.45937800
C	1.50659000	-1.09381100	-2.01921800
C	1.46855900	-1.98230100	-0.92409300
C	2.52675100	-1.15090900	-2.93174700
C	2.48238300	-2.94669700	-0.75392900
C	3.54594200	-2.11580700	-2.76033000
H	2.56126500	-0.45091000	-3.76030200
C	0.42855700	-2.57641500	1.07032600
C	2.41130300	-3.75393900	0.40213700
C	3.52620600	-2.99519100	-1.70750900
H	4.35998000	-2.14905700	-3.48069000
C	1.39571200	-3.56944400	1.30692400
H	-0.37749200	-2.37957300	1.77376100
H	3.18173700	-4.50530300	0.57304600

H	4.32279100	-3.72668100	-1.57827200
H	1.33068400	-4.16226500	2.21450900
N	0.45776600	-1.82691700	-0.01764300
C	-1.00695500	1.69485000	-0.71926500
S	2.12697600	0.88500200	1.29017100
O	1.40583200	1.90476400	0.30382400
O	3.05514800	-0.07507500	0.55454700
C	3.27435400	2.07896300	2.23038000
O	1.16187500	0.32120400	2.32771100
H	0.06495200	1.62098800	0.00615800
F	4.09552900	2.64558000	1.37199600
F	2.54144400	2.99067800	2.83363900
F	3.95498800	1.38423700	3.11984100

TS19-24

S	1.12934100	2.60196400	1.09592800
O	0.15836300	1.68046700	1.95745900
O	2.15134100	3.45290900	1.79752500
C	-0.05914200	3.78234200	0.15535400
O	1.58351600	1.53863700	0.01253100
Ni	0.30676300	0.23019000	0.71357200
F	0.67861200	4.56082800	-0.60040000
F	-0.71011400	4.47960500	1.05405400
F	-0.87234400	3.05787400	-0.56628100
C	-1.46048600	-3.15191700	3.30383900
C	-0.55427700	-2.29955900	1.25962900
C	-0.94941900	-0.99369400	1.60343100
C	-1.57218600	-0.78154800	2.83879400
C	-1.83629700	-1.85975700	3.67676200
H	-1.66754600	-3.98637900	3.97133800
H	-1.87496800	0.22922800	3.11099200
H	-2.33411200	-1.69766000	4.63114500
C	0.25081700	-2.46452800	0.04098400
O	0.70069700	-3.48084700	-0.40775400
N	0.48732900	-1.14938300	-0.60463900
H	-0.33793000	-0.91663900	-1.20634400
C	1.68341700	-1.05339200	-1.38368500
C	2.91997300	-1.21088700	-0.70472400
C	1.63549500	-0.74701300	-2.71942900
C	4.11809200	-1.07255100	-1.45160400
C	2.83488400	-0.61402200	-3.45134700
H	0.67029500	-0.60157900	-3.20384700
C	4.05165800	-1.58164600	1.24419800
C	5.33293000	-1.22419500	-0.74640000

C	4.04949300	-0.77952400	-2.83519700
H	2.78513600	-0.37749400	-4.51177700
C	5.30442500	-1.47845500	0.60020000
H	4.01086500	-1.77288300	2.31794700
H	6.27667300	-1.12833900	-1.28351900
H	4.97780400	-0.67758200	-3.39686800
H	6.22015500	-1.59369200	1.17497400
N	2.89726300	-1.45899500	0.62809700
C	-0.80783200	-3.37963000	2.09644100
H	-0.46672600	-4.37211500	1.80737300
S	-2.83439900	0.42564500	-1.30275600
O	-2.48918000	0.65953900	0.22740800
O	-3.61853900	1.55565100	-1.92585600
C	-3.98787600	-1.08387400	-1.17799700
O	-1.62043600	-0.14355700	-2.06413900
H	-1.57589400	-0.19658500	0.76155900
F	-4.34563300	-1.46010800	-2.38481700
F	-5.04224600	-0.77491200	-0.45902800
F	-3.30076800	-2.04950700	-0.58584300

TS19-25

S	2.96725100	-0.29323800	-0.96823500
O	2.31367100	-1.52876000	-1.70886400
O	3.87879800	0.59066600	-1.77612900
C	3.97888200	-1.11676600	0.42977400
O	1.79274500	0.35625700	-0.14494900
S	-0.70895400	2.96053500	-0.33746400
O	-0.08814600	1.83199800	-1.28401500
O	-1.01929000	4.20095200	-1.14665600
C	0.77824600	3.40445600	0.77839700
O	-1.73945500	2.40040700	0.64009700
Ni	0.00424400	0.03321200	-0.74240400
F	0.48189000	4.50620800	1.43899300
F	1.84668500	3.58465900	0.03992000
F	0.97472700	2.41597600	1.63601300
F	3.23816600	-2.08182600	0.91906300
F	5.08515000	-1.59357900	-0.09044600
F	4.23907700	-0.21108600	1.33843800
C	-0.98248100	-4.51916500	0.29150900
C	-0.14140700	-2.33538200	0.84522900
C	0.02468500	-2.01804000	-0.52004000
C	-0.36907700	-2.98681700	-1.46010300
C	-0.87197700	-4.22082800	-1.06418500
H	-1.36294500	-5.48939300	0.60642100

H	1.16980300	-1.65251500	-1.07058500
H	-0.21625500	-2.77917600	-2.52123100
H	-1.16105200	-4.95863200	-1.81056800
C	0.05773100	-1.25135300	1.85704200
O	0.90057900	-1.24837600	2.72496500
N	-0.81912400	-0.18563000	1.63801400
H	-0.63758600	0.62634300	2.22648600
C	-2.19922400	-0.38868700	1.32116300
C	-2.68300700	-0.33000000	-0.01539100
C	-3.09734800	-0.58175800	2.34518400
C	-4.07937300	-0.44843800	-0.25519800
C	-4.48070300	-0.71401900	2.10839000
H	-2.71555300	-0.61619500	3.36469600
C	-2.29102700	-0.01593300	-2.29832300
C	-4.54095300	-0.34180100	-1.58484400
C	-4.96470400	-0.64678300	0.82978100
H	-5.15612300	-0.86060400	2.94806400
C	-3.65613700	-0.11624900	-2.60709000
H	-1.54757400	0.18073100	-3.06883000
H	-5.60999600	-0.42758300	-1.77704400
H	-6.03090900	-0.73432400	0.62527200
H	-3.98237900	-0.00822400	-3.63729800
N	-1.83378600	-0.14058300	-1.06620200
C	-0.61662800	-3.57605700	1.24948500
H	-0.72611400	-3.79022100	2.31234000

TS19-22

S	1.56454600	2.29644000	-0.02753100
O	1.56121600	2.03990000	1.48533900
O	2.80842200	2.78953300	-0.73384100
C	0.26365700	3.66906800	-0.25855100
O	0.85924300	1.08317900	-0.79686400
Ni	-0.32832000	0.11919000	0.30653200
F	-0.84614000	3.30589900	0.36121200
F	0.03340600	3.82948400	-1.54182300
F	0.72592900	4.78304800	0.26891000
C	-2.42430500	-0.61693000	4.41353300
C	-0.68277400	-1.02675500	2.82010500
C	-1.49358100	-0.58011600	1.75809300
C	-2.77825100	-0.11927100	2.07092400
C	-3.23475200	-0.13505500	3.38700400
H	-2.79330900	-0.62871000	5.43711900
H	-3.43458200	0.23115600	1.27608200
H	-4.23453400	0.23018000	3.61531100

C	0.70815000	-1.36306600	2.51103900
O	1.48654900	-1.99098800	3.17198900
N	1.11423100	-0.76192400	1.21195700
H	1.77729700	0.01878600	1.41532700
C	1.74794300	-1.67077300	0.29377500
C	3.01566600	-1.30139900	-0.22524700
C	1.12193900	-2.82286900	-0.11588400
C	3.62508000	-2.14535400	-1.18939400
C	1.74586100	-3.66313100	-1.06045800
H	0.13726900	-3.08213300	0.27362700
C	4.71662000	0.22213800	-0.30869100
C	4.87148600	-1.72080300	-1.70569700
C	2.96912700	-3.33250200	-1.58957300
H	1.23753500	-4.57088900	-1.37669300
C	5.41515900	-0.53926100	-1.27372200
H	5.11482500	1.17736500	0.03539300
H	5.37645000	-2.33602100	-2.45045000
H	3.44522000	-3.97339000	-2.33116600
H	6.36379600	-0.17713300	-1.66258600
N	3.56916800	-0.14820600	0.20985600
C	-1.13882500	-1.06633000	4.13350600
H	-0.47038700	-1.41623500	4.91859500
S	-2.19190400	-0.78311300	-1.58496300
O	-2.24435400	-1.87763200	-0.43053600
O	-1.79891500	0.57176100	-0.87936600
C	-4.03494200	-0.49705700	-1.99001800
O	-1.49237000	-1.18878800	-2.85523700
H	-1.68945300	-1.28569000	0.59430300
F	-4.52305300	-1.61876500	-2.45967000
F	-4.10694800	0.45979100	-2.88066400
F	-4.64998500	-0.15121800	-0.88095400

TS19-23

S	-0.52322900	-2.50878100	0.11093800
O	-1.11020700	-1.69405400	1.26025700
O	-1.31027600	-3.62433300	-0.54809000
C	1.04020700	-3.37614700	0.81057500
O	0.08850400	-1.51909800	-0.99100600
Ni	0.23073500	0.26636300	-0.41156800
F	1.60810500	-2.60917600	1.71439100
F	1.86942400	-3.61382800	-0.18054000
F	0.65302500	-4.50884600	1.36256200
C	-0.38042400	4.73973400	0.93117500
C	-0.71549600	2.90973000	-0.57370600

C	0.38660000	2.21532900	-0.04172400
C	1.05810500	2.80176000	1.03998300
C	0.67520500	4.04919900	1.52484400
H	-0.66666900	5.72049400	1.30693500
H	1.90674900	2.28323100	1.48185300
H	1.20515300	4.49139500	2.36655000
C	-1.59050500	2.19353400	-1.50807000
O	-2.42185500	2.63668400	-2.24670800
N	-1.33271100	0.70737000	-1.46442200
H	-1.04397700	0.42381900	-2.40789500
C	-2.51092400	-0.07149900	-1.14174200
C	-3.26007500	0.30334500	0.00190100
C	-2.84435400	-1.18419200	-1.86763500
C	-4.35108900	-0.51222700	0.39824400
C	-3.93411900	-1.98741200	-1.46779900
H	-2.23466200	-1.48636700	-2.71791400
C	-3.57513200	1.75737500	1.73884300
C	-5.05574600	-0.11260800	1.55409300
C	-4.67150900	-1.66362400	-0.35968700
H	-4.16060300	-2.88463700	-2.03784700
C	-4.66996900	1.01729200	2.23133600
H	-3.25097400	2.66666000	2.25063700
H	-5.89858600	-0.71368200	1.89525800
H	-5.50270000	-2.29166000	-0.04122700
H	-5.19077900	1.34642600	3.12723900
N	-2.89563200	1.42072200	0.66612500
C	-1.08730600	4.16886200	-0.12246300
H	-1.95609600	4.65692300	-0.56172900
S	3.01801200	0.15326500	-0.69082300
O	2.60657700	1.53885900	-1.34924700
O	1.92438300	-0.12294200	0.41655000
C	4.54352000	0.59829800	0.36936200
O	3.42708900	-0.95525300	-1.62302500
H	1.41569300	1.80795200	-0.83382300
F	5.53610400	0.85571500	-0.44635100
F	4.81693800	-0.42894700	1.13433100
F	4.25230300	1.65547100	1.09416900

TS38-39

S	-4.21332400	1.31304800	0.95809900
O	-3.94621100	2.42006200	1.96966500
O	-4.42981600	1.66528000	-0.50802800
C	-5.83839900	0.49863700	1.53038100
O	-3.21310400	0.08821700	1.14417500

Ni	-1.70297800	0.16918000	-0.06004100
F	-6.14015400	-0.49806800	0.71771800
F	-6.79417200	1.40466200	1.49743600
F	-5.68489600	0.04684300	2.75815400
C	-2.99826800	-3.13743200	-0.20954600
C	-1.88362500	-1.37377800	-1.42505200
C	-3.12698400	-0.91625400	-1.90881300
C	-4.29578700	-1.56531800	-1.53271900
C	-4.22176100	-2.67650300	-0.70041300
H	-2.97548700	-3.98785700	0.47012800
H	-3.17703200	-0.04037600	-2.55430200
H	-5.25808100	-1.17924300	-1.86003600
H	-5.13936800	-3.17931400	-0.39781500
C	-0.55767400	-0.81100400	-1.89577100
O	0.18707500	-1.31901100	-2.71664600
N	-0.63873100	0.68791200	-1.75864600
H	-0.94635600	1.08438900	-2.65299200
C	0.48996200	1.40413300	-1.26053800
C	0.39724200	1.86555900	0.07440600
C	1.60544000	1.70050100	-2.00653000
C	1.42750100	2.65846900	0.62994100
C	2.64651100	2.47645800	-1.45030400
H	1.67529600	1.32289500	-3.02516500
C	-0.84654000	1.94792300	2.04639000
C	1.25213000	3.11052300	1.95882300
C	2.55980400	2.95429900	-0.16600900
H	3.52263200	2.69927200	-2.05561600
C	0.11996100	2.77253400	2.65585200
H	-1.75401200	1.64242500	2.56450300
H	2.02514600	3.72972200	2.41364800
H	3.35662300	3.56341300	0.25910100
H	-0.04550300	3.11612700	3.67305100
N	-0.70354200	1.51103400	0.80907000
C	-1.82171200	-2.49353900	-0.55822100
C	-0.44031700	-2.79456500	-0.03537000
C	0.31294000	-1.44757700	0.00438300
C	0.60290100	-1.25353800	1.49815500
C	-0.40433900	-3.25875600	1.43155900
H	0.83121500	-0.22750700	1.81144900
H	0.03923100	-3.53285700	-0.69832300
H	1.23655700	-1.41035900	-0.58521700
H	-1.12018900	-4.05562700	1.67111300
C	1.05008600	-3.61894100	1.76658400
H	1.49429100	-4.27919600	1.00922700

H	1.10519200	-4.14508000	2.72893000
C	-0.57781700	-1.93794300	2.19333200
H	-1.54792500	-1.44818100	2.02943600
H	-0.42262800	-2.05625500	3.27543400
C	1.74411400	-2.23607900	1.84203600
H	2.59288100	-2.14209500	1.15211100
H	2.12315300	-2.03704300	2.85582000

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S	-0.58298400	3.74782500	-1.55098600
O	0.57457700	4.75276000	-2.25740400
O	0.21748900	2.56514300	-1.02996300
C	-0.89031500	5.06730000	-0.14245400
O	-1.74432700	3.67365500	-2.50643400
Ni	-2.47169100	-0.90393900	0.33403500
C	-2.35902500	-1.39811000	-4.35888700
C	-2.12537800	-2.12506700	-2.08302500
C	-2.23199100	-0.80401400	-1.59557400
C	-2.36711900	0.22031800	-2.54539700
C	-2.40953000	-0.07875700	-3.91085500
H	-2.41943900	-1.61776900	-5.42431900
H	-0.56327200	-5.16681900	-1.86644100
H	-2.43332200	1.26342500	-2.23834900
H	-2.49713000	0.73829400	-4.62819500
C	-1.90633600	-3.17402800	-1.06260700
O	-1.95365300	-4.39076800	-1.31181500
N	-1.70960600	-2.61526400	0.15775300
C	-1.63866800	-3.34273700	1.33060100
C	-1.97392500	-2.58632500	2.49021000
C	-1.27828400	-4.67238000	1.50103200
C	-1.90658400	-3.14376700	3.79061300
C	-1.24271000	-5.23197500	2.79410000
H	-1.02307100	-5.27137800	0.63460000
C	-2.61765300	-0.51372100	3.30472000
C	-2.19610600	-2.28010900	4.87149400
C	-1.53375100	-4.50137600	3.92430900
H	-0.95892700	-6.27938900	2.89319000
C	-2.53255800	-0.96961400	4.63451200
H	-2.91657100	0.50629500	3.06656200
H	-2.14024100	-2.66825700	5.88891400
H	-1.48534800	-4.94880500	4.91646000
H	-2.74985800	-0.28365700	5.44931800
N	-2.35403300	-1.29409700	2.27562200
C	-2.22896200	-2.43276700	-3.43542800

H	-2.18804700	-3.47883400	-3.74240700
F	-1.88210200	4.77667300	0.65372500
F	-1.14714100	6.19049900	-0.77763100
F	0.23294100	5.14748700	0.52754400
C	1.29452200	-4.90356400	-1.63557700
O	0.28501200	-5.59545100	-2.16103000
O	1.15204700	-3.92705700	-0.92888600
Ag	-0.05803000	-0.18170700	-0.70126100
C	2.30604600	0.11060900	1.67567600
C	3.16674200	-0.73987000	0.98937700
C	3.11471800	-2.15227600	1.19157800
C	2.14236800	-2.69018800	2.08155400
C	1.25332800	-1.80744100	2.73246400
C	1.33389300	-0.45163600	2.54205200
H	4.78053100	-2.65121200	-0.11067800
C	4.03562700	-3.04381000	0.58138300
C	2.11799100	-4.08310300	2.33079800
H	0.52237900	-2.22186700	3.42780200
H	0.65699300	0.20584000	3.08532300
C	3.03751100	-4.91378600	1.74594000
C	4.00759300	-4.38437800	0.86762600
H	1.35711600	-4.47231900	3.00834700
H	3.02469100	-5.98233200	1.95710800
H	4.73949100	-5.04898600	0.40972200
C	8.16477700	0.36855300	1.52886000
C	7.87496800	0.63989400	0.21605600
C	6.57090500	0.43388200	-0.29279200
C	5.54771700	-0.04943300	0.57138900
C	7.15973300	-0.13149600	2.38400900
H	7.04812300	1.02766700	-2.31773200
H	9.17047300	0.53083800	1.91331800
H	8.64287000	1.01603000	-0.46047400
C	6.25847400	0.68354200	-1.64913600
C	4.21589400	-0.21459300	0.07071300
H	7.39255300	-0.34426000	3.42616500
C	3.94115100	0.05381400	-1.26202100
C	4.98966100	0.48931000	-2.12016200
H	4.77683000	0.68096000	-3.17053500
P	2.52345400	1.96074300	1.44692800
P	2.23345400	-0.17081600	-1.94536200
C	5.88609500	-0.33799300	1.91770400
H	5.11631500	-0.71757600	2.58707000
C	2.41110200	-1.61448200	-3.09521000
C	1.23543500	-2.22437300	-3.54016600

C	3.63751900	-2.08095000	-3.57770500
C	1.27520700	-3.23526000	-4.49433100
H	0.27171700	-1.92564800	-3.12598800
C	3.67802100	-3.10304700	-4.52102300
H	4.57177900	-1.65412900	-3.21672600
C	2.49851700	-3.67230400	-4.99248400
H	0.34477100	-3.69657600	-4.82289000
H	4.64011200	-3.45660300	-4.88936700
H	2.53480000	-4.46969600	-5.73322600
C	2.09857100	1.22763400	-3.16957000
C	2.84531200	2.40557600	-3.06165400
C	1.14300000	1.13059500	-4.18513200
C	2.69368800	3.42738800	-3.99871500
H	3.55303700	2.53356000	-2.24348300
C	0.96135400	2.16912100	-5.09347800
H	0.51984600	0.23903900	-4.27099500
C	1.74691200	3.31402100	-5.01590600
H	3.30804400	4.32436400	-3.92147600
H	0.20168600	2.07650500	-5.86764500
H	1.61490100	4.12074900	-5.73410100
C	1.12269100	2.63309000	2.46388000
C	1.32318700	3.54295400	3.50709400
C	-0.19195700	2.32909300	2.08813600
C	0.23993800	4.11035500	4.17292900
H	2.33455900	3.81561400	3.80574800
C	-1.27169800	2.88158200	2.76587700
H	-0.40065200	1.67666700	1.23811700
C	-1.06098000	3.77479500	3.81265200
H	0.41811700	4.81935800	4.98063300
H	-2.27727900	2.63614700	2.42265900
H	-1.90670200	4.22035000	4.33493100
C	3.95366100	2.23592800	2.60612900
C	5.02062300	3.01230300	2.15007700
C	4.00988000	1.70024900	3.89819200
C	6.12443800	3.25162700	2.96484500
H	4.98981300	3.41625200	1.13632900
C	5.10554000	1.94500300	4.71644500
H	3.18293800	1.08744000	4.26127100
C	6.16580100	2.72080100	4.24894800
H	6.95565500	3.84871600	2.59248400
H	5.13659500	1.52814100	5.72242900
H	7.02631700	2.90991800	4.88939600
C	2.62310900	-5.49677700	-2.00960300
H	2.55769500	-6.03992600	-2.95741100

H	2.92966900	-6.20201600	-1.22632500
H	3.37472300	-4.70357000	-2.07489700
C	-5.65208200	4.45208700	-1.63870900
C	-4.60151800	2.44378600	-0.79869700
C	-5.52599100	1.67691400	-1.51476100
C	-6.50199900	2.29356200	-2.28719100
C	-6.57380600	3.68283500	-2.34234300
H	-5.69770100	5.53898300	-1.68782500
H	-5.46535100	0.58910500	-1.47770800
H	-7.20858300	1.68602200	-2.85056500
H	-7.34406700	4.16652200	-2.94152600
C	-3.47565400	1.78453100	-0.05362900
O	-2.34837000	2.29326400	-0.09231900
N	-3.68776300	0.58510900	0.54512400
H	1.27529300	4.14710600	-2.58804200
C	-4.92538200	0.29338600	1.10675200
C	-5.44524300	-1.04115600	1.03881300
C	-5.66752100	1.23551900	1.80807200
C	-6.69904700	-1.35310400	1.63553100
C	-6.91613100	0.92389700	2.37516900
H	-5.26939300	2.24575300	1.90788500
C	-5.13970400	-3.21317800	0.33225100
C	-7.14054800	-2.69350000	1.53513800
C	-7.43642000	-0.34501600	2.29647200
H	-7.46520300	1.70665700	2.89692100
C	-6.36999200	-3.62546000	0.88936900
H	-4.49289000	-3.93174700	-0.17938600
H	-8.09638500	-2.96762300	1.98345300
H	-8.39785300	-0.59314900	2.74542100
H	-6.68501000	-4.66315400	0.80438000
N	-4.70257600	-1.97610000	0.39733800
C	-4.66116600	3.83448100	-0.88484500
H	-3.92180100	4.42901600	-0.35428500

IM18

S	0.14415800	-4.09745800	1.78561300
O	1.14948800	-4.82740300	2.67650800
O	0.76622600	-2.89134100	1.00293200
C	-0.12687700	-5.33922600	0.35762600
O	-1.23939100	-3.81137300	2.36535400
Ni	-2.75706700	0.95716700	-0.27797000
C	-1.72414700	1.60937400	4.26490300
C	-2.10314100	2.31923100	2.00127800
C	-2.38574300	1.00299400	1.62248700

C	-2.33926000	-0.02064300	2.56586700
C	-1.97721400	0.29413800	3.88340400
H	-1.44864000	1.83110800	5.29424700
H	-1.01321500	5.73558900	1.73256900
H	-2.54400400	-1.06267900	2.32732000
H	-1.87292900	-0.51819300	4.60302600
C	-2.03305400	3.31523400	0.91101100
O	-2.08863700	4.54224100	1.06915900
N	-1.95166700	2.66291100	-0.27852100
C	-1.77638900	3.23140600	-1.53306400
C	-2.01930300	2.33569900	-2.61055500
C	-1.34186700	4.51407500	-1.83032000
C	-1.75578800	2.70320300	-3.95317500
C	-1.11424400	4.88608700	-3.16967000
H	-1.12725100	5.19993700	-1.01914800
C	-2.64604500	0.18683800	-3.22156200
C	-1.94470400	1.70578100	-4.93839900
C	-1.29824600	4.01354300	-4.21843900
H	-0.76420800	5.89808000	-3.36935900
C	-2.37151700	0.45106600	-4.57715400
H	-2.98024800	-0.79988600	-2.89998800
H	-1.73412200	1.94650800	-5.98035200
H	-1.09563200	4.31239000	-5.24606400
H	-2.49170700	-0.34501900	-5.30737400
N	-2.48609900	1.09828900	-2.28539100
C	-1.81088500	2.63171000	3.32592000
H	-1.61748600	3.67268600	3.58959600
F	-1.08283400	-4.90286400	-0.45405800
F	-0.48784100	-6.51000200	0.85251000
F	0.99236900	-5.46564500	-0.32750300
C	0.64091800	6.41839700	1.11709400
O	-0.31070000	6.36173800	2.05738500
O	0.58436900	5.82680200	0.06430500
Ag	-0.07135800	-0.74052600	0.98425000
C	2.24357900	-0.02478100	-1.65010100
C	3.10083300	0.62086500	-0.76075800
C	3.15160100	2.05199000	-0.73304400
C	2.27660000	2.80010500	-1.57804000
C	1.33966500	2.10929100	-2.38113500
C	1.33051200	0.73964200	-2.42058300
H	4.75877400	2.21813400	0.71208100
C	4.08590600	2.76896100	0.05736900
C	2.39751700	4.20712800	-1.63882100
H	0.66237700	2.68688400	-3.01364600

H	0.63905700	0.21394000	-3.08155100
C	3.33095500	4.86395100	-0.88164600
C	4.16908500	4.13790200	-0.01040200
H	1.70689200	4.75549400	-2.27976100
H	3.41318200	5.94884800	-0.93730800
H	4.90498800	4.66336000	0.59900700
C	7.92166200	-1.17019300	-1.24765800
C	7.46842200	-1.66355400	-0.05129100
C	6.18378300	-1.32003900	0.43503000
C	5.33933300	-0.48194500	-0.35199900
C	7.10829400	-0.30298800	-2.00683400
H	6.37873200	-2.39535700	2.30237600
H	8.91311400	-1.43854100	-1.60945100
H	8.09559400	-2.31967600	0.55417300
C	5.72872300	-1.76191800	1.69703500
C	4.02535400	-0.16856700	0.11447200
H	7.47370100	0.09471800	-2.95239600
C	3.64168300	-0.57286300	1.38767400
C	4.50464200	-1.37412300	2.17339200
H	4.18347000	-1.69211800	3.16504200
P	2.41370000	-1.87829300	-1.87367500
P	2.05453300	0.07380600	2.07309900
C	5.84974800	0.02802200	-1.57436900
H	5.22694400	0.69181500	-2.17072900
C	2.51669500	1.78128900	2.56778300
C	1.58987900	2.81563500	2.46413100
C	3.73826500	2.00591400	3.21170000
C	1.86520400	4.04915900	3.05366300
H	0.64880600	2.66419900	1.92836800
C	4.03078700	3.24882300	3.75439900
H	4.46186300	1.19341700	3.29613500
C	3.08361400	4.26817200	3.68777000
H	1.12573200	4.84684500	3.01353900
H	4.98616100	3.41546800	4.24993000
H	3.29175200	5.23848400	4.13849500
C	1.80578300	-0.69363300	3.73445900
C	1.74373800	-2.08529000	3.85662600
C	1.49103200	0.10519000	4.84075100
C	1.35634100	-2.66994700	5.05742800
H	1.98651300	-2.73443200	3.01559300
C	1.11063100	-0.48543300	6.04186100
H	1.53633600	1.19180900	4.76458900
C	1.03486100	-1.87190200	6.15029000
H	1.29577900	-3.75522300	5.10999800

H	0.87069800	0.14469200	6.89672000
H	0.72463100	-2.32906200	7.08883000
C	0.89760000	-2.22944700	-2.90306200
C	0.85457800	-2.28827800	-4.30041500
C	-0.26653500	-2.52705300	-2.18870900
C	-0.32408000	-2.62109400	-4.96278300
H	1.75203900	-2.08681400	-4.88415500
C	-1.44798300	-2.85107900	-2.84963000
H	-0.26149900	-2.53706500	-1.09986500
C	-1.48200400	-2.90601200	-4.24056100
H	-0.33305200	-2.67086600	-6.05192400
H	-2.33423600	-3.09000800	-2.25662100
H	-2.39876000	-3.18077400	-4.76100200
C	3.73673600	-1.90188700	-3.18751400
C	4.63235300	-2.97280200	-3.13079900
C	3.89751400	-0.94144700	-4.19173700
C	5.65977500	-3.09131000	-4.06378000
H	4.53299900	-3.70742400	-2.33167600
C	4.92015900	-1.05971900	-5.12774500
H	3.22117500	-0.08457000	-4.23380900
C	5.80041700	-2.13775300	-5.06604000
H	6.35541200	-3.92694600	-4.00061800
H	5.03162700	-0.30555000	-5.90744200
H	6.60162600	-2.22763200	-5.79841000
C	1.78592500	7.30967500	1.50045200
H	1.85894300	7.44573600	2.58472600
H	1.64767000	8.29672300	1.04198700
H	2.70556500	6.86593900	1.10471700
C	-4.82214700	-5.03194700	1.41343100
C	-4.20899400	-2.77508900	0.83146800
C	-5.26880700	-2.29417300	1.60851000
C	-6.10125500	-3.18062200	2.27955500
C	-5.88852000	-4.55218200	2.16780400
H	-4.63735500	-6.10317300	1.34761200
H	-5.42479400	-1.21953300	1.70184000
H	-6.91436500	-2.79998000	2.89322700
H	-6.54543400	-5.24762200	2.68750200
C	-3.26378300	-1.82421600	0.17430400
O	-2.05374300	-2.07081900	0.20576400
N	-3.74548200	-0.65070700	-0.34030100
C	-5.02563100	-0.47884200	-0.85576900
C	-5.52005500	0.85721000	-0.86082200
C	-5.82175900	-1.46285300	-1.42257500
C	-6.82586500	1.15760700	-1.32108400

C	-7.11852900	-1.16259300	-1.88204400
H	-5.45315600	-2.48498800	-1.48971400
C	-5.05244500	3.08393200	-0.41853500
C	-7.22118400	2.51458300	-1.27278700
C	-7.63158200	0.11343500	-1.82425400
H	-7.71992500	-1.96875500	-2.29565300
C	-6.34712600	3.47182800	-0.81978600
H	-4.32339900	3.82312100	-0.08316900
H	-8.22262600	2.78711300	-1.60716700
H	-8.63387400	0.33705500	-2.18655500
H	-6.62786800	4.52094500	-0.77603000
N	-4.66416500	1.82622300	-0.43665600
C	-3.97021400	-4.14798000	0.76128300
H	-3.11691800	-4.53196700	0.20920700
H	-1.54068400	0.16236600	-0.19969200