

Supporting Information

Highly Active Nickel Catalysts for Enantioselective Reductive Alkenylation of N-Sulfonyl Aldimines

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DFT calculations

Computational methods

DFT calculations were performed using the Gaussian 16 software package.¹ All computations were conducted at the Shenzhen Bay Laboratory Supercomputing Center. The geometries of the intermediates and transition states were optimized using the M06-L functional with a mixed basis set: SDD for nickel and 6-31G(d,p) for other atoms.² Harmonic vibrational frequencies were calculated at the same level as the optimization to confirm the local minima or transition states of the optimized structures. For insertion of neutral complex (bisoxazoline **L7**)Ni(cyclohexenyl) to (*E*)-*N*-benzenesulfonyl benzylimine, higher-level single-point electronic energies for the optimized structures were calculated at the M06-L/Def2TZVP level in 1,4-dioxane solvent using the SMD solvation model at 298 K.^{2a, 3} Three-dimensional visualizations of key transition states and intermediates were generated using CYLview (version 1.0).⁴ Gibbs free energies were employed for the discussion, and possible isomers of the intermediates and transition states were carefully considered. Cartesian coordinates and energies of all computed structures are provided in the “**Energies and Optimized Structures**” section.

Computational details

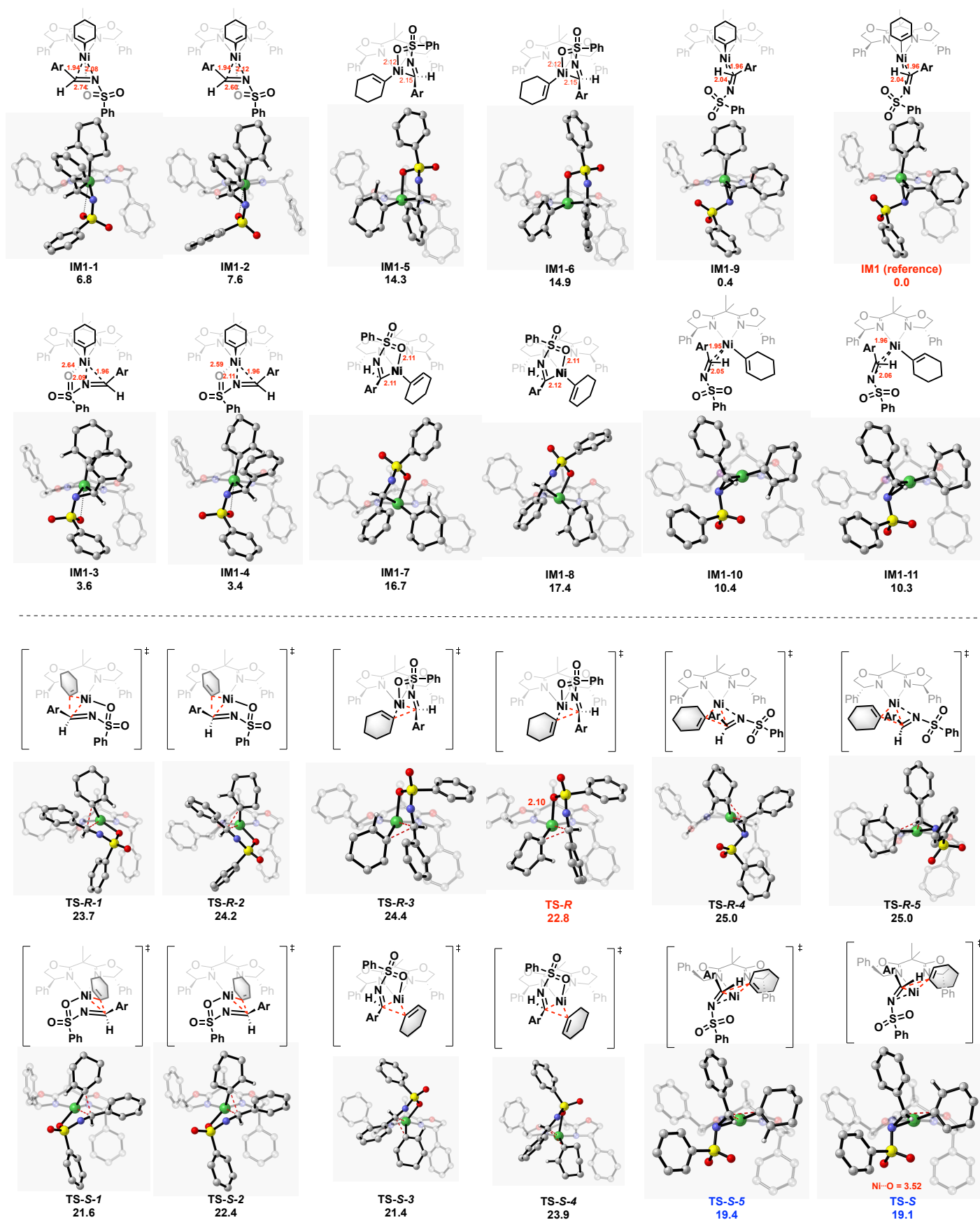


Fig S1 Relative Gibbs free energies for ground state and transition structures for different alkenyl addition modes of neutral complex (bisoxazoline **L7**)Ni(cyclohexenyl) with bound (*E*)-benzenesulfonyl benzylimine.

Energies and optimized structures

Species	IM1	IM1-1	IM1-2	IM1-3
Imaginaries	0	0	0	0
Zero-point Energy Correction (Hartree)	0.7437	0.7425	0.7427	0.7432
Thermal Correction to Energy (Hartree)	0.7885	0.7878	0.7879	0.7881
H Correction (Hartree)	0.7895	0.7887	0.7889	0.7891
G Correction (Hartree)	0.6631	0.6600	0.6604	0.6627
Solvated Electronic Energy (Hartree)	-3921.6963	-3921.6823	-3921.6814	-3921.6902

Species	IM1-4	IM1-5	IM1-6	IM1-7
Imaginaries	0	0	0	0
Zero-point Energy Correction (Hartree)	0.7430	0.7429	0.7436	0.7429
Thermal Correction to Energy (Hartree)	0.7880	0.7879	0.7884	0.7879
H Correction (Hartree)	0.7890	0.7888	0.7893	0.7888
G Correction (Hartree)	0.6623	0.6628	0.6641	0.6621
Solvated Electronic Energy (Hartree)	-3921.6901	-3921.6732	-3921.6736	-3921.6687

Species	IM1-8	IM1-9	IM1-10	IM1-11
Imaginaries	0	0	0	0
Zero-point Energy Correction (Hartree)	0.7425	0.7439	0.7432	0.7431
Thermal Correction to Energy (Hartree)	0.7877	0.7887	0.7885	0.7884
H Correction (Hartree)	0.7887	0.7896	0.7895	0.7893
G Correction (Hartree)	0.6612	0.6630	0.6605	0.6605
Solvated Electronic Energy (Hartree)	-3921.6667	-3921.6955	-3921.6771	-3921.6772

Species	TS-R	TS-R-1	TS-R-2	TS-R-3
Imaginaries	1	1	1	1
Zero-point Energy Correction (Hartree)	0.7424	0.7416	0.7421	0.7426
Thermal Correction to Energy (Hartree)	0.7867	0.7863	0.7864	0.7868
H Correction (Hartree)	0.7876	0.7872	0.7873	0.7877
G Correction (Hartree)	0.6643	0.6609	0.6643	0.6657
Solvated Electronic Energy (Hartree)	-3921.6611	-3921.6564	-3921.6589	-3921.6600

Species	TS-R-4	TS-R-5	TS-S	TS-S-1
Imaginaries	1	1	1	1
Zero-point Energy Correction (Hartree)	0.7430	0.7429	0.7429	0.7426
Thermal Correction to Energy (Hartree)	0.7874	0.7872	0.7873	0.7868
H Correction (Hartree)	0.7883	0.7882	0.7882	0.7877
G Correction (Hartree)	0.6636	0.6629	0.6628	0.6637
Solvated Electronic Energy (Hartree)	-3921.6571	-3921.6561	-3921.6655	-3921.6625

Species	TS-S-2	TS-S-3	TS-S-4	TS-S-5
Imaginaries	1	1	1	1
Zero-point Energy Correction (Hartree)	0.7423	0.7417	0.7417	0.7430
Thermal Correction to Energy (Hartree)	0.7866	0.7862	0.7862	0.7874
H Correction (Hartree)	0.7875	0.7872	0.7871	0.7884
G Correction (Hartree)	0.6627	0.6602	0.6620	0.6626
Solvated Electronic Energy (Hartree)	-3921.6602	-3921.6593	-3921.6570	-3921.6649

IM1							
C	-2.10051800	0.82820800	-2.21574500	C	4.71937400	1.98102400	-2.14294900
C	-0.82241700	2.69820200	-1.16924600	H	3.56544000	0.56940300	-3.29479100
C	-2.03756100	2.31415800	-1.97113200	H	5.59324300	3.44745100	-0.82484500
C	-2.75575100	-0.97505700	-3.35545500	H	5.64974900	1.77768900	-2.66622500
C	-2.18408000	-1.39352700	-1.99425600	Ni	-0.51082200	0.03958900	0.22019400
H	-2.09084800	-1.22388200	-4.18795400	C	-1.75706500	0.46956500	1.65274600
H	-3.75921400	-1.35577100	-3.55448100	C	-2.37339700	-0.72195000	2.34843500
N	-1.63972500	-0.11359400	-1.47807900	C	-2.04022100	1.71397400	2.07643100
N	-0.06205500	1.95456200	-0.45278400	C	-3.59178400	-0.36102300	3.19473800
O	-2.83920100	0.47174200	-3.28490100	C	-2.95304700	2.05622200	3.22667500
H	-1.36089200	-2.10362300	-2.10641000	C	-3.28126000	0.83659400	4.08000000
C	-3.20803100	-1.94244700	-1.03154500	H	-4.42820400	-0.11031900	2.52548000
C	-3.07443900	-3.23108700	-0.51443300	H	-3.88694100	2.50425700	2.84581000
C	-4.30581700	-1.16341500	-0.65018600	H	-4.11088900	1.05487200	4.76277600
C	-4.02429300	-3.73299300	0.37320700	H	-3.91815500	-1.22473600	3.78756300
C	-5.25423600	-1.66464300	0.23343200	H	-2.41528500	0.59409900	4.71343700
H	-4.41026900	-0.15114800	-1.03924800	H	-2.49593900	2.84116900	3.84577500
C	-5.11276600	-2.95196100	0.75031500	H	-1.58491900	2.57399500	1.57487100
H	-6.09907700	-1.04831000	0.52888700	H	-2.63645700	-1.50378800	1.62238800
H	-5.84784400	-3.34042100	1.44984400	C	3.87482500	-2.51982800	-0.89648900
C	-3.29654900	2.69532900	-1.15954500	C	2.66811200	-3.06110500	-0.45230200
H	-3.28598300	3.76791500	-0.94808100	C	2.63125100	-4.24030900	0.28509300
H	-4.19210900	2.46636900	-1.74425800	C	3.82685600	-4.89475700	0.57405500
H	-3.32638200	2.14673700	-0.21199900	C	5.03704600	-4.36703400	0.13297000
C	-2.02375200	3.07534800	-3.30460100	C	5.06082000	-3.18003900	-0.60009700
H	-2.90704600	2.81419900	-3.88787500	H	3.87111100	-1.58959100	-1.45893500
H	-2.02495900	4.14972000	-3.11952400	H	1.67291000	-4.62828200	0.61582200
H	-1.13782100	2.82991300	-3.89667700	H	3.81123700	-5.81832100	1.14583100
O	-0.52739400	4.01304600	-1.22169800	H	6.00717600	-2.76860600	-0.93947000
C	0.52441900	4.20928100	-0.24380400	S	1.15405200	-2.18790600	-0.81390600
H	1.25399900	4.90085700	-0.66807600	O	0.04673800	-2.98291300	-0.23907800
H	0.06492300	4.64940900	0.64836600	O	1.12637700	-1.89947100	-2.25258700
C	1.06138100	2.79310900	-0.00571200	N	1.35950900	-0.75652700	-0.04589000
H	1.23887400	2.61292700	1.06215700	C	0.96527300	-0.67280900	1.28921100
H	-3.90604000	-4.73397000	0.77864300	H	0.51136900	-1.55561100	1.76285700
H	-2.20356000	-3.82069900	-0.78513000	C	1.73071000	0.21509000	2.17685700
C	2.32465500	2.49186600	-0.78620300	C	3.00369400	0.67627000	1.81339400
C	2.35961500	1.56216800	-1.82525600	C	1.19345300	0.61777600	3.41028300
C	3.49738100	3.16996600	-0.43946800	C	3.70921200	1.53443700	2.65183400
C	3.55364300	1.30831300	-2.49735500	H	3.42114500	0.35798300	0.86110900
H	1.46713900	0.99815200	-2.07867500	C	1.90062800	1.47393500	4.24359700
C	4.68818400	2.91839200	-1.11105400	H	0.19881000	0.27477900	3.68752600
H	3.48021100	3.88215200	0.38532000	C	3.16107000	1.94135500	3.86604100
				H	4.69402000	1.88539000	2.35162000

H	1.46655800	1.78392200	5.19072400
H	5.96714400	-4.87933000	0.36267800
H	3.71313900	2.61142100	4.51969900
H	-1.60514100	-1.19027000	2.98902300

IM1-1

C	-1.03259000	-1.86572300	-2.25359300
C	-2.72039900	-1.94827400	-0.41579300
C	-2.14507000	-2.66190900	-1.61345900
C	0.21588900	-1.23352100	-3.99689400
C	0.76041900	-0.61284200	-2.69526400
H	-0.07216800	-0.50181900	-4.75378300
H	0.90514300	-1.96036300	-4.43986700
N	-0.11567100	-1.19634100	-1.65908500
N	-2.22267400	-0.97077600	0.24945800
O	-0.97775200	-1.94762800	-3.59756100
H	0.59362500	0.47184900	-2.66772000
C	2.22026500	-0.89448400	-2.45672500
C	3.15401800	0.14313400	-2.47977100
C	2.66466300	-2.20151100	-2.23899900
C	4.50820500	-0.11713200	-2.28393600
C	4.01453200	-2.46374200	-2.02924700
H	1.93918000	-3.01424100	-2.21437900
C	4.93972400	-1.42077500	-2.05425800
H	4.34478400	-3.48157600	-1.84161900
H	5.99366300	-1.62431800	-1.88746900
C	-1.54024800	-3.99737800	-1.12671600
H	-2.32805700	-4.62255900	-0.69875500
H	-1.09849000	-4.53039300	-1.97420900
H	-0.76890600	-3.81794400	-0.37028300
C	-3.26604000	-2.93441800	-2.62545400
H	-2.87044100	-3.48530200	-3.47934800
H	-4.05068300	-3.52701500	-2.15447300
H	-3.70999200	-2.00714600	-2.99703400
O	-3.90235600	-2.44065100	0.00517900
C	-4.16969600	-1.78127200	1.26815500
H	-5.22724200	-1.51441000	1.29009000
H	-3.94889800	-2.49940800	2.06582700
C	-3.21548600	-0.57534600	1.26445800
H	-2.70818300	-0.47037600	2.23019800
H	5.22255600	0.70082100	-2.29448200
H	2.81064300	1.16560400	-2.63352300
C	-3.89053600	0.72837000	0.91101500
C	-4.40119100	1.52610700	1.93631500

C	-4.07281800	1.12299000	-0.41451800
C	-5.08883000	2.69806200	1.64314700
H	-4.24426700	1.23093400	2.97246100
C	-4.75663000	2.29812600	-0.70797600
H	-3.64002500	0.53303900	-1.21879400
C	-5.26927500	3.08549400	0.31803300
H	-5.47153900	3.31658300	2.45008000
H	-4.87483700	2.60679900	-1.74277700
H	-5.79515600	4.00755000	0.08709200
Ni	-0.29046000	-0.39001600	0.26701100
C	0.35310400	-1.81499300	1.43738500
C	-0.03938700	-1.64687800	2.88164000
C	1.13103700	-2.83623500	1.05041000
C	0.86114800	-2.43313000	3.83276900
H	-0.03077800	-0.57842100	3.14924200
C	1.68790900	-3.89124800	1.97009100
H	1.45555500	-2.89333800	0.00804700
C	1.02341700	-3.86505100	3.34175200
H	1.84527600	-1.94375200	3.86517800
H	1.59448200	-4.89046800	1.51975100
H	1.59642400	-4.46582100	4.05799500
C	1.21999100	0.79467400	0.59464400
H	1.59826200	0.99203500	-0.42166500
N	0.09851200	1.50207500	1.04624900
C	2.27014100	0.47189900	1.57059500
C	3.33375700	-0.36095300	1.19254900
C	2.23793900	0.97343000	2.87743100
C	4.33907700	-0.68030200	2.09320700
H	3.34224300	-0.77710200	0.18771900
C	3.24678600	0.64855600	3.78137000
H	1.41546500	1.62487300	3.16130300
C	4.30042300	-0.17657700	3.39526400
H	5.15346300	-1.33072600	1.78124900
H	3.21255300	1.04785100	4.79204400
H	2.77371900	-3.72611300	2.08104300
H	0.02949600	-4.33205500	3.27239700
H	0.46289700	-2.40853800	4.85484100
H	-1.08878600	-1.96771100	3.01350600
S	-0.56878800	2.49979300	-0.08509700
O	-0.81462200	1.75959200	-1.34925200
O	-1.66985400	3.22575700	0.53763300
C	0.74612400	3.66126200	-0.44844100
C	1.31612300	3.69490400	-1.71793000
C	1.20979500	4.49295600	0.57030700

C	2.36450700	4.57655700	-1.97228900
H	0.92082800	3.04094300	-2.49057300
C	2.25697500	5.36860800	0.30757900
H	0.75039700	4.44377900	1.55366700
C	2.83501500	5.41003600	-0.96124200
H	2.81223200	4.61301000	-2.96191100
H	2.62588900	6.01992400	1.09466700
H	3.65445200	6.09487100	-1.16047200
H	5.08750900	-0.42589600	4.10198700

IM1-2

C	-0.83197700	-2.04502000	-2.13099300
C	-2.40852700	-2.15200200	-0.21086100
C	-1.80127100	-2.91211200	-1.36291700
C	0.23745900	-1.39965400	-3.98289500
C	0.71655300	-0.57318400	-2.77362600
H	-0.15411000	-0.80416400	-4.80913400
H	1.01070400	-2.07889300	-4.35896500
N	0.01699400	-1.21515200	-1.64608400
N	-2.04658600	-1.02050400	0.27613000
O	-0.84637300	-2.21044300	-3.46845100
H	0.34940800	0.46083600	-2.82020300
C	2.21399600	-0.55820300	-2.62248500
C	2.94916200	0.55772800	-3.02805400
C	2.89205100	-1.67791600	-2.13568000
C	4.34079200	0.55069200	-2.96166600
C	4.28038900	-1.68024900	-2.04980500
H	2.31962100	-2.54031600	-1.79974900
C	5.00871100	-0.56907500	-2.47131300
H	4.79353800	-2.54833300	-1.64475200
H	6.09312700	-0.57120900	-2.40554200
C	-1.03310900	-4.12280600	-0.79423300
H	-1.73729800	-4.81025500	-0.31925500
H	-0.52034300	-4.65322000	-1.60219300
H	-0.30286100	-3.79967200	-0.04863900
C	-2.92951500	-3.39832800	-2.28437100
H	-2.51302800	-3.98007100	-3.10762100
H	-3.61863400	-4.02615100	-1.71891100
H	-3.49270100	-2.56341200	-2.70942000
O	-3.46530600	-2.76067000	0.35864700
C	-3.73850800	-1.98485700	1.55713700
H	-4.82026300	-1.94505100	1.69047400
H	-3.26580100	-2.50762700	2.39719300
C	-3.08310000	-0.63565900	1.25075700

H	-2.60331700	-0.20606000	2.13757500
H	4.90194200	1.42408200	-3.28155000
H	2.42289200	1.43559900	-3.39971900
C	-4.05681100	0.36477700	0.66354400
C	-4.98388600	0.96773200	1.51681900
C	-4.07544100	0.68362200	-0.69291500
C	-5.91229100	1.87683300	1.02504000
H	-4.96404100	0.73479000	2.58074400
C	-5.00346800	1.59687400	-1.18576900
H	-3.32783700	0.25708400	-1.35612100
C	-5.92405600	2.19439400	-0.33159800
H	-6.62098400	2.34574600	1.70214300
H	-4.99626300	1.85115200	-2.24209300
H	-6.64308400	2.91157300	-0.71755200
Ni	-0.08770900	-0.41291000	0.25919700
C	0.64183400	-1.84948400	1.40712700
C	-0.01055500	-2.10219800	2.55566100
C	1.89973300	-2.60835800	1.07087300
C	0.40567500	-3.11741500	3.58972200
C	2.50358000	-3.35785700	2.25927400
H	2.64716800	-1.92390900	0.64749600
C	1.42361300	-4.10289400	3.02995600
H	0.83724600	-2.59867200	4.46326700
H	3.29412000	-4.04091500	1.92320000
H	1.85662600	-4.71094700	3.83318600
C	1.31624500	0.95155300	0.53936400
H	1.57904800	1.27211900	-0.48095500
N	0.14175700	1.42984200	1.11628500
C	2.46486500	0.64610400	1.39023800
C	3.71768900	0.45498400	0.79288000
C	2.34991500	0.50937800	2.78211200
C	4.82823100	0.11957800	1.55955800
H	3.80660800	0.56642100	-0.28626700
C	3.46235300	0.18378700	3.54608200
H	1.37613500	0.65721200	3.23968400
C	4.70475100	-0.01834800	2.94042500
H	5.79136000	-0.02996900	1.07667900
H	3.36245400	0.07968400	4.62381200
H	2.98406200	-2.62903700	2.92654100
H	0.91435800	-4.80366500	2.35061800
H	-0.47295800	-3.65156100	3.97993600
S	-0.76244400	2.39659300	0.12049200
O	-0.78685000	1.83557800	-1.25208500
O	-2.01841200	2.67725800	0.80889900

C	0.16618200	3.91799300	0.02371100
C	1.08051300	4.10763800	-1.01101500
C	-0.00855100	4.87946600	1.01711000
C	1.83276800	5.27777600	-1.04656800
H	1.17561400	3.34911300	-1.78288000
C	0.74618600	6.04663000	0.97006900
H	-0.73863000	4.70536000	1.80168600
C	1.66753500	6.24452900	-0.05725300
H	2.54466900	5.43828100	-1.85140600
H	0.61376900	6.80539000	1.73600500
H	2.25518200	7.15767700	-0.08904200
H	5.57022700	-0.27842800	3.54397200
H	1.68977600	-3.32372100	0.25500400
H	-0.89045500	-1.50266200	2.81632900

IM1-3

C	2.10135600	-1.88523000	-1.63696100
C	0.87760000	-2.99858900	0.23670900
C	2.12674700	-2.99251300	-0.61006600
C	2.64979400	-0.95812500	-3.59805900
C	1.99559900	0.09052700	-2.68609200
H	2.03117700	-1.22510300	-4.45869200
H	3.64996600	-0.68362400	-3.94192000
N	1.61141700	-0.71054800	-1.49964900
N	0.02754200	-2.05420500	0.39961300
O	2.77769400	-2.14606700	-2.77270800
H	1.08003900	0.49805700	-3.12841900
C	2.88734600	1.22498800	-2.24935100
C	2.36753000	2.51616500	-2.14730900
C	4.20731000	0.98166200	-1.85857800
C	3.16457500	3.55193100	-1.66400000
C	5.00274900	2.01660400	-1.38040400
H	4.61078200	-0.02973600	-1.91099700
C	4.48006700	3.30540600	-1.28061100
H	6.02633100	1.81770900	-1.07439300
H	5.09867800	4.11378800	-0.90045800
C	3.33140900	-2.70674200	0.31729600
H	3.37710700	-3.45573800	1.11251700
H	4.25616600	-2.76183500	-0.26433900
H	3.24948000	-1.70694400	0.75760000
C	2.29526000	-4.35942100	-1.28440200
H	3.20964300	-4.37074300	-1.87821100
H	2.35528000	-5.14138700	-0.52671000
H	1.45711400	-4.58747600	-1.94846100

O	0.68869000	-4.13353100	0.94052500
C	-0.48476200	-3.91332100	1.75961600
H	-1.19541800	-4.71583300	1.54589200
H	-0.17338400	-3.97066900	2.80622600
C	-0.99615600	-2.51402900	1.34483700
H	-0.99128000	-1.82869900	2.20358800
H	2.75177600	4.55351900	-1.58121700
H	1.33050500	2.69231600	-2.42429200
C	-2.37972000	-2.51939200	0.74246000
C	-3.48607700	-2.23721400	1.54766000
C	-2.58192200	-2.85708000	-0.59732700
C	-4.77662200	-2.30683600	1.02907000
H	-3.33143400	-1.96217200	2.59025100
C	-3.87024800	-2.92463400	-1.11792800
H	-1.72224600	-3.02679400	-1.24032100
C	-4.97046000	-2.65693200	-0.30528700
H	-5.62816500	-2.08107900	1.66503800
H	-4.01427500	-3.17034000	-2.16600200
H	-5.97534800	-2.70471300	-0.71592800
Ni	0.40765100	-0.05884200	-0.01565600
C	1.64685100	0.22012600	1.49056700
C	2.62578300	1.12712800	1.34567200
C	1.49117500	-0.54354200	2.77982000
C	3.65614400	1.45755700	2.39423100
H	2.68740500	1.71089600	0.42515800
C	2.28820200	0.05362300	3.94042300
H	0.42837000	-0.57843000	3.06371400
C	3.69993800	0.40750100	3.49644900
H	3.42748800	2.44486800	2.83175100
H	2.30072600	-0.63420700	4.79545800
H	4.30404400	0.75577700	4.34273800
C	-1.07982200	0.99019100	0.70315100
H	-1.92669400	0.28802900	0.63198900
N	-0.67459400	1.67704100	-0.44851500
C	-0.96844200	1.65529100	2.00234800
C	-1.63310600	1.10948300	3.10902200
C	-0.19051800	2.80857500	2.18632000
C	-1.51891700	1.68760400	4.36945400
H	-2.25420300	0.22460300	2.96223500
C	-0.08254700	3.38799000	3.44278800
H	0.32660600	3.22555900	1.32646100
C	-0.74134100	2.83027800	4.54094400
H	-2.04430600	1.25253500	5.21572400
H	0.52351100	4.28130400	3.57210900

H	1.77862200	0.96642500	4.28030200
H	4.19441900	-0.49952900	3.11591600
H	4.64530700	1.57300400	1.92837700
S	-1.43350100	1.18545400	-1.82526500
O	-1.43590400	-0.29589000	-1.89465600
O	-0.85447400	1.93649000	-2.94469400
C	-3.13532500	1.68267600	-1.64801500
C	-4.04573600	0.79686000	-1.07235100
C	-3.51747800	2.96519300	-2.03641000
C	-5.36054800	1.21012400	-0.88088900
H	-3.72434700	-0.20630100	-0.80393800
C	-4.83619200	3.36365100	-1.84510700
H	-2.78445500	3.62400000	-2.49206500
C	-5.75507000	2.49010500	-1.26472400
H	-6.07876300	0.52566800	-0.43675600
H	-5.14867900	4.35810500	-2.15068500
H	-6.78339000	2.80768700	-1.11599000
H	-0.65216300	3.28794400	5.52240300
H	1.78460200	-1.59998700	2.62926000

IM1-4

C	2.10014200	-2.05517100	-1.47548300
C	0.87504200	-3.01139600	0.48208800
C	2.10248100	-3.10388900	-0.39022500
C	2.65980000	-1.26453500	-3.49272900
C	2.02249200	-0.15043800	-2.65123600
H	2.03089300	-1.58336200	-4.32793300
H	3.65939200	-1.02523300	-3.86309700
N	1.62071300	-0.86919100	-1.41769900
N	0.01070100	-2.06858700	0.54460900
O	2.78167700	-2.39317300	-2.58782500
H	1.11458500	0.24339400	-3.12099500
C	2.93001000	0.99554000	-2.28261600
C	2.41289900	2.29022400	-2.21648800
C	4.26257100	0.76747200	-1.92498300
C	3.22427200	3.34446000	-1.80319400
C	5.07215300	1.82160600	-1.51510800
H	4.66634000	-0.24481400	-1.95064800
C	4.55163500	3.11374500	-1.45289100
H	6.10590700	1.63564100	-1.23688700
H	5.18162200	3.93736000	-1.12816700
C	3.34766700	-2.84187500	0.48796000
H	3.39570300	-3.58162100	1.29132700
H	4.24939300	-2.93361400	-0.12424200

H	3.30359700	-1.84090000	0.92946000
C	2.18010000	-4.51070000	-1.00003100
H	3.07882500	-4.60330500	-1.61044100
H	2.21304500	-5.25645100	-0.20502300
H	1.31544100	-4.72167100	-1.63552300
O	0.71079800	-4.06362900	1.30989500
C	-0.48700800	-3.79634300	2.07594400
H	-1.19771300	-4.60341400	1.87553500
H	-0.21481900	-3.80620700	3.13420400
C	-0.97763700	-2.41919800	1.57110400
H	-0.90341000	-1.66357100	2.36648600
H	2.81342100	4.34880300	-1.74763900
H	1.36734500	2.45523500	-2.46934600
C	-2.38898200	-2.43190300	1.03950100
C	-3.44048200	-1.97209400	1.83524300
C	-2.67087500	-2.95450700	-0.22510200
C	-4.75667100	-2.05225800	1.38593300
H	-3.22369400	-1.54742000	2.81440100
C	-3.98385300	-3.03375500	-0.67642500
H	-1.85065000	-3.26732700	-0.86679600
C	-5.03053300	-2.59099000	0.13123200
H	-5.56532400	-1.68837400	2.01375400
H	-4.19012600	-3.42863500	-1.66692900
H	-6.05551300	-2.65070500	-0.22465100
Ni	0.38947800	-0.10209900	-0.01278800
C	1.60014900	0.31817200	1.46710400
C	2.38092800	1.58082200	1.23228100
C	1.77558400	-0.39766000	2.58901000
C	3.02092500	2.14121400	2.49976000
H	1.73736100	2.33830100	0.76155900
C	2.73764700	-0.03966400	3.69358600
H	1.18996500	-1.30604900	2.76571500
C	3.73182100	1.03066900	3.25983500
H	2.23654500	2.57582100	3.13677100
H	3.27109100	-0.93648300	4.04211700
H	4.27550700	1.42444200	4.12691900
C	-1.06881300	1.03710600	0.62884200
H	-1.90142000	0.31506300	0.64409200
N	-0.69831900	1.62244100	-0.58960500
C	-0.95609000	1.85570800	1.84169100
C	-1.28725400	1.30320100	3.08746800
C	-0.51151100	3.18352000	1.79692600
C	-1.15663100	2.04108800	4.25502400
H	-1.64147500	0.27299400	3.12636900

C	-0.38373400	3.92503200	2.96748000
H	-0.27768300	3.61578800	0.82803000
C	-0.69888600	3.35847800	4.20041200
H	-1.41319600	1.59270100	5.21143100
H	-0.03864700	4.95465900	2.91616900
H	2.16868700	0.31681300	4.56928200
H	4.48658000	0.57696000	2.59925400
H	3.71320300	2.95536800	2.24824900
H	3.16066900	1.37601000	0.48241500
S	-1.43672900	0.98093100	-1.90880200
O	-1.42770200	-0.50030700	-1.81130100
O	-0.84689800	1.60785000	-3.09711900
C	-3.14366400	1.47870100	-1.80963300
C	-4.04717300	0.66951300	-1.12130100
C	-3.53810200	2.69152200	-2.37115300
C	-5.36717300	1.08988000	-0.99190800
H	-3.71683400	-0.28393900	-0.71756100
C	-4.86223300	3.09675400	-2.24072300
H	-2.81027700	3.28990100	-2.91076900
C	-5.77424600	2.30041200	-1.54905100
H	-6.07884600	0.46361100	-0.45992900
H	-5.18446200	4.03598400	-2.68121100
H	-6.80677500	2.62328200	-1.44890400
H	-0.59720900	3.93951600	5.11287900

IM1-5

C	0.53586700	-2.67141500	-1.84187900
C	-0.96972300	-3.15795000	0.09679500
C	0.15332500	-3.66269400	-0.77189600
C	1.37916000	-2.14839500	-3.83575700
C	1.15327000	-0.87895600	-3.00063800
H	0.63992000	-2.28009800	-4.63391800
H	2.38545700	-2.23817900	-4.24713600
N	0.39276800	-1.39649700	-1.84370800
N	-1.29081800	-1.94848300	0.37333200
O	1.18694100	-3.22451500	-2.88640100
H	0.53654300	-0.14769700	-3.53544200
C	2.45014400	-0.21697000	-2.59379000
C	3.18108400	-0.65451100	-1.49028500
C	2.96188400	0.81470400	-3.38420500
C	4.38598400	-0.04086000	-1.15872900
C	4.17371700	1.41674500	-3.06465000
H	2.38946500	1.16689900	-4.24162200
C	4.88520800	0.99574100	-1.94238700

H	4.55258700	2.22800100	-3.68061100
H	5.82355100	1.47655200	-1.67995900
C	1.38554900	-3.85715500	0.14448800
H	1.15433900	-4.60690600	0.90556500
H	2.23001500	-4.21517800	-0.45102700
H	1.64900700	-2.91670000	0.63578600
C	-0.23217100	-5.00396600	-1.41092400
H	0.60015300	-5.38142600	-2.00485200
H	-0.47017700	-5.73093100	-0.63467900
H	-1.10246800	-4.90692700	-2.06569000
O	-1.66892500	-4.14068800	0.69345200
C	-2.63647700	-3.49534300	1.55263900
H	-3.62974600	-3.85000700	1.26369200
H	-2.42246400	-3.80138500	2.57932200
C	-2.42152600	-1.98913600	1.30896000
H	-2.09288400	-1.50999600	2.24024200
H	4.92758500	-0.36858600	-0.27516400
H	2.78005400	-1.43270200	-0.84944100
C	-3.62378500	-1.25782800	0.76263500
C	-3.74905700	-0.96026800	-0.59715100
C	-4.63865400	-0.86150100	1.63861700
C	-4.86560800	-0.27280300	-1.06920100
H	-2.95709500	-1.24843900	-1.28651800
C	-5.75860100	-0.18498400	1.16622300
H	-4.53654800	-1.06733900	2.70278500
C	-5.87315400	0.11434900	-0.19046300
H	-4.93926500	-0.02997600	-2.12574200
H	-6.53430000	0.12529900	1.86038100
H	-6.73975000	0.65643600	-0.55789900
Ni	-0.41839600	-0.14842700	-0.30544700
C	-0.14106900	1.48887900	-1.26426200
C	-1.25434700	1.84277100	-2.21927000
C	0.95642100	2.24317500	-1.14466900
C	-1.14390700	3.27485600	-2.74407800
C	1.22243900	3.48277800	-1.95134600
H	1.71003700	1.96743000	-0.40194600
C	0.28933100	3.58533200	-3.15190500
H	-1.44902500	3.96205900	-1.94288500
H	2.27221400	3.50678700	-2.27700800
H	0.36124800	4.57619700	-3.61584200
C	-0.99514300	1.10096400	1.34642300
H	-1.73402200	0.35259900	1.67410700
N	0.17446300	1.20731500	2.10775100
C	-1.65543000	2.38634500	1.05748400

C	-3.01161200	2.41305700	0.70726000
C	-0.96301800	3.60395500	1.13412500
C	-3.65704500	3.61278500	0.42612600
H	-3.56121400	1.47599400	0.65986100
C	-1.60966200	4.80322400	0.86427400
H	0.08749900	3.58031100	1.41056700
C	-2.95883700	4.81593000	0.50375700
H	-4.71095200	3.60506900	0.15609200
H	-1.05855300	5.73842900	0.93201400
H	-2.23029500	1.70986400	-1.72674000
H	-1.83832500	3.43401700	-3.57835000
H	0.60815900	2.86047400	-3.91819400
H	1.09379000	4.36964600	-1.30658200
S	0.91983300	-0.17731800	2.23622900
O	1.30006800	-0.64831600	0.83549500
O	0.29261900	-1.25806100	3.03130500
C	2.45035700	0.26622100	3.01958900
C	2.86554800	-0.43532000	4.14582700
C	3.23687900	1.27106800	2.45737800
C	4.09185400	-0.11911400	4.72611000
H	2.22137800	-1.20964600	4.55069800
C	4.45830100	1.57838600	3.04486100
H	2.88035600	1.80006000	1.57742400
C	4.88555500	0.88434600	4.17734000
H	4.42529300	-0.65583900	5.60978100
H	5.07885600	2.36211300	2.61936900
H	5.84117600	1.12917200	4.63290300
H	-1.26233400	1.12890300	-3.06431400
H	-3.46033500	5.75634700	0.29082800

IM1-6

C	0.58608700	-2.98725800	-1.35442500
C	-0.93976800	-3.11109800	0.61936300
C	0.20734700	-3.75593500	-0.11485900
C	1.45815600	-2.86473600	-3.40255000
C	1.11943000	-1.45974000	-2.87983100
H	0.77263700	-3.21458800	-4.18213800
H	2.48824700	-2.97462900	-3.74534800
N	0.39080500	-1.74890700	-1.62755100
N	-1.30830300	-1.88308400	0.62321600
O	1.27693300	-3.72148800	-2.25103700
H	0.44979900	-0.92238200	-3.55966600
C	2.34434300	-0.61114500	-2.64166000
C	3.12716700	-0.76621300	-1.49695500

C	2.73792200	0.30719900	-3.61617900
C	4.27797300	-0.00189800	-1.32477700
C	3.89295700	1.06475600	-3.45030300
H	2.11538700	0.44679900	-4.49913900
C	4.66566000	0.91238600	-2.30079200
H	4.17860200	1.78728700	-4.21016000
H	5.55950700	1.51375700	-2.16139300
C	1.42819600	-3.76533100	0.83516300
H	1.18828900	-4.35119000	1.72602300
H	2.27805800	-4.23159500	0.32890300
H	1.68540000	-2.74728900	1.13704300
C	-0.15804200	-5.19984100	-0.49190300
H	0.68455100	-5.67322900	-0.99569300
H	-0.39846100	-5.76854000	0.40601600
H	-1.02183700	-5.23837800	-1.16148200
O	-1.61662800	-3.97048100	1.40206100
C	-2.67187500	-3.21113100	2.03257500
H	-3.62717000	-3.62902000	1.69901200
H	-2.57467900	-3.33832100	3.11237400
C	-2.44125600	-1.76488700	1.56003500
H	-2.10093200	-1.15228900	2.40440300
H	4.86466200	-0.11129600	-0.41650200
H	2.81014200	-1.44813200	-0.71265100
C	-3.63428700	-1.11716300	0.90480300
C	-3.91447900	-1.33554500	-0.44728900
C	-4.47364800	-0.28330400	1.64648100
C	-5.01713100	-0.73071300	-1.04513300
H	-3.24802300	-1.96389800	-1.03582700
C	-5.57899000	0.31729100	1.05143300
H	-4.23961600	-0.08420400	2.69062400
C	-5.85255600	0.09513100	-0.29620100
H	-5.21805200	-0.89672200	-2.09989200
H	-6.21503500	0.97604100	1.63543000
H	-6.70719800	0.57478900	-0.76475600
Ni	-0.36276600	-0.21443000	-0.33514000
C	0.04044900	1.26971200	-1.49002500
C	-0.69159200	1.32271500	-2.61606100
C	1.05878200	2.31482900	-1.15809500
C	-0.58602200	2.41584200	-3.64914000
C	0.85744000	3.59714800	-1.96587000
H	1.03387500	2.52947700	-0.08053500
C	0.64906700	3.28649400	-3.44141600
H	-1.49455300	3.03915800	-3.60114200
H	1.71129900	4.27244600	-1.82916900

H	0.56503200	4.20828600	-4.02971300
C	-1.02178100	1.22114200	1.08306900
H	-1.77195100	0.49751900	1.42852700
N	0.06820600	1.44788400	1.93443900
C	-1.69355700	2.44846800	0.61205200
C	-2.86690200	2.34868100	-0.15073600
C	-1.20966300	3.72386800	0.92680900
C	-3.53251900	3.48314400	-0.58988200
H	-3.24181100	1.35999000	-0.41206900
C	-1.87885300	4.86381000	0.48714200
H	-0.30587100	3.80058100	1.52503500
C	-3.03913200	4.75105800	-0.27407400
H	-4.43945800	3.37953700	-1.18170000
H	-1.49050200	5.84699900	0.74191900
H	-0.58563500	1.98825700	-4.66355300
H	1.53535900	2.75805600	-3.81845600
H	-0.02690000	4.12311300	-1.57892100
S	0.86771200	0.12324600	2.23955400
O	1.31389200	-0.51734600	0.93071600
O	0.25204100	-0.87369400	3.14647800
C	2.35953700	0.72782300	2.98875500
C	3.52522500	-0.01827300	2.82661600
C	2.34917100	1.89076100	3.75518300
C	4.69782300	0.40958800	3.44053000
H	3.50695000	-0.91347000	2.21036000
C	3.52840600	2.30949500	4.36349100
H	1.42821100	2.45756100	3.84642900
C	4.70024100	1.57140800	4.20943800
H	5.61261800	-0.16290800	3.31420900
H	3.53241400	3.21943000	4.95687000
H	5.61810200	1.90493400	4.68537000
H	-1.46380300	0.56663800	-2.80638600
H	-3.55860700	5.64197200	-0.61708500
H	2.06420300	1.90316400	-1.33929700

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C	-1.44485600	2.81688700	0.82129300
C	0.71685100	2.25800600	1.90540700
C	-0.65045200	2.85851700	2.09720100
C	-2.86683600	3.65168700	-0.67694600
C	-2.59336500	2.16512600	-0.96645900
H	-2.38575200	4.32869000	-1.39052700
H	-3.92635100	3.89795600	-0.59173100
N	-1.50841900	1.84483200	-0.01859900

N	1.24751600	1.80186200	0.82866800
O	-2.24976200	3.87305400	0.61257600
H	-2.22116100	2.03370200	-1.99128700
C	-3.81516300	1.29595000	-0.76604500
C	-4.04053100	0.60481500	0.42464700
C	-4.76028700	1.21610400	-1.79337500
C	-5.18807200	-0.16877200	0.57791500
C	-5.91470400	0.45763700	-1.63251600
H	-4.58081200	1.74216200	-2.73083300
C	-6.12958700	-0.23878200	-0.44449800
H	-6.63848300	0.39696900	-2.44036900
H	-7.02209000	-0.84618000	-0.32451300
C	-1.42745900	2.02495300	3.14080800
H	-0.90806900	2.07029000	4.10032900
H	-2.42964400	2.44536000	3.26791500
H	-1.50847800	0.97904300	2.83219000
C	-0.48726100	4.30029800	2.59984800
H	-1.46400400	4.74395700	2.79816700
H	0.09248300	4.29619900	3.52392800
H	0.02841600	4.92808900	1.86829000
O	1.44433400	2.23624400	3.03751400
C	2.75565000	1.76788200	2.64614700
H	3.44000600	2.62474600	2.67272100
H	3.07814900	1.02156300	3.37375300
C	2.54383900	1.22070200	1.22636700
H	2.39314100	0.13299000	1.25683300
H	-5.32625700	-0.73155200	1.49629600
H	-3.29415600	0.61315800	1.21410200
C	3.68175700	1.52618300	0.29409900
C	3.62754200	2.57670600	-0.62186900
C	4.85483400	0.77174200	0.39211800
C	4.72513100	2.86363700	-1.43082300
H	2.70993600	3.15360900	-0.70665900
C	5.95569400	1.06507000	-0.40494000
H	4.89415500	-0.06390200	1.08981700
C	5.89295300	2.11403400	-1.32108600
H	4.66663200	3.67643800	-2.14990800
H	6.85849900	0.46614000	-0.32189400
H	6.74796200	2.33919200	-1.95216600
Ni	-0.01727000	0.38813400	-0.32393200
C	1.41342700	-0.39168700	-1.33146500
C	1.63814800	0.26934800	-2.66717400
C	2.20021400	-1.37970500	-0.88848600
C	2.59807400	-0.51731800	-3.56264800

C	3.39745200	-1.90493200	-1.63366600
H	1.96322100	-1.85707700	0.06756800
C	3.81206100	-0.97390100	-2.76783700
H	2.06884800	-1.39344500	-3.96110200
H	4.23983700	-2.05649500	-0.94246300
H	4.54505500	-1.46550100	-3.41883300
C	-1.24657200	-1.23244000	-0.90760700
H	-2.13562600	-0.61544400	-0.70527100
N	-0.95972400	-2.24189800	0.00887100
C	-1.14695500	-1.60525500	-2.32425200
C	-1.83139800	-0.85609800	-3.29223200
C	-0.36763300	-2.69162800	-2.74943400
C	-1.72888100	-1.16639700	-4.64400100
H	-2.46947200	-0.03453000	-2.96566500
C	-0.27280100	-3.00680800	-4.09829600
H	0.15948500	-3.27166700	-1.99732900
C	-0.94444400	-2.24246000	-5.05398900
H	-2.27061700	-0.57550700	-5.37828600
H	0.33570000	-3.85195500	-4.41151700
H	2.89776400	0.08996800	-4.42559000
H	4.31146900	-0.09153000	-2.34351300
H	3.17073000	-2.90807700	-2.03589900
S	-0.94085400	-1.71794900	1.49876000
O	0.02080100	-0.53166300	1.58705700
O	-2.21470800	-1.40981000	2.18294400
C	-0.18496800	-3.06703600	2.37738500
C	-0.49317300	-3.21814100	3.72732400
C	0.72592600	-3.91153600	1.74466400
C	0.12889800	-4.22642500	4.45721700
H	-1.22673100	-2.55839700	4.18045700
C	1.33520500	-4.92091000	2.48324200
H	0.92418100	-3.77781700	0.68549100
C	1.04214800	-5.07597900	3.83709200
H	-0.10774800	-4.35462800	5.50967200
H	2.03824700	-5.59188100	1.99782100
H	1.52146300	-5.86631700	4.40821600
H	0.67664200	0.40281800	-3.18873200
H	-0.86320600	-2.48983800	-6.10885400
H	2.03048800	1.28752300	-2.50278800

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C	-1.53767600	2.87700200	-0.60653100
C	0.70462600	2.90589600	0.46945800
C	-0.65221200	3.55133500	0.40541700

C	-3.15348600	2.87445000	-2.14333900
C	-2.79035600	1.43399400	-1.74360000
H	-2.79791000	3.15028600	-3.14155200
H	-4.21679100	3.10299000	-2.05525400
N	-1.60185200	1.62316200	-0.88766400
N	1.19968200	2.01155500	-0.30559200
O	-2.43884000	3.68954700	-1.18740000
H	-2.50389400	0.84857600	-2.62701400
C	-3.91183600	0.72340700	-1.01973900
C	-4.03122100	0.76994400	0.37033900
C	-4.86952500	0.03058900	-1.76527200
C	-5.08399000	0.11769300	1.00545900
C	-5.93124600	-0.60641400	-1.13156200
H	-4.77053400	-0.02314000	-2.84900500
C	-6.03858900	-0.56520200	0.25705500
H	-6.66435700	-1.15012700	-1.72059900
H	-6.85628300	-1.07897900	0.75428100
C	-1.35240800	3.41750800	1.77605600
H	-0.77306400	3.95083400	2.53243200
H	-2.34863900	3.86597200	1.72148800
H	-1.43890700	2.36946400	2.07472400
C	-0.46243000	5.03816300	0.06491800
H	-1.42270200	5.55570800	0.07595400
H	0.19259600	5.49556800	0.80835100
H	-0.01365200	5.17129600	-0.92302400
O	1.46962100	3.38392900	1.47342600
C	2.77058100	2.78478500	1.28238100
H	3.44549400	3.55271500	0.88400300
H	3.13420000	2.45196500	2.25626600
C	2.50481600	1.65208400	0.28051400
H	2.33155000	0.71623700	0.83272500
H	-5.13555000	0.12832800	2.08988100
H	-3.26757200	1.25810800	0.97019700
C	3.61543700	1.43814500	-0.70889600
C	3.43173700	1.60643100	-2.08100900
C	4.87493900	1.05923900	-0.23366300
C	4.48996600	1.39974100	-2.96211600
H	2.44590200	1.87769900	-2.44696600
C	5.93461000	0.85787800	-1.11300200
H	5.02296000	0.90770100	0.83507300
C	5.74328300	1.02681800	-2.48232900
H	4.33200200	1.52484000	-4.03022400
H	6.90656400	0.56026500	-0.72943100
H	6.56610800	0.86310000	-3.17247000

Ni	-0.11223500	0.17596000	-0.52758200
C	1.29295100	-1.01518500	-1.06251400
C	1.50411400	-1.02550700	-2.38869200
C	2.10845700	-1.85520400	-0.12723600
C	2.61176900	-1.78383300	-3.07034200
C	2.94408900	-2.90624600	-0.85843100
H	2.77899000	-1.21027500	0.46731800
C	3.63849500	-2.28903600	-2.06509800
H	2.18241500	-2.62905800	-3.63360500
H	3.67101800	-3.36099000	-0.17443300
H	4.31927900	-3.00609200	-2.53917600
C	-1.31948900	-1.51467700	-0.08982400
H	-2.20128900	-0.86319200	-0.17760600
N	-0.94072500	-1.91057000	1.18901200
C	-1.28691300	-2.55702000	-1.12258700
C	-1.92941900	-2.33648200	-2.34950000
C	-0.59218800	-3.76040600	-0.94037600
C	-1.84971800	-3.26671400	-3.37693700
H	-2.49558800	-1.41485100	-2.48618300
C	-0.51272300	-4.69181600	-1.96870200
H	-0.11103500	-3.94142200	0.01713200
C	-1.13200500	-4.44854200	-3.19397600
H	-2.35253300	-3.07578600	-4.32178000
H	0.03753700	-5.61700500	-1.81408500
H	3.09800800	-1.14477600	-3.82213300
H	4.25636600	-1.44266200	-1.73021500
H	2.27989300	-3.71393000	-1.19874200
S	-0.83757000	-0.69861100	2.20299000
O	-0.03085000	0.42763400	1.56587700
O	-2.07411300	-0.18867100	2.82612600
C	0.21505100	-1.35443200	3.47550400
C	1.07156200	-0.47426400	4.13459300
C	0.15629700	-2.70204400	3.82375800
C	1.87979100	-0.95451300	5.16025000
H	1.10262900	0.56882000	3.82980800
C	0.97069700	-3.16996400	4.84992800
H	-0.50528200	-3.36517200	3.27552800
C	1.82941800	-2.29968200	5.51897000
H	2.55355100	-0.27746200	5.67800600
H	0.93777600	-4.22035800	5.12479800
H	2.46428500	-2.67182700	6.31806400
H	0.84465300	-0.45387800	-3.05378200
H	-1.06561400	-5.17807000	-3.99640100
H	1.44330300	-2.32659700	0.61163200

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C	-2.11944000	0.40514700	-2.30623000
C	-0.96156500	2.44680100	-1.48413600
C	-2.19068900	1.90551400	-2.16787300
C	-2.58456100	-1.54558500	-3.28084100
C	-2.04807700	-1.78339400	-1.86429800
H	-1.86320300	-1.81760500	-4.05697600
H	-3.54550900	-2.02336800	-3.48097800
N	-1.61445700	-0.42015400	-1.46674100
N	-0.16129500	1.83382400	-0.69143400
O	-2.78367500	-0.10791200	-3.35978800
H	-1.17549000	-2.44154800	-1.86819800
C	-3.07227100	-2.28413000	-0.87495700
C	-2.79469700	-3.37780600	-0.05481500
C	-4.30091000	-1.62749000	-0.74669200
C	-3.73460100	-3.80695800	0.88146200
C	-5.23709200	-2.05485800	0.18645500
H	-4.52089500	-0.76700100	-1.37816400
C	-4.95298100	-3.14637900	1.00652500
H	-6.18520200	-1.53264900	0.28265300
H	-5.68065900	-3.47728600	1.74248500
C	-3.41109200	2.20753600	-1.26619700
H	-3.46667100	3.28033800	-1.05991200
H	-4.32758200	1.90807000	-1.78312700
H	-3.34118400	1.65853200	-0.32070100
C	-2.36658700	2.57703600	-3.53385900
H	-3.26056300	2.18891000	-4.02286100
H	-2.47108500	3.65511600	-3.40852100
H	-1.51188900	2.38956400	-4.18867000
O	-0.72161400	3.75256300	-1.71527100
C	0.34140800	4.11751100	-0.79859300
H	1.04419900	4.75648000	-1.33571900
H	-0.11587600	4.67504800	0.02641600
C	0.92562900	2.76608200	-0.36127300
H	1.09465400	2.74254900	0.72351700
H	-3.50759300	-4.65591200	1.52034400
H	-1.82862300	-3.86715500	-0.13719700
C	2.21300000	2.40843000	-1.07359100
C	2.29097000	1.36900800	-1.99989800
C	3.36174100	3.15116300	-0.78287500
C	3.50318500	1.07622200	-2.62178400
H	1.41958800	0.75279000	-2.20040200
C	4.57165900	2.85814900	-1.40229900
H	3.30975200	3.95293700	-0.04639200

C	4.64518000	1.81525600	-2.32477600	H	4.25019500	2.44606100	2.50965100
H	3.54873000	0.25095200	-3.32806400	H	1.09346700	1.82528600	5.36232700
H	5.45789600	3.43887700	-1.16130400	H	6.51604900	-4.06107700	0.69255500
H	5.59015700	1.58004700	-2.80698800	H	3.19248700	2.98065700	4.69661200
Ni	-0.55686700	0.01814400	0.23279900				
C	-1.86161400	0.62259400	1.55509600			IM1-10	
C	-2.71680900	-0.26035500	2.10192400	C	0.51775300	2.76799800	-1.36076400
C	-1.85632800	2.06174300	2.00967200	C	2.70382600	2.08063100	-0.77107700
C	-3.71199600	0.05861600	3.18864900	C	1.74310200	3.24037200	-0.61576200
C	-3.07778500	2.44778200	2.84552600	C	-0.76176900	2.49653500	-3.16123500
H	-0.93316300	2.25397100	2.58254100	C	-1.23658100	1.57782400	-2.01327500
C	-3.38602800	1.37581500	3.88028500	H	-0.36200400	1.95158600	-4.02072900
H	-4.73032900	0.10102700	2.76613900	H	-1.52586100	3.19979900	-3.50253200
H	-3.94895300	2.55892900	2.18160100	N	-0.25793100	1.84420700	-0.93586500
H	-4.20678400	1.68629500	4.53765000	N	2.38009200	0.85357100	-0.56935900
H	-3.74379400	-0.76345700	3.91703200	O	0.32900700	3.27057500	-2.59503300
H	-2.50483800	1.24028300	4.52482800	H	-1.15675600	0.51887700	-2.28232700
H	-2.92533600	3.42536900	3.31964500	C	-2.64964900	1.85780400	-1.57361700
H	-1.78797100	2.73675400	1.14205500	C	-3.62044700	0.86056800	-1.65562800
H	-2.71128300	-1.29977000	1.76404700	C	-3.00416100	3.11698100	-1.07979700
C	4.10082700	-2.03089900	-0.56345000	C	-4.92683900	1.11413400	-1.24204500
C	2.98785600	-2.78444400	-0.18936600	C	-4.30706500	3.37201600	-0.66584800
C	3.12460500	-3.98449900	0.50077300	H	-2.24411300	3.89394100	-0.99637200
C	4.40276100	-4.44235600	0.81407300	C	-5.27172300	2.36784900	-0.74416500
C	5.52153600	-3.70169700	0.44315600	H	-4.57065100	4.35148000	-0.27527300
C	5.37008600	-2.49651300	-0.24341300	H	-6.28885600	2.56440300	-0.41672900
H	3.96069100	-1.08808000	-1.08753200	C	1.39880800	3.41809300	0.87238700
H	2.23452200	-4.53942100	0.78011800	H	2.29507500	3.68325300	1.44041300
H	4.52301900	-5.37905300	1.35099800	H	0.66328100	4.21928400	0.98920600
H	6.24401900	-1.91667800	-0.52717200	H	0.96792900	2.50513900	1.29939200
S	1.36168700	-2.17118500	-0.59909300	C	2.31536100	4.52839700	-1.19836200
O	0.38536300	-3.10286700	0.00207600	H	1.58018700	5.33210200	-1.11555100
O	1.30921500	-1.95499300	-2.05031800	H	3.21163900	4.82228700	-0.64855800
N	1.35181000	-0.69073700	0.10005800	H	2.57983300	4.41668500	-2.25039200
C	0.89265400	-0.57314000	1.40912600	O	3.96719100	2.34230700	-1.14177000
H	0.44286300	-1.45315900	1.89156000	C	4.56106500	1.03632300	-1.39407000
C	1.54394600	0.38808600	2.30480800	H	4.59490900	0.89450000	-2.48059000
C	2.73889700	1.02893000	1.94688900	H	5.57590500	1.04805500	-0.99495700
C	0.96962000	0.67794400	3.55294700	C	3.60605000	0.05326800	-0.70387100
C	3.32250200	1.95881300	2.80191900	H	3.95794000	-0.16582200	0.31636600

C	4.44291900	-2.18865500	-1.41755900
C	2.03891500	-2.80973400	-2.66968800
H	1.37242700	-0.86757800	-2.03979100
C	4.28667900	-3.41723500	-2.04919500
H	5.37424700	-1.95707200	-0.90114400
C	3.08094500	-3.73087400	-2.67463700
H	1.08030600	-3.04839900	-3.12008500
H	5.10082700	-4.13687600	-2.03980400
H	2.95189900	-4.69822600	-3.15194900
Ni	0.69735900	0.16206900	0.39604900
C	1.89706000	-0.64255300	1.72613400
C	2.16438300	-1.95578300	1.79366700
C	2.64054800	0.35480500	2.58378700
C	3.19215500	-2.56676200	2.70979600
C	3.88083300	-0.23327000	3.26283200
H	1.95498000	0.76934500	3.34191900
C	3.58879300	-1.61382400	3.82937700
H	4.08644200	-2.85460400	2.13078500
H	4.68967000	-0.32312300	2.52000400
H	4.45042200	-1.99996200	4.38648600
H	2.80932300	-3.50881900	3.12381200
H	2.76107100	-1.53637300	4.54938200
H	4.25227800	0.44858700	4.03775000
H	2.93888500	1.22828000	1.98131600
H	1.61989400	-2.64542100	1.14607500
C	-3.81976600	-1.92035200	0.28664600
C	-2.84440400	-2.73483100	-0.28499300
C	-3.10222900	-4.07881600	-0.55650400
C	-4.35553600	-4.60543600	-0.26630000
C	-5.34070500	-3.79742500	0.29982500
C	-5.07030800	-2.46084700	0.57899900
H	-3.59780200	-0.87914200	0.50318900
H	-2.31723700	-4.70042000	-0.97718900
H	-4.56177600	-5.65129400	-0.47533800
H	-5.83211800	-1.83093100	1.03068100
S	-1.22081600	-2.10785600	-0.72077700
O	-0.26127900	-3.10920400	-0.23757000
O	-1.22478700	-1.79356100	-2.15940100
N	-1.16084500	-0.65869800	0.06310300
C	-0.76441900	-0.68263300	1.38751600
H	-0.45415400	-1.62953700	1.83669500
C	-1.23472900	0.35906700	2.30672400
C	-2.11339100	1.37276100	1.89665400
C	-0.76739600	0.36347700	3.63200800

C	-2.49087200	2.37623700	2.78030500
H	-2.48435200	1.35502800	0.87686100
C	-1.14609500	1.36937200	4.51093900
H	-0.08919600	-0.42731400	3.94964500
C	-2.00451000	2.38524000	4.08739200
H	-3.17561200	3.15247500	2.44618500
H	-0.77379500	1.36232500	5.53205400
H	-6.31742000	-4.21369000	0.53013800
H	-2.30049100	3.17146900	4.77653800

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C	0.54813400	2.76255500	-1.29972000
C	2.70380300	2.10298800	-0.58232500
C	1.71706200	3.24656000	-0.47604800
C	-0.59588800	2.46035700	-3.18456300
C	-1.13759600	1.54025700	-2.06765500
H	-0.12229700	1.91773600	-4.00733200
H	-1.34564800	3.14608000	-3.58748600
N	-0.23921200	1.82623500	-0.92710400
N	2.38374200	0.86589400	-0.45164300
O	0.43491100	3.25972900	-2.54501900
H	-1.02443600	0.48035200	-2.32216100
C	-2.58235600	1.80173900	-1.72990700
C	-3.52675900	0.78329300	-1.85189000
C	-2.99216500	3.06337600	-1.28807900
C	-4.86146500	1.01853500	-1.52732400
C	-4.32363500	3.30007200	-0.96361500
H	-2.25438600	3.85751100	-1.17214400
C	-5.26176700	2.27481600	-1.08012100
H	-4.63024200	4.28180400	-0.61212600
H	-6.30119900	2.45697600	-0.82174600
C	1.28250000	3.40723600	0.99002700
H	2.14510200	3.64935100	1.61694200
H	0.55157500	4.21681600	1.07341000
H	0.81248500	2.49454800	1.37322400
C	2.30490700	4.54793400	-1.01257200
H	1.55126000	5.33785200	-0.97518400
H	3.15639200	4.85417100	-0.40187300
H	2.64157100	4.44793100	-2.04507100
O	3.98859000	2.39772800	-0.83085200
C	4.64877400	1.11738800	-1.02828500
H	4.87801400	1.02375300	-2.09557700
H	5.57828000	1.13289400	-0.45718300
C	3.61785600	0.07817500	-0.55176000

H	3.85748500	-0.25440200	0.47078600
H	-5.58596200	0.21269500	-1.61570600
H	-3.19733700	-0.20182000	-2.17863000
C	3.48771100	-1.13475300	-1.43536100
C	2.27928500	-1.48903800	-2.03689300
C	4.60431200	-1.95789500	-1.61502200
C	2.18459500	-2.65294900	-2.79592800
H	1.39281800	-0.87439700	-1.89194200
C	4.51419700	-3.11106400	-2.38664900
H	5.54694400	-1.70197100	-1.13176400
C	3.30099500	-3.46290900	-2.97638200
H	1.22279100	-2.92237200	-3.22189700
H	5.38859100	-3.74294300	-2.51668900
H	3.22664500	-4.37246200	-3.56577500
Ni	0.66530800	0.17757700	0.44839800
C	1.78107900	-0.63431900	1.84206300
C	2.19200300	-2.07652100	1.71783800
C	2.25612900	0.14193200	2.83035100
C	3.43000900	-2.41279900	2.54732100
C	3.20045900	-0.32638100	3.90994500
C	3.30009200	-1.84592100	3.95375400
H	4.32223600	-1.98062300	2.06517400
H	4.20194900	0.10816500	3.75177500
H	4.13517200	-2.16077000	4.59042800
H	3.59124900	-3.49697100	2.56874500
H	2.38771500	-2.25339200	4.41301300
H	2.87411900	0.06370200	4.88448700
H	1.93205200	1.18379200	2.91117500
H	1.34942100	-2.71597100	2.02277600
C	-3.80779100	-2.01509200	0.14766800
C	-2.74871800	-2.82162200	-0.26495800
C	-2.90614200	-4.20094700	-0.39773600
C	-4.14457800	-4.77396200	-0.13029200
C	-5.21280000	-3.97555400	0.27546700
C	-5.04183700	-2.60106500	0.41859800
H	-3.65972500	-0.94497100	0.26277700
H	-2.05665600	-4.80960900	-0.69324500
H	-4.27428100	-5.84776400	-0.23132100
H	-5.86925900	-1.97801800	0.74770500
S	-1.14802500	-2.12584500	-0.67616000
O	-0.14765500	-3.06292100	-0.14869600
O	-1.13017200	-1.83860800	-2.12062200
N	-1.17389700	-0.65939000	0.07420000
C	-0.83738200	-0.63127300	1.41709900

H	-0.56566200	-1.56464400	1.91971200
C	-1.35747400	0.44557600	2.26716700
C	-2.21207700	1.43673300	1.76065800
C	-0.96540000	0.51576600	3.61492700
C	-2.63749000	2.48216900	2.56985400
H	-2.52677400	1.36831400	0.72485400
C	-1.39130800	1.56513100	4.41911000
H	-0.30278300	-0.25089600	4.01080400
C	-2.22294500	2.55760500	3.89957200
H	-3.30302900	3.23843700	2.15964000
H	-1.07546800	1.60933400	5.45815500
H	-6.17736100	-4.42781600	0.48850600
H	-2.55525500	3.37663100	4.53177300
H	2.34586200	-2.34903500	0.66575300

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C	1.74795700	-2.61489000	-1.35550400
C	-0.72251000	-2.83565600	-1.03398100
C	0.60786200	-3.55037000	-1.04018900
C	3.82141400	-2.18023800	-2.07879800
C	3.18999100	-0.91722700	-1.45295700
H	4.04085400	-2.08540700	-3.14543500
H	4.71908300	-2.51677100	-1.55365300
N	1.84559300	-1.37110500	-1.06513000
N	-0.96005600	-1.58342400	-0.89393000
O	2.81169800	-3.20822000	-1.93105100
H	3.07191600	-0.12020600	-2.20037000
C	3.96769400	-0.36274300	-0.28571700
C	4.99436600	0.55471500	-0.52081500
C	3.69001400	-0.75730400	1.02371000
C	5.72128300	1.08840800	0.53917100
C	4.40951200	-0.21511300	2.08543400
H	2.86715900	-1.43670300	1.22243500
C	5.42438300	0.70829000	1.84656600
H	4.15435200	-0.50057800	3.10197600
H	5.97654000	1.13915000	2.67692200
C	0.86177100	-4.10071600	0.38269500
H	0.05308000	-4.78204700	0.66300300
H	1.80240200	-4.65830200	0.39518700
H	0.91733300	-3.28189800	1.10572100
C	0.57087300	-4.71050900	-2.04384500
H	1.52059700	-5.24548300	-2.02926300
H	-0.22894700	-5.40229400	-1.77952100
H	0.39498400	-4.35843500	-3.06383100

O	-1.78268000	-3.66685600	-1.14175900	H	3.66845300	2.72311500	-1.43505100
C	-2.94570500	-2.81133300	-1.23521600	H	1.61873900	4.46428700	0.01311900
H	-3.30219000	-2.84473300	-2.27176700	S	-0.18695300	-0.25737700	2.70181100
H	-3.71406300	-3.20563500	-0.56722700	O	0.61208700	-1.01212000	1.64905100
C	-2.42382200	-1.42440900	-0.83138400	O	0.32253000	-0.38931500	4.06252300
H	-2.68566300	-1.22031300	0.21533400	C	-1.77928800	-1.11221500	2.62815700
H	6.50694300	1.81338500	0.34491800	C	-2.96185700	-0.37797400	2.70180100
H	5.20868300	0.87143800	-1.54087100	C	-1.81535600	-2.49432700	2.44472100
C	-2.93683400	-0.29397900	-1.67822300	C	-4.18632200	-1.03333200	2.57325500
C	-4.09734000	0.38099800	-1.29253600	H	-2.90628100	0.69967400	2.83706100
C	-2.28976700	0.07862000	-2.85884000	C	-3.03915500	-3.14412000	2.31876200
C	-4.61195700	1.40647000	-2.08023800	H	-0.88178400	-3.04642700	2.38708200
H	-4.58330100	0.10738300	-0.35660900	C	-4.22669300	-2.41237300	2.37437300
C	-2.79765200	1.11272700	-3.64143200	H	-5.11057500	-0.46355700	2.62359200
H	-1.37122100	-0.43015200	-3.14464100	H	-3.06729800	-4.22115100	2.16890100
C	-3.96226100	1.77389100	-3.25663100	H	-5.18264500	-2.91884200	2.26978800
H	-5.50801100	1.93320200	-1.76509400	H	-0.02198900	1.63163000	-2.08987700
H	-2.27895800	1.40725600	-4.54958700	H	1.47828600	2.62443000	1.61331900
H	-4.35488900	2.58383900	-3.86485800	H	-2.29509300	6.49198100	-0.13220500
Ni	0.43310000	-0.08881600	-0.22648300				
C	1.01937800	1.70776600	-0.23773200			TS-R-1	
C	0.84494300	2.01918800	-1.54646000	C	1.14820400	-2.22380200	1.82952700
C	1.97153100	2.43646300	0.64952800	C	2.59067500	-2.47446000	-0.09992000
C	1.70625000	3.00778200	-2.28474200	C	1.78395900	-3.24796700	0.91912000
C	2.44476800	3.73743300	0.00263800	C	0.76267700	-1.20735200	3.77026100
H	2.82892100	1.79559200	0.89409300	C	0.17390700	-0.38456800	2.61480100
C	2.87930000	3.48864300	-1.43687300	H	1.42486100	-0.64880100	4.43330300
H	1.07197200	3.86738100	-2.56225900	H	-0.01625100	-1.69680000	4.36764500
H	3.26375800	4.17531800	0.58548400	N	0.34997000	-1.28537000	1.45340600
H	3.31984700	4.38931100	-1.87995700	N	2.22500600	-1.36302500	-0.62766900
C	-0.81502600	1.43608700	0.95377500	O	1.54050100	-2.23836200	3.12271100
H	-1.55062300	0.73040200	0.52022100	H	0.79453600	0.50123200	2.41054300
N	-0.44302300	1.23238600	2.28789400	C	-1.23115700	0.08439300	2.87474600
C	-1.23471100	2.82832100	0.66743200	C	-1.50118900	1.45323000	2.93302300
C	-1.89034300	3.14151500	-0.53141500	C	-2.25886100	-0.82315400	3.15099100
C	-0.98798800	3.85819000	1.58356400	C	-2.76523300	1.91151100	3.29795800
C	-2.26864300	4.44495700	-0.81832400	C	-3.52324900	-0.36774900	3.51025600
H	-2.08644600	2.34725500	-1.24798500	H	-2.06483300	-1.89229700	3.07727100
C	-1.36431000	5.16750800	1.29173400	C	-3.77456900	1.00166800	3.60075400
H	-0.50929200	3.60833700	2.52574900	H	-4.31582400	-1.08149700	3.71757300
C	-2.00045900	5.46997800	0.09102700	H	-4.76172800	1.35570000	3.88463200
H	-2.77757900	4.66184900	-1.75521300	C	0.69534300	-4.00846700	0.13804000
H	-1.16291400	5.95592200	2.01289200	H	1.16519600	-4.74265000	-0.52282500
H	2.06189700	2.59405500	-3.23988200	H	0.03057500	-4.53866500	0.82632800

H	0.10173700	-3.31736600	-0.47015000
C	2.66135500	-4.22379600	1.70049200
H	2.05804400	-4.76485100	2.43226000
H	3.11166200	-4.94489300	1.01677300
H	3.46328800	-3.71294200	2.23685500
O	3.73729700	-3.03779600	-0.52614200
C	4.20743300	-2.19056800	-1.60776700
H	5.25841600	-1.96175700	-1.41632200
H	4.12449500	-2.76678700	-2.53365800
C	3.28672500	-0.95347700	-1.57292400
H	2.82279700	-0.76205800	-2.54474900
H	-2.95876500	2.97997600	3.33944200
H	-0.70705600	2.16069800	2.69898500
C	3.96151900	0.30708600	-1.09177600
C	3.94067100	1.46837900	-1.86459500
C	4.58756300	0.33116000	0.15853600
C	4.52799500	2.63902000	-1.39248700
H	3.41728700	1.46475600	-2.81693700
C	5.17853500	1.49936600	0.63057500
H	4.60213100	-0.57083700	0.77109900
C	5.14605900	2.65754900	-0.14472100
H	4.48388600	3.54177600	-1.99476900
H	5.66054200	1.50802700	1.60477100
H	5.59642700	3.57368500	0.22713000
Ni	0.27975300	-0.62387900	-0.48926700
C	-1.51087800	-1.16989800	-1.13366100
C	-1.43139000	-1.40917800	-2.46395500
C	-2.40574000	-2.01767500	-0.26407300
C	-2.11608400	-2.53806300	-3.17775700
C	-3.44684700	-2.79017700	-1.06925700
H	-1.79316200	-2.71955100	0.32413500
C	-2.77127200	-3.52676400	-2.21893500
H	-2.88535600	-2.10188800	-3.83936300
H	-3.99801600	-3.48760400	-0.42600700
H	-3.48202400	-4.16513400	-2.75655200
C	-1.91437000	1.09760400	-0.99991100
H	-1.53879500	1.23600900	0.02425100
N	-1.34635000	1.75203600	-2.03888400
C	-3.35761000	0.86342600	-1.09135600
C	-4.10990800	0.68723500	0.07459000
C	-4.01434000	0.83844400	-2.33189200
C	-5.48211700	0.46720200	0.01128000
H	-3.60075700	0.72278300	1.03340700
C	-5.38408800	0.62585900	-2.39315300

H	-3.42454600	0.98783700	-3.23205600
C	-6.12469600	0.43349400	-1.22354400
H	-6.04864400	0.32799400	0.92949000
H	-5.88368300	0.60763800	-3.35840100
H	-4.18511700	-2.08029700	-1.47058800
H	-2.00536400	-4.20087900	-1.80554500
H	-1.42363400	-3.05416200	-3.85767300
S	0.21258400	2.06410700	-1.91913200
O	1.00328900	0.78604400	-1.84778600
O	0.63390300	2.99536600	-2.95863700
C	0.48985400	2.86175000	-0.32599600
C	1.50941500	2.43113800	0.52035500
C	-0.31666600	3.94623700	0.02068300
C	1.74024500	3.11518400	1.71383500
H	2.11683400	1.57478400	0.23596300
C	-0.08763800	4.61517100	1.21946100
H	-1.11622100	4.25422100	-0.64834500
C	0.94614700	4.20622300	2.06240000
H	2.54819400	2.79305600	2.36685700
H	-0.71270600	5.46043200	1.49390300
H	1.12885900	4.73655600	2.99312400
H	-7.19673300	0.26414900	-1.27827600
H	-2.89959700	-1.39264100	0.49182500
H	-0.90793800	-0.68285800	-3.09290300

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C	1.09049100	-1.26888200	2.50443300
C	2.34018600	-2.40138300	0.79631100
C	1.61007800	-2.63199700	2.10174400
C	1.05664100	0.57841600	3.75476100
C	0.23930800	0.78601200	2.47165900
H	1.85024300	1.31345000	3.90203200
H	0.43187500	0.54077800	4.65431300
N	0.24643400	-0.55937700	1.84146900
N	1.95545100	-1.59730200	-0.12932700
O	1.67568100	-0.71636400	3.58747300
H	0.77164500	1.45191100	1.77536400
C	-1.13590700	1.35043400	2.69350800
C	-1.54114800	2.47861800	1.97876700
C	-2.02262600	0.76102300	3.59945100
C	-2.81434000	3.01140500	2.16186700
C	-3.29244700	1.29670900	3.78917900
H	-1.72340300	-0.13280500	4.14522700
C	-3.69001300	2.42332900	3.06987600

H	-3.97814800	0.82884800	4.49023800	C	-3.22242000	0.17913000	-0.87494900
H	-4.68656500	2.83250300	3.20918200	C	-3.75586900	0.10011600	0.41550800
C	0.44443300	-3.59837400	1.84310200	C	-4.08519700	0.03766900	-1.96947000
H	0.83615600	-4.56364400	1.50957700	C	-5.11110600	-0.13592500	0.61270800
H	-0.12304700	-3.75806900	2.76434000	H	-3.09122200	0.21035700	1.26881300
H	-0.22891600	-3.20496100	1.07622400	C	-5.43952800	-0.20556000	-1.77040200
C	2.55261400	-3.20626200	3.15888800	H	-3.67141200	0.12248500	-2.97023500
H	2.01969500	-3.32892500	4.10400800	C	-5.96078200	-0.29667000	-0.48035700
H	2.91752200	-4.18223400	2.83521500	H	-5.50453300	-0.19008300	1.62565700
H	3.41446500	-2.56076900	3.33757700	H	-6.09619500	-0.31916600	-2.62956800
O	3.49327500	-3.07032500	0.60981600	H	-3.72538300	-3.75056700	-0.63673800
C	3.90935000	-2.74081000	-0.74318700	H	-1.06751600	-4.76442500	-1.75336400
H	4.98308200	-2.54697000	-0.72031600	H	-1.76990000	-3.67782600	-3.93462900
H	3.70472800	-3.61397500	-1.37088500	H	-0.05833800	-2.49410600	-2.66358200
C	3.05204100	-1.52018400	-1.11608700	S	0.05782800	1.32048700	-2.51028200
H	2.63890100	-1.59990800	-2.12483600	O	0.96881900	0.23211100	-1.97903000
H	-3.12064000	3.88034900	1.58590800	O	0.34158000	1.77594800	-3.86608500
H	-0.85321600	2.92924900	1.26517600	C	0.37701300	2.71026800	-1.40406100
C	3.77034500	-0.19783200	-0.97306900	C	1.45698700	2.69888400	-0.52388900
C	4.00201600	0.60687300	-2.08912200	C	-0.49247700	3.80138000	-1.44987300
C	4.20444800	0.24102100	0.28235500	C	1.67483800	3.79709900	0.30903100
C	4.65959800	1.82649900	-1.95670100	H	2.11892500	1.83678100	-0.50181300
H	3.62125700	0.29300700	-3.05765300	C	-0.26780200	4.89290800	-0.61699900
C	4.86285100	1.46036200	0.41664800	H	-1.34005400	3.77828900	-2.13002700
H	4.01643100	-0.36900100	1.16626500	C	0.81679500	4.89297300	0.26217300
C	5.09166500	2.25622100	-0.70421800	H	2.52087500	3.79025600	0.99298900
H	4.81567000	2.45096800	-2.83136800	H	-0.94043000	5.74568800	-0.65099400
H	5.19356800	1.79110600	1.39794400	H	0.98744600	5.74650100	0.91247300
H	5.59502000	3.21328200	-0.59950100	H	-7.02081900	-0.48233100	-0.32891700
Ni	0.12421200	-0.67761400	-0.30713900				
C	-1.31686800	-1.75358100	-1.10158100			TS-R-3	
C	-1.10238500	-2.16802300	-2.52820300	C	1.95087300	-2.37170100	-1.36583300
C	-2.05342800	-2.49841700	-0.25349500	C	-0.46341000	-2.81729400	-1.05228300
C	-2.05733200	-3.28210800	-2.95352700	C	0.92442200	-3.41538200	-1.00586100
H	-1.21181800	-1.28943300	-3.17824600	C	3.83904100	-1.63786000	-2.30386900
C	-2.62666000	-3.84540100	-0.58541300	C	3.20089500	-0.53155400	-1.43584700
H	-2.31246000	-2.09307500	0.72766400	H	3.80911800	-1.42587300	-3.37703700
C	-2.09003400	-4.38592000	-1.90478300	H	4.86168200	-1.88492600	-2.01055400
H	-3.06804100	-2.86456800	-3.06523700	N	1.93716500	-1.14107700	-1.00274700
H	-2.44023300	-4.55864200	0.23177300	N	-0.81004400	-1.60420500	-0.80464700</

C	3.74738900	-0.34009700	1.04710100	H	3.46423200	4.32944000	-1.23697300
C	6.10595500	1.02008900	0.43761500	C	-1.12826600	1.37540900	1.06031300
C	4.58908000	0.09912700	2.06727800	H	-1.74793600	0.59913000	0.58323300
H	2.81531400	-0.84060500	1.29659000	N	-0.74023100	1.21079700	2.37164100
C	5.76837500	0.77554900	1.76771100	C	-1.59075600	2.73608800	0.72596200
H	4.30966500	-0.08417300	3.10092000	C	-2.47601800	2.94483400	-0.33776500
H	6.42036600	1.11719300	2.56662800	C	-1.16573700	3.84514500	1.47338300
C	1.20636800	-3.86079900	0.44771400	C	-2.91013900	4.22593600	-0.66496300
H	0.47656400	-4.62053000	0.74514100	H	-2.82063500	2.08981200	-0.91288000
H	2.20444600	-4.30436000	0.50709000	C	-1.60476200	5.12183000	1.14879400
H	1.14752100	-3.01233000	1.13600800	H	-0.49095600	3.67700300	2.30800600
C	1.02104300	-4.62089800	-1.94516900	C	-2.47430500	5.32212500	0.07468200
H	2.02366500	-5.04709500	-1.89551100	H	-3.59623100	4.36191300	-1.49821900
H	0.29946100	-5.38247900	-1.64883300	H	-1.26803200	5.97132600	1.73797100
H	0.82046200	-4.34640100	-2.98355400	H	-0.47358100	2.67657300	-1.86396600
O	-1.43831500	-3.70117000	-1.34153100	H	1.47030400	4.12490500	-2.69588700
C	-2.66842400	-2.94373700	-1.40112100	H	3.28015900	2.64457200	-1.69954200
H	-3.01792000	-2.95677100	-2.43896600	H	2.56561200	3.93420200	0.97413700
H	-3.40238600	-3.43707000	-0.75954900	S	-0.42491300	-0.26557500	2.86340300
C	-2.27514500	-1.53475600	-0.91701200	O	0.58624400	-0.95724000	1.97894600
H	-2.67855000	-1.36259100	0.08959600	O	-0.13521000	-0.28652200	4.29301900
H	7.02071300	1.55326700	0.19403200	C	-1.91584300	-1.24557100	2.58497800
H	5.51463900	0.80519200	-1.61979200	C	-3.16765200	-0.63124800	2.59961500
C	-2.75774800	-0.43252600	-1.82110900	C	-1.80010800	-2.61220900	2.33255800
C	-1.90680600	0.21995100	-2.71402200	C	-4.30755200	-1.39054400	2.33945800
C	-4.10921000	-0.07548400	-1.77776200	H	-3.23379200	0.43649700	2.79319300
C	-2.40257600	1.21902500	-3.54950800	C	-2.94185100	-3.36718100	2.08156000
H	-0.84840800	-0.03257200	-2.72195800	H	-0.81317500	-3.06553300	2.32291000
C	-4.60565300	0.91369200	-2.62058100	C	-4.19628800	-2.75504900	2.07555400
H	-4.76812400	-0.56793900	-1.06293600	H	-5.28402400	-0.91379200	2.33966100
C	-3.75062600	1.56421300	-3.50924000	H	-2.85255800	-4.43283700	1.88205900
H	-1.72674100	1.73730400	-4.22471100	H	-5.08730800	-3.34345600	1.87228800
H	-5.65552600	1.18850600	-2.57327900	H	0.90066200	1.76059700	-2.43921800
H	-4.13295600	2.34694100	-4.15829300	H	-2.81348900	6.32363100	-0.17610000
Ni	0.45335400	-0.13115500	-0.04860200				
C	0.67312600	1.75396900	-0.31388000			TS-R-4	
C	0.57837900	2.45021300	-1.63894600	C	-1.72986900	-2.51510000	-0.16997500
C	1.61080900	2.08147400	0.60252900	C	-0.21322700	-2.43502600	-2.08831100
C	1.41926800	3.72638000	-1.67554900	C	-1.52923800	-2.98659300	-1.58986100
C	2.73447100	3.04285600	0.34603700	C	-1.88898200	-2.72032100	2.03781500</

N	0.37407400	-1.37049600	-1.67805100	C	-3.64452800	1.86996800	-1.87471100
O	-1.90900700	-3.45110800	0.77893600	H	-1.67407900	2.63007300	-2.36471200
H	-1.30995000	-0.62181100	2.13268200	C	-4.11653700	2.99707800	-0.96685100
C	-3.43472100	-0.68932400	1.89375400	H	-4.43733500	1.97743500	0.91326200
C	-3.65839000	0.07481000	3.04170400	H	-4.07808600	0.92063000	-1.52414300
C	-4.51023000	-0.96841600	1.04741600	H	-5.19828600	3.14748100	-1.05680000
C	-4.93531700	0.53640400	3.34780900	H	-3.85832400	3.61308000	1.09786000
C	-5.78784700	-0.50455800	1.34925900	H	-3.64377300	3.93465600	-1.29369100
H	-4.33882100	-1.54113100	0.13780000	H	-3.99371900	2.01695400	-2.90393800
C	-6.00529000	0.24339300	2.50444000	H	-1.78246100	0.88992300	-2.41269100
H	-6.61515800	-0.72528900	0.67988100	H	-1.91339600	2.15093700	1.61429700
H	-7.00168400	0.60654000	2.74007000	C	3.68001200	1.86145700	1.65148700
C	-2.64807900	-2.39852600	-2.47263700	C	3.05586300	0.71889700	2.14706100
H	-2.47949200	-2.66411200	-3.52000100	C	3.72338100	-0.14185500	3.01502600
H	-3.61759000	-2.80425700	-2.16850800	C	5.03149600	0.14704700	3.39130900
H	-2.68273600	-1.30902100	-2.37990200	C	5.66511600	1.28752200	2.90110300
C	-1.53437400	-4.51342600	-1.67652100	C	4.98904600	2.14296800	2.03239200
H	-2.48254300	-4.90255800	-1.30061800	H	3.15065400	2.50299900	0.95153900
H	-1.40881900	-4.83011400	-2.71285100	H	3.22232700	-1.04255200	3.35679600
H	-0.73264500	-4.95407100	-1.08017700	H	5.56118900	-0.52495800	4.06136500
O	0.37376600	-3.13464300	-3.08241700	H	5.48435800	3.02878900	1.64438200
C	1.50989400	-2.33080200	-3.49490700	S	1.36758800	0.33219100	1.69091000
H	2.35780200	-3.00323100	-3.63725400	O	0.48021100	1.03643200	2.64397800
H	1.24922000	-1.85784700	-4.44766400	O	1.28457500	-1.13861300	1.67406700
C	1.69647700	-1.32460900	-2.34954500	N	1.26628200	0.93033500	0.16443500
H	1.86418800	-0.30943300	-2.72381000	C	0.34302500	2.00338600	-0.00349700
H	-5.09384200	1.13328300	4.24178500	H	0.06560000	2.49618600	0.93045800
H	-2.81547800	0.31818700	3.68661800	C	0.71433900	2.96528000	-1.07833500
C	2.79326600	-1.69884400	-1.38202000	C	1.68422000	2.65946600	-2.03812000
C	3.74725600	-0.76502500	-0.98166600	C	0.08580400	4.21620800	-1.13732800
C	2.85870300	-2.99813800	-0.87121500	C	2.00812600	3.57190900	-3.03801500
C	4.75025500	-1.11992500	-0.08459700	H	2.19114200	1.70067100	-1.96723500
H	3.68421000	0.25659300	-1.35020300	C	0.41148800	5.13008300	-2.13254800
C	3.85786600	-3.35532400	0.02611800	H	-0.67751100	4.45263700	-0.39733500
H	2.11400700	-3.73489600	-1.17148500	C	1.37118100	4.80940800	-3.09209300
C	4.80591200	-2.41447700	0.42220500	H	2.76801200	3.31951400	-3.77349000
H	5.47014300	-0.37361600	0.24268700	H	-0.08416200	6.09695600	-2.16039900
H	3.89338000	-4.36651200	0.42198300	H	6.68861000	1.50778200	3.19209300
H	5.58054900	-2.68538300	1.13490900	H	1.62483600	5.52253600	-3.87155800
Ni	-0.43214300	0.11960900	-0.51757800				
C	-1.60831200	1.71307000	-0.41767600			TS-R-5	
C	-2.33997600	2.18393700	0.60907300	C	-2.93012400	1.33413300	0.82526000
C	-2.12080100	1.77098300	-1.84106800	C	-1.18331300	2.59685900	1.83840300
C	-3.73745100	2.71103500	0.48183200	C	-2.47947300	1.88565200	2.15985700

C	-4.07417300	1.35231600	-1.07576200	Ni	-0.13925600	0.20044500	0.28420000
C	-3.07965100	0.17609900	-1.05340000	C	-0.13708900	-1.45381800	-0.85048300
H	-3.75723500	2.17419100	-1.72840400	C	0.19604100	-1.10261500	-2.27976500
H	-5.10044800	1.06740700	-1.31221600	C	-0.83849200	-2.56438400	-0.55271300
N	-2.27775000	0.45696900	0.14746300	C	-0.68573200	-1.85908000	-3.27161100
N	-0.21640200	2.04034100	1.21006100	C	-1.33532600	-3.56160200	-1.55845300
O	-4.04815500	1.85239600	0.28612200	C	-0.71764000	-3.34240900	-2.93491100
H	-2.42083900	0.20132400	-1.93240200	H	-1.71484100	-1.46832900	-3.23116500
C	-3.78437800	-1.15989200	-0.99415700	H	-2.43326500	-3.51994100	-1.62533000
C	-4.39049800	-1.64727600	-2.15613100	H	-1.26542000	-3.91020600	-3.69581800
C	-3.90492900	-1.88770000	0.18911700	H	-0.33084500	-1.68982800	-4.29489400
C	-5.10743800	-2.83928900	-2.13728900	H	0.31232300	-3.72648000	-2.94107600
C	-4.61430700	-3.08624600	0.20730900	H	-1.11504200	-4.57662000	-1.19652700
H	-3.41074200	-1.52788000	1.08775400	H	-1.04292400	-2.79829400	0.49321000
C	-5.22092800	-3.56300400	-0.95191100	H	0.12432100	-0.01649300	-2.43880500
H	-4.68991200	-3.65138500	1.13216500	C	4.85761000	-0.95258900	0.81372600
H	-5.77356000	-4.49789900	-0.93443200	C	4.30528300	-0.60279600	-0.41872400
C	-2.17498800	0.70910300	3.10244500	C	4.68769900	-1.25538300	-1.58684700
H	-1.73737100	1.07502300	4.03569800	C	5.64631800	-2.26489700	-1.52130500
H	-3.09881500	0.17477500	3.34282100	C	6.20576700	-2.61809200	-0.29644300
H	-1.47217000	0.00872800	2.63834100	C	5.81029500	-1.96312200	0.87027700
C	-3.51044600	2.82767400	2.77066600	H	4.52904700	-0.43693000	1.71229900
H	-4.44530500	2.29296600	2.95204300	H	4.23177000	-0.95842500	-2.52691100
H	-3.14113200	3.21288000	3.72304900	H	5.95382200	-2.77769700	-2.42867400
H	-3.72364800	3.67684000	2.12041800	H	6.24498800	-2.24336600	1.82576400
O	-1.06413500	3.89094300	2.17211400	S	3.05516600	0.68551800	-0.48145800
C	0.29099900	4.25805600	1.77489800	O	2.61556800	0.75771800	-1.88471900
H	0.23530600	5.21893100	1.26019600	O	3.63771200	1.89295600	0.12367800
H	0.87666500	4.36526800	2.69309800	N	1.92225200	0.16156300	0.57268300
C	0.76294600	3.08829800	0.89095500	C	1.43108600	-1.15012100	0.39031700
H	1.76624900	2.74561300	1.16762300	H	1.97065400	-1.76828900	-0.33978800
H	-5.56917900	-3.20748000	-3.04909000	C	1.19574300	-1.88289900	1.66877900
H	-4.29176000	-1.08792500	-3.08604100	C	1.00064200	-1.19101600	2.87190400
C	0.75469900	3.38230500	-0.59427000	C	1.19444800	-3.28214300	1.69444200
C	1.85441200	4.02455900	-1.16811200	C	0.77438600	-1.88116200	4.05753700
C	-0.32711300	3.03824700	-1.40928000	H	1.04591000	-0.10399500	2.85411900
C	1.87205400	4.31410000	-2.52723800	C	0.97739800	-3.97343900	2.88260800
H	2.71946200	4.24907600	-0.55050500	H	1.36141700	-3.82578200	0.76615800
C	-0.30381600	3.31646200	-2.77374700	C	0.75695900	-3.27579800	4.06799600
H	-1.18605900	2.53098400	-0.97631800	H	0.62222700	-1.32825400	4.98175000
C	0.79609400	3.95543100	-3.33627400	H	0.98420900	-5.06029300	2.88338100
H	2.74133000	4.79914400	-2.96193700	H	1.25695100	-1.31629000	-2.47745700
H	-1.14648800	3.02576600	-3.39778500	H	6.95008500	-3.40827000	-0.24782800
H	0.81997000	4.16599600	-4.40181000	H	0.58600700	-3.81465400	4.99601200

TS-S				C	3.29583700	-3.42355800	-2.70154600
C	0.84327700	2.87087000	-1.20357500	H	5.15708500	-4.07940300	-1.83398600
C	2.92272700	2.08936800	-0.29186800	H	1.44915100	-2.51479600	-3.35551700
C	1.97668000	3.26725000	-0.28377700	H	3.17115400	-4.31693600	-3.30671200
C	-0.39435700	2.92447900	-3.04815700	Ni	0.66991500	0.16756700	0.20646200
C	-0.92832100	1.85221800	-2.08299200	C	1.24458900	-1.03915900	1.72680900
H	0.10915300	2.50477100	-3.92470800	C	1.74149300	-2.43224000	1.42693600
H	-1.14592300	3.64829000	-3.36933700	C	1.64002500	-0.38367200	2.83741600
N	0.10716900	1.83777600	-1.02145900	C	2.99304100	-2.79296700	2.22265600
N	2.55421800	0.87327900	-0.12044200	C	2.62851200	-0.91725800	3.83614900
O	0.61158900	3.64525500	-2.28051000	C	2.82822200	-2.42077700	3.68847400
H	-0.96498200	0.85792500	-2.53936800	H	3.86530700	-2.26129000	1.81081600
C	-2.28062500	2.18502200	-1.50404200	H	3.59793900	-0.40099200	3.72711400
C	-3.32109900	1.25977400	-1.56891200	H	3.68402200	-2.75676200	4.28515800
C	-2.50240600	3.41940100	-0.88428000	H	3.21251100	-3.86067400	2.10462100
C	-4.56443500	1.55945800	-1.01723000	H	1.94608900	-2.94126000	4.08831200
C	-3.74361300	3.72069700	-0.33331400	H	2.29221200	-0.67047200	4.85310700
H	-1.69227300	4.14676500	-0.82591600	H	1.20613000	0.59298600	3.06400900
C	-4.77745300	2.78719500	-0.39622500	H	1.90503100	-2.57418900	0.35410500
H	-3.90466200	4.68124300	0.14922100	C	-3.85285700	-1.76795800	-0.11943800
H	-5.74574000	3.01839100	0.03900200	C	-2.91873300	-2.48671900	-0.86227200
C	1.40873900	3.42124800	1.14077700	C	-3.27117800	-3.68662100	-1.48175800
H	2.21266100	3.64422200	1.84812100	C	-4.57259000	-4.16058800	-1.36666900
H	0.68584900	4.24222300	1.16795100	C	-5.51589000	-3.44518700	-0.62941600
H	0.89974400	2.50338500	1.45549400	C	-5.15407800	-2.25502800	-0.00528500
C	2.66335400	4.55005100	-0.73889600	H	-3.55737200	-0.83815300	0.35958100
H	1.94623700	5.37339600	-0.74189800	H	-2.52154100	-4.24175700	-2.03844400
H	3.47800000	4.80086600	-0.05685400	H	-4.85159200	-5.09348400	-1.84872700
H	3.07599200	4.45766100	-1.74463800	H	-5.88411900	-1.69963400	0.57800700
O	4.22943700	2.32920000	-0.48759200	S	-1.22924000	-1.91086600	-1.06526800
C	4.86197800	1.02177700	-0.55920300	O	-0.38075300	-3.06141900	-0.71361700
H	5.21410600	0.88077600	-1.58611400	O	-1.11802900	-1.38179600	-2.43824400
H	5.71759400	1.03045900	0.11856300	N	-1.12883700	-0.64289800	-0.05202500
C	3.74737000	0.02782700	-0.17041900	C	-0.73377700	-0.90893500	1.28619000
H	3.90967900	-0.35951800	0.84766700	H	-0.75162500	-1.96679100	1.57398200
H	-5.36357300	0.82397900	-1.06593600	C	-1.34816800	-0.02232800	2.31024500
H	-3.13681700	0.29398100	-2.03562400	C	-1.89016900	1.22331200	1.97350600
C	3.59139400	-1.14755300	-1.10286100	C	-1.38007400	-0.42906800	3.65026600
C	4.55117200	-2.16329800	-1.07301600	C	-2.43796500	2.04453300	2.95415300
C	2.49190500	-1.27453700	-1.95587500	H	-1.88036200	1.53319600	0.93209200
C	4.40881600	-3.29253000	-1.87253600	C	-1.92945100	0.39026700	4.62964400
H	5.40246000	-2.07887800	-0.39782800	H	-0.95466100	-1.39552100	3.91788300
C	2.33859900	-2.41471000	-2.74116500	C	-2.45702400	1.63446500	4.28605400
H	1.72241000	-0.50328100	-1.97923200	H	-2.85878400	3.00652900	2.67019300

H	-1.94800900	0.05758400	5.66424700
H	0.94261200	-3.15202100	1.66134700
H	-6.53140100	-3.82061100	-0.53794900
H	-2.88607700	2.27564100	5.05145700

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C	-2.53531600	1.44896800	-1.86091500
C	-1.12306000	3.03449200	-0.56772400
C	-2.49466900	2.76686500	-1.13061400
C	-3.38896000	-0.00037700	-3.32596600
C	-2.44425600	-0.72421500	-2.35622500
H	-2.98061000	0.09577900	-4.33688600
H	-4.38970100	-0.43409500	-3.37606300
N	-1.83975000	0.40319200	-1.60144700
N	-0.25056000	2.17368000	-0.18433100
O	-3.51676200	1.33940600	-2.78101900
H	-1.64492300	-1.25896900	-2.87396600
C	-3.13567400	-1.66156200	-1.39638900
C	-4.27418700	-1.24025100	-0.70009400
C	-2.63728500	-2.94398900	-1.17667400
C	-4.91139500	-2.09532500	0.19129000
C	-3.26647200	-3.79694600	-0.27284500
H	-1.73110900	-3.26385800	-1.68109500
C	-4.40667600	-3.37829500	0.40588500
H	-2.84844400	-4.78365600	-0.09533200
H	-4.89824500	-4.04338300	1.11099000
C	-3.46656800	2.62896000	0.06574100
H	-3.43247800	3.53030400	0.68438100
H	-4.48807900	2.50016900	-0.30300400
H	-3.20047300	1.76183500	0.67945900
C	-2.93928200	3.91736900	-2.03816900
H	-3.93801000	3.71576600	-2.42645800
H	-2.95970100	4.85188000	-1.47648800
H	-2.26327400	4.04572900	-2.88728100
O	-0.83138000	4.33906300	-0.38372200
C	0.40694800	4.36479300	0.36513400
H	1.06737700	5.10050500	-0.09803500
H	0.16632000	4.67726200	1.38683000
C	0.92276000	2.91606500	0.28867000
H	1.18221000	2.54853200	1.29099500
H	-5.79605500	-1.75999300	0.72660900
H	-4.66723200	-0.23613700	-0.86159000
C	2.11736100	2.72857400	-0.61968100
C	3.36235300	3.20729800	-0.19727800

C	2.01722100	2.11053600	-1.86755000
C	4.48603700	3.07488900	-1.00526700
H	3.45005500	3.67632100	0.78282500
C	3.14420500	1.97854300	-2.67780600
H	1.05890600	1.71194500	-2.19485200
C	4.37841100	2.45838100	-2.25051600
H	5.44708300	3.44490100	-0.66006400
H	3.05518400	1.48446700	-3.64201300
H	5.25556200	2.34806000	-2.88202700
Ni	-0.39927300	0.12993300	-0.17387500
C	-0.80176800	-0.16204700	1.73553900
C	-1.48727000	-1.29812100	1.96484100
C	-0.95636600	1.04095500	2.63658200
C	-2.54679500	-1.45088100	3.01487700
H	-1.22692700	-2.19485800	1.39730400
C	-1.70350800	0.71159600	3.92879900
H	0.03120600	1.45893400	2.88121800
C	-2.94502800	-0.11668000	3.62947500
H	-2.16450300	-2.12247200	3.80300300
H	-1.95867600	1.63354400	4.46523800
H	-3.54550400	-0.27082600	4.53344000
C	1.18350200	-0.75528700	1.16860000
H	1.61324600	-0.14008300	0.34119200
N	1.15802400	-2.13287500	0.98452300
C	1.78580000	-0.33350600	2.45614600
C	2.66176600	0.75527600	2.50407500
C	1.49658700	-1.01382600	3.64630100
C	3.20403300	1.18749300	3.71285800
H	2.94414000	1.24421900	1.57256800
C	2.03990200	-0.58657100	4.85094500
H	0.83210900	-1.87294000	3.59991300
C	2.88558400	0.52377100	4.89364300
H	3.88666500	2.03427600	3.72740700
H	1.80184600	-1.12015200	5.76780600
H	-1.03756100	0.13727200	4.58869700
H	-3.58490200	0.43288600	2.92106500
H	-3.41996900	-1.96925200	2.59989900
S	0.92619800	-2.61928200	-0.50203100
O	0.17379200	-1.56126400	-1.29302700
O	0.38502300	-3.97929500	-0.54719900
C	2.52092400	-2.68251100	-1.30879000
C	3.08524100	-1.51366100	-1.82121000
C	3.22781900	-3.88350000	-1.32771800
C	4.36997300	-1.55163700	-2.35376700

H	2.51171300	-0.59020800	-1.81377700
C	4.50882200	-3.91247500	-1.86970100
H	2.75917400	-4.77818000	-0.92951600
C	5.08262200	-2.74882400	-2.37924000
H	4.81216500	-0.64168500	-2.75286900
H	5.06132700	-4.84776000	-1.89608400
H	6.08410900	-2.77645000	-2.79979800
H	-1.48714100	1.84707200	2.10474200
H	3.30419500	0.85641700	5.83954700

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C	-2.55362000	1.45667100	-1.75639000
C	-1.20883200	3.08358300	-0.47537500
C	-2.60188400	2.70753400	-0.91253600
C	-3.24180800	0.10514000	-3.38933500
C	-2.31685500	-0.65687700	-2.43310100
H	-2.77559500	0.33108300	-4.35379100
H	-4.20643300	-0.37873100	-3.55339400
N	-1.79820800	0.43520300	-1.56368700
N	-0.28285500	2.27782400	-0.10145900
O	-3.49150000	1.37032900	-2.72230200
H	-1.47222800	-1.12018900	-2.94794200
C	-3.02064600	-1.68645500	-1.58344500
C	-2.46756500	-2.95179500	-1.39377900
C	-4.21780700	-1.35909900	-0.93545900
C	-3.09182700	-3.87375700	-0.55714900
C	-4.84595100	-2.28153300	-0.10577700
H	-4.65630800	-0.37089800	-1.07515800
C	-4.27974400	-3.54169900	0.08738500
H	-5.77133600	-2.01542800	0.39818600
H	-4.76220500	-4.25790800	0.74697200
C	-3.40616300	2.35410700	0.36032900
H	-3.45148800	3.22132000	1.02613300
H	-4.42825300	2.07725900	0.08552100
H	-2.93349200	1.52216600	0.89395600
C	-3.27409100	3.85788800	-1.66232200
H	-4.28507800	3.56874200	-1.95140900
H	-3.32893900	4.73914400	-1.02203600
H	-2.72666700	4.12970900	-2.56786600
O	-0.95404300	4.40560600	-0.41266700
C	0.37527900	4.53384200	0.14366900
H	0.96355800	5.15854900	-0.53282100
H	0.28218300	5.03474100	1.11129600
C	0.89101700	3.08118300	0.25197800

H	1.16592700	2.84780800	1.28991400
H	-2.62691600	-4.84196500	-0.39587300
H	-1.52000100	-3.20100000	-1.86026400
C	2.07182200	2.78655900	-0.64290000
C	3.35680000	3.12835500	-0.21165300
C	1.90767600	2.22796300	-1.91328000
C	4.45952400	2.92345700	-1.03463800
H	3.49167500	3.55147300	0.78344100
C	3.01178000	2.02508400	-2.73878900
H	0.91423000	1.93226800	-2.24536900
C	4.28749900	2.37419800	-2.30326400
H	5.45288700	3.18684500	-0.68338500
H	2.87482900	1.57675600	-3.71931000
H	5.14710700	2.21224200	-2.94784300
Ni	-0.33994200	0.19104500	-0.15641800
C	-0.84994000	-0.27686900	1.70409700
C	-1.62019700	-1.56113900	1.80367500
C	-1.05594000	0.72933600	2.57996100
C	-2.32635200	-1.71733300	3.14875300
H	-0.94890000	-2.40940400	1.61378500
C	-2.11437700	0.72445100	3.64481700
H	-0.38809500	1.59539700	2.57190400
C	-3.08356600	-0.44251600	3.49313000
H	-1.58521900	-1.92021300	3.93536700
H	-2.65999100	1.68049600	3.65197000
H	-3.68037500	-0.56322200	4.40467300
C	1.19568300	-0.69488100	1.25797900
H	1.60752900	-0.03433200	0.45400700
N	1.26776900	-2.06675000	1.04474200
C	1.74065900	-0.26541000	2.56781600
C	2.47153700	0.91939800	2.67614900
C	1.53511900	-1.03426100	3.72080200
C	2.94424200	1.36068700	3.91080200
H	2.70100400	1.47754800	1.77026100
C	2.00672700	-0.59766800	4.95056600
H	0.99751400	-1.97423200	3.62632200
C	2.70284600	0.60912500	5.05580200
H	3.51580800	2.28424300	3.97284700
H	1.83359600	-1.20089100	5.83827900
H	-1.62001800	0.67344100	4.63070700
H	-3.79572600	-0.22663700	2.68123400
H	-3.00126200	-2.58131000	3.11938500
H	-2.36799300	-1.59584100	0.99982700
S	1.04060900	-2.54167400	-0.44651100

O	0.26645900	-1.48731900	-1.22519700
O	0.52392400	-3.91015800	-0.51298400
C	2.63498500	-2.56689400	-1.25495700
C	3.19741800	-1.37387800	-1.71141300
C	3.33973400	-3.76622700	-1.33757100
C	4.47699700	-1.38815000	-2.25647500
H	2.62837100	-0.44903200	-1.65313700
C	4.61708800	-3.76997400	-1.88932000
H	2.87203300	-4.67855200	-0.98062800
C	5.18769000	-2.58356200	-2.34670000
H	4.91563700	-0.46004500	-2.61530200
H	5.16818000	-4.70331600	-1.96526600
H	6.18532800	-2.59146900	-2.77712700
H	3.06836100	0.94779600	6.02134600

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C	0.20413000	-2.21568000	1.93072500
C	1.82534200	-2.74345600	0.15565400
C	0.71207900	-3.29921700	1.00372500
C	-0.41070400	-1.39009700	3.90060700
C	-0.80964800	-0.43432500	2.76841800
H	0.46083100	-1.04400600	4.46729700
H	-1.22237000	-1.64243700	4.58449700
N	-0.11515800	-1.01007300	1.60402700
N	1.88769600	-1.53486400	-0.25390800
O	-0.02016900	-2.59749200	3.20203000
H	-0.42339900	0.57509100	2.95297800
C	-2.30805300	-0.36049900	2.56647500
C	-3.06437300	0.33408500	3.51733700
C	-2.95889100	-0.95192400	1.48310700
C	-4.44311100	0.44415500	3.38554400
C	-4.34282100	-0.84137000	1.35114200
H	-2.38482300	-1.47492500	0.72023400
C	-5.08604500	-0.14410000	2.29731700
H	-4.83111000	-1.29572400	0.49380800
H	-6.16266400	-0.05297300	2.18653400
C	-0.44412800	-3.65279300	0.04040800
H	-0.12391000	-4.43435300	-0.65468700
H	-1.30868300	-4.01951600	0.60253500
H	-0.73943400	-2.77082100	-0.53975000
C	1.16856800	-4.53489700	1.77664700
H	0.33949000	-4.94614500	2.35418900
H	1.52249100	-5.29453400	1.07838100
H	1.98099400	-4.30352700	2.46929900

O	2.77260000	-3.60173500	-0.26120800
C	3.56166200	-2.85679200	-1.23194000
H	4.61473000	-3.01527900	-0.99216300
H	3.33945000	-3.27351500	-2.21831700
C	3.09437900	-1.39161600	-1.07300200
H	2.80084300	-0.95920700	-2.03613900
H	-5.01504700	0.99679600	4.12560300
H	-2.55962500	0.81354900	4.35554300
C	4.11883200	-0.50593400	-0.40485800
C	4.31215100	-0.54583700	0.97873100
C	4.95220900	0.30055900	-1.18118100
C	5.33080100	0.19444600	1.57118400
H	3.64993700	-1.15273600	1.59434700
C	5.97151200	1.04243600	-0.59074400
H	4.79005700	0.35379700	-2.25632600
C	6.16784800	0.98525800	0.78687600
H	5.46924000	0.15780000	2.64831500
H	6.60679600	1.67258100	-1.20700300
H	6.96070700	1.56591900	1.24947500
Ni	0.36041500	-0.18855300	-0.26668400
C	0.97856000	1.65982700	-0.14561600
C	1.20158600	2.15715000	1.25835000
C	1.69771300	2.12943300	-1.18281900
C	1.98179900	3.47063300	1.28740800
C	2.81186400	3.12445700	-1.05105100
H	1.40008200	1.84493300	-2.19441700
C	3.21309100	3.36469500	0.39886800
H	1.32732300	4.27567800	0.92348900
H	3.68485100	2.81248500	-1.64207900
H	3.83734600	4.26253800	0.47883500
C	-1.01857500	1.46361300	-0.86556200
H	-1.59247500	0.63112300	-0.39120600
N	-1.01064600	1.48883400	-2.26549500
C	-1.43377000	2.75481200	-0.26366100
C	-2.14450100	2.78801800	0.93942600
C	-1.12379600	3.96847800	-0.89325300
C	-2.51445800	3.99823100	1.52055700
H	-2.42127900	1.85037600	1.41395400
C	-1.50024300	5.17554300	-0.31800200
H	-0.58836200	3.93633600	-1.83823600
C	-2.18892000	5.19897300	0.89647100
H	-3.06882800	3.99672200	2.45683200
H	-1.25447600	6.10896500	-0.81844300
H	0.23642400	2.28893400	1.76776900

H	2.25927000	3.72841900	2.31671600
H	3.82965700	2.52376700	0.74616300
H	2.48148100	4.07254200	-1.51013500
S	-0.89201400	0.08160200	-2.95657100
O	0.13187600	-0.80369400	-2.25533200
O	-0.73674400	0.18114800	-4.40449600
C	-2.43142400	-0.81130300	-2.64385800
C	-3.60678700	-0.09681200	-2.42105400
C	-2.44064100	-2.20579400	-2.66075800
C	-4.80049200	-0.78678100	-2.22261100
H	-3.56907300	0.98971400	-2.40123300
C	-3.63418400	-2.88943900	-2.44874700
H	-1.51060900	-2.73954300	-2.83751000
C	-4.81585000	-2.18033100	-2.23414200
H	-5.71997200	-0.23354600	-2.04954400
H	-3.64529400	-3.97652900	-2.45944200
H	-5.74864900	-2.71509200	-2.07522100
H	1.74690700	1.38600400	1.83079300
H	-2.47823100	6.14627800	1.34354300

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C	0.07675200	-2.25773500	1.90306300
C	1.71402800	-2.80645800	0.15926700
C	0.54028600	-3.33343800	0.94412300
C	-0.47406700	-1.45184400	3.89952900
C	-0.83447300	-0.44977400	2.79259900
H	0.41414300	-1.16124900	4.47120100
H	-1.29398900	-1.68333100	4.58107400
N	-0.19265800	-1.03425200	1.60420200
N	1.81092900	-1.60930000	-0.27896100
O	-0.14196500	-2.65797900	3.16946900
H	-0.38780500	0.53226400	2.99422900
C	-2.32894600	-0.28272200	2.61830800
C	-3.02709400	0.43397000	3.59672100
C	-3.03034000	-0.80928700	1.53312000
C	-4.39838700	0.62942500	3.49130000
C	-4.40704200	-0.61403500	1.42902300
H	-2.50055600	-1.34850600	0.74928000
C	-5.09254900	0.10436200	2.40247000
H	-4.93606500	-1.02189900	0.57257200
H	-6.16350900	0.26097100	2.31233100
C	-0.60317900	-3.56756000	-0.06744600
H	-0.30963200	-4.33072900	-0.79437200
H	-1.50458500	-3.91009700	0.45032100

H	-0.83005300	-2.64229100	-0.60903000
C	0.89067500	-4.62830700	1.67285700
H	0.01839400	-5.00455100	2.20940900
H	1.21049500	-5.38130100	0.95126400
H	1.69660800	-4.48493700	2.39534600
O	2.68768100	-3.67618700	-0.16007300
C	3.54961000	-2.96161800	-1.08824000
H	4.58287300	-3.12524600	-0.77683600
H	3.38810200	-3.39549900	-2.07943500
C	3.08705400	-1.49061300	-0.98646000
H	2.88967200	-1.07292000	-1.98109900
H	-4.92411800	1.19879900	4.25253800
H	-2.48120800	0.86271900	4.43674600
C	4.06706500	-0.60881800	-0.24367000
C	3.88687800	-0.26782400	1.09819800
C	5.22545800	-0.18484900	-0.90211500
C	4.86234900	0.46205700	1.77451500
H	2.97148700	-0.56190000	1.60630700
C	6.19915600	0.54363300	-0.22682300
H	5.36286300	-0.43026400	-1.95434700
C	6.02201600	0.86370600	1.11796700
H	4.71017400	0.72343300	2.81840900
H	7.09336700	0.86713800	-0.75192600
H	6.77941500	1.43499000	1.64687500
Ni	0.36209200	-0.17171500	-0.28372600
C	1.06357100	1.64532400	-0.30593400
C	1.33230200	2.14737700	0.91721900
C	1.83734000	2.07769400	-1.51611200
C	2.45856500	3.09351400	1.21580800
C	2.58558700	3.38604500	-1.27125700
H	1.15468400	2.16505800	-2.37136300
C	3.38376200	3.29628000	0.02102400
H	2.01619300	4.05863100	1.51952300
H	3.23958100	3.61540900	-2.12066200
H	4.00344200	4.18823500	0.17101600
C	-1.00698500	1.52048100	-0.87830600
H	-1.55287900	0.68811900	-0.37121200
N	-1.06871400	1.54319800	-2.27374700
C	-1.36403600	2.81492800	-0.25248100
C	-1.87497400	2.86008900	1.04814300
C	-1.17904400	4.02010900	-0.94227500
C	-2.16121200	4.07335300	1.66347800
H	-2.05065200	1.92739700	1.57698600
C	-1.45964800	5.23328500	-0.32444600

H	-0.81314400	3.98177900	-1.96457500
C	-1.94571100	5.26964500	0.98257900
H	-2.56398300	4.08121700	2.67438900
H	-1.30365500	6.16108100	-0.86956900
H	3.03479200	2.75314100	2.08978300
H	4.07431100	2.44509800	-0.05325500
H	1.85763100	4.20690000	-1.19945400
S	-0.90538100	0.14370600	-2.97357500
O	0.15794400	-0.70434400	-2.28774800
O	-0.76677600	0.25310800	-4.42177600
C	-2.40993300	-0.80363800	-2.65482700
C	-3.58958200	-0.13903400	-2.32779800
C	-2.38730400	-2.19309900	-2.77664900
C	-4.75499000	-0.87495400	-2.12256400
H	-3.57891300	0.94444600	-2.23764500
C	-3.55142300	-2.92249400	-2.55762600
H	-1.45471100	-2.68861400	-3.03403000
C	-4.73682800	-2.26382800	-2.23100000
H	-5.67911100	-0.36004700	-1.87227500
H	-3.53681500	-4.00589500	-2.64756700
H	-5.64703000	-2.83407800	-2.06553300
H	0.64214300	1.95061000	1.74180400
H	-2.16723800	6.22075100	1.45918600
H	2.55659000	1.28950500	-1.79599700

TS-S-5

C	1.03420800	2.76646300	-1.37764800
C	3.08057400	1.87732300	-0.45440100
C	2.24587200	3.13265400	-0.54977200
C	-0.35301400	2.87631000	-3.11111100
C	-0.87055800	1.85686500	-2.08221000
H	0.04073000	2.41004800	-4.01960100
H	-1.07920900	3.64603200	-3.37977400
N	0.24673600	1.79043200	-1.10928300
N	2.62441000	0.72767500	-0.11499800
O	0.76253500	3.53565700	-2.44853000
H	-1.00511800	0.86140200	-2.51591300
C	-2.14634000	2.28380500	-1.40181100
C	-3.26384100	1.45073300	-1.41860200
C	-2.22364000	3.51443700	-0.74235500
C	-4.43934300	1.83456700	-0.77893500
C	-3.39751800	3.90136600	-0.10317700
H	-1.35304900	4.17029200	-0.72272500
C	-4.50770500	3.05811600	-0.11745100

H	-3.44599200	4.85820300	0.41021800
H	-5.42241400	3.35513400	0.38818200
C	1.75324500	3.50194200	0.86317900
H	2.60205400	3.68389800	1.52880200
H	1.14906200	4.41291800	0.81938800
H	1.13773800	2.69645700	1.27851700
C	3.03149300	4.28577300	-1.16562900
H	2.39676100	5.17099700	-1.23598200
H	3.89602600	4.52370300	-0.54303600
H	3.38970600	4.04591400	-2.16789100
O	4.38687800	1.97767800	-0.74978300
C	4.91740400	0.62755300	-0.66022000
H	5.25343700	0.33752700	-1.66026300
H	5.77533700	0.65451200	0.01518400
C	3.73698500	-0.22876700	-0.15149100
H	3.91847400	-0.56715200	0.87917800
H	-5.29825000	1.16826900	-0.78998500
H	-3.19310500	0.48550200	-1.91628300
C	3.44376000	-1.44823600	-0.98887900
C	4.29317000	-2.55320600	-0.88083400
C	2.34904600	-1.51318400	-1.85264700
C	4.04593200	-3.70830100	-1.61518600
H	5.14287600	-2.51262400	-0.19921500
C	2.09151300	-2.67557200	-2.57536900
H	1.66448300	-0.66956600	-1.93736800
C	2.93852100	-3.77282900	-2.45908000
H	4.70846200	-4.56388200	-1.51574400
H	1.20493700	-2.71944500	-3.20012800
H	2.73141100	-4.68263700	-3.01532600
Ni	0.66827600	0.17208600	0.20101500
C	1.22728200	-0.91196000	1.80688000
C	1.73153800	-2.15120500	1.65086900
C	1.65928500	-0.01338100	2.94018400
C	2.80772100	-2.73213700	2.52233600
C	2.94724200	-0.48921000	3.61642300
H	0.85506900	0.05077300	3.68718000
C	2.92139900	-1.99210700	3.84899700
H	3.77669300	-2.70071200	1.99114700
H	3.81120900	-0.24258100	2.97948100
H	3.80896200	-2.31909100	4.40287500
H	2.61808200	-3.80076700	2.68739300
H	2.05308700	-2.24074800	4.47576300
H	3.10135900	0.05498000	4.55596600
H	1.78846200	1.01780500	2.58061800

H	1.35377800	-2.77786800	0.84058300
C	-3.91186500	-1.63458000	-0.13269300
C	-3.03086000	-2.30787800	-0.97610300
C	-3.46977600	-3.37886700	-1.75632500
C	-4.80151500	-3.77113600	-1.69528400
C	-5.69092600	-3.10213000	-0.85460200
C	-5.24493300	-2.03902800	-0.07530700
H	-3.55512200	-0.79756000	0.46216300
H	-2.76552100	-3.89761700	-2.40068400
H	-5.14700700	-4.60298200	-2.30285800
H	-5.93411200	-1.51767800	0.58407400
S	-1.29719300	-1.85103500	-1.09660900
O	-0.54528200	-3.05351100	-0.69897300
O	-1.09483000	-1.34414300	-2.46697800
N	-1.15893400	-0.59102700	-0.07312400
C	-0.79383500	-0.91835600	1.25574000
H	-0.77404300	-1.98600300	1.47787400
C	-1.44243800	-0.11471500	2.31917600
C	-1.90716700	1.18445400	2.07943900
C	-1.59747100	-0.66059000	3.59927400
C	-2.50753300	1.91688000	3.09705300
H	-1.79863700	1.60268600	1.08136700
C	-2.19636100	0.07406000	4.61793400
H	-1.23261800	-1.66928400	3.78956500
C	-2.65217300	1.36738600	4.37091700
H	-2.87060500	2.92085200	2.88966400
H	-2.31144200	-0.36515200	5.60542900
H	-6.73096500	-3.41289800	-0.80716200
H	-3.12177600	1.94164700	5.16494800

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