

Supporting Information for

Origin and Stabilization of Axial Chirality on the Construction of Naphthyl-C2-Indoles: A DFT Study

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1. Test results of computational methods

M062X method was employed for optimization and the frequency calculation of all intermediates, and transition states. In order to test the reliability of the selected method, different computational levels including M06-2X/6-31G(d, p) (L1), B3LYP/6-31G(d, p) (L2), and ω B97X-D/6-31G(d, p) (L3) were used for additionally computing the key step, and the calculated results had been shown in **Table S1**. There are small differences between the calculated results obtained by L1-3, but the trend and conclusions should be the same, indicating the computational method is reliable.

Table S1. Comparison of relative Gibbs free energies ($\Delta\Delta G^\ddagger$) of the key step calculated by using different levels including M06-2X/6-31G(d, p) (L1), B3LYP/6-31G(d, p) (L2) and ω B97X-D/6-31G(d, p) (L3) (Unit: kcal/mol).

	L1	L2	L3
Int2	0.0	0.0	0.0
TS1R	20.1	18.8	19.5
$\Delta\Delta G^\ddagger$	20.1	18.8	19.5

2. NCI and topology analyses of TS1S.

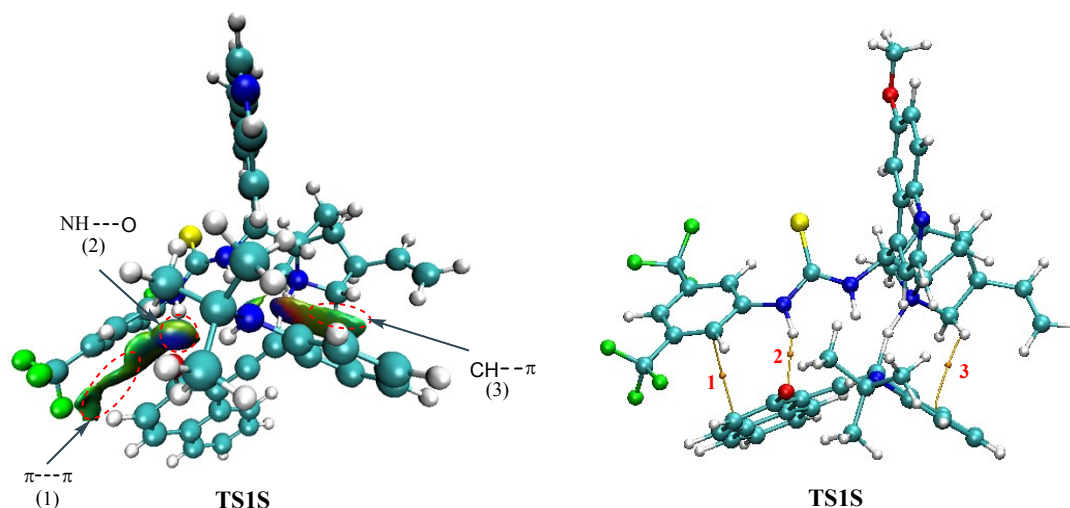


Fig. S1 NCI analysis and topological analysis of bond critical points (BCPs) along the bond paths for the transition state **TS1S**.

Table S2. Summary of distances, types of interaction, electron densities (ρ_{bcp}), Lagrangian kinetic energies (G_{b}), potential energy densities (V_{b}), energy densities (H_{b}), and Laplacian of electron densities ($\nabla^2\rho$) at the bond critical points (BCPs) along the bond paths in **TS1S** (bond lengths in Å,

other values in a.u.).

BCP index	Type of interaction	Distance	$\rho_{\text{bcp}} \times 10^{-2}$	$G_{\text{b}} \times 10^{-2}$	$V_{\text{b}} \times 10^{-2}$	$H_{\text{b}} \times 10^{-3}$	$\nabla^2\rho \times 10^{-1}$
1	$\pi \cdots \pi$	3.15	0.8182	0.5433	-0.4094	1.3390	0.2709
2	N-H \cdots O	1.89	2.8975	2.4994	-2.4617	0.3770	1.0148
3	C-H \cdots π	2.70	0.8860	0.5641	-0.4558	1.0826	0.2689

Table S3. Summary of distances, types of interaction, electron densities (ρ_{bcp}), Lagrangian kinetic energies (G_{b}), potential energy densities (V_{b}), energy densities (H_{b}), and Laplacian of electron densities ($\nabla^2\rho$) at the bond critical points (BCPs) along the bond paths in **TS1R** (bond lengths in Å, other values in a.u.).

BCP index	Type of interaction	Distance	$\rho_{\text{bcp}} \times 10^{-2}$	$G_{\text{b}} \times 10^{-2}$	$V_{\text{b}} \times 10^{-2}$	$H_{\text{b}} \times 10^{-3}$	$\nabla^2\rho \times 10^{-1}$
1	$\pi \cdots \pi$	3.40	0.6100	0.3549	-0.2833	0.7165	0.1706
2	$\pi \cdots \pi$	3.19	0.7747	0.4849	-0.3724	1.1252	0.2390
3	N-H \cdots O	2.00	2.2874	1.9351	-1.8042	1.3096	0.8264
4	N-H \cdots O	1.83	3.3297	2.8490	-2.9987	1.4969	1.0797
5	C-H \cdots π	3.10	0.5062	0.2756	-0.2344	0.4128	0.1268
6	C-H \cdots π	2.62	0.8556	0.5810	-0.4564	1.2464	0.2823
7	C-H \cdots π	2.64	0.8517	0.5637	-0.4504	1.1332	0.2708

3. The structures of intermediates.

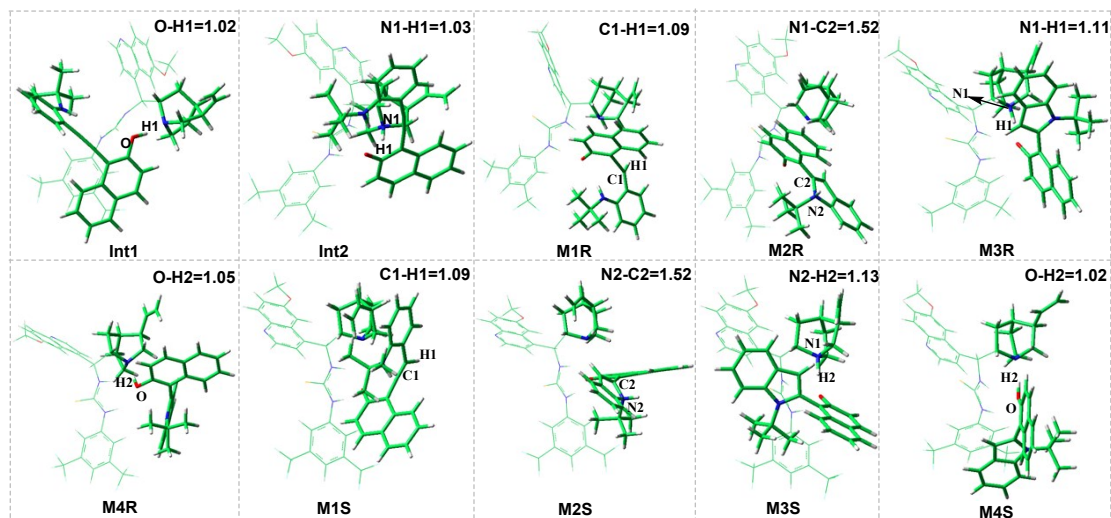


Fig. S2. Optimized geometries of intermediates for the catalytic cycle (Distances are in angstroms).

4. The volume of R

To obtain the relationship of substituents and transformation barriers, the three typical functional group H, methyl and tert-butyl were employed. The volume can be obtained from the output files of Gaussian. For function group H, the volume can be calculated from the H₂ molecule. When R=Me, the volume can be calculated from the CH₄ and H. So the tert-butyl is.

H₂

Molar volume = 131.562 bohr³/mol (11.740 cm³/mol)

1/2 Molar volume = 1/2 * [131.562 bohr³/mol (11.740 cm³/mol)] = 5.9 cm³/mol

5.9*10²⁴/6.02*10²³=9.8 Å³

Cavity volume = 1/2 *22.672 Å³=11.4 Å³

CH₄

Molar volume = 297.037 bohr³/mol (26.507 cm³/mol)

Molar volume = [297.037 bohr³/mol (26.507 cm³/mol)] -1/2 H₂ Molar volume = 20.6 cm³/mol

20.6*10²⁴/6.02*10²³=34.4 Å³

Cavity volume = 51.165 Å³-1/2 H₂ Cavity volume=39.8 Å³

t-Bu

Molar volume = 777.335 bohr³/mol (69.369 cm³/mol)

Molar volume = [777.335 bohr³/mol (69.369 cm³/mol)] -1/2 H₂ Molar volume = 63.5 cm³/mol

63.5*10²⁴/6.02*10²³=10.5*10⁻²³=63.5*10²⁴/6.02*10²³=105.5 Å³

Cavity volume = 128.663 Å³-1/2 H₂ Cavity volume=117.3 Å³

5. Energies of optimized structures

Table S4. The single-point, Gibbs free energy corrections (GFEC) and GFE (=E+GFEC) energies

of the stationary points involved in cinchonine-thiourea catalyzed asymmetric annulation. (unit: a.u.).

	GFE (M06-2X/6-31G(d, p) /IEF-PCM _{chloroform})	E (M06-2X/6-311+G(2df, 2pd)/IEF-PCM _{chloroform})	GFE
Cat	0.471086	-2413.3639	-2412.892814
R1	0.325829	-980.8502521	-980.5244231
Int1	0.826473	-3394.2600676	-3393.433595
TS1	0.820546	-3394.2461878	-3393.425642
Int2	0.829187	-3394.2575679	-3393.428381
TS1R	0.824422	-3394.2208551	-3393.396433
M1R	0.820802	-3394.2281904	-3393.407388
TS2R	0.821669	-3394.2167512	-3393.395082
M2R	0.827528	-3394.2431104	-3393.415582
TS3R	0.829126	-3394.2371851	-3393.408059
M3R	0.831019	-3394.2964493	-3393.46543
TS4R	0.828251	-3394.2883365	-3393.460086
M4R	0.831043	-3394.2890416	-3393.457999
PR	0.330127	-980.8990688	-980.5689418
TS1S	0.822346	-3394.2110924	-3393.388746
M1S	0.818661	-3394.2258934	-3393.407232
TS2S	0.825318	-3394.2192505	-3393.393933
M2S	0.829665	-3394.2475838	-3393.417919
TS3S	0.832034	-3394.241718	-3393.409684
M3S	0.8271	-3394.3018981	-3393.474798
TS4S	0.826067	-3394.3008051	-3393.474738
M4S	0.828133	-3394.3048107	-3393.476678
PS	0.330099	-980.8990694	-980.5689704

6. Cartesian coordinates of all the stationary points

Cat

0 1

C	-1.67154100	-0.30487500	2.35581100
C	-2.23148500	-0.53149200	1.12714300
C	-3.29762800	-1.48303800	1.04191500
C	-3.72559600	-2.09696600	2.25442100
C	-2.17059900	-0.97892000	3.49716600
H	-3.62054400	-1.43770800	-1.12145200
H	-0.84308200	0.38626700	2.46879700
C	-3.92840500	-1.85258900	-0.16815400
C	-4.78452900	-3.03527900	2.20862200
H	-1.71862600	-0.78357800	4.46789800
C	-5.39445800	-3.37276500	1.02711700
C	-4.95329900	-2.77633000	-0.18121600
H	-5.09775500	-3.48461200	3.14520100
H	-6.20143200	-4.09524900	1.02632800
O	-5.48898800	-3.06333500	-1.39486000
C	-6.52963100	-4.02390800	-1.45378300
H	-7.40391000	-3.70074800	-0.87876100
H	-6.80108100	-4.10789300	-2.50512200
H	-6.19194300	-4.99889000	-1.08683500
C	-1.77697100	0.22056600	-0.11087700
H	-1.73905900	-0.48313600	-0.95047500
C	-2.79838700	1.31682500	-0.50171700
C	-2.33859300	2.20575400	-1.69234400
H	-3.68281400	0.75260100	-0.81470400
C	-2.26003900	3.09519600	1.08438000
C	-4.44860200	2.87943900	0.18675700
C	-2.61606300	3.66822100	-1.32339800

H	-1.27269100	2.07827100	-1.91244800
H	-2.88544700	1.92845900	-2.59714700
H	-2.71909300	3.68485100	1.88302200
H	-1.43086300	2.55601400	1.55211700
C	-1.79331500	4.01970000	-0.07684600
C	-4.12088800	3.84119400	-0.99259500
H	-4.82486900	3.44654000	1.04320400
H	-5.22408500	2.15784600	-0.08225400
H	-2.34293900	4.32449200	-2.15597500
H	-1.93364600	5.07210600	0.18807100
H	-0.72521900	3.89396600	-0.29766200
H	-4.25185500	4.87765700	-0.65434000
N	-3.26786700	2.12811100	0.63289500
C	-4.95325700	3.67625000	-2.23907800
C	-5.75209200	2.66328100	-2.56760800
H	-4.83478000	4.48645700	-2.95987300
H	-6.27273800	2.65645000	-3.51959600
H	-5.92621900	1.80918900	-1.91998800
N	-0.42492400	0.74669100	0.03000700
H	-0.31319900	1.75185700	0.05439800
C	0.69035800	-0.00589300	-0.09182700
S	0.64463900	-1.65807700	-0.39475200
N	1.83716100	0.72103500	0.09251800
H	1.72620800	1.62959400	0.52631800
C	5.88639400	-0.37378400	-0.26651300
C	4.94240100	-0.88206700	-1.15400600
C	3.59788900	-0.54900500	-1.06124900
C	3.17393100	0.30068400	-0.03594800
C	4.10904000	0.82347900	0.85758100
C	5.45250300	0.48828200	0.73104700

H	6.93349900	-0.63992700	-0.35533600
H	2.88488900	-0.94314800	-1.77248700
H	3.78821500	1.48983900	1.65226900
C	6.43498800	1.01684500	1.73779000
F	7.67395200	1.08504700	1.23219900
F	6.09850600	2.24444900	2.16023500
F	6.49674200	0.23378200	2.82606400
C	5.40831900	-1.75145400	-2.28834900
F	4.42702500	-2.53172300	-2.75784400
F	5.85471400	-1.01503000	-3.31912500
F	6.42039600	-2.54772200	-1.91418700
N	-3.16178900	-1.83511800	3.47032500

R1

0 1

C	1.94626500	2.87928300	0.08292700
C	1.78741000	1.50601300	-0.15679000
C	2.91381000	0.69352100	-0.43642200
C	4.17235000	1.30743400	-0.47196300
C	4.31982900	2.66329100	-0.20550300
C	3.20654900	3.45737700	0.07282200
H	1.06423500	3.47743500	0.28837300
H	5.03531100	0.71016300	-0.74239600
H	5.30952300	3.10769200	-0.23995400
H	3.32170800	4.51802000	0.26738300
C	0.48810600	0.91154200	-0.12635500
C	-0.58665900	0.34753600	-0.11780600
C	-1.83073200	-0.34638000	-0.11097500
C	-3.07826800	0.34981000	-0.00067500
C	-1.82597300	-1.72973100	-0.21912700

C	-3.14206500	1.76230200	0.11271000
C	-4.29078200	-0.39252400	-0.00314000
C	-3.03684900	-2.46099600	-0.22107100
C	-4.35327600	2.40020900	0.21727600
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H	-3.00193500	-3.54331600	-0.30705900
C	-5.56129300	1.66256500	0.21453400
H	-4.38675300	3.48160200	0.30340100
H	-6.44571800	-0.28423200	0.10289900
H	-5.16310800	-2.37076500	-0.11813500
H	-6.51022700	2.18162200	0.29848600
O	-0.62552600	-2.35346500	-0.32092000
H	-0.75480700	-3.30950100	-0.36706100
N	2.76532500	-0.67385800	-0.74539100
C	3.19779400	-1.69801600	0.24789600
C	4.69741800	-1.61041900	0.52409600
H	4.95841700	-0.69560900	1.06189200
H	4.99668400	-2.45989100	1.14495500
H	5.26649800	-1.64777800	-0.40974400
C	2.41346400	-1.54526400	1.55693700
H	1.34082700	-1.65724900	1.36797300
H	2.72388100	-2.30160100	2.28519800
H	2.58618800	-0.55663800	1.99561400
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H	3.44655200	-3.17255300	-1.32221100
H	3.13979000	-3.86431900	0.28773900
H	1.81387900	-3.12042700	-0.62443900
H	1.78091100	-0.85956800	-0.93557000

Int1

0 1

C	4.20202000	3.41555300	0.50767900
C	5.49366600	2.39486500	-1.07841000
C	4.80363900	1.15248200	-0.94610200
C	3.74215300	1.09550400	0.01098700
C	3.45543300	2.23268200	0.72391900
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H	3.96295100	4.30919800	1.08085800
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C	5.20162000	0.06344900	-1.75594500
H	2.65042100	2.24621700	1.45435800
C	6.24093000	0.19043800	-2.65403300
C	6.93083100	1.42388800	-2.78316900
H	4.69750600	-0.89536500	-1.71156100
H	7.74569000	1.53067000	-3.48836900
N	5.18627900	3.50776500	-0.35264600
O	6.54280000	-0.91206400	-3.38191200
C	7.59934600	-0.82499500	-4.32360200
H	8.55018500	-0.58951600	-3.83374100
H	7.66741100	-1.80710800	-4.78888800
H	7.38790000	-0.07366100	-5.09160400
C	2.92972000	-0.16878000	0.25783000
H	3.13014600	-0.89104100	-0.53391400
N	1.50577000	0.10550400	0.21241800
H	1.06104400	0.32831700	1.09822800
C	0.68437000	-0.19188300	-0.81394700
S	1.21405100	-0.79384700	-2.29595900
N	-0.61421200	0.10541400	-0.53415400

H	-0.80337200	0.47913600	0.39344800
C	3.26818600	-0.78878700	1.62840300
C	4.74568000	-1.26012800	1.70964000
H	3.07824000	-0.02415800	2.39314200
C	2.43755300	-2.97542300	0.91263200
C	2.77104900	-2.48481700	3.25053900
C	4.75909900	-2.79086900	1.78962400
H	5.30890600	-0.92683800	0.83214300
H	5.23255800	-0.83171600	2.59083400
H	1.88983600	-3.84081600	1.29749000
H	1.91917200	-2.63907500	0.00886700
C	3.91258300	-3.34957500	0.63942000
C	4.11977700	-3.23052300	3.12619200
H	1.97733000	-3.14686700	3.61022800
H	2.84210800	-1.64507800	3.94777000
H	5.78634200	-3.16201700	1.72583800
H	4.02092400	-4.43560400	0.57050100
H	4.25735900	-2.93139900	-0.31340300
H	3.92417300	-4.30984100	3.04589400
N	2.34973800	-1.91806100	1.94778500
C	5.06312400	-3.04445200	4.28539200
C	4.82928100	-2.41894400	5.43629900
H	6.04211100	-3.50158600	4.13598900
H	5.59721000	-2.36235300	6.20061800
H	3.87826700	-1.95342100	5.67540500
C	-1.77776300	-0.37496300	-1.17980500
C	-2.86662400	0.48892600	-1.25906800
C	-1.90765100	-1.70945100	-1.56138300
C	-4.09237200	0.00224000	-1.70076600
H	-2.76074100	1.51935300	-0.92651500

C	-3.13677500	-2.16316400	-2.02369000
H	-1.07041500	-2.38929300	-1.45092900
C	-4.24104200	-1.32027000	-2.09519900
H	-5.20594800	-1.69867000	-2.41048100
C	-3.26777700	-3.60320100	-2.42918300
C	-5.27228700	0.93075600	-1.70229800
F	-6.43287200	0.26864900	-1.80843400
F	-5.22053700	1.80719700	-2.71769900
F	-5.32442800	1.65483200	-0.57131300
F	-2.56896700	-4.41207200	-1.61520500
F	-4.54158900	-4.01908700	-2.41035300
F	-2.80328400	-3.81371500	-3.67134400
C	-5.89465400	-1.54183600	0.90072000
C	-4.78876000	-0.86080800	1.34954400
C	-3.54854300	-1.52761700	1.51818600
C	-3.47791700	-2.91779400	1.23032000
C	-4.63399700	-3.59308100	0.76326300
C	-5.81957400	-2.92118500	0.59761600
H	-4.84333100	0.20363700	1.55353800
C	-2.36049100	-0.83684700	1.93336400
C	-2.23486400	-3.58950500	1.37969700
H	-4.55703200	-4.65051400	0.52530400
H	-6.69747300	-3.44284900	0.23087300
C	-1.11407900	-2.92265600	1.79412200
C	-1.16184800	-1.53019300	2.06745000
H	-2.18417000	-4.65088500	1.15506500
H	-0.17207700	-3.44665800	1.92091000
C	-2.37359500	0.58652500	2.07903800
C	-2.42853800	1.80238400	2.09997300
C	-2.58231700	3.22549800	2.18801000

C	-3.34331000	3.75289100	3.23898800
C	-2.01675700	4.08542100	1.20490900
C	-3.57240400	5.11661500	3.34843000
H	-3.75591400	3.06208400	3.96726300
C	-2.26864500	5.46249000	1.33286000
C	-3.03029400	5.96112200	2.38214800
H	-4.16456500	5.51170500	4.16573900
H	-1.86973600	6.15724700	0.60823600
H	-3.19786500	7.03211700	2.44094900
H	-6.83112900	-1.01122900	0.75994100
O	-0.05307200	-0.85637600	2.42459900
H	0.80619500	-1.37999600	2.23947000
N	-1.29976600	3.52433700	0.16404200
H	-0.98715500	2.58484400	0.37105300
C	-0.40321200	4.22058500	-0.78000100
C	0.33332000	3.11384000	-1.54189800
H	0.98556800	3.55283800	-2.30047000
H	0.95963400	2.52329700	-0.86249900
H	-0.37519600	2.44170300	-2.03758600
C	0.64166400	5.08521000	-0.05949100
H	1.35527200	5.48581500	-0.78553100
H	0.20032800	5.92625500	0.47813900
H	1.19401000	4.47382000	0.66121500
C	-1.21550800	5.03405900	-1.79522600
H	-1.77801700	5.85063600	-1.34047000
H	-0.53977100	5.46761600	-2.53804000
H	-1.92387600	4.37816500	-2.30902000

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C	-3.56801600	-1.22556400	1.91270300
C	-3.47650100	-1.48610800	0.56990100
C	-4.46376400	-2.33449700	-0.02332100
C	-5.48723300	-2.83384800	0.83586000
C	-4.62679800	-1.77802000	2.67242300
H	-3.711171000	-2.37724800	-2.07898700
H	-2.82894600	-0.60350900	2.40895000
C	-4.47804200	-2.70806400	-1.38723300
C	-6.48713100	-3.67659100	0.29150000
H	-4.68970400	-1.56078100	3.73661100
C	-6.48959800	-4.02152800	-1.03494000
C	-5.46651800	-3.53036200	-1.88674600
H	-7.25384700	-4.04383900	0.96526600
H	-7.26653600	-4.67037700	-1.42005400
O	-5.38971400	-3.82733100	-3.20719400
C	-6.37855200	-4.68033900	-3.76038000
H	-7.37872500	-4.24543900	-3.66263500
H	-6.13044400	-4.78124000	-4.81580900
H	-6.36096500	-5.66778400	-3.28723100
C	-2.35873200	-0.84106000	-0.23955100
H	-2.28342400	-1.34184600	-1.20691700
C	-2.66719400	0.65125100	-0.44356200
C	-4.01242300	0.88690300	-1.16282100
H	-2.68854200	1.13533800	0.54258200
C	-1.64232000	1.03730300	-2.65879800
C	-1.76047100	2.83503300	-1.01962700
C	-3.85185200	2.07012000	-2.12490200
H	-4.30907900	-0.00342600	-1.72806300
H	-4.79201700	1.07262700	-0.41993500
H	-0.73137900	1.43891800	-3.10936100

H	-1.60502400	-0.04957300	-2.76003000
C	-2.92306600	1.64404100	-3.26935200
C	-3.20270200	3.25409600	-1.37685700
H	-1.01808100	3.31999600	-1.65761300
H	-1.49198400	3.06152500	0.01366300
H	-4.82691900	2.37030600	-2.51813000
H	-2.67792200	2.50869200	-3.89283400
H	-3.41752800	0.90710100	-3.90684000
H	-3.15049200	4.09506400	-2.08061500
N	-1.58372000	1.36110700	-1.20368900
C	-4.05476100	3.69792600	-0.21014200
C	-3.64897300	4.08135200	0.99828200
H	-5.12263300	3.72790200	-0.43123200
H	-4.36870200	4.40838700	1.74187800
H	-2.60380800	4.12370400	1.29517000
N	-1.06506300	-0.96399700	0.40563100
H	-0.68755300	-0.13580800	0.85270800
C	-0.18994800	-1.96728000	0.17043200
S	-0.65854700	-3.42982900	-0.51387200
N	1.08287800	-1.60545400	0.51728100
H	1.24585900	-0.59790500	0.38740400
C	4.58634200	-3.92063000	0.76721700
C	3.36113000	-4.45264000	1.16743700
C	2.18551500	-3.72208000	1.08779800
C	2.22081900	-2.41842900	0.57785700
C	3.44045000	-1.86887700	0.18566200
C	4.60694000	-2.62236600	0.28294800
H	5.49767500	-4.50300400	0.83704700
H	1.25092700	-4.15136000	1.42406100
H	3.47899000	-0.85549900	-0.20652800

C	5.89601600	-1.97729400	-0.13905200
F	6.91008200	-2.85084200	-0.17627500
F	5.79069800	-1.42612500	-1.35871300
F	6.24899700	-0.98920900	0.69852700
C	3.32948600	-5.86810600	1.67085800
F	3.44623800	-6.75012800	0.66501000
F	4.34549700	-6.11073400	2.51377900
F	2.19121000	-6.15121500	2.31708200
N	-5.55927900	-2.54789200	2.16772600
C	-0.73124000	6.19489400	0.83876700
C	0.05669300	5.11716100	1.26944700
C	0.01232400	4.69656900	2.62363400
C	-0.85275300	5.36951800	3.49577100
C	-1.65233000	6.41443500	3.04557300
C	-1.58985500	6.83929300	1.71809800
H	-0.67325800	6.49909500	-0.20162500
H	-0.86084300	5.09598300	4.54424300
H	-2.31213600	6.91718300	3.74565300
H	-2.20515500	7.66351900	1.37466500
C	0.87017700	4.38748800	0.34282500
C	1.49879200	3.66615200	-0.40651900
C	2.13781800	2.75488300	-1.30025200
C	3.17658300	3.18047000	-2.19086900
C	1.70747800	1.42400600	-1.28805000
C	3.64149400	4.52015400	-2.22071800
C	3.76954900	2.23338800	-3.07049600
C	2.30738000	0.49999400	-2.19867800
C	4.64387700	4.89602700	-3.08175500
H	3.19219800	5.24260500	-1.54598700
C	4.80120300	2.65142600	-3.94841600

C	3.30620600	0.88786400	-3.04858300
H	1.93910000	-0.52330600	-2.19090600
C	5.23291100	3.95470400	-3.95785100
H	4.98930300	5.92505600	-3.08996800
H	5.24401700	1.91665000	-4.61559300
H	3.75638700	0.16919500	-3.72836900
H	6.02385000	4.26580700	-4.63215100
O	0.76789600	0.99696100	-0.45027200
N	0.87195100	3.67899900	3.07166800
C	0.32401400	2.37077200	3.51611400
C	-0.27900800	2.46688700	4.91758000
H	-1.21006000	3.03884700	4.91746100
H	-0.51005100	1.46366500	5.28827300
H	0.42828900	2.93953800	5.60475000
C	-0.72318400	1.84718400	2.52400400
H	-0.28057400	1.82015500	1.51860700
H	-1.04113600	0.83935900	2.81770500
H	-1.61172100	2.48854300	2.50841100
C	1.51853800	1.41468500	3.53299900
H	2.29982200	1.79124200	4.19900900
H	1.21026000	0.42416200	3.87766100
H	1.93672700	1.30852100	2.52462500
H	-0.46317900	1.13691900	-0.83529400
H	1.54749100	3.48771500	2.33563600

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C	2.42931300	1.32177500	1.35455000
C	1.97042200	1.90563000	0.20171500
C	2.07555100	3.32775600	0.07238000

C	2.67201900	4.03112800	1.16224800
C	3.00294100	2.12007900	2.37630800
H	1.14707600	3.58097700	-1.89334500
H	2.36365100	0.24876000	1.51091100
C	1.64421900	4.06007800	-1.05745000
C	2.81363900	5.43683800	1.07341700
H	3.36732400	1.63846300	3.28255300
C	2.39409500	6.13104100	-0.03215500
C	1.79811800	5.43056500	-1.11183600
H	3.27134800	5.94778100	1.91373800
H	2.51793000	7.20626500	-0.07047800
O	1.34890800	6.03905100	-2.23719500
C	1.46945600	7.44873800	-2.32901900
H	2.51864400	7.76137700	-2.29829700
H	1.03921500	7.72401300	-3.29078000
H	0.91576000	7.94881100	-1.52756200
C	1.38765600	1.03127800	-0.90326900
H	1.12254200	1.65029400	-1.75906400
C	2.45406500	0.01012500	-1.33980500
C	3.65683300	0.68769800	-2.03393900
H	2.76410900	-0.58709300	-0.47543000
C	1.23483200	-0.36393800	-3.50172700
C	3.00278400	-1.91499700	-2.75482800
C	3.62471500	0.36236200	-3.53342400
H	3.60151800	1.76957300	-1.88037500
H	4.59549900	0.34068300	-1.59406200
H	1.00592300	-1.17875500	-4.19131800
H	0.29918500	0.09290800	-3.17588900
C	2.22542600	0.65444600	-4.09312300
C	3.91387600	-1.14274100	-3.72276500

H	2.55451300	-2.80482300	-3.19962800
H	3.52531200	-2.21109900	-1.84454900
H	4.37540900	0.95701800	-4.05948800
H	2.22263800	0.56958100	-5.18189700
H	1.92011800	1.67658500	-3.84615800
H	3.63739100	-1.40008100	-4.75442800
N	1.88417300	-1.00843500	-2.30671600
C	5.37538500	-1.47069800	-3.55885400
C	5.90910700	-2.41728900	-2.79112400
H	6.03483800	-0.85565700	-4.17050600
H	6.98313600	-2.56711000	-2.76970900
H	5.31590200	-3.08859800	-2.17582000
N	0.16772200	0.36298100	-0.49781000
H	0.21178800	-0.25234900	0.32023700
C	-1.08901300	0.72175300	-0.91069600
S	-1.35251100	1.92497500	-2.07226400
N	-2.03038800	-0.02946900	-0.30295900
H	-1.62629600	-0.80405100	0.30727000
C	-6.23382300	-0.27096400	-0.24500300
C	-5.62206100	0.75651600	-0.95207100
C	-4.23904100	0.89700400	-1.01673100
C	-3.42557100	-0.03047600	-0.35556500
C	-4.03336200	-1.07068200	0.36615900
C	-5.41467900	-1.17955000	0.41500200
H	-7.31238700	-0.35773000	-0.20189400
H	-3.79961200	1.71729500	-1.56561600
H	-3.40454000	-1.78633300	0.89225100
C	-6.00674600	-2.29823600	1.22429500
F	-7.34348800	-2.32439900	1.14789400
F	-5.55618800	-3.49491600	0.81535100

F	-5.68082100	-2.18910900	2.52192500
C	-6.46859600	1.73043300	-1.72263000
F	-5.95781400	2.96971600	-1.69008600
F	-6.56283300	1.38479500	-3.01741000
F	-7.71918100	1.79491500	-1.24354000
N	3.12837000	3.42139400	2.29501100
C	4.04045000	-1.53530700	4.06873500
C	2.75056900	-1.39174500	3.54321300
C	1.80270900	-0.51195500	4.15624000
C	2.22986600	0.16674700	5.31767900
C	3.51554200	0.00585400	5.81761700
C	4.43795600	-0.83920600	5.20056500
H	4.72593600	-2.20935300	3.56431600
H	1.55598800	0.83268400	5.83599500
H	3.79657400	0.55509100	6.71110700
H	5.43918800	-0.95637500	5.59866300
C	2.34480600	-2.09437800	2.37211600
C	1.85345500	-2.61132600	1.38593900
C	1.13379000	-3.10764800	0.26411800
C	1.70566500	-4.01017800	-0.68676000
C	-0.20651500	-2.66301300	0.15093200
C	3.03238800	-4.50242700	-0.56095200
C	0.94036800	-4.40431500	-1.82070400
C	-0.93628100	-3.07143200	-1.02273600
C	3.56968100	-5.32807300	-1.52017000
H	3.61620800	-4.20863700	0.30702600
C	1.51935600	-5.26331700	-2.78864200
C	-0.38463700	-3.89865300	-1.96185600
H	-1.95562800	-2.71140700	-1.13499100
C	2.81096400	-5.71242600	-2.65155500

H	4.58549600	-5.69464200	-1.40721800
H	0.92065800	-5.55536700	-3.64748300
H	-0.96094000	-4.18984500	-2.83633300
H	3.24717000	-6.36698100	-3.39837200
O	-0.73604100	-1.86846400	1.02968600
N	0.57253700	-0.35340400	3.57650200
C	-0.52858900	0.50501500	4.03745900
C	-1.05499100	0.06579300	5.41276400
H	-0.30474800	0.14447400	6.20105700
H	-1.90976300	0.68602000	5.69867900
H	-1.38528100	-0.97586000	5.36413400
C	-0.12461600	1.98766000	4.01992700
H	0.15047600	2.27820000	3.00105400
H	-0.97359300	2.60038700	4.33766800
H	0.71969200	2.21788500	4.67148800
C	-1.65510600	0.33036000	3.01610500
H	-1.94868100	-0.72013100	2.92795500
H	-2.52559000	0.91950900	3.31560600
H	-1.32337400	0.68022300	2.03425900
H	1.18198900	-1.56776600	-1.79986200
H	0.33324500	-1.00981200	2.83491100

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C	5.37381900	-2.12303400	-2.29521700
C	4.31211500	-2.11167400	-1.34174400
C	3.51798600	-0.92420800	-1.26707100
C	3.81477100	0.10879000	-2.12057500
H	6.99236100	-3.25910600	-3.12750500
H	5.11251000	0.81197900	-3.70708400

C	6.19013800	-3.27570500	-2.39727700
C	4.10557300	-3.25695900	-0.53811100
H	3.23782600	1.03096300	-2.11706800
C	4.91688300	-4.36538800	-0.66492600
C	5.97816200	-4.37538000	-1.60665600
H	3.29838600	-3.31394800	0.18390100
H	6.61944400	-5.24209200	-1.70941200
N	5.64908500	-1.07707800	-3.12664400
O	4.63499000	-5.41122000	0.15044900
C	5.42005200	-6.58568100	0.02871600
H	6.47182100	-6.38730400	0.26011000
H	5.01820900	-7.29088900	0.75439700
H	5.34081500	-7.01446700	-0.97574300
C	2.37116800	-0.78152800	-0.27634600
H	2.21712700	-1.72049400	0.25185300
N	1.13334900	-0.50106300	-0.97096300
H	1.09620900	0.32477300	-1.57411900
C	-0.00261300	-1.21484000	-0.86425600
S	-0.09735800	-2.65673400	0.02336500
N	-1.03437200	-0.63262600	-1.53921900
H	-0.78776900	0.27131000	-1.95178300
C	2.71467600	0.31686800	0.74872300
C	4.02584800	-0.02467700	1.49950000
H	2.82514800	1.26835400	0.21185900
C	1.53932700	-0.53457100	2.74108100
C	1.94026700	1.83265300	2.45973500
C	3.86430800	0.34418100	2.97810400
H	4.24474800	-1.09644400	1.41640300
H	4.85951600	0.51435100	1.04290300
H	0.64316900	-0.33619800	3.33438800

H	1.36602300	-1.46605000	2.19645700
C	2.82045600	-0.58775500	3.60446500
C	3.35265100	1.79694500	3.08671500
H	1.16625900	1.96045600	3.22143600
H	1.82339400	2.64609600	1.74142400
H	4.82265400	0.24804800	3.49660900
H	2.60807800	-0.27478900	4.63142800
H	3.20421800	-1.61072200	3.64528000
H	3.26416900	2.02959700	4.15574800
N	1.62931800	0.56222800	1.74566100
C	4.35990800	2.75959700	2.50648300
C	4.20078400	3.64286600	1.52369900
H	5.34166700	2.68612100	2.97688700
H	5.03135000	4.26759700	1.21121600
H	3.26230300	3.79945900	0.99909300
C	-2.41873500	-0.85246600	-1.46231300
C	-3.02475300	-2.06548300	-1.12769200
C	-3.22434700	0.25288300	-1.76789300
C	-4.41287100	-2.13077300	-1.05177400
H	-2.42742400	-2.93876100	-0.91483900
C	-4.60425900	0.15209800	-1.70551600
H	-2.76079900	1.20189000	-2.02222000
C	-5.22100000	-1.03797500	-1.33308600
H	-6.30186000	-1.10750600	-1.26324200
C	-5.46756300	1.32047900	-2.08568600
C	-5.08292600	-3.42016400	-0.67180300
F	-4.20800600	-4.37305900	-0.32633900
F	-5.82855300	-3.90636200	-1.67733900
F	-5.91829500	-3.24760000	0.36880000
F	-6.45704600	1.51921800	-1.19993000

F	-4.77330400	2.46118800	-2.18402900
F	-6.06065700	1.11644800	-3.27546700
C	1.22783900	6.07559000	1.46689700
C	0.70032300	4.88987800	0.98320600
C	1.04444500	4.42283400	-0.29688800
C	1.90670300	5.20560200	-1.09576900
C	2.43217500	6.40709200	-0.58883500
C	2.10573700	6.83837000	0.68409800
H	0.01598000	4.30578800	1.59275200
C	0.56054200	3.14276900	-0.81890200
C	2.23114600	4.75389600	-2.43027400
H	3.09882100	6.99355700	-1.21521000
H	2.51620200	7.76480000	1.07060100
C	1.74250600	3.60652500	-2.95330800
C	0.87413000	2.72768600	-2.18184100
H	2.89056300	5.38065900	-3.02626700
H	1.98709600	3.28700400	-3.96078600
C	-0.18152100	2.31084400	-0.04147500
C	-0.73575900	1.50057000	0.77445700
C	-2.17076500	1.39969300	1.10872600
C	-3.00224100	2.43807600	0.65932300
C	-2.73708900	0.31734900	1.83479300
C	-4.37004600	2.44287500	0.87331700
H	-2.53813200	3.26019300	0.11941000
C	-4.13708400	0.32154000	2.00344600
C	-4.93360900	1.35660200	1.53660600
H	-4.98451800	3.25719600	0.50669600
H	-4.62055700	-0.50897900	2.49313400
H	-6.00767300	1.30258600	1.68633100
C	-2.37558700	-1.82661100	3.16870200

H	0.95463700	6.41638800	2.46037100
O	0.46852100	1.64895700	-2.67775900
H	0.39914300	0.85274300	1.24620700
N	-1.91493900	-0.66702100	2.37476600
H	-1.14080200	-0.91414700	1.76471600
C	-3.08811400	-1.36705100	4.45080300
H	-2.47876700	-0.61231000	4.95655300
H	-4.08218400	-0.95126100	4.29146000
H	-3.19606800	-2.22558300	5.12003600
C	-1.11214100	-2.57164600	3.61905300
H	-0.52051800	-1.95954200	4.30606400
H	-1.39761900	-3.48930600	4.14029800
H	-0.49225200	-2.84751100	2.76114400
C	-3.22779600	-2.80860700	2.34796000
H	-2.62006200	-3.22938500	1.54145900
H	-3.57350300	-3.62921100	2.98514900
H	-4.10382400	-2.34098400	1.89525600
C	4.88801100	-0.01441600	-3.03596700

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C	1.96027400	0.40514600	-2.20442600
C	2.43595900	-0.74707500	-1.63784900
C	3.79259500	-1.11630400	-1.93625500
C	4.57563500	-0.18964800	-2.68350400
C	2.82321800	1.24600200	-2.95520400
H	3.81467200	-3.11210600	-1.04209400
H	0.92356400	0.69348600	-2.09277300
C	4.37942200	-2.34452100	-1.55832500
C	5.92810000	-0.50192200	-2.95995200

H	2.42606600	2.17216100	-3.36852900
C	6.49192000	-1.68472100	-2.55220300
C	5.69883700	-2.62662600	-1.85176500
H	6.50537500	0.22725600	-3.51849400
H	7.52944100	-1.89368200	-2.78204300
O	6.15965400	-3.83097400	-1.43375500
C	7.50858800	-4.16529900	-1.71542700
H	8.19954900	-3.45918100	-1.24267800
H	7.66451500	-5.15807800	-1.29635500
H	7.69528500	-4.19243600	-2.79417600
C	1.56023900	-1.63263800	-0.75622500
H	1.43669800	-2.59657100	-1.26390700
C	2.21492000	-1.94553200	0.62319300
C	2.03593000	-3.41456400	1.05909700
H	3.28047700	-1.74755900	0.51617500
C	0.55003000	-1.55333400	2.41963900
C	2.89998600	-1.12096500	2.76702200
C	2.11559000	-3.47419600	2.59026600
H	1.06932500	-3.80033800	0.71509500
H	2.81766600	-4.02632600	0.59733300
H	0.22543300	-0.77204800	3.11076000
H	-0.21710800	-1.65866400	1.65385100
C	0.81303900	-2.88920600	3.14651900
C	3.28776800	-2.58772700	3.07800000
H	2.52888700	-0.61946000	3.66447200
H	3.73660000	-0.53164500	2.38238400
H	2.25882000	-4.50308300	2.93189000
H	0.89659000	-2.73691700	4.22734400
H	-0.01962100	-3.57570800	2.97226200
H	3.34705100	-2.69950900	4.16811400

N	1.79999900	-1.07020800	1.75986900
C	4.59736700	-3.08173500	2.51068900
C	5.47504600	-2.43325200	1.74874800
H	4.81121300	-4.12015800	2.76761800
H	6.37189100	-2.92967800	1.39284500
H	5.34780800	-1.39913900	1.43967900
N	0.22882600	-1.07737500	-0.62533100
H	0.15841300	-0.09987700	-0.34048900
C	-0.93146800	-1.69901300	-0.95158600
S	-1.02538200	-3.32805000	-1.37465300
N	-1.98656400	-0.83998500	-0.89514900
H	-1.73351100	0.15075200	-0.89112400
C	-6.15995000	-1.25118900	-1.20557800
C	-5.39304500	-2.32558600	-0.76847200
C	-4.00860400	-2.24950200	-0.66241700
C	-3.36132200	-1.06806800	-1.03368200
C	-4.11911100	0.01617200	-1.48796600
C	-5.50192800	-0.07789100	-1.55344400
H	-7.23957500	-1.32342200	-1.26517200
H	-3.44211500	-3.09022600	-0.28689800
H	-3.61725000	0.93733300	-1.77209500
C	-6.28832600	1.14319500	-1.93393100
F	-7.50345100	0.83220500	-2.40278000
F	-6.46925700	1.95416100	-0.87683200
F	-5.66141800	1.86779200	-2.87206300
C	-6.07748600	-3.62062900	-0.43171600
F	-6.19657600	-4.41069500	-1.51064400
F	-5.40127700	-4.31942300	0.49087300
F	-7.31647900	-3.41804600	0.04000000
N	4.08750000	0.99065300	-3.17062000

C	1.86037300	1.97693800	4.11369000
C	0.85670100	1.78941200	3.15919600
C	-0.50079600	1.72234000	3.55179700
C	-0.77910200	1.79828100	4.92672000
C	0.22561400	2.01177900	5.86275400
C	1.55471400	2.11699800	5.46253400
H	2.89277900	2.01827900	3.77697600
H	-1.79516100	1.65310800	5.26754200
H	-0.03473300	2.07190200	6.91477500
H	2.34351200	2.27972100	6.18867500
C	1.25203900	1.56428100	1.74469400
C	1.17404000	2.30968500	0.71842800
C	1.01520200	2.99442500	-0.43945100
C	1.97987100	3.97285000	-0.93132300
C	-0.20277800	2.69575600	-1.18286300
C	3.19223600	4.23203300	-0.27346000
C	1.67826200	4.68227200	-2.11413900
C	-0.45268700	3.47982400	-2.37981500
C	4.07776800	5.16882500	-0.77791400
H	3.42820100	3.68589400	0.63517600
C	2.58832800	5.63254600	-2.61011500
C	0.43793600	4.40709000	-2.80472500
H	-1.36894600	3.27481800	-2.92283300
C	3.77846400	5.87704700	-1.95091700
H	5.01312400	5.35506300	-0.26002400
H	2.34129700	6.17070400	-3.52099100
H	0.23339400	4.97103300	-3.71197000
H	4.47817300	6.60938200	-2.33847700
O	-0.97729200	1.77344500	-0.83233800
N	-1.51485500	1.46835100	2.60988000

C	-2.65934100	2.40912700	2.43639400
C	-3.54185300	2.50720000	3.68239800
H	-3.07139500	3.08681900	4.47925800
H	-4.47128400	3.01751700	3.41367000
H	-3.79407600	1.51198200	4.06094100
C	-2.14298900	3.80009500	2.05177900
H	-1.54665000	3.74112400	1.13443000
H	-2.97269900	4.49344700	1.88197700
H	-1.51166900	4.20719700	2.84870000
C	-3.49289800	1.82266100	1.29491800
H	-3.82564600	0.81012300	1.54572600
H	-4.37389600	2.44061800	1.09898100
H	-2.89560200	1.78434400	0.38003100
H	1.61850300	0.29498900	1.55146600
H	-1.09836400	1.35675500	1.68566600

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C	-3.71534600	-0.57599600	-2.00526200
C	-4.03442500	-0.52796200	-0.67247000
C	-5.41853300	-0.46063700	-0.31713600
C	-6.36569700	-0.46869100	-1.38343800
C	-4.73802000	-0.56503700	-2.98260000
H	-5.21791800	-0.32557700	1.85627000
H	-2.67495900	-0.61715700	-2.31525600
C	-5.89422800	-0.36929400	1.01119800
C	-7.74658800	-0.41033200	-1.07392300
H	-4.46895600	-0.59998600	-4.03674500
C	-8.18902100	-0.33511800	0.22170900
C	-7.24519200	-0.30837200	1.27959100

H	-8.44534200	-0.42257800	-1.90373000
H	-9.25171400	-0.28896100	0.42561500
O	-7.59423600	-0.22208500	2.58951700
C	-8.96944500	-0.10610300	2.90608900
H	-9.53012000	-0.99104400	2.58530600
H	-9.02223000	-0.02099300	3.99063600
H	-9.40944100	0.78809400	2.45125200
C	-2.92577300	-0.63799000	0.36192800
H	-3.30984900	-0.35294600	1.34759400
C	-2.42373800	-2.09923000	0.38817400
C	-3.48311600	-3.09188900	0.92262500
H	-2.16977400	-2.35967100	-0.64828900
C	-1.40733000	-2.14773600	2.58419400
C	-0.55146800	-3.51126200	0.81223100
C	-2.75614200	-4.10341300	1.82053900
H	-4.25155700	-2.57369900	1.50917700
H	-3.99091900	-3.58842800	0.09121900
H	-0.43608000	-2.11058200	3.08658800
H	-1.91205700	-1.20227400	2.80476200
C	-2.24686000	-3.36275700	3.06412700
C	-1.53372700	-4.68671400	1.06914700
H	0.34815600	-3.61747500	1.42777200
H	-0.21738800	-3.48180400	-0.22834100
H	-3.43464600	-4.91332900	2.10741500
H	-1.63994700	-4.03840800	3.67640500
H	-3.09046600	-3.03406400	3.67897500
H	-1.05937100	-5.40850400	1.74788900
N	-1.15934900	-2.21265500	1.13551500
C	-1.98223300	-5.45926400	-0.14607600
C	-1.70974600	-5.22284500	-1.42723400

H	-2.62888100	-6.30642200	0.08979500
H	-2.11732000	-5.86126100	-2.20439800
H	-1.07534500	-4.40596200	-1.75851400
N	-1.77533400	0.18461000	0.04208500
H	-0.89090000	-0.29717400	0.21822800
C	-1.76669000	1.53987600	0.04752400
S	-3.15356600	2.45409100	0.31761400
N	-0.51022700	2.01781400	-0.18782900
H	0.20923900	1.28372600	-0.24920200
C	1.36267600	5.78675500	-0.20517400
C	-0.01931600	5.70898600	-0.32302300
C	-0.70089500	4.49514600	-0.32055000
C	0.02327300	3.30647300	-0.17832600
C	1.42004400	3.37195800	-0.06140000
C	2.06976700	4.59563600	-0.07969700
H	1.87387300	6.74162800	-0.21418300
H	-1.77585100	4.46890400	-0.43102500
H	1.98787700	2.45063700	0.04909700
C	3.56886700	4.60282300	0.00201800
F	4.01782300	3.75693800	0.94331300
F	4.12981200	4.21295200	-1.15774700
F	4.05423000	5.81810000	0.28439700
C	-0.82435100	6.97536800	-0.40751200
F	-0.09727300	7.99932600	-0.87927700
F	-1.89115100	6.83570300	-1.20681600
F	-1.28696500	7.34686900	0.79737000
N	-6.01744500	-0.52343800	-2.70185100
C	5.24932900	-1.66145800	3.58684600
C	4.87143000	-1.68604900	2.24523100
C	5.83711200	-1.58366700	1.23379900

C	7.18731400	-1.54209700	1.57063100
C	7.56229800	-1.52200300	2.91416400
C	6.59705700	-1.56204200	3.91810900
H	4.49329300	-1.73992300	4.36200200
H	7.94275400	-1.52531600	0.79250600
H	8.61443500	-1.47592300	3.17431500
H	6.89723900	-1.54053700	4.96030100
C	3.51249300	-1.96497300	1.78856900
C	3.18263300	-2.04023300	0.51966800
C	2.33668000	-2.16633000	-0.53542800
C	2.39110000	-3.33262900	-1.41107800
C	1.39429400	-1.08162500	-0.78443500
C	3.31231700	-4.37445700	-1.21208900
C	1.50205100	-3.41271900	-2.50550800
C	0.50277700	-1.24298600	-1.93091100
C	3.33812100	-5.46516100	-2.06492700
H	3.99960800	-4.32120500	-0.37252400
C	1.53962700	-4.52899400	-3.35858900
C	0.56586300	-2.33229000	-2.72982100
H	-0.19431500	-0.43359600	-2.12854000
C	2.44806000	-5.54935600	-3.14442900
H	4.05408700	-6.26251800	-1.89292500
H	0.84344600	-4.57679000	-4.19183200
H	-0.10295300	-2.41341700	-3.58456100
H	2.47273600	-6.40838800	-3.80583100
O	1.33379900	-0.06665700	-0.05806900
N	5.30939800	-1.59695800	-0.09739900
C	5.39176000	-0.33024900	-0.89949400
C	4.79121400	-0.64445700	-2.27113300
H	4.84297200	0.24526900	-2.90376900

H	5.35346300	-1.44378800	-2.76727300
H	3.74749700	-0.95258000	-2.19651400
C	4.60691000	0.77130600	-0.19005300
H	4.67734400	1.69617000	-0.76954100
H	3.55181900	0.50589900	-0.07882800
H	5.02471500	0.97016300	0.80222600
C	6.84483600	0.12358200	-1.09151800
H	7.45780700	-0.67673300	-1.52070200
H	6.86610500	0.97075400	-1.78300600
H	7.29395600	0.45083000	-0.15089600
H	2.74341700	-2.22075800	2.51602100
H	5.72327900	-2.35338400	-0.64242400

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C	-3.66473800	-0.43426300	-1.99131500
C	-3.99111900	-0.42628900	-0.65946900
C	-5.37771100	-0.37859300	-0.31018400
C	-6.31920200	-0.35743600	-1.38122100
C	-4.68241400	-0.39901800	-2.97308000
H	-5.19073100	-0.32200200	1.86818800
H	-2.62211300	-0.46280700	-2.29532400
C	-5.86177100	-0.33783100	1.01799500
C	-7.70205700	-0.31756600	-1.07756000
H	-4.40741200	-0.40238200	-4.02632200
C	-8.15235800	-0.29035100	0.21734400
C	-7.21453800	-0.29574200	1.28065300
H	-8.39603600	-0.30569900	-1.91142000
H	-9.21642300	-0.25813300	0.41682200
O	-7.57142100	-0.25980000	2.59131200

C	-8.94944300	-0.16940700	2.90277500
H	-9.49907100	-1.04735500	2.54534500
H	-9.01025500	-0.12538400	3.98936600
H	-9.39570800	0.73664400	2.47853000
C	-2.88766700	-0.56258700	0.37735400
H	-3.27593300	-0.29813200	1.36766800
C	-2.39307500	-2.02692800	0.36696200
C	-3.46514700	-3.04014700	0.83329800
H	-2.11393300	-2.24516900	-0.67275900
C	-1.43194800	-2.18806200	2.58100200
C	-0.52927800	-3.45359800	0.75680100
C	-2.75491700	-4.10134800	1.68678000
H	-4.23902300	-2.55025200	1.43702500
H	-3.96443000	-3.48830700	-0.03032600
H	-0.47502700	-2.17019600	3.11126700
H	-1.95090600	-1.25912600	2.83633000
C	-2.27169700	-3.43114200	2.97904700
C	-1.51605900	-4.64213500	0.93006800
H	0.35938700	-3.59202500	1.38258200
H	-0.17341800	-3.36319200	-0.27296800
H	-3.43840400	-4.92604300	1.91412600
H	-1.67120900	-4.13783000	3.56225500
H	-3.12701800	-3.14140900	3.59745500
H	-1.05535100	-5.39902000	1.57988000
N	-1.14789500	-2.17599900	1.13862500
C	-1.93780100	-5.35015200	-0.33321300
C	-1.62942200	-5.05192900	-1.59324000
H	-2.59508300	-6.20374400	-0.15570400
H	-2.01936300	-5.64896400	-2.41163000
H	-0.98328600	-4.22281500	-1.86623300

N	-1.72946000	0.25343000	0.07875800
H	-0.84400500	-0.23417800	0.23945800
C	-1.69786000	1.60777600	0.06229300
S	-3.07377000	2.55375700	0.30501700
N	-0.43163700	2.05080000	-0.16919600
H	0.28062800	1.27830500	-0.21735300
C	1.58799800	5.74209200	-0.22387600
C	0.20051100	5.72395700	-0.28837300
C	-0.53566800	4.54089400	-0.27076400
C	0.13909200	3.31879200	-0.16982600
C	1.54286200	3.32654100	-0.10139100
C	2.24537900	4.51839300	-0.13417900
H	2.13822800	6.67476300	-0.24533400
H	-1.61458900	4.56343600	-0.33925300
H	2.06665700	2.37802800	-0.01256200
C	3.74477600	4.45344800	-0.12033800
F	4.19543100	3.53568500	0.75317900
F	4.23872600	4.10228200	-1.32193100
F	4.30112100	5.62726000	0.20460000
C	-0.55442900	7.02239500	-0.33510300
F	0.20828300	8.03079200	-0.78506700
F	-1.63011200	6.94483700	-1.13174400
F	-0.99831100	7.38105200	0.88110500
N	-5.96383200	-0.37000300	-2.69889400
C	4.76902700	-1.33599100	3.75396700
C	4.42353800	-1.49110200	2.41499700
C	5.40899500	-1.82931100	1.48574400
C	6.71437000	-2.10765300	1.84264200
C	7.04835000	-1.95691900	3.19150900
C	6.09336000	-1.55943100	4.12717000

H	4.01792500	-1.06970900	4.48948500
H	7.45523300	-2.43590700	1.12386900
H	8.06519800	-2.15819300	3.50874800
H	6.38178900	-1.44626100	5.16669800
C	3.13930900	-1.49768900	1.73046500
C	3.29643700	-1.83544900	0.44235300
C	2.33071600	-1.99820500	-0.62573900
C	2.34463500	-3.15655000	-1.46294600
C	1.39074300	-0.95366900	-0.81399000
C	3.14963100	-4.29614200	-1.19118800
C	1.49821200	-3.20575500	-2.60540900
C	0.54021300	-1.05286800	-1.98480800
C	3.16130200	-5.38242700	-2.03778800
H	3.71043600	-4.34719000	-0.25958500
C	1.52932900	-4.33225300	-3.45695800
C	0.60821200	-2.11049800	-2.83958900
H	-0.14085500	-0.22612600	-2.17117500
C	2.35707200	-5.40071600	-3.19553500
H	3.77731200	-6.24324800	-1.79670500
H	0.87532600	-4.34263500	-4.32557600
H	-0.03095800	-2.14332600	-3.71939800
H	2.37235200	-6.26130400	-3.85510400
O	1.30930100	0.05322900	-0.02521200
N	4.78936000	-1.89744100	0.14971000
C	5.25827600	-0.74895300	-0.84559400
C	4.76489400	-1.10185800	-2.25004500
H	5.27667000	-0.43714700	-2.95002400
H	5.01865400	-2.13184500	-2.52255200
H	3.69242100	-0.96048400	-2.36737400
C	4.68570700	0.57083600	-0.34966100

H	5.04825200	1.36589000	-1.00658600
H	3.59272900	0.56846100	-0.36957300
H	5.02578700	0.79697400	0.66537600
C	6.78470700	-0.71808900	-0.85618400
H	7.21519400	-1.69541100	-1.09839600
H	7.08806200	-0.02416400	-1.64283000
H	7.20092400	-0.35564700	0.08363800
H	2.17079300	-1.32305700	2.17859100
H	5.02186600	-2.78135400	-0.31993500

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C	0.68453800	0.43348400	-2.38004100
C	1.37957900	-0.62757700	-1.85757300
C	2.67159500	-0.90943700	-2.41604700
C	3.19322100	0.01723400	-3.36620700
C	1.28745800	1.27538700	-3.34888100
H	3.05653300	-2.82752000	-1.44123900
H	-0.31255200	0.67756400	-2.03352200
C	3.43717900	-2.05449200	-2.09903100
C	4.48645100	-0.20162500	-3.89855300
H	0.73268200	2.13730200	-3.71628200
C	5.23101600	-1.30132000	-3.54977300
C	4.68945300	-2.25062700	-2.64683600
H	4.86602400	0.52479900	-4.60937500
H	6.21391900	-1.44313600	-3.98189600
O	5.33746900	-3.38132700	-2.27315300
C	6.61617100	-3.63228500	-2.83161000
H	7.32995000	-2.84728200	-2.55912600
H	6.94641700	-4.58105300	-2.41143600

H	6.56419400	-3.71639300	-3.92218000
C	0.75923600	-1.51477800	-0.77488900
H	0.54177400	-2.47291000	-1.25843800
C	1.68558200	-1.82727600	0.45856700
C	1.76934500	-3.36764700	0.70926600
H	2.68126300	-1.44668000	0.21656500
C	0.05153200	-1.51518000	2.38153900
C	2.39856200	-1.70196800	2.72999500
C	1.14448200	-3.71287700	2.06300000
H	1.24511700	-3.90931600	-0.08275100
H	2.81498500	-3.69667200	0.69426200
H	0.14716900	-1.29760000	3.45037600
H	-0.73950000	-0.87612000	2.00816900
C	-0.21524500	-3.01134500	2.16794500
C	2.06141700	-3.14207200	3.15997700
H	2.46019000	-1.04227800	3.59698400
H	3.35741100	-1.67932300	2.21281000
H	1.04034800	-4.79674900	2.16641500
H	-0.79787800	-3.40341100	3.00680600
H	-0.79382100	-3.18072300	1.25185500
H	1.48865400	-3.12251400	4.09810400
N	1.37562300	-1.13729700	1.78110400
C	3.27086900	-4.00315100	3.40859000
C	4.55002500	-3.63576500	3.38293800
H	3.03290300	-5.03987200	3.64867300
H	5.33544800	-4.35489200	3.59027100
H	4.87071800	-2.61997900	3.16733200
N	-0.49583600	-0.96855200	-0.35299500
H	-0.44960500	-0.09265300	0.22948100
C	-1.71925200	-1.43460000	-0.63301300

S	-2.01191500	-2.83395900	-1.54232500
N	-2.67421400	-0.64518800	-0.04393900
H	-2.27835900	0.09981200	0.54429700
C	-6.88264500	-0.56365300	-0.01684300
C	-6.21288900	-1.22697200	-1.03742200
C	-4.82467400	-1.29078400	-1.09342200
C	-4.06976700	-0.68700600	-0.08220500
C	-4.73442700	-0.00885600	0.94973900
C	-6.11977300	0.05070000	0.97015000
H	-7.96567800	-0.52209300	0.00769200
H	-4.33329200	-1.79668400	-1.91186000
H	-4.15949500	0.46515600	1.73998600
C	-6.81487200	0.83337900	2.04751900
F	-7.96578200	0.25177800	2.41519400
F	-6.05643900	0.96296700	3.14453800
F	-7.12275600	2.07369500	1.63414800
C	-7.01836700	-1.93745500	-2.08893900
F	-6.33796900	-2.08353900	-3.23322100
F	-7.37759900	-3.16759500	-1.68546200
F	-8.15216100	-1.27788100	-2.37257700
N	2.50272600	1.11104500	-3.81025500
C	5.18423400	0.51877100	-0.11168700
C	3.96620700	1.03826400	0.33112100
C	3.60256200	0.98687700	1.67744100
C	4.49487200	0.50893100	2.63100600
C	5.73133600	0.03468000	2.19248700
C	6.06430000	0.01056300	0.83424000
H	5.42528900	0.52311100	-1.17103400
H	4.27525800	0.48572000	3.68915200
H	6.43986300	-0.33129600	2.92783000

H	7.02241000	-0.39192300	0.52293400
C	2.89392700	1.68233800	-0.38092700
C	1.88592400	1.99377300	0.45884500
C	0.65894200	2.69145800	0.03917000
C	0.77848200	3.84613400	-0.81223100
C	-0.60654700	2.17027500	0.35490200
C	2.00759600	4.51865400	-1.07212000
C	-0.39462300	4.39723100	-1.40984100
C	-1.76362800	2.77291200	-0.24504500
C	2.06879100	5.61229600	-1.90280500
H	2.91650100	4.17315100	-0.59398500
C	-0.29893000	5.51547200	-2.27397600
C	-1.66010000	3.82149000	-1.10880200
H	-2.73354300	2.34989000	0.00489500
C	0.90898400	6.11386700	-2.53212900
H	3.02457900	6.09965900	-2.06952400
H	-1.21295400	5.89672100	-2.72232300
H	-2.54843400	4.24660000	-1.56940800
H	0.97236000	6.97055600	-3.19455300
O	-0.75462500	1.14390800	1.14922900
N	2.20687300	1.44858100	1.81316800
H	1.63596100	0.35322900	1.82791200
C	1.95088600	2.35508900	3.05332900
C	0.68173600	3.20019600	2.92562200
H	-0.19210200	2.58210200	2.72488800
H	0.54741200	3.69504100	3.89102100
H	0.77661600	3.97495400	2.16500600
C	1.75445800	1.45084400	4.27090700
H	2.62489500	0.85046900	4.52941200
H	1.53493100	2.08104800	5.13583300

H	0.89497100	0.79096300	4.11314600
C	3.13404800	3.31414800	3.20857900
H	3.32850900	3.82495200	2.25896100
H	2.86886800	4.07211800	3.94940300
H	4.05102800	2.82584500	3.53757200
H	2.89256200	1.90187600	-1.43984700

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C	-1.06869500	2.61157400	-2.33773300
C	-0.64011600	3.13871700	-1.14649800
C	-0.54442400	4.56127200	-1.03370600
C	-0.93538100	5.32810100	-2.17227400
C	-1.42566300	3.46730500	-3.40695300
H	0.25648700	4.70945900	0.99872800
H	-1.12845500	1.53634900	-2.47825800
C	-0.08559900	5.24158600	0.11837900
C	-0.86651700	6.74136100	-2.10314000
H	-1.76929600	3.03530700	-4.34461600
C	-0.42873000	7.38323800	-0.97415900
C	-0.02823200	6.61931100	0.15273100
H	-1.17124600	7.30112600	-2.98089800
H	-0.38615900	8.46512100	-0.95305700
O	0.42637400	7.17190600	1.30379800
C	0.53687900	8.58411500	1.37226200
H	-0.43967800	9.06621100	1.25783500
H	0.93437900	8.80472900	2.36177700
H	1.22537300	8.96652100	0.61152900
C	-0.31673900	2.19945400	0.00741500
H	0.21453600	2.75404900	0.78402600

C	-1.62789400	1.63504400	0.58934800
C	-2.45079000	2.70548600	1.34466700
H	-2.21124500	1.19058300	-0.22250500
C	-0.44632900	0.90087200	2.65248000
C	-2.65840700	0.02334500	2.10590100
C	-2.44334000	2.38640100	2.84556600
H	-2.02263900	3.69700200	1.17243800
H	-3.47673200	2.72806600	0.96839800
H	-0.41867400	0.05424400	3.34121200
H	0.55777300	1.02737900	2.24323700
C	-0.99582900	2.18033800	3.31259000
C	-3.22248600	1.06852600	3.08837000
H	-2.44706200	-0.92972200	2.59552100
H	-3.32066500	-0.16609400	1.25805700
H	-2.91059200	3.20295500	3.40163500
H	-0.95367000	2.08138100	4.39969400
H	-0.38676300	3.04869100	3.04215600
H	-2.99903500	0.74433200	4.11132000
N	-1.35980100	0.49561800	1.53806200
C	-4.71340900	1.27570000	2.98763500
C	-5.46552500	1.12743800	1.89915400
H	-5.17971400	1.63363900	3.90406000
H	-6.52820000	1.34683000	1.92419600
H	-5.07216900	0.78986600	0.94366800
N	0.54326100	1.09623000	-0.38506200
H	0.12362200	0.16926900	-0.46379400
C	1.88289300	1.10738400	-0.17134000
S	2.75872200	2.53554000	-0.00186800
N	2.38586400	-0.15364900	-0.05454000
H	1.68103300	-0.85778500	0.21932600

C	6.39851100	-1.37472600	0.27680600
C	6.03237900	-0.40433600	-0.65207900
C	4.71748000	0.02186200	-0.78112800
C	3.73697700	-0.51283400	0.05884300
C	4.09079200	-1.47728400	1.00172400
C	5.41055300	-1.90811600	1.09296600
H	7.42668100	-1.70699200	0.35787600
H	4.44852800	0.75751300	-1.52939300
H	3.33923300	-1.87545800	1.67684000
C	5.74331000	-3.00320800	2.06572500
F	7.04341200	-3.01337600	2.38603000
F	5.04402100	-2.88163200	3.20429000
F	5.45053500	-4.21273800	1.56045900
C	7.08663000	0.23015900	-1.51508600
F	6.60968300	0.55285100	-2.72540100
F	7.55636700	1.36174200	-0.96637100
F	8.13749500	-0.58236500	-1.69608400
N	-1.37488500	4.77511500	-3.33878100
C	-4.63362100	0.52286000	-1.92415400
C	-3.98214700	-0.57224600	-1.33043800
C	-4.70699000	-1.49633600	-0.53344600
C	-6.10121900	-1.35901600	-0.39496500
C	-6.72356000	-0.28604800	-1.01186500
C	-5.99901700	0.66247300	-1.75758200
H	-4.06611100	1.23525700	-2.51724300
H	-6.70081900	-2.06384800	0.16569800
H	-7.79858900	-0.17684000	-0.91116800
H	-6.52019500	1.49637900	-2.21590800
C	-2.63328700	-1.03427400	-1.35904300
C	-2.55851100	-2.17565300	-0.60191300

C	-1.37241400	-3.05981100	-0.58393100
C	-1.41907100	-4.28618200	-1.32083700
C	-0.18650300	-2.64409300	0.02389200
C	-2.56093000	-4.67380000	-2.07726900
C	-0.29456000	-5.15837500	-1.32702000
C	0.93034900	-3.54717500	0.00124800
C	-2.59019000	-5.86674300	-2.75996500
H	-3.41455800	-4.00420200	-2.12626400
C	-0.35502400	-6.38425400	-2.03464200
C	0.87726600	-4.75463200	-0.62952400
H	1.83303600	-3.23838300	0.52082100
C	-1.48129500	-6.74279400	-2.73380300
H	-3.47221900	-6.13440600	-3.33384400
H	0.51628800	-7.03405300	-2.01793500
H	1.73888000	-5.41719100	-0.62086400
H	-1.51885600	-7.68262700	-3.27443300
O	-0.01407200	-1.47744800	0.62020700
N	-3.81662800	-2.45161800	-0.04720900
H	-0.90725400	-0.38762200	1.04733000
C	-4.20695600	-3.47043200	0.97976700
C	-2.99717200	-4.21559300	1.55029100
H	-2.23312700	-3.52132200	1.91089200
H	-3.35343800	-4.80509900	2.39974600
H	-2.54469100	-4.89692400	0.83029800
C	-4.87476200	-2.76607300	2.17598500
H	-5.67282300	-2.07957200	1.90021200
H	-5.29266900	-3.52684700	2.84050100
H	-4.13370200	-2.20053000	2.74551400
C	-5.15577000	-4.49516000	0.34290300
H	-4.63734100	-5.04937700	-0.44309300

H	-5.48467900	-5.20709900	1.10501100
H	-6.04161500	-4.02942200	-0.09200900
H	-1.81892900	-0.65574600	-1.96298100

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C	-3.93287400	-0.27917600	-2.45202700
C	-4.03564300	-0.01789200	-1.10941600
C	-5.29629000	0.43046000	-0.60359200
C	-6.36424800	0.55216400	-1.54221800
C	-5.05777700	-0.11643300	-3.29515600
H	-4.75985800	0.70878000	1.50039900
H	-2.99039600	-0.60309800	-2.88481400
C	-5.54128200	0.75699400	0.75064800
C	-7.63338800	0.98332200	-1.08381500
H	-4.96265600	-0.32781500	-4.35817200
C	-7.85452500	1.28515100	0.23477300
C	-6.78959700	1.17230900	1.16562300
H	-8.42849700	1.06834600	-1.81683500
H	-8.83602500	1.61259000	0.55429800
O	-6.91892700	1.45753200	2.48426800
C	-8.18270200	1.89661500	2.95483300
H	-8.95246700	1.13354800	2.79891600
H	-8.05934500	2.07204600	4.02238500
H	-8.48712800	2.82840900	2.46691000
C	-2.82220700	-0.23559300	-0.21565000
H	-2.98747900	0.25284500	0.74703000
C	-2.59368900	-1.74643000	-0.00319700
C	-3.71309000	-2.42125000	0.82640700
H	-2.50558500	-2.21328600	-0.99169700

C	-1.17196500	-1.32043800	1.98247300
C	-1.13388400	-3.48175100	0.85120900
C	-3.13325400	-2.85059800	2.18185600
H	-4.54528200	-1.72761000	0.97600000
H	-4.10720200	-3.29190500	0.29460300
H	-0.24396700	-1.67742000	2.43798000
H	-1.05760600	-0.24750400	1.80653000
C	-2.41679100	-1.65622300	2.82869800
C	-2.09633900	-3.97270900	1.95017900
H	-0.08635200	-3.68135700	1.08457900
H	-1.35330700	-3.93251000	-0.12016500
H	-3.93467400	-3.21072300	2.83255300
H	-2.11908300	-1.89556700	3.85252400
H	-3.09450900	-0.79759600	2.88196000
H	-1.53530900	-4.09078200	2.88798100
N	-1.27608700	-2.00776200	0.66469300
C	-2.75089800	-5.29788700	1.65926600
C	-2.50410600	-6.12210200	0.64440300
H	-3.49739400	-5.59199000	2.39754000
H	-3.03972600	-7.06122800	0.55553000
H	-1.76150600	-5.91931000	-0.12159500
N	-1.61122400	0.33577700	-0.77606400
H	-0.97309700	-0.29927400	-1.26129200
C	-1.08186500	1.50785700	-0.36939700
S	-1.98731300	2.70884900	0.39302100
N	0.26021100	1.58633900	-0.60586400
H	0.75060700	0.69681900	-0.73600700
C	2.51661500	5.12716700	-0.30977800
C	1.41609800	5.04906200	-1.16209800
C	0.66965000	3.88722500	-1.26217300

C	1.01622000	2.77354300	-0.49048000
C	2.11320200	2.83196700	0.36394700
C	2.85459500	4.01369000	0.44327700
H	3.09541700	6.04101700	-0.23673700
H	-0.18073800	3.83129700	-1.93195400
H	2.37206500	1.97282600	0.97968200
C	4.03950900	4.07297900	1.36520300
F	4.42769700	5.32962200	1.60657100
F	3.77653600	3.49249200	2.54419800
F	5.10605900	3.42803100	0.84928300
C	1.03066100	6.26628900	-1.95462400
F	0.21707900	5.96473100	-2.97444200
F	0.39604500	7.16980200	-1.19227600
F	2.11075100	6.87957800	-2.46260700
N	-6.23399900	0.27644900	-2.87142400
C	3.06978000	-1.50446300	3.84788800
C	3.08359900	-1.66192400	2.45355900
C	3.70348300	-0.70179200	1.60736300
C	4.29098300	0.43699600	2.19522100
C	4.25857700	0.57265800	3.57453600
C	3.66139500	-0.38870700	4.40659000
H	2.58860300	-2.25508000	4.46857700
H	4.75781200	1.22266300	1.62399900
H	4.70176600	1.46099700	4.01264600
H	3.65666600	-0.24464800	5.48200900
C	2.52610300	-2.66183600	1.60735900
C	2.78412600	-2.30209100	0.31353600
C	2.20442900	-3.01492400	-0.85365400
C	2.68481600	-4.29461600	-1.27142800
C	1.04314300	-2.49169400	-1.41346800

C	3.82712700	-4.90810200	-0.68495400
C	2.01204800	-4.99120200	-2.31677100
C	0.39239700	-3.19462800	-2.47146200
C	4.26986500	-6.13441100	-1.11494300
H	4.34417700	-4.38854300	0.11596300
C	2.49598200	-6.25553900	-2.74138900
C	0.86234700	-4.40202000	-2.90833700
H	-0.49302300	-2.74204900	-2.91032500
C	3.60091900	-6.82057900	-2.15683500
H	5.14350700	-6.58333300	-0.65273400
H	1.96974500	-6.76886000	-3.54190900
H	0.35604000	-4.93241000	-3.71058300
H	3.96386600	-7.78771900	-2.48842400
O	0.50205100	-1.35826200	-0.95208500
N	3.52501600	-1.11339500	0.28161300
H	-0.37261700	-1.66898500	-0.06356100
C	4.24105500	-0.63042900	-0.94656800
C	3.24961700	-0.08985900	-1.98145600
H	2.70708200	0.76667200	-1.56998800
H	3.80948500	0.26179400	-2.85329400
H	2.53648700	-0.84195400	-2.31216500
C	5.22055500	0.50139600	-0.63302100
H	5.94980700	0.21878700	0.12920100
H	5.76509600	0.72393400	-1.55371500
H	4.70789500	1.41726800	-0.33446300
C	5.06040300	-1.78711500	-1.53531400
H	4.42771700	-2.58529900	-1.92110700
H	5.66971100	-1.41131200	-2.36195900
H	5.72909600	-2.20228100	-0.77491300
H	1.98195200	-3.54568300	1.91185000

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C	-3.89105400	-0.57648100	-2.43850700
C	-4.01507900	-0.31083200	-1.09839500
C	-5.30361600	0.06379800	-0.60294300
C	-6.37172900	0.11740700	-1.54759800
C	-5.01919300	-0.48802200	-3.28826200
H	-4.79653900	0.37939400	1.50315000
H	-2.92870400	-0.84735800	-2.86424600
C	-5.57479800	0.38159400	0.74848700
C	-7.66569600	0.47902100	-1.09888600
H	-4.90631600	-0.70289600	-4.34893600
C	-7.91095700	0.77654100	0.21650600
C	-6.84700800	0.72767100	1.15397000
H	-8.46051900	0.51391300	-1.83650500
H	-8.91118500	1.05084500	0.52814600
O	-6.99998700	1.01037400	2.47096400
C	-8.28764600	1.38445500	2.93192100
H	-9.01708000	0.58355200	2.77142900
H	-8.18119400	1.56656900	4.00022000
H	-8.63556200	2.29945400	2.44112000
C	-2.79547600	-0.44181500	-0.19745200
H	-3.00108300	0.03587000	0.76211500
C	-2.44200200	-1.92787400	0.02183500
C	-3.53909200	-2.69221400	0.80927500
H	-2.30569600	-2.38314700	-0.96809200
C	-1.14412400	-1.40308800	2.03355200
C	-0.86892000	-3.51739400	0.89586700
C	-2.96088300	-3.10436900	2.16970800

H	-4.42355200	-2.06416700	0.95474900
H	-3.85873900	-3.57781000	0.25209300
H	-0.20207500	-1.66771800	2.52379600
H	-1.13322400	-0.31922200	1.88417600
C	-2.37034200	-1.86572000	2.85602800
C	-1.82281400	-4.12524200	1.94805400
H	0.18155000	-3.63579500	1.17493400
H	-1.00363600	-3.98605400	-0.08366500
H	-3.74537600	-3.54767700	2.79047600
H	-2.07394500	-2.09933200	3.88230300
H	-3.12691600	-1.07477500	2.91086300
H	-1.28761800	-4.21753300	2.90443300
N	-1.13111500	-2.07022400	0.71135200
C	-2.34722900	-5.49568700	1.60735400
C	-1.95724600	-6.28930000	0.61274500
H	-3.11951300	-5.85803000	2.28715000
H	-2.40304800	-7.26954800	0.48057900
H	-1.17901700	-6.01482200	-0.09363200
N	-1.63424700	0.23198600	-0.75331300
H	-0.98121100	-0.33457300	-1.28796900
C	-1.20104100	1.44497700	-0.35978400
S	-2.18186100	2.54658500	0.45800900
N	0.11452300	1.66187500	-0.66396500
H	0.68760600	0.83078900	-0.81656000
C	2.08777200	5.36497900	-0.32784700
C	0.92798300	5.23958700	-1.09146300
C	0.27263800	4.02544700	-1.20598300
C	0.77156000	2.90446700	-0.53446900
C	1.92711000	3.01070700	0.23361800
C	2.57670700	4.24465500	0.32416800

H	2.59493000	6.31930900	-0.24325300
H	-0.62204400	3.93566400	-1.81112700
H	2.30327800	2.14616800	0.77822200
C	3.82070200	4.35118800	1.15940200
F	4.18556400	5.62110100	1.36267000
F	3.65939200	3.77505800	2.35923800
F	4.86836900	3.73167200	0.57684700
C	0.37124600	6.46227600	-1.76459300
F	-0.49709400	6.14984300	-2.73446400
F	-0.27268300	7.25248000	-0.89216800
F	1.34415400	7.20575300	-2.31326700
N	-6.21864500	-0.16018000	-2.87414000
C	3.27641000	-1.21096900	3.82791000
C	3.29397100	-1.42141100	2.44050300
C	3.84410000	-0.45449000	1.55519200
C	4.34775300	0.74817000	2.09174300
C	4.30991300	0.93566500	3.46433800
C	3.78935100	-0.03464000	4.33751900
H	2.85118700	-1.96703700	4.48165700
H	4.74841600	1.54294700	1.48366900
H	4.68502900	1.87231700	3.86380100
H	3.77838600	0.15133700	5.40638800
C	2.79470700	-2.48535700	1.63624900
C	3.02169000	-2.15361800	0.32973500
C	2.44950700	-2.91645500	-0.80920500
C	2.95746000	-4.19273900	-1.20930400
C	1.28063200	-2.44685000	-1.37813500
C	4.12270400	-4.76170800	-0.62602900
C	2.28568300	-4.92277300	-2.23174400
C	0.62948400	-3.16449500	-2.41368600

C	4.58737100	-5.98644900	-1.03566200
H	4.63710200	-4.21053100	0.15502100
C	2.79257200	-6.18618900	-2.63450800
C	1.12013000	-4.37280800	-2.82831400
H	-0.26634600	-2.73502100	-2.85284400
C	3.91742100	-6.71028600	-2.05154800
H	5.47830000	-6.40536200	-0.57889300
H	2.26848900	-6.72910500	-3.41622000
H	0.61989100	-4.93006500	-3.61530700
H	4.29769900	-7.67650000	-2.36601800
O	0.71293900	-1.28778100	-0.92726400
N	3.69053800	-0.92695100	0.24770700
H	0.02141000	-1.55696300	-0.18510000
C	4.36340300	-0.43979900	-1.00261800
C	3.33327100	0.06721400	-2.01730700
H	2.74079800	0.87660000	-1.57933900
H	3.86238100	0.47337400	-2.88455900
H	2.66617800	-0.71979200	-2.36418300
C	5.32580000	0.71563500	-0.72091000
H	6.05091700	0.46932000	0.05767600
H	5.87504300	0.91374300	-1.64417300
H	4.79852500	1.63393100	-0.45948900
C	5.19602200	-1.58213600	-1.60141700
H	4.57727000	-2.40272200	-1.96210800
H	5.77029100	-1.19945300	-2.44946700
H	5.89704100	-1.97035100	-0.85618700
H	2.29312400	-3.38200500	1.97413700

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C	-3.33422700	-1.79803900	-1.64898400
C	-2.26622700	-1.04772300	-1.13052700
C	-2.45776000	-0.20409200	-0.00656000
C	-3.72663800	-0.11892000	0.59725000
C	-4.76232500	-0.86970800	0.06692000
C	-4.57528400	-1.70619400	-1.04930600
H	-3.17534900	-2.44147000	-2.50949500
H	-3.92149100	0.50582400	1.45851700
H	-5.74224400	-0.80734400	0.52941800
H	-5.41176400	-2.27958200	-1.43565700
C	-0.89622600	-0.92807800	-1.50033600
C	-0.30620400	-0.04951000	-0.63235400
C	1.14087900	0.27217300	-0.69019200
C	2.09290700	-0.58427700	-0.05956800
C	1.58571500	1.34427100	-1.43413600
C	1.69383800	-1.68818000	0.74406700
C	3.48427600	-0.31868700	-0.20352500
C	2.97031200	1.60720400	-1.58504900
C	2.62954400	-2.48240600	1.35852100
H	0.63414600	-1.89539600	0.85989500
C	4.42715500	-1.16459200	0.43703900
C	3.89249700	0.79292800	-0.98600300
H	3.28659600	2.46096400	-2.17808100
C	4.01293500	-2.22381700	1.20303300
H	2.30805000	-3.32034400	1.96891500
H	5.48529000	-0.95207800	0.30992000
H	4.95367200	0.99443400	-1.10106500
H	4.73970400	-2.86459700	1.69120400
O	0.65351300	2.17043500	-1.97863100
N	-1.24498900	0.40942500	0.29368000

C	-1.08711100	1.38395700	1.41049600
C	-1.38885900	0.66890800	2.73548000
H	-0.65713900	-0.12964700	2.89120200
H	-1.30497100	1.38029700	3.56166500
H	-2.38422800	0.22671900	2.76724800
C	0.33176500	1.94727100	1.51455000
H	0.60884700	2.51005200	0.62166900
H	0.33986000	2.63526900	2.36436000
H	1.07480600	1.17034500	1.70285500
C	-2.01793200	2.57953700	1.15657800
H	-3.06925900	2.30261400	1.08991900
H	-1.90828900	3.30437000	1.96795000
H	-1.73297900	3.06324800	0.21775900
H	-0.38351100	-1.43414900	-2.30594000
H	1.08889800	2.86887000	-2.48334400

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C	5.24472800	2.26801200	1.98457000
C	4.34349100	2.07350700	0.89511800
C	3.48048200	0.93641800	0.96315900
C	3.55959300	0.12662300	2.06614700
H	6.80762700	3.50183900	2.78633400
H	4.53250600	-0.22825300	3.97095900
C	6.13050300	3.37311200	1.94854600
C	4.35944600	2.99391400	-0.17792700
H	2.91266300	-0.74276600	2.15246900
C	5.23486600	4.05963100	-0.18236900
C	6.13698400	4.25182100	0.89601900
H	3.66807800	2.91302900	-1.00895000

H	6.82549200	5.08781100	0.89956100
N	5.30252700	1.44322200	3.06975300
O	5.16898600	4.88492800	-1.25575200
C	6.03864300	6.00414000	-1.29638800
H	7.08867400	5.69323200	-1.29715200
H	5.81551900	6.52261200	-2.22755600
H	5.85806500	6.67918000	-0.45322400
C	2.50163400	0.57979100	-0.14540600
H	2.47859000	1.38401900	-0.87852600
N	1.14009100	0.45132500	0.34554600
H	0.91038600	-0.41587400	0.83407400
C	0.18826800	1.39678700	0.18182300
S	0.51019500	2.89752200	-0.53699900
N	-1.02437000	1.02744200	0.66675500
H	-1.09859200	0.13475800	1.16593800
C	2.93790400	-0.72250200	-0.83942200
C	4.29485900	-0.55027200	-1.57401800
H	2.99565700	-1.51839500	-0.08425300
C	1.59456800	-0.12643300	-2.81608200
C	2.44643600	-2.37490000	-2.52615900
C	4.03797500	-0.56498700	-3.08801800
H	4.76708100	0.39266500	-1.28166000
H	4.98160400	-1.35722200	-1.30250200
H	0.96502900	-0.59846200	-3.57508900
H	1.00276500	0.65582100	-2.33484300
C	2.90882500	0.42057500	-3.42126200
C	3.57271700	-1.97945000	-3.49927200
H	1.60880400	-2.86320900	-3.03327500
H	2.80780400	-3.05148400	-1.74870500
H	4.95136900	-0.29688000	-3.62642600

H	2.80428100	0.53358000	-4.50356000
H	3.14206900	1.41095700	-3.01440400
H	3.16203700	-1.90192500	-4.51603400
N	1.91385400	-1.17992500	-1.82097900
C	4.71190800	-2.96318300	-3.55839000
C	4.79392000	-4.14995900	-2.96155600
H	5.54362100	-2.63928500	-4.18470800
H	5.67219500	-4.77293900	-3.09446000
H	4.00582700	-4.55889800	-2.33498800
C	-2.26797800	1.67044200	0.50929900
C	-2.64777300	2.32107600	-0.66414600
C	-3.18919300	1.53892900	1.55343300
C	-3.92838000	2.85745200	-0.76491800
H	-1.95149300	2.41100800	-1.48754900
C	-4.47232200	2.04428600	1.40962200
H	-2.90538900	1.00145200	2.45167500
C	-4.85688700	2.72371900	0.25775500
H	-5.85618300	3.13272100	0.15672400
C	-5.50275400	1.81014600	2.47564000
C	-4.32027500	3.52617100	-2.05210100
F	-5.40492000	4.29896900	-1.90504400
F	-4.60311100	2.62657700	-3.00861200
F	-3.33285800	4.29776800	-2.52905900
F	-4.98622100	1.22088600	3.56312400
F	-6.08648400	2.95085000	2.86782300
F	-6.48774800	1.00989000	2.02578600
C	-4.20671300	-2.92719100	-3.68653000
C	-3.23132200	-2.72439900	-2.72495700
C	-3.57694000	-2.26785900	-1.44367500
C	-4.93445500	-2.01324800	-1.15239100

C	-5.91089600	-2.21999100	-2.14215100
C	-5.55553400	-2.67352500	-3.39924900
H	-2.18635100	-2.91476300	-2.95333200
C	-2.57914400	-2.02413600	-0.40560600
C	-5.29891800	-1.55090800	0.16913200
H	-6.95135200	-2.01816300	-1.90251900
H	-6.31353400	-2.83046700	-4.15888600
C	-4.39201600	-1.34943400	1.15114200
C	-2.96824700	-1.54408000	0.91866900
H	-6.35191400	-1.36115100	0.36482100
H	-4.68526000	-1.00930300	2.13912300
C	-1.26690100	-2.32579600	-0.54736500
C	-0.01445800	-2.54853100	-0.55916700
C	0.72460200	-3.68507300	0.05196300
C	1.05716400	-4.81572100	-0.69055600
C	1.13185400	-3.56717300	1.40434600
C	1.81149300	-5.84535700	-0.13261800
H	0.71913300	-4.87938300	-1.72108000
C	1.88551000	-4.61516700	1.95014600
C	2.22547800	-5.73149600	1.18915800
H	2.06347000	-6.72026700	-0.72186700
H	2.20376600	-4.57653600	2.98193200
H	2.81048200	-6.52167900	1.64893100
H	-3.92206300	-3.28188800	-4.67200400
O	-2.13078700	-1.30692700	1.82183100
H	0.82940000	-1.69592600	-1.17014400
C	4.48118700	0.42137900	3.09889800
N	0.77976300	-2.38757500	2.09180800
H	-0.15399500	-2.09350400	1.79284000
C	0.82380500	-2.25997700	3.57192000

C	0.36743700	-0.82361700	3.86117000
H	1.06325400	-0.09905300	3.42414500
H	-0.63376500	-0.64681000	3.45749200
H	0.33549000	-0.65610400	4.94122300
C	-0.16437100	-3.23466600	4.22587000
H	0.08227100	-4.27217100	3.98298400
H	-0.14395200	-3.12352900	5.31431100
H	-1.17885800	-3.02491000	3.87204000
C	2.24901100	-2.45290800	4.14008700
H	2.36068800	-3.41204400	4.65238200
H	3.01192600	-2.40561700	3.35885400
H	2.46649500	-1.67202100	4.87430900

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C	-2.69909800	-1.25462200	-2.07541000
C	-3.35879100	-1.46167300	-0.89077500
C	-4.70167500	-1.95213100	-0.94676000
C	-5.25196300	-2.19636300	-2.23965300
C	-3.34450800	-1.52866500	-3.30444700
H	-5.14448300	-2.00251800	1.19435100
H	-1.68406200	-0.86912300	-2.07599300
C	-5.50860000	-2.18749000	0.19043400
C	-6.57991700	-2.67804400	-2.33873600
H	-2.80881900	-1.35926600	-4.23673900
C	-7.34578200	-2.90579100	-1.22437100
C	-6.80055800	-2.65277500	0.06034400
H	-6.97504200	-2.85769800	-3.33312000
H	-8.35868000	-3.27259800	-1.33462800
O	-7.49088100	-2.84274100	1.21412700

C	-8.83567200	-3.28034600	1.12283400
H	-8.90385700	-4.26873100	0.65554400
H	-9.20159800	-3.34063800	2.14676100
H	-9.44909100	-2.56864600	0.56004700
C	-2.62267400	-1.24779000	0.42084700
H	-3.34044700	-1.16109000	1.24302600
C	-1.65826700	-2.42653400	0.65512000
C	-2.32752000	-3.81505500	0.71393100
H	-0.96510300	-2.41404800	-0.19660400
C	-1.56045600	-2.57468200	3.06446800
C	0.37236500	-3.03273900	1.73259200
C	-1.51440900	-4.65974900	1.70979100
H	-3.36649700	-3.74553200	1.05921300
H	-2.34552200	-4.26671400	-0.28229900
H	-0.99106000	-2.22462900	3.93037600
H	-2.51497800	-2.03928500	3.07421300
C	-1.78334000	-4.10927400	3.11669300
C	-0.00042500	-4.50551900	1.41601300
H	0.91222800	-2.97036700	2.68410300
H	1.02892200	-2.59924200	0.97439900
H	-1.80131200	-5.71391200	1.64184900
H	-1.10402200	-4.57871600	3.83680300
H	-2.80584900	-4.34148700	3.43033700
H	0.53456100	-5.16624100	2.11234100
N	-0.82701400	-2.18966300	1.84806300
C	0.32519700	-4.99063400	0.02457800
C	0.93123400	-4.33505400	-0.96255900
H	0.00756300	-6.01812400	-0.16470800
H	1.10707600	-4.81703500	-1.91951100
H	1.29906900	-3.31662800	-0.86725400

N	-1.78329200	-0.06358200	0.39540400
H	-0.83287600	-0.23243500	0.72502500
C	-2.22637900	1.20685300	0.34457000
S	-3.86404700	1.59670100	0.24450500
N	-1.19043500	2.09678200	0.40405500
H	-0.27131500	1.65954200	0.51218000
C	-0.78322800	6.28419000	0.27839400
C	-1.94031900	5.68968200	-0.21475400
C	-2.13835100	4.31420000	-0.18770200
C	-1.15507100	3.49314600	0.37827900
C	0.00449700	4.08281900	0.89582200
C	0.18724700	5.45706500	0.82744800
H	-0.63920900	7.35666700	0.22837000
H	-3.03500700	3.88087900	-0.60721700
H	0.76854100	3.45544300	1.34817600
C	1.49084000	6.02043700	1.31546500
F	1.46873800	7.35682100	1.38645800
F	1.80969800	5.55365700	2.53197700
F	2.50286500	5.68047500	0.49735200
C	-3.02569000	6.56965100	-0.76905600
F	-3.77356100	5.93258400	-1.67969400
F	-3.85793300	6.99343900	0.19585800
F	-2.52077100	7.66655500	-1.35452100
N	-4.56860900	-1.98684000	-3.40250200
C	3.50221400	-4.47958000	1.95840900
C	3.77197500	-3.37113900	1.14935000
C	4.15806200	-3.56048400	-0.20740200
C	4.22917700	-4.88132200	-0.68485700
C	3.92994800	-5.96111500	0.13472300
C	3.56466200	-5.77539100	1.46557000

H	3.22514800	-4.30502500	2.99546800
H	4.52314000	-5.07132300	-1.70714400
H	3.99457500	-6.96365700	-0.27706200
H	3.33917400	-6.62010600	2.10664300
C	3.64826500	-2.04125000	1.77003700
C	3.57832900	-0.85831800	1.21346900
C	3.60637500	0.34513400	0.65676600
C	4.88777500	1.00751200	0.32508100
C	2.31658700	0.97088700	0.24946000
C	6.11931600	0.49773600	0.74873700
C	4.86448700	2.15648700	-0.48934000
C	2.40301100	2.13494500	-0.62991300
C	7.30529700	1.10995300	0.36282800
H	6.14284300	-0.38203000	1.38546800
C	6.06804900	2.76453700	-0.87019700
C	3.59160800	2.68369700	-0.95261400
H	1.46942100	2.54804200	-0.99945100
C	7.28384600	2.24522100	-0.45152900
H	8.25219400	0.70289000	0.70170100
H	6.03599400	3.64728800	-1.50219700
H	3.61938100	3.56411800	-1.58993800
H	8.21174800	2.71928600	-0.75204700
O	1.23168200	0.53221000	0.64153800
N	4.41084700	-2.44340400	-0.97724000
H	4.78571800	-1.66829300	-0.44575800
C	4.81676400	-2.37558500	-2.38935200
C	6.17429400	-3.04540100	-2.65146600
H	6.15442800	-4.12338500	-2.48261600
H	6.47938800	-2.87357700	-3.68809400
H	6.93411700	-2.61185700	-1.99384600

C	3.71446200	-2.94626000	-3.28840700
H	2.77750800	-2.41106800	-3.10911400
H	3.99519100	-2.81561000	-4.33740000
H	3.53490400	-4.00932300	-3.11985600
C	4.95233200	-0.87623700	-2.68711200
H	5.75949200	-0.43160400	-2.09239600
H	5.18395100	-0.72114300	-3.74369100
H	4.01964700	-0.35211300	-2.45057500
H	3.57631300	-2.03998200	2.86030300

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C	5.55501100	1.31387300	2.10375600
C	4.95186900	1.17186700	0.81866200
C	3.63543900	0.61323100	0.77391400
C	3.04845000	0.25522800	1.96055700
H	7.29414300	1.95835200	3.18120800
H	3.25398600	0.16479300	4.11445000
C	6.85781700	1.86230900	2.19252000
C	5.67380900	1.60158200	-0.31893100
H	2.04773000	-0.16631700	1.96893400
C	6.94089500	2.13296900	-0.19906500
C	7.54618900	2.26384900	1.07666700
H	5.25544900	1.53768000	-1.31623500
H	8.54008900	2.68172900	1.17923700
N	4.94405300	0.95081600	3.26901200
O	7.54436000	2.51238900	-1.35479600
C	8.83507900	3.09207200	-1.27580700
H	9.56252600	2.39049800	-0.85362900
H	9.11879400	3.33240200	-2.29941700

H	8.82436300	4.00962100	-0.67806200
C	2.92432100	0.30766100	-0.53415000
H	3.39883200	0.85506100	-1.35603800
N	1.50596000	0.61773400	-0.51272300
H	0.94199500	-0.11623800	-0.95170200
C	0.96813100	1.84355700	-0.35094900
S	1.87371700	3.20182900	0.07310500
N	-0.37958600	1.83333000	-0.56127200
H	-0.77023000	0.94496100	-0.89656100
C	3.01942800	-1.21568600	-0.76834400
C	4.45521300	-1.71872800	-1.02666300
H	2.64207100	-1.68252800	0.15081100
C	2.70084400	-1.41362600	-3.15533600
C	1.88761300	-3.10027600	-1.65968600
C	4.34689600	-2.89133900	-2.01558600
H	5.08053400	-0.93038000	-1.46409400
H	4.92536400	-2.02238900	-0.08675800
H	1.93111300	-1.58738600	-3.91220300
H	2.97416200	-0.35536400	-3.21529900
C	3.93648600	-2.32381800	-3.38033700
C	3.23756500	-3.86387800	-1.54072900
H	1.31934300	-3.45550000	-2.52571100
H	1.25494400	-3.25114800	-0.78030200
H	5.30115900	-3.42267500	-2.08654400
H	3.69831600	-3.14306000	-4.06767000
H	4.76109500	-1.75559400	-3.82153500
H	3.23101300	-4.71274200	-2.23876300
N	2.10466700	-1.65652700	-1.83208500
C	3.57921900	-4.41739200	-0.17812300
C	2.84307300	-4.41887800	0.93083200

H	4.57392100	-4.86493200	-0.12831000
H	3.22562200	-4.85726600	1.84718300
H	1.83386500	-4.01673800	0.98043800
C	-1.35239500	2.79062300	-0.24042100
C	-2.58108300	2.28021300	0.19843600
C	-1.20452000	4.16891100	-0.39303500
C	-3.64533600	3.12672700	0.45423800
H	-2.69246300	1.21054000	0.33736000
C	-2.28095900	5.00411400	-0.09265900
H	-0.26846600	4.58001000	-0.74663100
C	-3.50792600	4.50708200	0.32338600
H	-4.33497200	5.17436200	0.53804800
C	-2.07353400	6.48715700	-0.21859400
C	-4.97773000	2.55456100	0.84457400
F	-5.86830500	2.65616300	-0.15866000
F	-5.50746900	3.20209900	1.89231500
F	-4.89717400	1.25532100	1.16694500
F	-1.31317600	6.96424200	0.77907200
F	-1.44904900	6.80200700	-1.36395100
F	-3.23134300	7.16178600	-0.19204700
C	-6.59818300	-3.32016700	-0.26328000
C	-5.22926700	-3.26410700	-0.46643200
C	-4.63152100	-2.11308800	-1.00819500
C	-5.45590100	-1.01533900	-1.34053500
C	-6.84198000	-1.08806400	-1.12470600
C	-7.41400900	-2.22774800	-0.58901700
H	-4.60662900	-4.11802700	-0.21420400
C	-3.18794900	-2.00100400	-1.19830600
C	-4.85084700	0.17027500	-1.90471100
H	-7.45709100	-0.23054500	-1.38391100

H	-8.48453600	-2.27735700	-0.42241300
C	-3.51770900	0.28587600	-2.09190900
C	-2.58815100	-0.76537400	-1.68490000
H	-5.50741400	0.99450000	-2.17232500
H	-3.07810400	1.18673000	-2.50963700
C	-2.35988200	-3.02582400	-0.84910600
C	-1.53321400	-4.01435300	-1.10948400
C	-0.88138900	-4.78640000	-0.05553000
C	-0.05022700	-5.88137600	-0.28628200
C	-1.25081900	-4.43502500	1.25064700
C	0.39749400	-6.63974500	0.79107500
H	0.23102900	-6.14152800	-1.30261500
C	-0.83823200	-5.22519000	2.32054600
C	-0.00509200	-6.32008100	2.08594300
H	1.05121700	-7.48824100	0.61949100
H	-1.17296700	-5.00332300	3.32742000
H	0.32352100	-6.92742100	2.92254500
H	-7.04065500	-4.21908900	0.15414500
O	-1.35193500	-0.57929400	-1.74706800
H	-1.41015600	-4.30548100	-2.15097600
N	-2.13759400	-3.30854700	1.32776100
H	-3.03116300	-3.59111200	1.73223000
C	-1.67734700	-2.05804300	2.01722900
C	-2.87421100	-1.10340400	2.01146700
H	-2.59251000	-0.15508600	2.47749600
H	-3.22906000	-0.90435300	0.99890000
H	-3.70816800	-1.52349800	2.58531700
C	-0.49484300	-1.46556100	1.25343100
H	-0.73651300	-1.29440000	0.20115800
H	-0.22057500	-0.50705800	1.70732700

H	0.37876100	-2.12741100	1.31132800
C	-1.26309100	-2.31796700	3.47041600
H	-2.05905200	-2.82434900	4.02604800
H	-0.34958000	-2.91425700	3.52858700
H	-1.06724900	-1.35926700	3.95942700
C	3.73648700	0.44851100	3.18080900

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C	6.31465700	-0.02943300	2.17817100
C	5.50115700	-0.15989100	1.01371500
C	4.09702100	-0.35038600	1.21514300
C	3.63069100	-0.37285400	2.50502100
H	8.30724100	0.24919500	2.92217100
H	4.14363500	-0.25358200	4.60643500
C	7.70963600	0.15692200	2.02127000
C	6.11643300	-0.07910400	-0.25728100
H	2.56926600	-0.49262900	2.69939500
C	7.47789800	0.10558800	-0.37671400
C	8.29004600	0.22123600	0.78052100
H	5.53977900	-0.14721900	-1.17251000
H	9.35992100	0.36641500	0.69538600
N	5.82254200	-0.07054200	3.45080100
O	7.96838800	0.16870700	-1.64153700
C	9.36371300	0.35176500	-1.80682000
H	9.92931300	-0.47243200	-1.35891000
H	9.53929700	0.36717700	-2.88149400
H	9.69645600	1.30029500	-1.37176400
C	3.12576900	-0.59042200	0.06987700
H	3.57076000	-0.24064100	-0.86630900

N	1.86342400	0.09447000	0.26576900
H	1.02930000	-0.50390600	0.29837600
C	1.65025400	1.40074500	0.02750200
S	2.89762400	2.47664900	-0.36629900
N	0.32230500	1.70879600	0.10442100
H	-0.29387800	0.87216700	0.22360300
C	2.79304800	-2.09408100	-0.02340300
C	4.01182400	-2.99484700	-0.33017400
H	2.37939000	-2.37934200	0.95428800
C	2.22820200	-2.27651400	-2.36765600
C	1.13743700	-3.64764200	-0.74610200
C	3.53315300	-4.10023300	-1.28587900
H	4.81473100	-2.42666600	-0.81497800
H	4.42128900	-3.41105100	0.59476700
H	1.36820300	-2.30880600	-3.04384800
H	2.71554300	-1.30854600	-2.52207500
C	3.20751500	-3.45027000	-2.63653600
C	2.23540900	-4.74975700	-0.73803800
H	0.40117700	-3.83564500	-1.53516400
H	0.58411900	-3.60832900	0.19696600
H	4.30819000	-4.86463000	-1.40211400
H	2.75710800	-4.19030100	-3.30710500
H	4.12507500	-3.09170100	-3.11393700
H	1.95491000	-5.54209000	-1.44563400
N	1.71286100	-2.32210400	-0.99354300
C	2.50575900	-5.42293600	0.58464500
C	1.96027300	-5.17369000	1.77296900
H	3.26724700	-6.20317400	0.52755000
H	2.26394300	-5.73648300	2.64961600
H	1.19785500	-4.41625000	1.92796900

C	-0.33130100	2.92146800	-0.10616300
C	-1.62121900	2.85447500	-0.64717200
C	0.18888600	4.16985400	0.25475300
C	-2.37050900	4.01198100	-0.81923400
H	-2.02245300	1.88749100	-0.94434400
C	-0.57510500	5.31293100	0.05299500
H	1.17537900	4.23933100	0.69313400
C	-1.85854100	5.25853700	-0.48039900
H	-2.44154500	6.16024400	-0.62443500
C	0.02608800	6.64789400	0.39108800
C	-3.76754300	3.89248000	-1.35401900
F	-3.84300000	3.00561100	-2.35868800
F	-4.24257500	5.05851900	-1.80312700
F	-4.62859600	3.46097400	-0.40508200
F	-0.91531100	7.56503300	0.65914200
F	0.83396100	6.57425200	1.45862000
F	0.76380800	7.13010000	-0.62187600
C	-4.74850400	-4.07004100	-2.84575800
C	-4.21514300	-3.54206600	-1.69002300
C	-3.14182300	-2.61179300	-1.73118700
C	-2.59666500	-2.28833000	-3.00372300
C	-3.16112800	-2.84410700	-4.17261000
C	-4.23008200	-3.71006000	-4.10569500
H	-4.58017100	-3.89951100	-0.72872100
C	-2.59578500	-2.00523900	-0.55505300
C	-1.47133400	-1.40663900	-3.05542000
H	-2.72940300	-2.57593800	-5.13374700
H	-4.65636300	-4.12995100	-5.01026600
C	-0.90419200	-0.90884300	-1.92278500
C	-1.43339100	-1.19888400	-0.60444800

H	-1.06064100	-1.15028600	-4.02965000
H	-0.02620200	-0.26984600	-1.97175000
C	-3.30182200	-2.10519800	0.70832600
C	-2.90185500	-2.43939600	1.94323400
C	-4.02725400	-2.41510500	2.86750800
C	-4.15311500	-2.80017100	4.19869900
C	-5.16381700	-2.03405500	2.15209900
C	-5.42728200	-2.82321000	4.76398700
H	-3.28168300	-3.09655400	4.77193000
C	-6.44014500	-2.10087200	2.67615300
C	-6.55609400	-2.49745200	4.01162400
H	-5.54675200	-3.12370400	5.79940500
H	-7.31928200	-1.86685400	2.08861400
H	-7.54068300	-2.55601900	4.46134800
H	-5.56196700	-4.78613900	-2.78190000
O	-0.89867500	-0.67969000	0.44533100
H	-1.89395700	-2.75102500	2.17871600
N	-4.75334100	-1.64762700	0.79178500
H	-5.31730100	-2.13659700	0.08559000
C	-4.91679200	-0.09903900	0.47739600
C	-4.73959700	0.11497700	-1.02757500
H	-5.05495800	1.13697400	-1.24451100
H	-3.70968600	-0.00232600	-1.36192400
H	-5.37703600	-0.56132700	-1.60765000
C	-3.88838900	0.66014900	1.30234400
H	-2.86254000	0.38307300	1.04469700
H	-4.03119700	1.72493900	1.10291000
H	-4.04390200	0.49123000	2.37241300
C	-6.33313600	0.32926400	0.85319800
H	-7.09261500	-0.27456100	0.34653300

H	-6.50492700	0.31423500	1.92937900
H	-6.45133100	1.36054500	0.51228900
C	4.52878300	-0.22922800	3.58865300

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C	2.70370200	-1.38696400	-2.67786800
C	3.01409800	-1.59545300	-1.35632700
C	3.84144400	-2.71377500	-1.02291700
C	4.29748400	-3.52738900	-2.10318100
C	3.20796800	-2.26511100	-3.66636400
H	3.88941300	-2.48245500	1.15190100
H	2.07313600	-0.54743300	-2.96573800
C	4.23532400	-3.04810500	0.29413600
C	5.12988300	-4.63795400	-1.81969300
H	2.95864200	-2.08948400	-4.71122900
C	5.50729300	-4.94206900	-0.53744400
C	5.05066500	-4.13378000	0.53562400
H	5.46107400	-5.24237100	-2.65753200
H	6.14512100	-5.79771400	-0.35286000
O	5.37093600	-4.36858300	1.83339400
C	6.19877600	-5.48125000	2.12579700
H	7.17993200	-5.38460900	1.64859800
H	6.32339900	-5.48618100	3.20758900
H	5.73075600	-6.41988400	1.81063000
C	2.46519900	-0.62683100	-0.31005700
H	2.69633600	-0.99357400	0.68831200
C	3.09670900	0.76545300	-0.52557700
C	4.61997900	0.69907900	-0.23220800
H	2.90519900	1.07409700	-1.55421300

C	2.48957500	1.36210800	1.76081500
C	3.31225200	3.04449500	0.20597500
C	4.89974500	1.38265000	1.10879300
H	4.95283400	-0.34260100	-0.19894200
H	5.18570300	1.19241000	-1.02883900
H	2.20374100	2.20727100	2.38456600
H	1.72306200	0.59108600	1.88275400
C	3.90185800	0.86688900	2.15162300
C	4.66118400	2.89515200	0.93201400
H	2.75436000	3.89141400	0.60507700
H	3.44792200	3.20696700	-0.86797000
H	5.92833700	1.19389600	1.42989100
H	4.15902900	1.24658300	3.14453800
H	3.94538100	-0.22595200	2.20780900
H	4.57270100	3.33222600	1.93746400
N	2.46436000	1.82589200	0.33711800
C	5.81721900	3.58213600	0.25527100
C	5.78251500	4.36901600	-0.81720700
H	6.77934100	3.40292700	0.73605100
H	6.69250400	4.81447700	-1.20493500
H	4.86544000	4.61325000	-1.34491400
N	1.02461700	-0.53637500	-0.42216200
H	0.75132100	0.14278900	-1.16253000
C	0.15714700	-1.34676400	0.19111700
S	0.58643400	-2.38191600	1.46317600
N	-1.10461800	-1.27878700	-0.34488700
H	-1.17702400	-0.77716400	-1.22601400
C	-4.92845200	-2.09841000	1.21025700
C	-3.86457900	-1.87152500	2.06842900
C	-2.57731400	-1.63027000	1.59441500

C	-2.34292600	-1.61438700	0.21943300
C	-3.41132000	-1.83681400	-0.66225300
C	-4.68086400	-2.07539600	-0.16185500
H	-5.92454000	-2.28476300	1.59528200
H	-1.76681300	-1.43694600	2.28655500
H	-3.24291600	-1.81512600	-1.73485900
C	-5.83376700	-2.35114700	-1.08524700
F	-6.35981600	-3.56454300	-0.84597800
F	-6.82953700	-1.46658100	-0.90746300
F	-5.48445100	-2.31538300	-2.37562000
C	-4.06775700	-1.84529200	3.55643600
F	-5.34631600	-2.04267700	3.89966300
F	-3.33351600	-2.78247500	4.17283300
F	-3.69247900	-0.66235500	4.07807000
N	3.97735900	-3.29518900	-3.40868900
C	-1.11042400	2.22925600	3.38337700
C	-0.91008500	2.35297100	2.00872000
C	-0.01183000	3.28631500	1.48419400
C	0.71986800	4.11151400	2.33440800
C	0.49752000	4.00364900	3.70781700
C	-0.40240300	3.07121600	4.23069300
H	-1.80232600	1.48679100	3.76798800
H	1.45965700	4.81672000	1.98490100
H	1.05150100	4.65262000	4.37708100
H	-0.54169600	3.00293100	5.30426200
C	-1.47575200	1.62389100	0.90316600
C	-0.96109300	2.05917600	-0.26388200
C	-1.39723200	1.61645400	-1.59869000
C	-2.80364500	1.41220000	-1.85473700
C	-0.42961800	1.23446900	-2.55731400

C	-3.84701200	1.81564600	-0.97318500
C	-3.20145700	0.77835900	-3.07086300
C	-0.88743500	0.64987100	-3.79458200
C	-5.16743100	1.53867700	-1.24429300
H	-3.60143400	2.36066400	-0.06952200
C	-4.56584900	0.50259900	-3.32017200
C	-2.20665000	0.41465800	-4.02668600
H	-0.12309800	0.36813800	-4.51270500
C	-5.54097300	0.85636000	-2.41999500
H	-5.93187500	1.85713000	-0.54187900
H	-4.82595700	-0.00787900	-4.24399600
H	-2.52804500	-0.06387800	-4.94886800
H	-6.58209400	0.62099400	-2.61024200
O	0.83214500	1.31834800	-2.31322600
N	0.08799000	3.09242100	0.02497200
C	-0.09811200	4.39924400	-0.82197200
C	-1.58777000	4.75358000	-0.79883700
H	-2.18783800	4.05205600	-1.38000400
H	-1.96301300	4.78294100	0.23009900
H	-1.71589900	5.74920100	-1.23135100
C	0.66765200	5.59005900	-0.23538700
H	1.74010800	5.40731800	-0.14011500
H	0.55016100	6.41191300	-0.94434800
H	0.25709700	5.92728600	0.71539300
C	0.41071900	4.19033600	-2.24730700
H	1.41212600	3.75554400	-2.25389600
H	-0.24638100	3.55370200	-2.83354400
H	0.44599600	5.17013600	-2.73009400
H	-2.22672800	0.85168900	0.99138300
H	1.16165500	2.45103600	-0.04561700

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C	2.96279100	0.08386300	1.94249600
C	3.23207500	0.66613400	0.73117100
C	4.40882700	1.47483800	0.61458800
C	5.23280400	1.58892100	1.77301600
C	3.84552700	0.28146400	3.03318900
H	4.19513600	2.13621000	-1.46204200
H	2.07442100	-0.52528500	2.08840100
C	4.79729900	2.15866500	-0.56111800
C	6.41734600	2.36169500	1.70046000
H	3.61532700	-0.18633000	3.98763900
C	6.78436800	3.00632100	0.54766800
C	5.95656300	2.90637400	-0.59953900
H	7.02742400	2.42590500	2.59526100
H	7.69594100	3.59021800	0.52451900
O	6.23567800	3.51915300	-1.77643000
C	7.40323700	4.32027200	-1.85357400
H	8.30659600	3.72624600	-1.67862700
H	7.42540000	4.72060400	-2.86594900
H	7.36579000	5.14721500	-1.13669900
C	2.29826700	0.41640500	-0.44558300
H	2.50286800	1.15844400	-1.22053500
C	2.50790500	-1.00398300	-1.00544000
C	3.90882200	-1.22286500	-1.62488000
H	2.31620300	-1.71738900	-0.19476400
C	1.50238800	-0.32014800	-3.17437400
C	1.76176800	-2.68534600	-2.60685600
C	3.77445700	-1.33944200	-3.15008800

H	4.56816500	-0.38967300	-1.36801700
H	4.36042800	-2.13253000	-1.21898200
H	0.83264600	-0.71069400	-3.94322100
H	1.06783800	0.61053900	-2.80252300
C	2.94819600	-0.15945100	-3.67876600
C	3.02281600	-2.64634500	-3.48985400
H	0.87053700	-3.01542400	-3.14530300
H	1.90029700	-3.32891300	-1.73732000
H	4.76526800	-1.34694400	-3.61187700
H	2.95869900	-0.14023300	-4.77103300
H	3.38062200	0.78542100	-3.33459300
H	2.72099000	-2.58312900	-4.54458800
N	1.47977300	-1.32136100	-2.06285700
C	3.90943400	-3.85679100	-3.35553400
C	3.67864500	-4.96373600	-2.65459900
H	4.83629800	-3.78644100	-3.92481300
H	4.40156500	-5.77236000	-2.64842900
H	2.77279000	-5.12795400	-2.07876100
N	0.89587500	0.55382800	-0.09440600
H	0.34925800	-0.30054600	0.01503700
C	0.18008400	1.68574600	-0.30569000
S	0.90206500	3.19446500	-0.47413400
N	-1.15180200	1.40913200	-0.41546800
H	-1.33471100	0.45197200	-0.77310100
C	-4.55765800	3.86400800	-0.24117700
C	-3.40745100	4.21682500	0.45752200
C	-2.25593000	3.44104300	0.41500600
C	-2.24101000	2.27993200	-0.36449400
C	-3.39443900	1.90424700	-1.05944600
C	-4.53463600	2.69482000	-0.99150400

H	-5.45129300	4.47413000	-0.18780700
H	-1.38238300	3.72469300	0.98801400
H	-3.39573700	0.98888400	-1.64561600
C	-5.73805400	2.29756900	-1.79842200
F	-5.62109300	2.68737400	-3.07842700
F	-5.90739300	0.96714800	-1.81393300
F	-6.86343100	2.84597400	-1.32133400
C	-3.39291100	5.48884200	1.25795400
F	-2.93268400	6.52242400	0.53545600
F	-4.62076100	5.82362800	1.68070100
F	-2.60578300	5.38807500	2.33821300
N	4.94331400	0.99265600	2.96524000
C	2.50023200	-3.56961200	2.37099000
C	1.22068800	-3.19214500	1.93187300
C	0.38993700	-2.37515500	2.74160900
C	0.82684200	-1.98582200	4.02202800
C	2.08490200	-2.38852800	4.44011200
C	2.92833700	-3.16187500	3.61965300
H	3.13263700	-4.18085600	1.73323400
H	0.21475100	-1.39844200	4.69246200
H	2.42480800	-2.09532300	5.42855000
H	3.91249500	-3.44463800	3.97843900
C	0.48347000	-3.46599400	0.74388200
C	-0.72503700	-2.82558300	0.83884900
C	-1.79491600	-2.97929100	-0.17344800
C	-2.75531800	-4.02413700	-0.03403000
C	-1.80951100	-2.13879900	-1.28056600
C	-2.77224200	-4.89247600	1.09321500
C	-3.75751600	-4.19365900	-1.03122100
C	-2.81590200	-2.33514900	-2.27807300

C	-3.72715000	-5.87248000	1.21397500
H	-2.01047000	-4.77532300	1.85914700
C	-4.72644300	-5.21784800	-0.88011400
C	-3.75524700	-3.32040600	-2.15435300
H	-2.81095800	-1.66526900	-3.13288700
C	-4.71725400	-6.04274100	0.21751800
H	-3.72208700	-6.52485100	2.08164700
H	-5.48153500	-5.33579500	-1.65312100
H	-4.51906200	-3.44959200	-2.91694100
H	-5.46481200	-6.82152700	0.32572000
O	-0.95630400	-1.12721600	-1.40885200
N	-0.79415600	-2.12950700	2.04950500
C	-1.88247700	-1.25953300	2.59149700
C	-2.48250600	-1.93759600	3.83026100
H	-3.26741900	-1.30247100	4.25006900
H	-2.92825000	-2.89477000	3.54317600
H	-1.74292400	-2.12560500	4.60957500
C	-1.30221600	0.12863900	2.90802300
H	-2.09959300	0.76940200	3.29417900
H	-0.49878800	0.11392100	3.64220500
H	-0.91552600	0.58361800	1.99145400
C	-3.01371500	-1.03685400	1.58492200
H	-3.55675900	-1.95373600	1.35361300
H	-3.71355900	-0.32829100	2.03635400
H	-2.64129800	-0.59885000	0.65672700
H	0.75645700	-4.13258900	-0.06180800
H	0.41580700	-1.32443200	-1.68025600

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C	2.97011000	0.11925000	1.94013800
C	3.22055800	0.69820100	0.72298800
C	4.38905900	1.51654700	0.59041800
C	5.22427000	1.64415200	1.73929600
C	3.86297300	0.32988800	3.02022200
H	4.14903100	2.16452600	-1.48762200
H	2.08897900	-0.49718000	2.09947600
C	4.75967600	2.19747500	-0.59276900
C	6.40108300	2.42693300	1.65054700
H	3.64767400	-0.13560000	3.97931900
C	6.75052300	3.06883000	0.49074700
C	5.91168200	2.95527400	-0.64706600
H	7.01980500	2.50082600	2.53866900
H	7.65685500	3.66024100	0.45533200
O	6.17286600	3.56437400	-1.83022300
C	7.33334300	4.37357000	-1.92458900
H	8.24304300	3.78750200	-1.75563200
H	7.34178800	4.76779300	-2.93960200
H	7.29737000	5.20479500	-1.21256400
C	2.27645200	0.43747700	-0.44261500
H	2.47005100	1.17540200	-1.22396600
C	2.47867400	-0.98582400	-0.99959900
C	3.87983300	-1.20438700	-1.62164500
H	2.29691200	-1.69369000	-0.18136100
C	1.46595000	-0.31343600	-3.15583500
C	1.72265700	-2.66633400	-2.58242000
C	3.73737200	-1.33234800	-3.14496200
H	4.53967400	-0.36808900	-1.37519200
H	4.33600400	-2.11008500	-1.21139400
H	0.79115700	-0.70304800	-3.92154500

H	1.03751800	0.62395800	-2.79180300
C	2.90815200	-0.15553400	-3.67575400
C	2.98207500	-2.64021800	-3.47074600
H	0.83158400	-3.00061400	-3.12007000
H	1.86175100	-3.31108500	-1.71348000
H	4.72560900	-1.34403500	-3.61285200
H	2.91125400	-0.14340600	-4.76844100
H	3.34490300	0.79106100	-3.34091400
H	2.67726500	-2.58437800	-4.52537100
N	1.44258200	-1.30530900	-2.04140900
C	3.86596900	-3.85201600	-3.33106300
C	3.61935900	-4.96434300	-2.64408300
H	4.80305000	-3.77997100	-3.88358300
H	4.33837400	-5.77641800	-2.63130400
H	2.70176500	-5.12805200	-2.08695800
N	0.87736500	0.57760900	-0.07600400
H	0.34100700	-0.27887200	0.05663900
C	0.15547500	1.70225200	-0.29533400
S	0.86630100	3.21175700	-0.49544600
N	-1.17938800	1.42223300	-0.38414600
H	-1.36784000	0.46766600	-0.72886700
C	-4.57640800	3.89129300	-0.22997500
C	-3.42560600	4.24296600	0.46848400
C	-2.27799100	3.46126400	0.43240300
C	-2.26768300	2.29610100	-0.34079000
C	-3.42094100	1.92199300	-1.03607400
C	-4.55787200	2.71811800	-0.97384800
H	-5.46729600	4.50584700	-0.18135700
H	-1.40386600	3.74379000	1.00511000
H	-3.42551400	1.00496600	-1.61946800

C	-5.76206700	2.32263700	-1.78058800
F	-5.64331800	2.70896300	-3.06133300
F	-5.93539000	0.99261000	-1.79278900
F	-6.88586400	2.87555800	-1.30518500
C	-3.40672100	5.51981000	1.26113600
F	-2.94600400	6.54780400	0.53117800
F	-4.63314100	5.85951500	1.68411700
F	-2.61768000	5.42388500	2.34035300
N	4.95315600	1.05109900	2.93749600
C	2.53833100	-3.52331900	2.44812700
C	1.25845800	-3.17506400	1.98706600
C	0.40412800	-2.35626700	2.76947000
C	0.81876300	-1.93609000	4.04811900
C	2.07793400	-2.30991500	4.48842300
C	2.94421400	-3.08485100	3.69352500
H	3.18793700	-4.13557700	1.82912600
H	0.18934900	-1.34699100	4.70073900
H	2.40105700	-1.99227900	5.47491900
H	3.92860600	-3.34341000	4.06962000
C	0.54297600	-3.48442300	0.79501800
C	-0.67562900	-2.86064900	0.86008400
C	-1.72442700	-3.04590800	-0.17029000
C	-2.64936400	-4.12665500	-0.05260200
C	-1.75879300	-2.20574600	-1.27307000
C	-2.65156900	-5.00183500	1.06889700
C	-3.62983300	-4.32336300	-1.06584300
C	-2.73828300	-2.42522500	-2.28728700
C	-3.57357900	-6.01493700	1.16948200
H	-1.90478800	-4.86370400	1.84580400
C	-4.56526100	-5.38136200	-0.93524700

C	-3.64385400	-3.44434900	-2.18371600
H	-2.74429900	-1.74760400	-3.13560200
C	-4.54273100	-6.21199200	0.15737400
H	-3.55884800	-6.67264400	2.03287500
H	-5.30507800	-5.51964900	-1.71933400
H	-4.39214200	-3.59497200	-2.95737700
H	-5.26455800	-7.01663900	0.24991100
O	-0.94360900	-1.14857600	-1.38097500
N	-0.77441800	-2.14327800	2.05646100
C	-1.89787300	-1.30841800	2.58129100
C	-2.48895900	-2.00251900	3.81550800
H	-3.29870800	-1.39268600	4.22544800
H	-2.90001300	-2.97460100	3.52663900
H	-1.75137000	-2.16441200	4.60263300
C	-1.37107700	0.10027900	2.90035200
H	-2.19652900	0.71322500	3.27267600
H	-0.57851400	0.11737200	3.64584500
H	-0.98819400	0.56684400	1.98818200
C	-3.02346200	-1.12841800	1.56008600
H	-3.52988200	-2.06469100	1.32276200
H	-3.75430700	-0.44577900	2.00178900
H	-2.65625200	-0.67684100	0.63606200
H	0.84328200	-4.15720600	0.00434800
H	0.28760000	-1.30899000	-1.64376800

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C	3.51255300	0.48018100	-2.44285900
C	3.81856300	-0.21795700	-1.30209600
C	4.92667000	-1.12164700	-1.34388100

C	5.64882300	-1.20796600	-2.57178300
C	4.29166100	0.30991500	-3.61147900
H	4.80216000	-1.92214700	0.68762300
H	2.66979900	1.16579400	-2.46642600
C	5.33935000	-1.92301900	-0.25385000
C	6.76085900	-2.08202100	-2.65158400
H	4.03808100	0.87199200	-4.50784800
C	7.15164800	-2.84397600	-1.58124600
C	6.42557600	-2.76532700	-0.36438100
H	7.29526200	-2.12920000	-3.59452500
H	8.00547400	-3.50380400	-1.67407900
O	6.73708000	-3.49109700	0.73770900
C	7.82865800	-4.39229100	0.65932400
H	8.76604800	-3.86545200	0.45119100
H	7.89364700	-4.86980400	1.63585000
H	7.66084600	-5.15584700	-0.10738600
C	2.98767300	0.00894200	-0.04548700
H	3.23308600	-0.75544000	0.69167100
C	3.29480200	1.40164500	0.54807200
C	4.73454500	1.44950900	1.12972000
H	3.18542800	2.14532900	-0.25275100
C	2.27045200	0.76489200	2.67274100
C	2.76386200	3.06805100	2.19226600
C	4.64351700	1.53004400	2.66283800
H	5.29862000	0.55732600	0.84035200
H	5.28084000	2.30788900	0.72860800
H	1.66441800	1.18687500	3.47952500
H	1.74648700	-0.12179800	2.30541900
C	3.69952900	0.42744800	3.16195100
C	4.02496500	2.88291900	3.07687400

H	1.93508400	3.49894100	2.76208400
H	2.99534900	3.75523500	1.37086100
H	5.63696500	1.41902400	3.10543500
H	3.72221900	0.37138900	4.25382800
H	4.02580900	-0.54840900	2.78455200
H	3.72387000	2.81060200	4.12944800
N	2.31315300	1.78754100	1.59711500
C	4.96547700	4.04457300	2.94169300
C	5.32557700	4.84017800	3.94476000
H	5.36290400	4.23273100	1.94305400
H	6.01230500	5.66704900	3.79710800
H	4.94314100	4.68770500	4.95089800
N	1.56568600	-0.13355100	-0.30670500
H	1.03896300	0.70487000	-0.52088100
C	0.84974600	-1.23765600	-0.00586300
S	1.57148300	-2.71362900	0.39558300
N	-0.49419200	-1.03088100	-0.02942600
H	-0.82572300	-0.06552000	-0.02215100
C	-3.47194400	-3.94977700	0.52439700
C	-2.53174700	-4.08588600	-0.49016100
C	-1.53279200	-3.13869500	-0.67807300
C	-1.47419500	-2.03101400	0.16423900
C	-2.42168000	-1.86766000	1.17287700
C	-3.40849800	-2.83149300	1.34697700
H	-4.25536500	-4.68806700	0.65498100
H	-0.81089700	-3.24540600	-1.47967200
H	-2.38747800	-0.99087700	1.81252300
C	-4.37420200	-2.71905200	2.49076900
F	-5.59091600	-3.18224700	2.16926300
F	-3.95775600	-3.43885800	3.54747400

F	-4.51677900	-1.45548100	2.91680200
C	-2.58988100	-5.28314200	-1.39379400
F	-1.84893900	-6.30066100	-0.92777400
F	-3.84461800	-5.74119400	-1.52377300
F	-2.13385600	-4.99945500	-2.62275600
N	5.32594600	-0.49190600	-3.68680300
C	-4.21106200	-1.19392400	-1.82756400
C	-3.71230700	0.00953000	-1.30088500
C	-4.33850500	0.62241100	-0.18728700
C	-5.47244200	0.02703700	0.39624900
C	-5.95225300	-1.15142800	-0.14878800
C	-5.32921200	-1.76483700	-1.25278300
H	-3.71280800	-1.66562100	-2.66982800
H	-5.97938500	0.45423200	1.25099600
H	-6.82298900	-1.61779600	0.29990300
H	-5.72238800	-2.69984900	-1.64002400
C	-2.60827000	0.83876200	-1.65398500
C	-2.59074900	1.90035600	-0.78605600
C	-1.63277200	3.02389100	-0.92666500
C	-1.92202000	4.09809900	-1.82142200
C	-0.41964100	2.98868100	-0.26886000
C	-3.16492300	4.19383700	-2.50714700
C	-0.95696200	5.12513500	-2.02264900
C	0.54424500	4.00840600	-0.47978400
C	-3.42194500	5.24798100	-3.34807400
H	-3.90817400	3.41593800	-2.35980000
C	-1.25067200	6.19890800	-2.90311800
C	0.28005900	5.04526400	-1.33283700
H	1.48761300	3.96008500	0.05127600
C	-2.45610500	6.26287300	-3.55358900

H	-4.37555700	5.30550800	-3.86331000
H	-0.49983700	6.97075800	-3.04891600
H	1.02087500	5.82452800	-1.48730100
H	-2.67468100	7.08750500	-4.22379900
O	-0.18147000	1.97429600	0.60192100
N	-3.63956900	1.78616800	0.12622200
C	-3.99901700	2.66030100	1.27986700
C	-5.40801000	3.22544300	1.05019900
H	-5.69480400	3.84625100	1.90327900
H	-5.40625700	3.85097200	0.15247800
H	-6.16510400	2.45256300	0.92220500
C	-3.89212200	1.83657300	2.57156900
H	-4.18063200	2.45694100	3.42458300
H	-4.51651600	0.94489100	2.57040400
H	-2.85236600	1.52320700	2.71136300
C	-3.05293400	3.85176500	1.44014800
H	-3.06679100	4.51501900	0.57358400
H	-3.40107900	4.42106200	2.30648600
H	-2.02924900	3.52872500	1.63795500
H	-1.91555700	0.70269300	-2.47302000
H	0.75665200	2.00466900	1.00289500

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C	3.33494000	-1.79523800	-1.65097900
C	2.26670300	-1.04571200	-1.13190500
C	2.45759500	-0.20384900	-0.00650500
C	3.72612500	-0.11975900	0.59818900
C	4.76207400	-0.86975200	0.06724000
C	4.57566700	-1.70440300	-1.05045600

H	3.17647600	-2.43725400	-2.51262600
H	3.92051600	0.50352700	1.46061800
H	5.74170900	-0.80822800	0.53045800
H	5.41236500	-2.27716100	-1.43727100
C	0.89687800	-0.92556100	-1.50225900
C	0.30631800	-0.04850000	-0.63315700
C	-1.14086400	0.27272600	-0.69056600
C	-2.09245500	-0.58449200	-0.06029000
C	-1.58620600	1.34532500	-1.43345800
C	-1.69279300	-1.68901600	0.74219500
C	-3.48393400	-0.31906800	-0.20343400
C	-2.97093300	1.60800600	-1.58369000
C	-2.62807400	-2.48391800	1.35643400
H	-0.63301200	-1.89619000	0.85728500
C	-4.42635800	-1.16566400	0.43687200
C	-3.89269400	0.79307800	-0.98489900
H	-3.28763900	2.46208500	-2.17604100
C	-4.01157600	-2.22543100	1.20181200
H	-2.30617400	-3.32231600	1.96598100
H	-5.48459700	-0.95328600	0.31038800
H	-4.95396000	0.99441100	-1.09943400
H	-4.73800900	-2.86674400	1.68978700
O	-0.65438600	2.17213300	-1.97760900
N	1.24465300	0.40914500	0.29404200
C	1.08632700	1.38257300	1.41172300
C	2.01774700	2.57811000	1.15963000
H	1.73371000	3.06277800	0.22101500
H	1.90770100	3.30225700	1.97155700
H	3.06904400	2.30094100	1.09355500
C	-0.33238500	1.94641900	1.51537100

H	-1.07587000	1.16973800	1.70287300
H	-0.34058000	2.63390400	2.36559200
H	-0.60872000	2.50984800	0.62266500
C	1.38703800	0.66612100	2.73616400
H	2.38222300	0.22349800	2.76798500
H	1.30302800	1.37671600	3.56301900
H	0.65493400	-0.13231000	2.89073700
H	0.38463100	-1.43060800	-2.30880300
H	-1.09011300	2.87135200	-2.48094700