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## SUPPORTING INFORMATION FOR

### **A general mechanistic map of organocatalytic hydroboration of alkynes: Polarity controlled switchable selective pathways**

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## Part 1: Computational details

All calculations reported in this paper were performed with the Gaussian 16 suite of programs.<sup>1</sup> The M06-2X<sup>2</sup> functional was used for geometry optimization using the SMD<sup>3</sup> solvation model (solvent = toluene for case study A and solvent = dichloromethane for case study B) with the standard 6-31G(d,p) basis set. Harmonic vibrational frequency calculations of all of the stationary points were performed to confirm whether they are local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. The transition states were confirmed by intrinsic reaction coordinate calculations. The single-point energies were calculated at the M06-2X/6-311+G(d,p) level using the SMD solvation model (solvent = toluene for case study A and solvent = dichloromethane for case study B). The calculated three-dimensional stereoscopic structures were prepared using the CYLview.<sup>4</sup>

In addition, the extent of enantioselectivity, in terms of enantiomeric excess (ee), was also calculated by using the Boltzmann distribution of stereo-selective transition states with the following equation:

$$\frac{[R]}{[S]} = \frac{\exp(-\Delta G_{[R]}^\ddagger/RT)}{\exp(-\Delta G_{[S]}^\ddagger/RT)} = \exp(-\Delta\Delta G^\ddagger/RT) \quad (1)$$

$$ee = \frac{[R]-[S]}{[R]+[S]} \times 100\% = \frac{\frac{[R]}{[S]}-1}{\frac{[R]}{[S]}+1} \times 100\% \quad (2)$$

where  $\Delta G^\ddagger$  is the Gibbs free energy barrier of the competing stereo-selective transition states and  $\Delta\Delta G^\ddagger$  is the Gibbs free energy barrier difference between the two stereo-selective transition states.

For analyzing the local nucleophilicity and electrophilicity, we have also performed the Parr function analysis<sup>5</sup> at the M06-2X/6-31G(d,p)/SMD level (solvent = toluene for case study A and solvent = dichloromethane for case study B). Pioneered by Domingo and coworkers, the nucleophilic ( $P_k^-$ ) and electrophilic ( $P_k^+$ ) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studies molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P_k^- = \rho_s^{rc}(r) \text{ for the electrophilic attacks} \quad (3)$$

$$P_k^+ = \rho_s^{ra}(r) \text{ for the nucleophilic attacks} \quad (4)$$

Where  $\rho_s^{rc}(r)$  is the ASD of the radical cation and  $\rho_s^{ra}(r)$  is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic  $P_k^-$  and electrophilic  $P_k^+$  Parr functions of the neutral system, respectively.

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For the global reactivity index (GRI) analysis, the relevant parameters of GRI, i.e., global electrophilicity index  $\omega$ ,<sup>6</sup> electronic chemical potential  $\mu$ , chemical hardness  $\eta$ , one-electron energies of the frontier molecular orbital HOMO ( $E_L$ ) and LUMO ( $E_H$ ). The HOMO energies obtained within the Kohn–Sham scheme,<sup>7</sup> global nucleophilicity index  $N^8$  was generally utilized to judge the nucleophilicity character. In addition, according to Domingo’s definition, the local electrophilicity ( $\omega_k$ ) and local nucleophilicity ( $N_k$ ) index can be expressed by the following equations:

$$N_k = N \times P_k^- \quad (5)$$

$$\omega_k = \omega \times P_k^+ \quad (6)$$

To ensure that the selected stereoselective conformations with the lowest energies, we employed CREST (version 2.12)<sup>9</sup> in combination with the xTB package (version 6.4.0)<sup>10</sup> for the samplings of low-energy conformations of the transition states at the GFN2-xTB level with toluene (case study A) and dichloromethane (case study B) implicit solvation,<sup>11</sup> atoms in the forming/cleaving bonds were constrained by applying a force constant of 0.5 Hartree/Bohr. An energy window of 6.0 kcal/mol and an RMSD threshold of 0.5 Å were used. Fully relaxed TS optimizations were performed for the low-lying TSs as well as for those TSs with remarkably different structural features.

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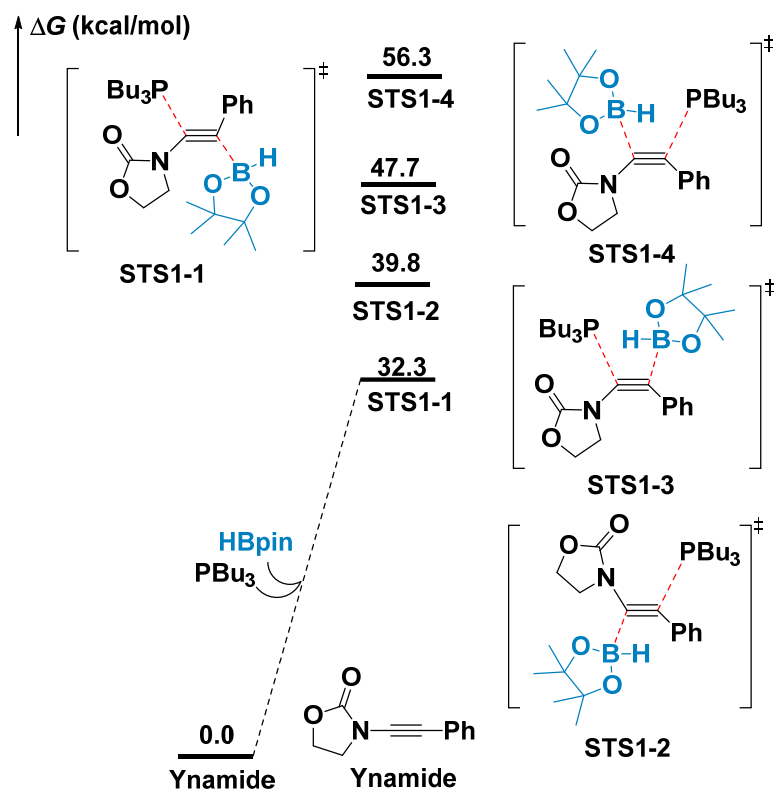
## Part 2: Test results of the different computational methods

We have compared the relative Gibbs free energy barriers ( $\Delta\Delta G^\ddagger$ ) between **M3** and **TS2R**, which are computed by the Gibbs free energy corrections at the M062x/6-31G(d,p)//SMD<sub>toluene</sub> plus the refined single-point energies at the M062x/6-311+G(d,p)//SMD<sub>toluene</sub> (denoted as L1); which are computed by the Gibbs free energy corrections at the B3LYP-D3(BJ)<sup>12</sup>/6-31G(d,p)//SMD<sub>toluene</sub> plus the refined single-point energies at the B3LYP-D3(BJ)/6-311+G(d,p)//SMD<sub>toluene</sub> (denoted as L2), and which are computed by the Gibbs free energy corrections at the  $\omega$ B97X-D<sup>13</sup>/6-31G(d,p)//SMD<sub>toluene</sub> plus the refined single-point energies at the  $\omega$ B97X-D/6-311+G(d,p)//SMD<sub>toluene</sub> (denoted as L3) levels, respectively. As shown in Table S1, there are small energy barrier differences between **M3** and **TS2R**, indicating the selected method should be proper and reliable in this kind of reaction system.

**Table S1** Comparison of relative Gibbs free energy barrier differences ( $\Delta\Delta G^\ddagger$ ) between **M3** and **TS2R** calculated by using the different levels (L1-3) (unit: kcal/mol).

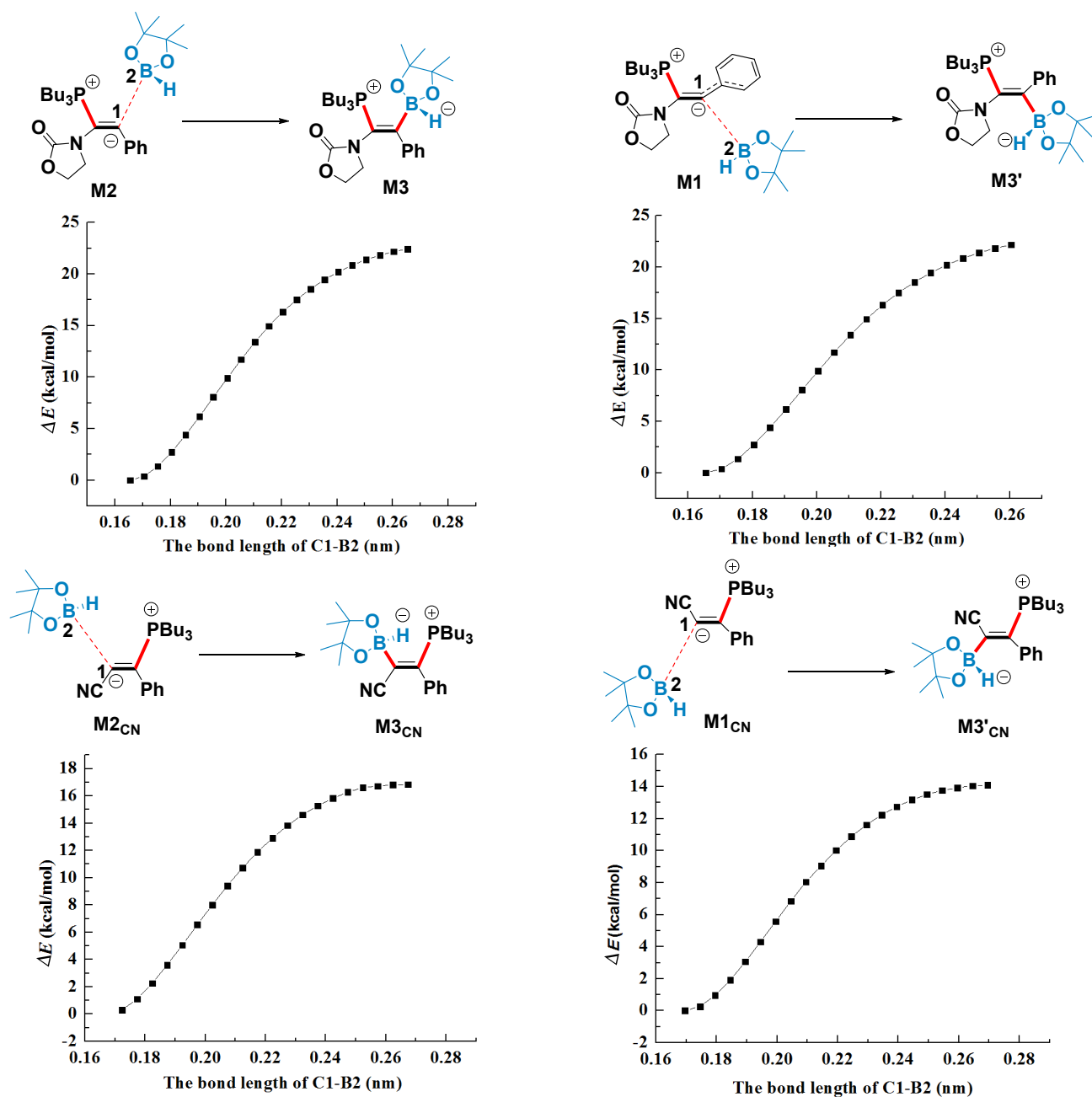
	$\Delta\Delta G^\ddagger$
<b>L1</b>	<b>12.5</b>
<b>L2</b>	<b>10.8</b>
<b>L3</b>	<b>11.7</b>

**Part 3: The one-step reaction processes of HBpin with ynamide in the presence of PBU<sub>3</sub>**



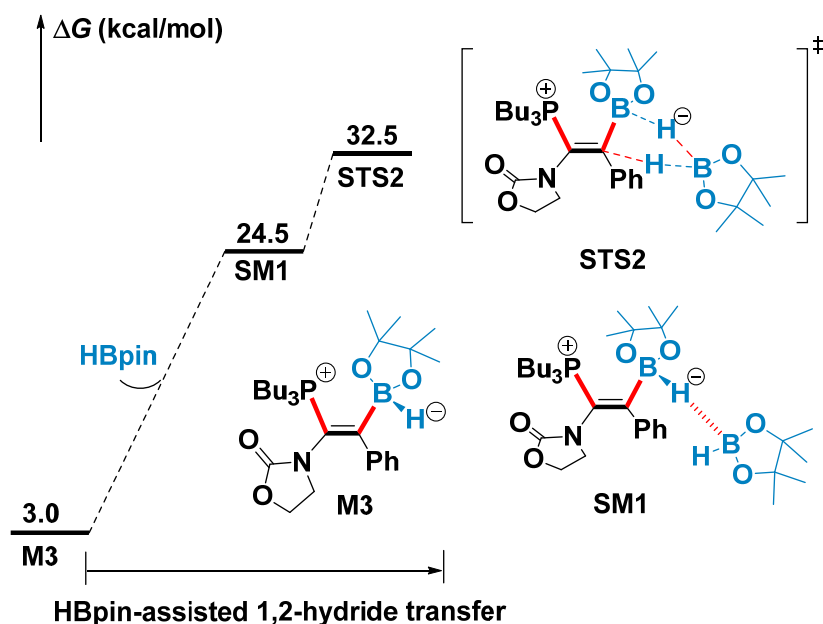
**Fig. S1** Free energy profiles of the one-step reaction processes of HBpin with ynamide in the presence of PBU<sub>3</sub> at the M06-2X/6-311+G(d,p)/SMD<sub>toluene</sub>//M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level.

## Part 4: The scan results of the barrier-less processes

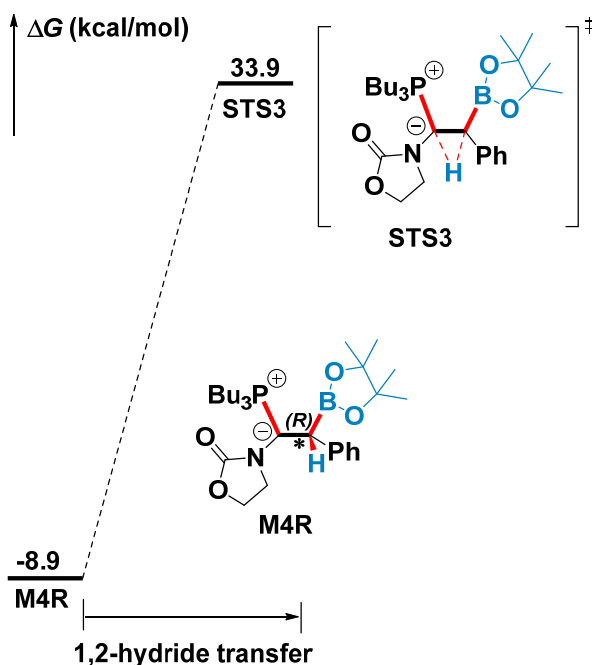


**Fig. S2** The scan profiles from **M2** and **M1** to **M3** and **M3'** at the M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level, and from **M2<sub>CN</sub>** and **M1<sub>CN</sub>** to **M3<sub>CN</sub>** and **M3'<sub>CN</sub>** at the M06-2X/6-31G(d,p)/SMD<sub>dichloromethane</sub> level.

**Part 5: The 1,2-hydride transfer assisted by HBpin and directly 1,2-proton transfer processes of PBU<sub>3</sub>-catalyzed hydroboration of ynamide**



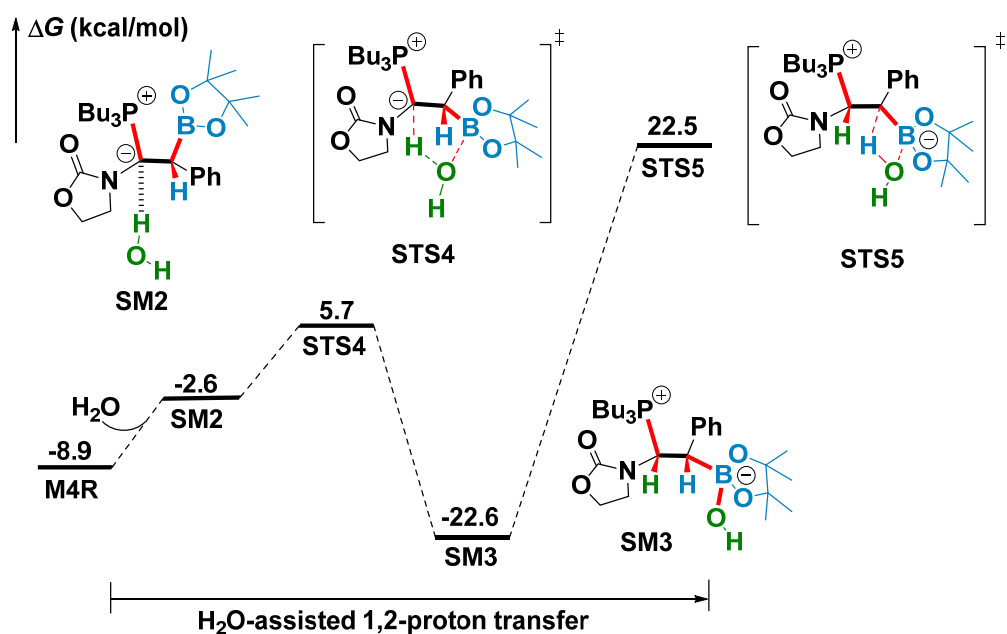
**Fig. S3** Free energy profiles of 1,2-hydride transfer process assisted by HBpin of PBU<sub>3</sub>-catalyzed hydroboration of ynamide at the M06-2X/6-311+G(d,p)/SMD<sub>toluene</sub>//M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level.



**Fig. S4** Free energy profiles of directly 1,2-proton transfer process of PBU<sub>3</sub>-catalyzed hydroboration of ynamide at the M06-2X/6-311+G(d,p)/SMD<sub>toluene</sub>//M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level.

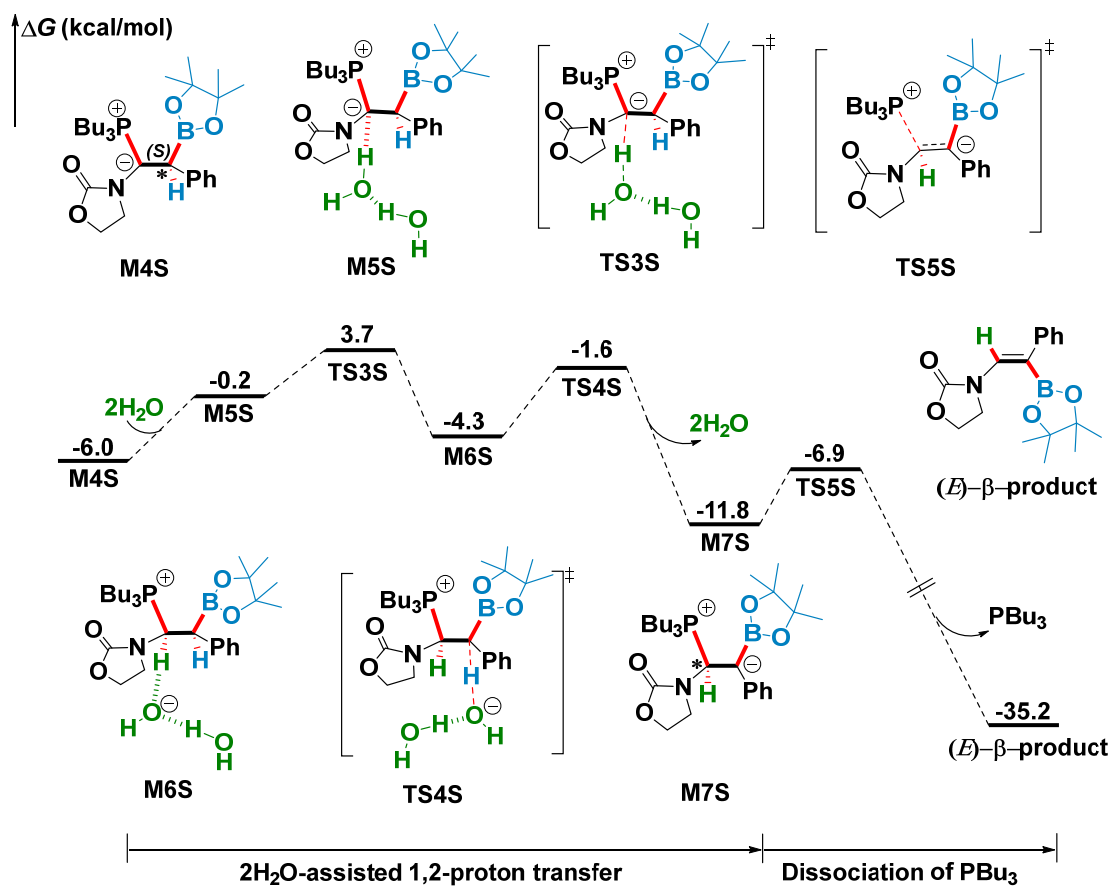


## Part 6: The H<sub>2</sub>O-assisted 1,2-hydride transfer process of PBu<sub>3</sub>-catalyzed hydroboration of ynamide



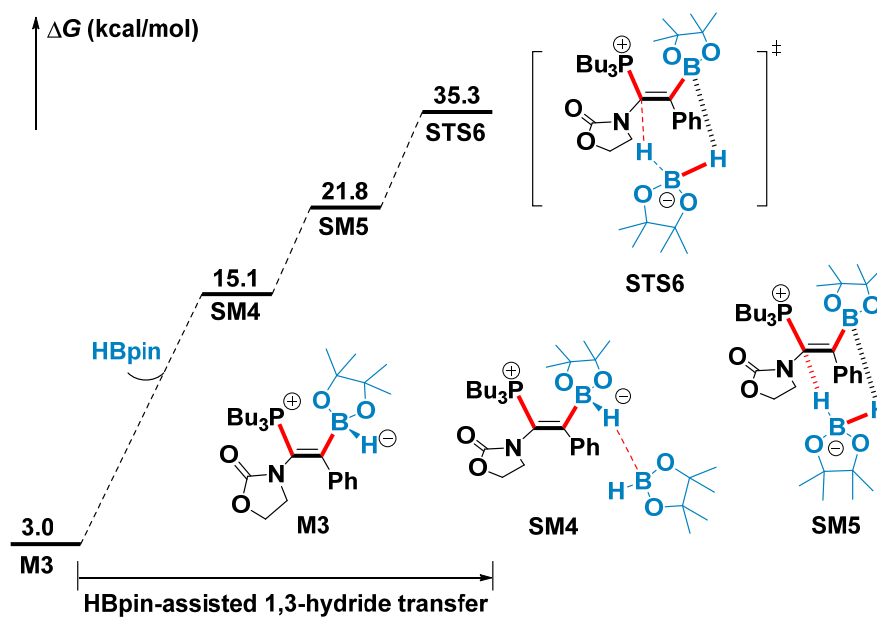
**Fig. S5** Free energy profiles of H<sub>2</sub>O-assisted 1,2-hydride transfer process leading to Z-isomer of PBu<sub>3</sub>-catalyzed hydroboration of ynamide at the M06-2X/6-311+G(d,p)/SMD<sub>toluene</sub>//M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level.

**Part 7: The 2H<sub>2</sub>O-assisted 1,2-proton transfer process leading to *E*-isomer of PBu<sub>3</sub>-catalyzed hydroboration of ynamide**



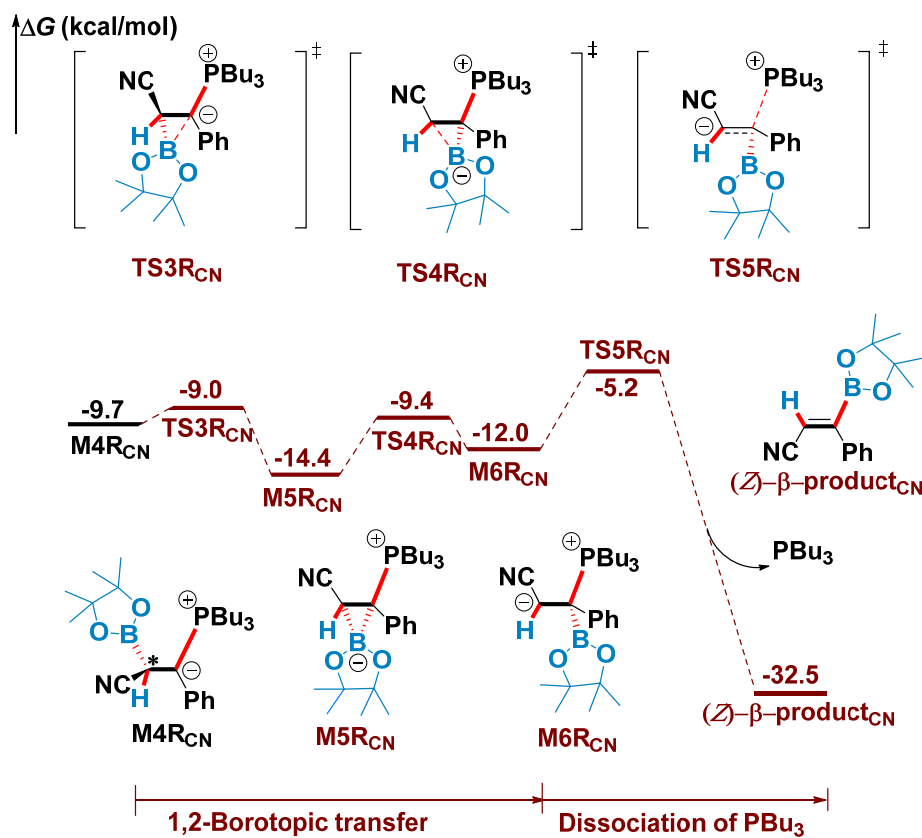
**Fig. S6** Free energy profiles of 2H<sub>2</sub>O-assisted 1,2-proton transfer process leading to *E*-isomer of PBu<sub>3</sub>-catalyzed hydroboration of ynamide at the M06-2X/6-311+G(d,p)/SMD<sub>toluene</sub>//M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level.

## Part 8: The 1,3-hydride transfer process assisted by HBpin of PBU<sub>3</sub>-catalyzed hydroboration of ynamide



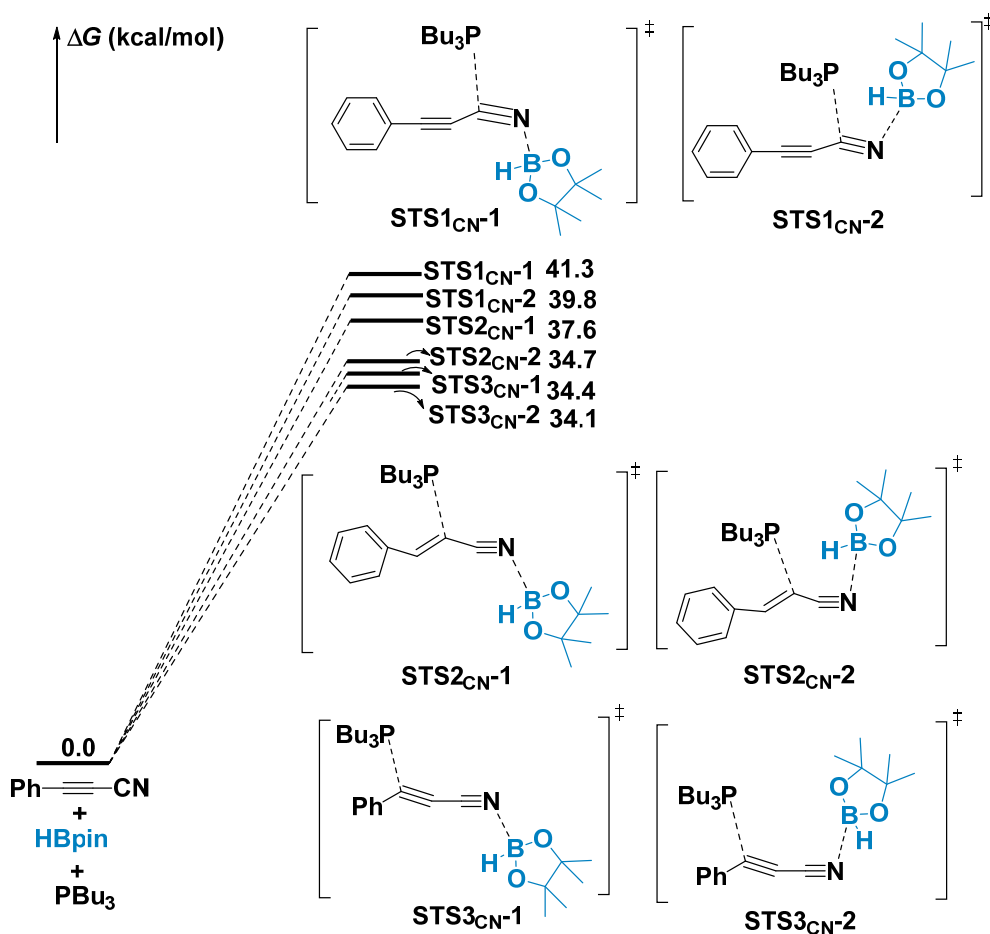
**Fig. S7** Free energy profiles of 1,3-hydride transfer process assisted by HBpin of PBU<sub>3</sub>-catalyzed hydroboration of ynamide at the M06-2X/6-311+G(d,p)/SMD<sub>toluene</sub>//M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level.

**Part 9: The 1,2-borotopic transfer leading to *Z*-isomer of PBU<sub>3</sub>-catalyzed hydroboration of propionitrile**



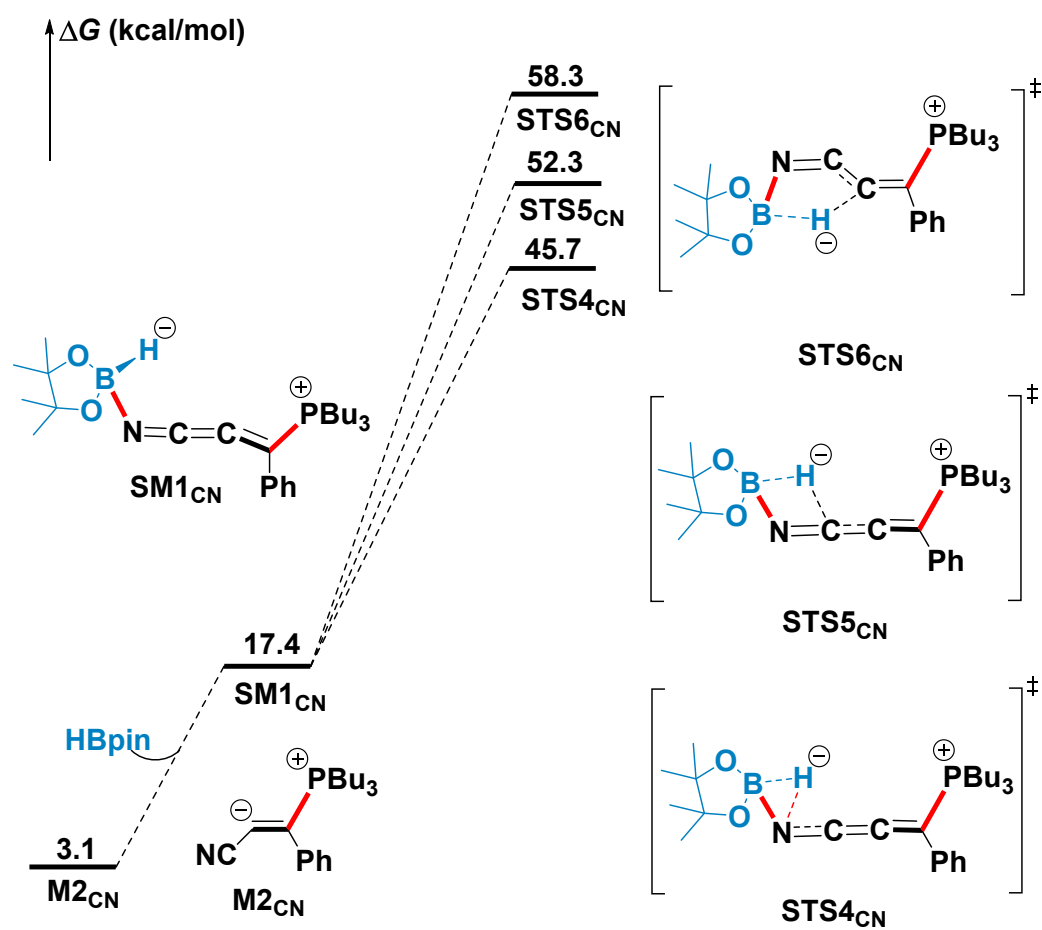
**Fig. S8** Free energy profiles of 1,2-borotopic transfer process leading to *Z*-isomer of PBU<sub>3</sub>-catalyzed hydroboration of propionitrile at the M06-2X/6-311+G(d,p)/SMD<sub>dichloromethane</sub>//M06-2X/6-31G(d,p)/SMD<sub>dichloromethane</sub> level.

**Part 10: The one-step reaction processes of HBpin with propiolonitrile in the presence of PBU<sub>3</sub>**



**Fig. S9** Free energy profiles of the one-step reaction processes of HBpin with propiolonitrile in the presence of PBU<sub>3</sub> at the M06-2X/6-311+G(d,p)/SMD<sub>dichloromethane</sub>//M06-2X/6-31G(d,p)/SMD<sub>dichloromethane</sub> level.

**Part 11: The 1,4-conjugate addition processes of HBpin with propiolonitrile in the presence of PBU<sub>3</sub>**



**Fig. S10** Free energy profiles of 1,4-conjugate addition processes of PBU<sub>3</sub>-catalyzed hydroboration of propiolonitrile at the M06-2X/6-311+G(d,p)/SMD<sub>dichloromethane</sub>//M06-2X/6-31G(d,p)/SMD<sub>dichloromethane</sub> level.

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## Part 12: The energies of all the optimized structures

**Table S2** The single-point energies ( $E$ ), Gibbs free energy corrections (GFEC), and Gibbs free energies (GFE) ( $=E+GFEC$ ) of the stationary points involved in the  $\text{PBU}_3$ -catalyzed hydroboration of ynamide. (Unit: a.u)

SP	GFEC (M06-2X/6-31G(d, p)/SMD <sub>toluene</sub> )	$E$ (M06-2X/6-311+G(d ,p)/SMD <sub>toluene</sub> )	GFE	Number of imaginary frequencies
Ynamide	0.141102	-629.668188	-629.527086	0
$\text{PBU}_3$	0.324634	-814.786738	-814.462104	0
HBpin	0.160138	-411.813457	-411.653319	0
$\text{H}_2\text{O}$	0.003282	-76.425306	-76.422024	0
$2\text{H}_2\text{O}$	0.020486	-152.85925	-152.838764	0
TS1	0.48747	-1444.438375	-1443.950905	1
M1	0.493283	-1444.458211	-1443.964928	0
M2	0.490555	-1444.45827	-1443.967715	0
TS1'	0.487995	-1444.432305	-1443.94431	1
TS1''	0.48946	-1444.419903	-1443.930443	1
M3	0.677531	-1856.315234	-1855.637703	0
TS2R	0.674025	-1856.291817	-1855.617792	1
M4R	0.677371	-1856.334057	-1855.656686	0
TS2S	0.671692	-1856.286687	-1855.614995	1
M4S	0.679541	-1856.331561	-1855.65202	0
M3'	0.679773	-1856.309277	-1855.629504	0
TS2R'	0.673795	-1856.29005	-1855.616255	1
TS2S'	0.673353	-1856.28305	-1855.609697	1
M5R	0.723991	-2009.210596	-2008.486605	0
TS3R	0.72158	-2009.202671	-2008.481091	1
M6R	0.723766	-2009.205418	-2008.481652	0

TS4R	0.722298	-2009.194048	-2008.47175	1
M7R	0.683129	-1856.34241	-1855.659281	0
TS5R	0.680424	-1856.327557	-1855.647133	1
(Z)- $\beta$ -product	0.327118	-1041.568318	-1041.2412	0
M5S	0.723359	-2009.204903	-2008.481544	0
TS3S	0.720426	-2009.19578	-2008.475354	1
M6S	0.726522	-2009.214694	-2008.488172	0
TS4S	0.721175	-2009.20494	-2008.483765	1
M7S	0.67959	-1856.340836	-1855.661246	0
TS5S	0.676887	-1856.330326	-1855.653439	1
(E)- $\beta$ -product	0.326964	-1041.563428	-1041.236464	0
TS6R	0.681416	-1856.322502	-1855.641086	1
M8R	0.682066	-1856.327059	-1855.644993	0
TS7R	0.678142	-1856.309567	-1855.631425	1
M9R	0.679058	-1856.315298	-1855.63624	0
TS8R	0.677964	-1856.302123	-1855.624159	1
(Z)- $\alpha$ -product	0.327472	-1041.563826	-1041.236354	0
STS1-1	0.668629	-1856.259643	-1855.591014	1
STS1-2	0.670994	-1856.250064	-1855.57907	1
STS1-3	0.670168	-1856.236612	-1855.566444	1
STS1-4	0.672361	-1856.225093	-1855.552732	1
SM1	0.862368	-2268.119216	-2267.256848	0
STS2	0.860122	-2268.104237	-2267.244115	1
STS3	0.674223	-1856.262775	-1855.588552	1
SM2	0.702184	-1932.770852	-1932.068668	0
STS4	0.705033	-1932.760434	-1932.055401	1
SM3	0.707002	-1932.807477	-1932.100475	0
STS5	0.699416	-1932.728062	-1932.028646	1
SM4	0.860072	-2268.131855	-2267.271783	0



SM5	0.858605	-2268.119702	-2267.261097	0
STS6	0.858071	-2268.097665	-2267.239594	1

**Table S3** The single-point energies (*E*), Gibbs free energy corrections (GFEC), and Gibbs free energies (GFE) (=E+GFEC) of the stationary points involved in the PBU<sub>3</sub>-catalyzed hydroboration of propiolonitrile. (Unit: a.u)

SP	GFEC (M06-2X/6-31G(d, p)/SMDdichloromet hane)	<i>E</i> (M06-2X/6-311+G(d, p)/SMDdichlorometha ne)	GFE	Number of imaginary frequencies
Propiolonitrile	0.076987	-400.59142	-400.514433	0
PBU <sub>3</sub>	0.323949	-814.789024	-814.465075	0
HBpin	0.159589	-411.816099	-411.65651	0
2H <sub>2</sub> O	0.020157	-152.864958	-152.844801	0
TS1 <sub>CN</sub>	0.420215	-1215.368219	-1214.948004	1
M1 <sub>CN</sub>	0.425798	-1215.39807	-1214.972272	0
TS1' <sub>CN</sub>	0.421234	-1215.358719	-1214.937485	1
M2 <sub>CN</sub>	0.425107	-1215.399753	-1214.974646	0
M3 <sub>CN</sub>	0.60895	-1627.244171	-1626.635221	0
M3' <sub>CN</sub>	0.608422	-1627.237764	-1626.629342	0
TS2 <sub>SCN</sub>	0.605747	-1627.215753	-1626.610006	1
TS2 <sub>RCN</sub>	0.607386	-1627.214805	-1626.607419	1
TS2' <sub>SCN</sub>	0.603355	-1627.211749	-1626.608394	1
TS2' <sub>RCN</sub>	0.603887	-1627.209181	-1626.605294	1
M4 <sub>SCN</sub>	0.611273	-1627.26266	-1626.651387	0
TS3 <sub>SCN</sub>	0.610425	-1627.261216	-1626.650791	1
M5 <sub>SCN</sub>	0.611388	-1627.268831	-1626.657443	0
TS4 <sub>SCN</sub>	0.611826	-1627.264296	-1626.65247	1

<b>M6<sub>CN</sub></b>	<b>0.612051</b>	<b>-1627.267547</b>	<b>-1626.655496</b>	<b>0</b>
<b>TS5<sub>CN</sub></b>	<b>0.609936</b>	<b>-1627.259456</b>	<b>-1626.64952</b>	<b>1</b>
<b>(E)-<math>\beta</math>-product<sub>CN</sub></b>	<b>0.261292</b>	<b>-812.482097</b>	<b>-812.220805</b>	<b>0</b>
<b>M4<sub>CN</sub></b>	<b>0.612198</b>	<b>-1627.263749</b>	<b>-1626.651551</b>	<b>0</b>
<b>TS3<sub>CN</sub></b>	<b>0.612474</b>	<b>-1627.262858</b>	<b>-1626.650384</b>	<b>1</b>
<b>M5<sub>CN</sub></b>	<b>0.613649</b>	<b>-1627.272625</b>	<b>-1626.658976</b>	<b>0</b>
<b>TS4<sub>CN</sub></b>	<b>0.61236</b>	<b>-1627.26333</b>	<b>-1626.65097</b>	<b>1</b>
<b>M6<sub>CN</sub></b>	<b>0.610265</b>	<b>-1627.265446</b>	<b>-1626.655181</b>	<b>0</b>
<b>TS5<sub>CN</sub></b>	<b>0.608798</b>	<b>-1627.253128</b>	<b>-1626.64433</b>	<b>1</b>
<b>(Z)-<math>\beta</math>-product<sub>CN</sub></b>	<b>0.260493</b>	<b>-812.483165</b>	<b>-812.222672</b>	<b>0</b>
<b>M7<sub>CN</sub></b>	<b>0.655752</b>	<b>-1780.148722</b>	<b>-1779.49297</b>	<b>0</b>
<b>TS6<sub>CN</sub></b>	<b>0.652357</b>	<b>-1780.134987</b>	<b>-1779.48263</b>	<b>1</b>
<b>M8<sub>CN</sub></b>	<b>0.655188</b>	<b>-1780.16982</b>	<b>-1779.514632</b>	<b>0</b>
<b>M9<sub>CN</sub></b>	<b>0.613315</b>	<b>-1627.294093</b>	<b>-1626.680778</b>	<b>0</b>
<b>TS7<sub>CN</sub></b>	<b>0.61032</b>	<b>-1627.270049</b>	<b>-1626.659729</b>	<b>1</b>
<b>(E)-<math>\alpha</math>-product<sub>CN</sub></b>	<b>0.261149</b>	<b>-812.484079</b>	<b>-812.22293</b>	<b>0</b>
<b>STS1<sub>CN</sub>-1</b>	<b>0.603261</b>	<b>-1627.173519</b>	<b>-1626.570258</b>	<b>1</b>
<b>STS1<sub>CN</sub>-2</b>	<b>0.603904</b>	<b>-1627.176575</b>	<b>-1626.572671</b>	<b>1</b>
<b>STS2<sub>CN</sub>-1</b>	<b>0.602614</b>	<b>-1627.178716</b>	<b>-1626.576102</b>	<b>1</b>
<b>STS2<sub>CN</sub>-2</b>	<b>0.602891</b>	<b>-1627.183631</b>	<b>-1626.58074</b>	<b>1</b>
<b>STS3<sub>CN</sub>-1</b>	<b>0.60549</b>	<b>-1627.186717</b>	<b>-1626.581227</b>	<b>1</b>
<b>STS3<sub>CN</sub>-2</b>	<b>0.603173</b>	<b>-1627.184817</b>	<b>-1626.581644</b>	<b>1</b>
<b>SM1<sub>CN</sub></b>	<b>0.606412</b>	<b>-1627.214761</b>	<b>-1626.608349</b>	<b>0</b>
<b>STS4<sub>CN</sub></b>	<b>0.602989</b>	<b>-1627.16624</b>	<b>-1626.563251</b>	<b>1</b>
<b>STS5<sub>CN</sub></b>	<b>0.607646</b>	<b>-1627.160364</b>	<b>-1626.552718</b>	<b>1</b>
<b>STS6<sub>CN</sub></b>	<b>0.603964</b>	<b>-1627.147037</b>	<b>-1626.543073</b>	<b>1</b>

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**Part 13: The geometries (Å) for all the optimized compounds and transition states of PBu<sub>3</sub>-catalyzed hydroboration of ynamide at M06-2X/6-31G(d,p)/SMD<sub>toluene</sub> level**

**Ynamide**

C	0.54095200	-0.14899300	-0.05193500
C	1.97152000	-0.08788100	-0.02502100
C	2.61991100	1.15542400	0.00791400
C	2.73616400	-1.26376700	-0.03072300
C	4.00766600	1.21540300	0.03455100
H	2.02587800	2.06326700	0.01318700
C	4.12356400	-1.19208100	-0.00167000
H	2.23443000	-2.22560800	-0.05833800
C	4.76373400	0.04477000	0.03027200
H	4.50102700	2.18193900	0.06060000
H	4.70736900	-2.10715000	-0.00550200
H	5.84755000	0.09636800	0.05237000
C	-0.66773500	-0.17657000	-0.06593600
C	-2.77293900	-1.46301000	0.16539100
C	-4.18752000	-0.94269200	-0.10316300
H	-2.63105900	-1.79117400	1.19991700
H	-2.48208900	-2.26184700	-0.51757800
H	-4.93201400	-1.34409900	0.58320900
H	-4.49620900	-1.12581200	-1.13601500
O	-4.10205900	0.47472300	0.10022800
N	-2.01111200	-0.24406800	-0.09285400
C	-2.82137900	0.88723900	-0.00351200
O	-2.47053200	2.03221900	-0.01008800

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**PBu<sub>3</sub>**

P	0.40955800	0.16243700	1.23356200
C	-0.29551000	1.27133600	-0.08632900
C	1.80096500	-0.62433000	0.27849200
C	-1.66814800	1.83248800	0.28682800
H	0.41139700	2.10018600	-0.21562200
H	-0.34606000	0.74288800	-1.04737100
C	-0.83396500	-1.22834300	1.24682600
C	3.00436900	0.30853700	0.12890200
H	2.10038200	-1.52518800	0.83008800
H	1.45756600	-0.95090500	-0.71121000
C	-2.20458500	2.82187000	-0.74737900
H	-1.60959000	2.32564400	1.26644000
H	-2.38795400	1.01001100	0.39950300
C	-1.29516100	-1.80966700	-0.08867100
H	-1.70039300	-0.86623100	1.81473200
H	-0.38792100	-2.01830600	1.86544600
C	4.17403100	-0.34690000	-0.60474700
H	2.70607200	1.21502100	-0.41492800
H	3.33650300	0.64034600	1.12116100
C	-3.57648600	3.37373600	-0.37296100
H	-2.25845400	2.32573300	-1.72472500
H	-1.49045600	3.64725700	-0.85872300
C	-2.30637300	-2.94362000	0.08744700
H	-1.75053400	-1.02166100	-0.70302800
H	-0.43324100	-2.18510900	-0.65469700
C	5.37009500	0.58834200	-0.75250500
H	3.83821100	-0.67847500	-1.59535100
H	4.47563200	-1.25173900	-0.06223700
H	-4.31221200	2.56778800	-0.28297800

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H	-3.53905700	3.89657900	0.58825200
H	-3.94457600	4.07940000	-1.12295100
C	-2.77496900	-3.52247500	-1.24386600
H	-3.16917600	-2.57043800	0.65350200
H	-1.85641500	-3.73610900	0.69846000
H	5.73828500	0.91090200	0.22682500
H	5.09780200	1.48684600	-1.31594500
H	6.19774300	0.10315700	-1.27744000
H	-1.93198700	-3.92563200	-1.81461500
H	-3.49699800	-4.33101500	-1.09923600
H	-3.25351400	-2.75335100	-1.85899900

**HBpin**

B	0.00000000	0.00000000	1.93256800
O	0.34859100	1.08916000	1.18561700
O	-0.34859100	-1.08916000	1.18561700
H	0.00000000	0.00000000	3.11912300
C	0.00000000	0.78170300	-0.18716400
C	1.02258800	1.42047900	-1.11063700
H	0.83128600	1.13644600	-2.15041900
H	0.95214200	2.50909900	-1.03836800
H	2.03996800	1.12725000	-0.84670500
C	-1.38503600	1.37531900	-0.43188200
H	-1.70049200	1.24071900	-1.47023800
H	-2.13227400	0.91609300	0.22257800
H	-1.35494600	2.44609300	-0.21466900
C	0.00000000	-0.78170300	-0.18716400
C	1.38503600	-1.37531900	-0.43188200
H	1.35494600	-2.44609300	-0.21466900
H	1.70049200	-1.24071900	-1.47023800
H	2.13227400	-0.91609300	0.22257800

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C	-1.02258800	-1.42047900	-1.11063700
H	-2.03996800	-1.12725000	-0.84670500
H	-0.83128600	-1.13644600	-2.15041900
H	-0.95214200	-2.50909900	-1.03836800
H <sub>2</sub> O			
O	0.00000000	0.11848400	0.00000000
H	0.75929700	-0.47399100	0.00000000
H	-0.75929700	-0.47388200	0.00000000
2H <sub>2</sub> O			
O	1.37152000	0.03387800	-0.11412100
H	1.67115600	-0.84198900	0.15712900
H	1.66955000	0.62299700	0.58907800
O	-1.49213700	-0.03542200	0.11418400
H	-1.84597500	0.23174600	-0.73964000
H	-0.52979200	-0.00040400	-0.00706800
TS1			
P	0.98949900	-0.09227600	-0.26504800
C	2.72428000	-0.63533100	0.10385500
C	-0.01749200	-1.62874200	-0.18480900
C	3.22928600	-1.88193300	-0.62541200
H	3.34911700	0.23448900	-0.12904400
H	2.78928100	-0.78126500	1.18917700
C	1.02041500	0.28152800	-2.06888700
C	-0.39867700	1.39489100	0.77272300
C	-0.08320400	-2.22370700	1.22119400
H	-1.02833100	-1.36480200	-0.51822500
H	0.37689300	-2.35913800	-0.90236900
C	4.68802100	-2.19418200	-0.28740900
H	3.13352700	-1.74708700	-1.71027800
H	2.60810600	-2.74783100	-0.36120500

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C	-0.30554100	0.84351300	-2.58416500
H	1.27580500	-0.63558700	-2.61485400
H	1.82701200	1.00531200	-2.22322100
N	0.42734200	2.34757300	1.36040100
C	-1.62737100	1.13478200	0.75263100
C	-0.98119500	-3.45790800	1.28786700
H	0.92573200	-2.48881600	1.56776900
H	-0.45945400	-1.45870200	1.91369600
C	5.19793300	-3.44075300	-1.00362500
H	4.78545100	-2.32337800	0.79775700
H	5.31059400	-1.33135100	-0.55354400
C	-0.29569400	1.08283100	-4.09287300
H	-1.12559600	0.15580600	-2.33579600
H	-0.52532800	1.78470400	-2.06554800
C	0.18416200	2.82634700	2.71307100
C	1.61182700	2.81480400	0.86031900
C	-2.76852600	0.34020200	0.46435200
C	-1.12699700	-3.99826200	2.70638500
H	-0.57214500	-4.23625400	0.63130300
H	-1.96833200	-3.19755300	0.88687500
H	4.60632000	-4.32055200	-0.73021500
H	5.13387700	-3.32228300	-2.09013800
H	6.24150900	-3.64872600	-0.75179400
C	-1.63085800	1.62360900	-4.59513900
H	-0.05920800	0.14359200	-4.60861200
H	0.50922400	1.78539900	-4.34169700
C	1.21341800	3.95785200	2.79436300
H	-0.84353900	3.17820600	2.81518400
H	0.36560800	2.02633500	3.43917900
O	2.15938400	3.67176100	1.75396600

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O	2.14199500	2.53978500	-0.19206600
C	-3.24122500	-0.62348000	1.38225200
C	-3.48247900	0.50425200	-0.74351400
H	-1.57986600	-3.24881000	3.36452600
H	-0.15326600	-4.26553100	3.13041200
H	-1.75895700	-4.89032000	2.73319000
H	-1.87878300	2.57064900	-4.10438400
H	-1.61417900	1.80090000	-5.67417800
H	-2.44175500	0.91784500	-4.38480800
H	1.74673200	3.99246700	3.74400400
H	0.76158000	4.93239700	2.59024900
C	-4.35404100	-1.40097900	1.08805600
H	-2.72296300	-0.74839500	2.32861400
C	-4.58909700	-0.28542100	-1.02795000
H	-3.15288000	1.26093300	-1.44900000
C	-5.03370500	-1.24619100	-0.12019600
H	-4.69164900	-2.13856000	1.81099100
H	-5.11348700	-0.14421500	-1.96875700
H	-5.90099400	-1.85745000	-0.34610200
M1			
P	-0.61421300	0.15312700	-0.41661600
C	-2.21286800	0.97796500	-0.09795000
C	0.60451000	1.46862500	-0.74375000
C	-2.63430400	1.97162600	-1.18418200
H	-2.95541700	0.18036900	0.00031100
H	-2.12575400	1.47117700	0.87731300
C	-0.77936800	-0.77175700	-1.98557900
C	-0.08253700	-0.80929600	1.04694400
C	0.67115100	2.53188500	0.35283200
H	1.58099400	0.99084900	-0.87833200



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H	0.32480100	1.91681800	-1.70528900
C	-3.97786500	2.62468500	-0.85826500
H	-2.70957600	1.45686800	-2.15041100
H	-1.87392800	2.75471700	-1.30047700
C	0.33738700	-1.79191500	-2.20069300
H	-0.78302300	-0.02581200	-2.78989500
H	-1.75346800	-1.26468700	-1.95789300
N	-1.21846000	-1.30764700	1.80525000
C	1.15142500	-0.96085300	1.51296100
C	1.77184000	3.55513300	0.07835000
H	-0.29456700	3.04859300	0.43473000
H	0.85270700	2.04496900	1.31758100
C	-4.41845800	3.60990800	-1.93562900
H	-3.90087900	3.13890900	0.10758300
H	-4.73633000	1.84240400	-0.73547800
C	0.18703200	-2.54088900	-3.52323000
H	1.31329700	-1.29063900	-2.17473000
H	0.32786600	-2.50742100	-1.36942500
C	-1.04680400	-1.68286000	3.20201400
C	-2.20006800	-2.07271400	1.24501800
C	2.41107800	-0.53992800	0.97356100
C	1.91479000	4.56488700	1.21168900
H	1.55530100	4.07539400	-0.86325100
H	2.71901000	3.02227500	-0.06540900
H	-3.68517200	4.41372100	-2.05714500
H	-4.52857100	3.10993400	-2.90320600
H	-5.37869600	4.06894100	-1.68619700
C	1.30328200	-3.56055200	-3.72598500
H	0.18513300	-1.82148100	-4.35167300
H	-0.78700600	-3.04437600	-3.54289900

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C	-2.43320500	-2.25191500	3.49297400
H	-0.24741400	-2.42309900	3.30182100
H	-0.79703700	-0.81601200	3.81608700
O	-2.90893100	-2.69736700	2.21196900
O	-2.46252900	-2.18741200	0.06399400
C	3.11313100	0.56419600	1.51724100
C	3.07823500	-1.27899300	-0.03412500
H	2.18122300	4.06229400	2.14745200
H	0.97879700	5.10781700	1.38028300
H	2.69369700	5.30081200	0.99474500
H	1.30206600	-4.30448700	-2.92299200
H	1.19370500	-4.09189600	-4.67526600
H	2.28380100	-3.07278600	-3.72533000
H	-3.12007100	-1.48662900	3.86783100
H	-2.42558300	-3.10401400	4.17241800
C	4.35310700	0.94850000	1.02423300
H	2.66744900	1.11219700	2.34303300
C	4.32612600	-0.89291600	-0.50968300
H	2.60244300	-2.17134300	-0.42950500
C	4.97253100	0.23355500	-0.00239700
H	4.84854100	1.81383000	1.45804100
H	4.79963200	-1.48397600	-1.28959200
H	5.94524300	0.53237900	-0.37814700
M2			
P	1.14131400	0.19517300	-0.38951300
C	2.31734100	0.11281500	1.00274400
C	1.58655400	-1.10676600	-1.58031000
C	3.78656600	0.08753600	0.57169400
H	2.11344200	0.98910000	1.62751600
H	2.06373800	-0.77778500	1.59006200

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C	1.40786300	1.78847300	-1.24975400
C	-0.55626300	-0.07057900	0.14175400
C	1.57861200	-2.51358800	-0.98422500
H	0.84595000	-1.03301000	-2.38246100
H	2.57143300	-0.84867700	-1.98772100
C	4.73165400	0.10616600	1.77290600
H	4.00244700	0.95233700	-0.06955700
H	3.98539500	-0.80852600	-0.03012600
C	0.15379000	2.30810100	-1.95665600
H	2.22497800	1.63288900	-1.96481000
H	1.73841900	2.50901600	-0.49655600
N	-0.84095700	0.33984600	1.49844900
C	-1.35381700	-0.64628400	-0.76618300
C	1.92856400	-3.57468200	-2.02656400
H	2.28972900	-2.57643500	-0.14896000
H	0.58005100	-2.71222800	-0.57898000
C	6.19820700	0.07702000	1.35595700
H	4.50986100	-0.75406600	2.41642700
H	4.53196700	1.00271200	2.37177600
C	0.44809000	3.56095500	-2.77936600
H	-0.27572700	1.52907000	-2.59895500
H	-0.59973600	2.53236700	-1.19388100
C	-1.76015600	-0.34547200	2.39759200
C	-0.52001500	1.57036500	1.97817900
C	-2.76860600	-0.83665900	-0.48643300
C	1.91782500	-4.98299900	-1.44143200
H	2.91619400	-3.35666100	-2.45233100
H	1.21044700	-3.50996100	-2.85246900
H	6.42515400	-0.82453700	0.77785200
H	6.44630700	0.94295900	0.73387800

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H	6.85964000	0.09093700	2.22619900
C	-0.80494000	4.11049100	-3.45354800
H	1.20645400	3.33009000	-3.53829100
H	0.88405800	4.32650500	-2.12557200
C	-1.51017600	0.44771100	3.68380200
H	-2.79403300	-0.26101200	2.05011800
H	-1.50401000	-1.40318800	2.49233100
O	-0.99905300	1.71335100	3.23685200
O	0.12490600	2.43363000	1.41467700
C	-3.66916500	0.24906700	-0.50397600
C	-3.30222000	-2.11745500	-0.23828500
H	0.93158600	-5.22900900	-1.03537400
H	2.64585400	-5.07744700	-0.62894500
H	2.16392700	-5.73204800	-2.19885800
H	-1.56375600	4.37399800	-2.71008000
H	-0.58384800	5.00685200	-4.03956000
H	-1.24456200	3.36823800	-4.12741000
H	-0.75127500	-0.02474100	4.31560000
H	-2.41347100	0.62662500	4.26615300
C	-5.02587000	0.06093500	-0.26491100
H	-3.28378900	1.24572400	-0.70381000
C	-4.65579700	-2.29455500	0.02274800
H	-2.63197200	-2.97319400	-0.24623900
C	-5.53177300	-1.20926400	0.01070300
H	-5.69430600	0.91767200	-0.28360800
H	-5.03373200	-3.29282500	0.22714600
H	-6.59025600	-1.35210200	0.20220100
TS1'			
P	0.00831300	-0.58843000	0.43997100
C	-0.94663100	-1.51036400	-0.83971400

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C	1.63647100	-1.47569300	0.46818200
C	-0.99346300	-3.03155500	-0.69503700
H	-1.95967000	-1.09625600	-0.80821700
H	-0.52085800	-1.22755100	-1.81046600
C	-0.75048100	-1.11831000	2.04337200
C	-0.89999000	2.02645700	-1.10106700
C	2.37997900	-1.44062500	-0.86828400
H	2.24586000	-0.99092900	1.24041100
H	1.47859300	-2.51255900	0.79253500
C	-1.84283800	-3.68876700	-1.78359100
H	-1.40033800	-3.30067600	0.28828600
H	0.02243200	-3.44613300	-0.73756300
C	-0.31756300	-0.22548200	3.20671500
H	-0.48014800	-2.16388900	2.23969700
H	-1.83464300	-1.06305900	1.91344300
N	-2.24772900	1.88284500	-1.26133900
C	0.10771200	1.50880500	-0.51939200
C	3.80686300	-1.97627300	-0.75682500
H	1.82715100	-2.02763800	-1.61457900
H	2.41971400	-0.41227000	-1.24724400
C	-1.89041200	-5.20742800	-1.64938100
H	-1.44002500	-3.41527300	-2.76691900
H	-2.85997200	-3.28020700	-1.74078600
C	-0.94867300	-0.64494900	4.53355800
H	0.77720100	-0.24485800	3.30898800
H	-0.59523000	0.81206300	2.98081200
C	-3.01105000	2.77782500	-2.13184200
C	-3.09092800	1.31365200	-0.32354000
C	1.52137100	1.87522200	-0.38414700
C	4.55858200	-1.89224700	-2.08114400

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H	3.78324100	-3.01444900	-0.40161100
H	4.34170900	-1.39614500	0.00552700
H	-0.88637000	-5.63896400	-1.71687500
H	-2.31410000	-5.50231600	-0.68386800
H	-2.50186900	-5.66076100	-2.43450100
C	-0.52141100	0.25152100	5.69133900
H	-0.67780500	-1.68602500	4.75032200
H	-2.04032200	-0.62310300	4.42966800
C	-4.41943300	2.22559200	-1.93089000
H	-2.91065800	3.81324900	-1.79043800
H	-2.66974100	2.70221800	-3.16452100
O	-4.37271200	1.60809400	-0.63567100
O	-2.78217000	0.66392800	0.64560800
C	2.20714000	2.37042600	-1.50466300
C	2.22306800	1.73857600	0.81878100
H	4.61998500	-0.85355900	-2.42251200
H	4.05066000	-2.47004100	-2.86047100
H	5.57821800	-2.27715300	-1.99068700
H	-0.80629400	1.29199000	5.50537100
H	-0.98489200	-0.05918200	6.63182700
H	0.56461700	0.22451900	5.82912900
H	-4.66648600	1.45862700	-2.67106800
H	-5.19568400	2.98995900	-1.91967700
C	3.55853500	2.68538800	-1.42709400
H	1.66070800	2.48838900	-2.43472500
C	3.57706600	2.05435000	0.89447800
H	1.69379300	1.38676000	1.70071100
C	4.25428700	2.51940800	-0.22973200
H	4.07372600	3.05539100	-2.30852400
H	4.10197200	1.94129100	1.83834600

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H	5.31147400	2.75804000	-0.17275800
TS1"			
C	1.17392500	0.47829000	0.59724600
C	1.31082800	1.91294500	0.88340100
C	2.34179700	2.63737500	0.26461300
C	0.45500200	2.59062600	1.76045200
C	2.49858700	3.99603300	0.51623000
H	3.02056100	2.11362900	-0.39793000
C	0.61705800	3.94913600	2.01235900
H	-0.33675100	2.04021000	2.26109300
C	1.63737000	4.66099200	1.38694000
H	3.29919100	4.53958100	0.02352100
H	-0.05402600	4.45090300	2.70309100
H	1.76155100	5.72233900	1.57748500
C	1.73901800	-0.61781600	0.29989300
C	2.85261200	-2.74844900	-0.28848500
C	4.34435700	-3.07038200	-0.23808800
H	2.42308200	-2.89447400	-1.28597900
H	2.27266300	-3.31768900	0.43954700
H	4.67368500	-3.75729800	-1.01731500
H	4.64500300	-3.45427100	0.74131400
O	4.98901100	-1.80645400	-0.44755200
N	2.86630000	-1.32793200	0.05587600
C	4.13704500	-0.79867300	-0.14394500
O	4.47569500	0.35249400	-0.08363200
P	-0.95420200	-0.00335900	0.48213300
C	-1.11273700	-0.20013600	-1.33861300
C	-1.07794200	-1.68857600	1.21120300
C	-1.18830000	1.14910600	-2.05618100
H	-0.21431400	-0.74467100	-1.65194200

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H	-1.97861100	-0.82379900	-1.58794000
C	-2.54385000	0.83002300	0.96544300
C	-1.54343400	-2.82610800	0.30101200
H	-0.06301800	-1.90733600	1.56738400
H	-1.73332700	-1.60514500	2.08722200
C	-1.21021100	0.99635700	-3.57668600
H	-0.32890200	1.76690700	-1.76384000
H	-2.08762700	1.69397000	-1.73800900
C	-3.83742400	0.20224300	0.44305000
H	-2.46512800	1.87542500	0.64178100
H	-2.55088800	0.85091500	2.06315100
C	-1.60196700	-4.16214500	1.04082000
H	-2.53198000	-2.60359100	-0.12176000
H	-0.85371300	-2.91249200	-0.54882400
C	-1.29228000	2.33911600	-4.29527100
H	-2.06312900	0.36809800	-3.86377200
H	-0.30808000	0.45966600	-3.89476900
C	-5.08309900	0.94819800	0.92382400
H	-3.82851000	0.19115000	-0.65474600
H	-3.89642700	-0.84605200	0.76570500
C	-2.03455800	-5.31210700	0.13688500
H	-2.29396600	-4.07506700	1.88783700
H	-0.61545900	-4.37752000	1.47079300
H	-2.20159700	2.88020600	-4.01376400
H	-0.43692700	2.97207800	-4.03872100
H	-1.30154600	2.21251600	-5.38140600
C	-6.37332000	0.32465000	0.40095200
H	-5.01927200	1.99523700	0.60277100
H	-5.09431200	0.96059200	2.02074100
H	-1.33953700	-5.43566200	-0.70006100



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H	-3.02892900	-5.12864200	-0.28292600
H	-2.07235700	-6.25894200	0.68251500
H	-6.47014900	-0.71387700	0.73394100
H	-7.25319700	0.87093900	0.75155200
H	-6.39362600	0.32557400	-0.69372600
M3			
P	-1.38831100	-0.05242800	-0.04406100
C	-3.07282900	-0.77138400	-0.03310400
C	-1.49028600	1.48565100	0.96232300
C	-4.18199300	0.22507800	-0.37473400
H	-3.06060900	-1.58316000	-0.76787500
H	-3.23556900	-1.21540500	0.95492200
C	-1.14411800	0.51908600	-1.79787600
C	-0.31274600	-1.18654200	0.64371200
C	-1.92443500	1.22725700	2.40375900
H	-0.50646800	1.96604100	0.93260800
H	-2.18432500	2.17283200	0.46431500
C	-5.55380400	-0.44762200	-0.43032500
H	-3.97507700	0.69556400	-1.34522900
H	-4.21073900	1.03421300	0.36699900
C	-1.31937500	2.00778900	-2.09300700
H	-1.80170000	-0.09882500	-2.42020200
H	-0.11763900	0.22494100	-2.03496200
N	-0.66164200	-2.56588300	0.49544900
C	1.12224300	-0.92099500	1.04186800
C	-1.94333700	2.50479300	3.24220400
H	-2.92525900	0.77350200	2.41390100
H	-1.24995300	0.49190200	2.85794000
C	-6.67057600	0.53558800	-0.76504400
H	-5.75724900	-0.92692900	0.53532200

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H	-5.52859300	-1.25106100	-1.17614200
C	-0.94924000	2.35192300	-3.53545700
H	-2.35213900	2.32834800	-1.89951500
H	-0.67696900	2.58672800	-1.41820400
C	-0.72920400	-3.47795900	1.62513800
C	-1.01624500	-3.19343100	-0.65508500
C	2.16551800	-1.76443800	0.29465900
C	-2.38528300	2.24874900	4.67949600
H	-2.61120700	3.23879200	2.77384900
H	-0.94066200	2.95104100	3.23786300
H	-6.73062300	1.33252300	-0.01656700
H	-6.49965800	1.00627100	-1.73865400
H	-7.64348200	0.03802000	-0.80145700
C	-1.07648500	3.84341300	-3.82878400
H	-1.58508600	1.77976200	-4.22228100
H	0.08040500	2.02064500	-3.72436900
C	-0.75203000	-4.82412000	0.89972800
H	0.14862700	-3.37246800	2.26884800
H	-1.63017800	-3.29179200	2.22453600
O	-1.24524800	-4.51359200	-0.40965700
O	-1.19040400	-2.70245400	-1.75545300
C	3.35807700	-2.12866400	0.93071700
C	1.98674300	-2.12532500	-1.04493800
H	-1.71599500	1.53672000	5.17282000
H	-3.39634800	1.82963400	4.70987100
H	-2.38771500	3.16982100	5.26882900
H	-0.43115700	4.42973400	-3.16517500
H	-0.79650300	4.07702600	-4.85977000
H	-2.10486700	4.18717500	-3.67602100
H	-1.41389200	-5.56231700	1.35325800

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H	0.25531600	-5.24175200	0.80263300
C	4.34661200	-2.83447000	0.25044700
H	3.51131000	-1.84345100	1.96913500
C	2.97315800	-2.83609500	-1.72511700
H	1.05776800	-1.86159600	-1.54414600
C	4.15705800	-3.19213600	-1.08300800
H	5.26454500	-3.10722400	0.76299000
H	2.81165700	-3.11575600	-2.76201600
H	4.92341600	-3.74758300	-1.61484100
B	1.72410300	0.50508400	0.75040000
O	1.44338600	1.24903500	-0.37561900
O	2.71786000	1.06311500	1.51317500
H	1.28960100	-1.11810500	2.11436900
C	2.55807100	2.15618000	-0.55458100
C	2.06321000	3.43243400	-1.21196600
H	2.87745700	4.15896800	-1.29971200
H	1.69927600	3.20804500	-2.21943200
H	1.24857900	3.88866600	-0.64488600
C	3.55501700	1.43436200	-1.45821900
H	4.41073900	2.06997700	-1.70241600
H	3.91973800	0.51530600	-0.98733700
H	3.04910900	1.15669300	-2.38715900
C	3.07816300	2.32648300	0.91027100
C	2.34257700	3.41778800	1.68264300
H	2.59696300	3.33306800	2.74224600
H	2.62597600	4.41562700	1.33604500
H	1.25784000	3.31060700	1.58358300
C	4.58146900	2.51416400	1.03003900
H	5.12144200	1.65479300	0.62882400
H	4.90140100	3.41487800	0.49646500

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H	4.85380000	2.62756500	2.08283500
TS2R			
P	-1.44367200	-0.14181300	-0.03728800
C	-2.82295600	-1.33427800	-0.12495900
C	-1.67720000	0.76475700	1.54503500
C	-4.20845900	-0.71606600	-0.32673700
H	-2.58078600	-2.01601700	-0.94713600
H	-2.79330500	-1.92292300	0.80070000
C	-1.60879100	1.01987200	-1.43262400
C	0.04436700	-1.06964900	-0.17148900
C	-1.06695700	-0.01171200	2.71375800
H	-1.17861300	1.73036800	1.44427800
H	-2.74989200	0.93556800	1.69686500
C	-5.30052300	-1.78632700	-0.35047000
H	-4.23297700	-0.16133100	-1.27369100
H	-4.43340000	0.00713800	0.46794800
C	-2.44654200	2.26763100	-1.15029100
H	-2.02119200	0.43233100	-2.26254500
H	-0.58903200	1.30459600	-1.70858600
N	-0.04384800	-2.45476700	0.17839300
C	1.30992200	-0.47807800	-0.29754300
C	-1.22948600	0.72298800	4.04303900
H	-1.52455400	-1.00817900	2.79143400
H	0.00181600	-0.16909100	2.51290900
C	-6.68736500	-1.19318800	-0.57485400
H	-5.28110000	-2.34044200	0.59595400
H	-5.07242900	-2.51209800	-1.13991600
C	-2.68689100	3.08199000	-2.42120400
H	-3.41382900	2.00253700	-0.70508700
H	-1.92013100	2.88367000	-0.41053500

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C	0.52856600	-3.00957700	1.39838000
C	-0.37235600	-3.44731500	-0.70535100
C	2.44909500	-1.37622800	-0.67687900
C	-0.60428200	-0.04258700	5.20455700
H	-2.29565300	0.89257400	4.23868000
H	-0.76619600	1.71370000	3.95780700
H	-6.94459100	-0.48273000	0.21758200
H	-6.73601800	-0.65926900	-1.52933200
H	-7.45558200	-1.97083500	-0.58829900
C	-3.37216500	4.41345100	-2.13381500
H	-3.29398600	2.48892000	-3.11628500
H	-1.72764700	3.25749100	-2.92411900
C	0.82965300	-4.44005700	0.94723500
H	1.43385900	-2.46607200	1.68533000
H	-0.18813300	-2.96968600	2.22825600
O	-0.03960700	-4.65146500	-0.17488300
O	-0.90819700	-3.33680600	-1.78560000
C	3.68431500	-1.37911600	-0.01764000
C	2.27859300	-2.23451500	-1.77253300
H	0.46645600	-0.19781900	5.03760600
H	-1.06920300	-1.02714900	5.32160400
H	-0.72138100	0.49582300	6.14890700
H	-2.75430900	5.03694400	-1.47862000
H	-3.55643200	4.97540600	-3.05324600
H	-4.33523600	4.26134200	-1.63549300
H	0.60972800	-5.19679800	1.70022600
H	1.86543500	-4.54246900	0.60764800
C	4.71561700	-2.21120800	-0.44208600
H	3.82996700	-0.72390400	0.83582900
C	3.31085800	-3.06768900	-2.19432000

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H	1.32588900	-2.23971400	-2.29428100
C	4.53426300	-3.06296800	-1.52937200
H	5.66443000	-2.19735700	0.08584600
H	3.15287100	-3.72390100	-3.04472700
H	5.33772900	-3.71705800	-1.85333500
B	1.69600200	0.99177700	-0.00036900
O	0.75080700	2.01753700	0.31686200
O	2.89704700	1.58492300	-0.45926700
H	1.89255100	0.13448800	1.06356600
C	1.38440400	3.27672500	0.04829800
C	0.94490300	4.28283900	1.10169300
H	1.48945100	5.22696200	0.99446300
H	-0.12298800	4.49757600	0.98693100
H	1.10732700	3.89563600	2.10989000
C	0.94763900	3.74314100	-1.34017000
H	1.35641300	4.72830300	-1.58435400
H	1.27074700	3.03057200	-2.10563600
H	-0.14371000	3.81521600	-1.36687000
C	2.90172700	2.90517800	0.08445800
C	3.44446200	2.84186500	1.51430400
H	4.43114000	2.37045000	1.49237100
H	3.54615700	3.83732300	1.95690900
H	2.79313400	2.23894300	2.15513400
C	3.79528400	3.78643800	-0.77434500
H	3.52323300	3.71480600	-1.82901600
H	3.73262600	4.83400600	-0.46116000
H	4.83476700	3.46244100	-0.67133800
M4R			
P	-1.43082200	-0.02477600	-0.04765700
C	-2.84238600	-1.18684300	-0.07204400

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C	-1.59600100	0.90217100	1.51143000
C	-4.19305400	-0.50939900	0.17853300
H	-2.83975800	-1.66258900	-1.05797100
H	-2.65453400	-1.96647200	0.67530400
C	-1.61491800	1.06760100	-1.50143300
C	0.07038500	-1.04956600	-0.11770900
C	-1.54457700	-0.00545000	2.74186500
H	-0.80131800	1.64987700	1.53368900
H	-2.55377100	1.43289200	1.45281800
C	-5.35443000	-1.48823900	0.00368400
H	-4.32526000	0.33245200	-0.51479000
H	-4.22459200	-0.09243000	1.19272800
C	-2.09294500	2.48379200	-1.18134700
H	-2.28764400	0.55104000	-2.19514700
H	-0.62523000	1.09409400	-1.96122400
N	-0.16766100	-2.38352000	-0.56342500
C	1.28775200	-0.60277200	0.26037400
C	-1.52719400	0.81438800	4.03110000
H	-2.40653900	-0.68704500	2.75050200
H	-0.63976900	-0.62447800	2.69939000
C	-6.70618600	-0.83381100	0.26775300
H	-5.21239800	-2.33699100	0.68406500
H	-5.32980400	-1.89670900	-1.01351400
C	-2.17148800	3.33932300	-2.44517100
H	-3.07983000	2.46087500	-0.69989900
H	-1.39023900	2.93687600	-0.47290400
C	0.01230900	-3.58522500	0.23548800
C	-0.63347300	-2.66930500	-1.81150800
C	2.44965200	-1.51577100	0.12327200
C	-1.48021300	-0.06580900	5.27522300

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H	-2.41346600	1.46067200	4.06322800
H	-0.65318300	1.47606400	4.00821300
H	-6.76189400	-0.44413700	1.28924800
H	-6.87787400	0.00217400	-0.41779700
H	-7.52484300	-1.54620300	0.13678200
C	-2.57781600	4.77706800	-2.13948700
H	-2.88271300	2.88950200	-3.14896100
H	-1.19448200	3.32694000	-2.94533400
C	-0.01743100	-4.64463800	-0.87251400
H	0.96679600	-3.57294700	0.76573000
H	-0.80430000	-3.70050400	0.95922700
O	-0.68907500	-4.01051400	-1.97451700
O	-0.98464100	-1.87228800	-2.65447700
C	3.30021700	-1.72712100	1.21600000
C	2.74075800	-2.15286200	-1.09129300
H	-0.58484200	-0.69540700	5.27254000
H	-2.35304900	-0.72530200	5.32647400
H	-1.46235900	0.53564800	6.18800000
H	-1.86257700	5.24771400	-1.45671300
H	-2.62228000	5.38219000	-3.04893500
H	-3.56356400	4.81389100	-1.66409400
H	-0.57133400	-5.54402100	-0.60513500
H	0.99386900	-4.91104400	-1.19263900
C	4.38090800	-2.59707000	1.11205900
H	3.10510400	-1.20102000	2.14543700
C	3.83769800	-3.00310000	-1.19995700
H	2.11268400	-1.95867100	-1.95713100
C	4.65164000	-3.24031700	-0.09414700
H	5.02345900	-2.76150000	1.97159200
H	4.05728400	-3.47924900	-2.15090000



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H	5.50203300	-3.90996900	-0.17646100
B	1.56106200	0.89800200	0.90051800
O	0.82175800	1.93457600	0.11521700
O	2.97515200	1.25078800	0.77563700
H	1.16403700	0.87383700	2.07458000
C	1.79333500	2.70920300	-0.57861500
C	1.26414600	4.12553100	-0.76877400
H	2.04609900	4.79095900	-1.15145600
H	0.44319300	4.12655400	-1.49466900
H	0.88744400	4.53189400	0.17321900
C	2.08007300	2.07204700	-1.94149900
H	2.79405900	2.66189500	-2.52542000
H	2.48192100	1.06154700	-1.81448000
H	1.15346500	2.00945900	-2.52080100
C	3.03333500	2.59994800	0.36268400
C	2.89019200	3.51530000	1.58470700
H	3.64594400	3.23123300	2.32270500
H	3.03379100	4.57091300	1.33108900
H	1.90408400	3.39406700	2.04316400
C	4.37306400	2.85132300	-0.31761100
H	4.56832700	2.09674700	-1.08242900
H	4.40822400	3.84469400	-0.77892500
H	5.17661900	2.79338700	0.42297900
TS2S			
P	-1.37306700	0.01176800	-0.02313700
C	-2.83513500	-1.06438800	0.23277300
C	-1.31164800	1.19861300	1.36026000
C	-4.03012000	-0.40238600	0.92694200
H	-3.12043900	-1.44404900	-0.75639100
H	-2.49647800	-1.92817500	0.81429800

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C	-1.64693500	0.94764400	-1.56898600
C	0.03319900	-1.03858400	-0.10620700
C	-0.95246600	0.53915900	2.69315300
H	-0.56940400	1.95234000	1.08182200
H	-2.29115300	1.68981400	1.41161300
C	-5.23727400	-1.33871900	0.97837600
H	-4.31528900	0.52386000	0.41446300
H	-3.75157600	-0.11729300	1.94945500
C	-2.96329300	1.71727800	-1.68999700
H	-1.54108500	0.20173300	-2.36635100
H	-0.78678200	1.62244300	-1.64124000
N	-0.28555900	-2.39427000	-0.43993200
C	1.35103600	-0.55385300	-0.19457600
C	-1.02736000	1.52775000	3.85572700
H	-1.62173100	-0.30957700	2.89440500
H	0.05808600	0.12037400	2.62072700
C	-6.42638000	-0.71170300	1.69848500
H	-4.94847100	-2.27118400	1.47909600
H	-5.52345000	-1.61168400	-0.04469100
C	-2.99093100	2.58026500	-2.95232100
H	-3.80795100	1.01688400	-1.71832600
H	-3.11432100	2.36186400	-0.81333400
C	-0.09300400	-3.52320200	0.45841400
C	-0.44022500	-2.81544400	-1.73208000
C	2.42653500	-1.59835200	-0.11682400
C	-0.61001500	0.89753200	5.18022900
H	-2.05060600	1.91669200	3.93424800
H	-0.38543700	2.38992600	3.63543400
H	-6.17053300	-0.45748300	2.73212100
H	-6.74690400	0.20814800	1.19893700

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H	-7.28099600	-1.39290400	1.72382600
C	-4.30766200	3.33201600	-3.11503700
H	-2.81498500	1.94091400	-3.82562600
H	-2.15637700	3.29124100	-2.91576200
C	-0.59847100	-4.67175200	-0.42065900
H	0.96318800	-3.63497400	0.72794600
H	-0.68001500	-3.40583100	1.37397400
O	-0.52496000	-4.16993600	-1.76192400
O	-0.51595400	-2.13232300	-2.72812000
C	3.11332000	-1.76276100	1.08891400
C	2.71200000	-2.45167300	-1.18536000
H	0.42126900	0.53389400	5.13165300
H	-1.25146800	0.04581000	5.42932900
H	-0.67359200	1.61533900	6.00244900
H	-4.49055000	3.99444900	-2.26252200
H	-4.30765200	3.94550000	-4.01999700
H	-5.15085700	2.63691400	-3.18320900
H	-1.64197700	-4.92334800	-0.20435100
H	0.01365400	-5.57134500	-0.35412200
C	4.05138700	-2.78105500	1.23318200
H	2.90596500	-1.08332200	1.91134200
C	3.65461300	-3.46776600	-1.04301300
H	2.18683500	-2.31248300	-2.12724300
C	4.32030800	-3.63968500	0.16852700
H	4.57875700	-2.90026700	2.17484600
H	3.86786000	-4.12520000	-1.88035600
H	5.05299400	-4.43298100	0.28024700
B	1.88120200	0.87657400	-0.41773600
O	3.23219600	1.24922200	-0.17195800
O	1.05858600	2.04544500	-0.39543600

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H	1.75591800	0.12178800	-1.56018100
C	3.23566200	2.63633700	0.15672000
C	4.52851700	3.26471900	-0.34185100
H	4.52182500	4.35000100	-0.19361100
H	5.37544100	2.85096300	0.21305800
H	4.68457900	3.05301100	-1.40130400
C	3.14294900	2.75485900	1.67974500
H	3.22630800	3.79103000	2.02231600
H	2.19448600	2.34053600	2.03875000
H	3.95674400	2.17556200	2.12443400
C	1.94568400	3.15959000	-0.55037200
C	2.16072000	3.39445400	-2.04532600
H	1.18920700	3.55029900	-2.52424100
H	2.78178900	4.27512800	-2.23397000
H	2.63463300	2.52419100	-2.50928600
C	1.30894800	4.38160700	0.09239200
H	1.02385500	4.18297700	1.12829600
H	1.99530800	5.23459800	0.07634000
H	0.40761000	4.66207500	-0.46193300
M4S			
P	1.32030600	0.12711900	-0.05035400
C	2.67013200	1.23136700	0.52456400
C	1.33907200	-1.34718500	1.04284500
C	3.84827300	0.55379200	1.22980900
H	3.01388200	1.78314900	-0.35960300
H	2.20753500	1.96400700	1.19273000
C	1.85399800	-0.51807200	-1.69389100
C	-0.15085200	1.04025400	0.03610000
C	0.78430100	-1.07973700	2.44115000
H	0.76573000	-2.13109000	0.53760900

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H	2.37719000	-1.69733600	1.09598900
C	4.96630100	1.54923500	1.53901400
H	4.25419000	-0.26153800	0.61926800
H	3.50436200	0.09664600	2.16669000
C	3.24152500	-1.15302300	-1.80367800
H	1.75672200	0.34079300	-2.36878700
H	1.07696700	-1.23588800	-1.98352400
N	0.10760500	2.44935300	-0.15772300
C	-1.42609100	0.57066700	-0.69618100
C	0.97593900	-2.27474400	3.37439400
H	1.26622100	-0.19438800	2.87824200
H	-0.27839600	-0.82006100	2.36147000
C	6.13325400	0.90183900	2.27726100
H	4.55908500	2.37401100	2.13695100
H	5.32046600	1.99300400	0.60034700
C	3.48790900	-1.74563400	-3.19217600
H	4.01398800	-0.40045200	-1.59793400
H	3.36484200	-1.94477700	-1.05207700
C	-0.26176000	3.45916700	0.82588300
C	0.25148000	3.01825500	-1.39080000
C	-2.56635000	1.49037500	-0.29590400
C	0.27971900	-2.08029800	4.71705100
H	2.04961600	-2.44242200	3.52854500
H	0.59345700	-3.18281100	2.88915000
H	5.80715100	0.47874100	3.23291300
H	6.56955000	0.09021200	1.68601100
H	6.92552900	1.62586800	2.48562300
C	4.87845900	-2.35719200	-3.32899800
H	3.34996600	-0.96021100	-3.94499800
H	2.72424300	-2.50649100	-3.39582300

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C	0.13428900	4.74166100	0.08964400
H	-1.33411100	3.41808200	1.04701400
H	0.29398100	3.32191900	1.75753700
O	0.17079500	4.37256800	-1.29482800
O	0.43949900	2.45782800	-2.45068100
C	-3.17401600	1.40071800	0.96205700
C	-2.94804800	2.53316100	-1.14329000
H	-0.80089600	-1.96650100	4.58080500
H	0.64584300	-1.18062100	5.22232200
H	0.44656800	-2.93052700	5.38410300
H	5.02806100	-3.16049100	-2.59990600
H	5.03475100	-2.77824900	-4.32600500
H	5.65619400	-1.60549900	-3.15888600
H	1.13129800	5.09002000	0.38036200
H	-0.58317100	5.55383300	0.21262900
C	-4.13886300	2.32181200	1.35537200
H	-2.87482100	0.60263300	1.63502100
C	-3.90745000	3.46627800	-0.74939900
H	-2.46772800	2.62447400	-2.11538900
C	-4.50650600	3.36332700	0.50221900
H	-4.60266900	2.23309300	2.33357100
H	-4.18132800	4.27441500	-1.42123000
H	-5.25442900	4.08641700	0.81307800
B	-1.78956900	-0.95270000	-0.51647300
O	-2.92649400	-1.43592700	0.07951000
O	-1.00463300	-1.96942600	-1.02365200
H	-1.28947200	0.69824600	-1.78690900
C	-2.80769200	-2.87292800	0.16278700
C	-4.18176600	-3.49372700	-0.02226500
H	-4.11032000	-4.58576600	-0.04756300

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H	-4.82471500	-3.21387500	0.81640600
H	-4.65546100	-3.14947400	-0.94304700
C	-2.26030400	-3.18779800	1.55219800
H	-2.20608800	-4.26531900	1.73215900
H	-1.26105700	-2.75980600	1.67794000
H	-2.91918100	-2.74149500	2.30193600
C	-1.78522400	-3.18730500	-0.97569300
C	-2.44654500	-3.33767300	-2.34304900
H	-1.67045600	-3.34632300	-3.11265600
H	-3.01561500	-4.26881200	-2.41272500
H	-3.11943100	-2.49959900	-2.54752000
C	-0.85939000	-4.36083700	-0.70326700
H	-0.28204600	-4.22031100	0.21325300
H	-1.43330400	-5.28860700	-0.61335100
H	-0.15876200	-4.47444900	-1.53535200
M3'			
P	-1.63658100	-0.25069500	-0.27154800
C	-2.16652000	-1.82462500	-1.01911400
C	-2.88447700	0.16028700	0.99633700
C	-3.62900200	-1.83575800	-1.47113200
H	-1.48068300	-1.99970200	-1.85581700
H	-1.97660600	-2.61587600	-0.28661000
C	-1.64444100	1.01682400	-1.59443700
C	0.04432700	-0.49655200	0.38245800
C	-2.86188000	-0.82799300	2.16468200
H	-2.68779600	1.17893700	1.34123000
H	-3.86251200	0.16660200	0.50048200
C	-3.94679700	-3.07925700	-2.30258500
H	-3.85995100	-0.93963200	-2.06364100
H	-4.29007100	-1.81165600	-0.59569400

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C	-2.37703700	2.31882500	-1.26377700
H	-2.08327500	0.53973100	-2.47861900
H	-0.59121800	1.20766700	-1.82537800
N	0.43565200	-1.86825500	0.40271100
C	0.89271700	0.49963800	0.70581400
C	-3.86259600	-0.44400200	3.25402600
H	-3.08429200	-1.84166900	1.80481400
H	-1.85131300	-0.86181500	2.59358500
C	-5.41093800	-3.13268100	-2.72486800
H	-3.69296300	-3.97343900	-1.72063300
H	-3.30089500	-3.09188700	-3.18816500
C	-2.17641800	3.36033500	-2.36279000
H	-3.44925600	2.12129500	-1.13459800
H	-2.00909900	2.72960000	-0.31684500
C	0.89781900	-2.52082200	1.62096900
C	1.03926700	-2.40350900	-0.71120500
C	0.39136800	1.89022200	0.83315000
C	-3.84722800	-1.42439500	4.42180500
H	-4.86887400	-0.39574000	2.82012300
H	-3.62864700	0.56631100	3.61192500
H	-6.07205000	-3.15119800	-1.85239300
H	-5.67841900	-2.25860500	-3.32735000
H	-5.61966300	-4.02482500	-3.32080400
C	-2.87237300	4.67601500	-2.03367600
H	-2.54529100	2.96551400	-3.31769600
H	-1.10020300	3.53209300	-2.48848200
C	1.82495400	-3.61193600	1.05344100
H	1.45046600	-1.81951400	2.24955400
H	0.05337800	-2.93723200	2.18081900
O	1.72723600	-3.50555600	-0.37354300



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O	0.91972900	-2.01132800	-1.85157000
C	0.79477700	2.89811300	-0.05475400
C	-0.42710600	2.23979900	1.91554000
H	-2.85622300	-1.46743400	4.88439700
H	-4.10486900	-2.43520200	4.08968100
H	-4.56415400	-1.13356700	5.19387400
H	-2.48926300	5.08787700	-1.09415100
H	-2.71252800	5.41983500	-2.81870600
H	-3.95228300	4.53449400	-1.92086100
H	1.51932100	-4.62133400	1.33451300
H	2.86239700	-3.43216100	1.33558700
C	0.33785300	4.20223700	0.10497500
H	1.47800400	2.64400100	-0.85701400
C	-0.86824200	3.55152200	2.08622000
H	-0.69481300	1.47592000	2.64206800
C	-0.49610600	4.53475500	1.17378500
H	0.64709400	4.96895100	-0.59938400
H	-1.49476600	3.80342500	2.93662700
H	-0.83737000	5.55734800	1.30206300
B	2.51205600	0.29614400	1.08125900
O	3.31457000	1.31698100	0.39009400
O	3.01539300	-1.00109100	0.58233000
H	2.56788900	0.42203500	2.31111300
C	4.06373200	0.67716900	-0.62833900
C	5.35950200	1.45103500	-0.84252800
H	6.02305000	0.93172900	-1.54328100
H	5.13431400	2.43848700	-1.25792700
H	5.88788200	1.59820500	0.10166500
C	3.25392600	0.65921000	-1.93024400
H	3.82291900	0.23214700	-2.76302000

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H	2.33554100	0.07479000	-1.80930700
H	2.99335300	1.68807800	-2.20092800
C	4.25691000	-0.76232300	-0.05872700
C	5.36841600	-0.80931300	0.99455300
H	5.31415900	-1.76778500	1.52051700
H	6.36536600	-0.71761800	0.55102800
H	5.23275900	-0.00900300	1.72806800
C	4.48559800	-1.83880400	-1.11202000
H	3.62070000	-1.92849000	-1.77323800
H	5.37618500	-1.61954300	-1.71235500
H	4.63798800	-2.80878900	-0.62673900
TS2R'			
P	-1.64287300	-0.37970500	-0.10961500
C	-2.48094900	-1.96148300	0.23452500
C	-2.60097600	0.91383000	0.76332000
C	-3.99003700	-1.93523800	-0.01677600
H	-1.99476700	-2.69890300	-0.41317600
H	-2.25471600	-2.23536300	1.27118600
C	-1.78950900	-0.05788200	-1.91533500
C	0.03761800	-0.52705000	0.42298600
C	-2.62563700	0.71351700	2.27799900
H	-2.17048700	1.88916300	0.51318200
H	-3.61614700	0.89656400	0.34877300
C	-4.61535600	-3.32043700	0.14857500
H	-4.19541800	-1.56834000	-1.03195400
H	-4.47735000	-1.23641400	0.67518100
C	-2.78771200	1.01724200	-2.34568900
H	-2.00933200	-1.02452500	-2.38160700
H	-0.77419800	0.19896200	-2.24050400
N	0.50543400	-1.87170600	0.53392100

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C	0.96157900	0.49831400	0.20429400
C	-3.32866000	1.86894300	2.98833000
H	-3.13043900	-0.23037800	2.52569600
H	-1.59654400	0.62517000	2.64665100
C	-6.12225000	-3.30732000	-0.08495700
H	-4.39783000	-3.69340500	1.15697600
H	-4.13546800	-4.01565500	-0.55032700
C	-2.74438600	1.25127400	-3.85554000
H	-3.80718000	0.73340600	-2.05233400
H	-2.56404900	1.96054400	-1.83140800
C	1.28685000	-2.34665000	1.66046500
C	0.67455300	-2.65877300	-0.56996900
C	0.47258600	1.90738500	0.27537600
C	-3.31535000	1.71053700	4.50481500
H	-4.36264500	1.94174900	2.62864400
H	-2.83341800	2.80633700	2.70596500
H	-6.62429700	-2.63869200	0.62179700
H	-6.35954500	-2.96188900	-1.09629600
H	-6.55233400	-4.30499900	0.03612000
C	-3.72368900	2.33165700	-4.30230300
H	-2.96251100	0.31020400	-4.37489100
H	-1.72368300	1.53263300	-4.14288800
C	1.99087600	-3.57232300	1.04842000
H	2.00704000	-1.58598500	1.97214300
H	0.64065200	-2.60618600	2.50654300
O	1.43317000	-3.73099000	-0.26243400
O	0.16161300	-2.49866700	-1.65817700
C	0.14900600	2.67062200	-0.84995000
C	0.29138300	2.47226500	1.54570600
H	-2.28876100	1.67333300	4.88364300

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H	-3.81564800	0.78541100	4.80936300
H	-3.82410300	2.54299600	4.99832800
H	-3.50237200	3.28655600	-3.81430800
H	-3.67756400	2.49013500	-5.38304500
H	-4.75332000	2.05940000	-4.04817200
H	1.80906100	-4.49257300	1.60647400
H	3.06491900	-3.41102900	0.94047600
C	-0.37288400	3.95732500	-0.70888200
H	0.30057100	2.24725400	-1.83888300
C	-0.22768900	3.75425600	1.68597100
H	0.56188600	1.89048300	2.42244400
C	-0.57432100	4.49858300	0.55696100
H	-0.62623800	4.53250600	-1.59456900
H	-0.36063300	4.17577700	2.67805100
H	-0.98654800	5.49665000	0.66618900
B	2.45461900	0.30458100	-0.17394400
O	3.11677100	-0.96325700	-0.21223200
O	3.41358100	1.33568600	0.01546200
H	1.65245100	0.49849700	-1.26737800
C	4.50679700	-0.71407300	0.01932800
C	5.32921500	-1.69918500	-0.79756300
H	6.39819500	-1.47008500	-0.72910500
H	5.17723100	-2.71526700	-0.41961800
H	5.02989300	-1.68440200	-1.84711100
C	4.78448500	-0.89986000	1.51253200
H	5.84767200	-0.78892200	1.74725000
H	4.21879100	-0.17028300	2.10063200
H	4.47688800	-1.90525000	1.81680600
C	4.65841300	0.78074100	-0.40830000
C	4.77043700	0.93309100	-1.92674900

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H	4.64307200	1.98875700	-2.18243100
H	5.74385100	0.60031000	-2.29989700
H	3.98680000	0.36224500	-2.43426300
C	5.78997400	1.53058300	0.27822800
H	5.63670500	1.57337100	1.35834800
H	6.75616300	1.05620000	0.07561100
H	5.83037800	2.55703800	-0.09766400
TS2S'			
P	-1.73696600	-0.26865900	-0.03761200
C	-2.38563300	-1.80875100	-0.77202900
C	-2.37179200	-0.18988400	1.68386900
C	-3.90310300	-1.86804800	-0.94985800
H	-1.87552000	-1.91057100	-1.73659500
H	-2.03626000	-2.63816500	-0.14624100
C	-2.51767600	1.11769600	-0.95340500
C	0.01072100	-0.37601100	-0.16881600
C	-1.65964300	-1.18269700	2.60326500
H	-2.22051100	0.83553600	2.03835800
H	-3.45461600	-0.36560100	1.66657800
C	-4.34758300	-3.21070200	-1.53143200
H	-4.23311800	-1.06303800	-1.61831800
H	-4.40945500	-1.70865400	0.01120900
C	-3.84888100	1.63418000	-0.40017900
H	-2.62493300	0.75902800	-1.98520600
H	-1.79362600	1.93514000	-0.98308900
N	0.51290300	-1.64677300	-0.57964700
C	0.91926000	0.64225200	0.16162200
C	-2.16501900	-1.10415100	4.04320400
H	-1.79691800	-2.20568000	2.22615800
H	-0.58002800	-0.98362700	2.57989300

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C	-5.85756500	-3.28315700	-1.73158200
H	-4.02130700	-4.01753600	-0.86385000
H	-3.83648200	-3.37297700	-2.48791300
C	-4.42337000	2.73807700	-1.28805800
H	-4.58192000	0.82307300	-0.30721100
H	-3.69219500	2.03497200	0.60868500
C	0.92912700	-2.65694800	0.38430900
C	1.23984300	-1.74447500	-1.74524600
C	0.43056400	2.04877400	0.25964900
C	-1.44870600	-2.08956800	4.96063900
H	-3.24509300	-1.29584700	4.06056000
H	-2.02483300	-0.08162400	4.41519300
H	-6.38699200	-3.14891300	-0.78272500
H	-6.20054600	-2.50227800	-2.41782600
H	-6.15794100	-4.24833800	-2.14766400
C	-5.73160400	3.30003400	-0.74197900
H	-4.58077800	2.34259800	-2.29914200
H	-3.68074100	3.54019500	-1.37933400
C	1.91980200	-3.49654100	-0.44044300
H	1.41853900	-2.18926800	1.24268400
H	0.07218200	-3.24697600	0.73110000
O	1.98421500	-2.87509300	-1.72573400
O	1.21702200	-0.99450200	-2.69071900
C	0.54709800	2.85409900	-0.88080100
C	-0.16960200	2.57646900	1.40358700
H	-0.37142000	-1.89669900	4.97615200
H	-1.59768200	-3.12015000	4.62229300
H	-1.81674300	-2.01877300	5.98762200
H	-5.58841600	3.72756400	0.25562300
H	-6.12795100	4.08737800	-1.38868400

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H	-6.49362400	2.51777000	-0.66278100
H	1.58933900	-4.52887900	-0.57777800
H	2.91959100	-3.48419800	-0.00267700
C	0.02916200	4.14375700	-0.88740600
H	1.02964300	2.44209600	-1.76288700
C	-0.68749800	3.87319300	1.39876300
H	-0.21756200	1.96676800	2.30287200
C	-0.59973000	4.65370700	0.25084200
H	0.11843000	4.75664600	-1.77908200
H	-1.15317400	4.27203600	2.29494100
H	-1.00403800	5.66111000	0.24430000
B	2.43319800	0.44082000	0.37054700
O	3.37721700	1.49841700	0.30534100
O	3.08133400	-0.80399000	0.13301400
H	1.66785000	0.49153900	1.55199100
C	4.54027000	0.94811400	-0.31719000
C	5.76564400	1.71413000	0.15548100
H	6.68529200	1.25360100	-0.22119100
H	5.72333300	2.74158900	-0.21745900
H	5.81035500	1.75209300	1.24588400
C	4.37015500	1.08505100	-1.83215700
H	5.26097600	0.75732100	-2.37722100
H	3.51124700	0.50015500	-2.17969700
H	4.18905800	2.13763300	-2.06839400
C	4.48804200	-0.54396500	0.13625500
C	5.00248200	-0.73276200	1.56302500
H	4.73099500	-1.73593700	1.90583700
H	6.09059200	-0.63196100	1.62246900
H	4.54358200	-0.00381200	2.23799400
C	5.16654900	-1.51916700	-0.81393600

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H	4.65023000	-1.54692900	-1.77552500
H	6.21406700	-1.24243700	-0.97559700
H	5.15109600	-2.52867500	-0.39052100
MSR			
P	-1.36627200	-0.36404300	-0.18897500
C	-2.68804100	-1.62713600	-0.26456500
C	-1.95320500	0.92362800	0.98106300
C	-4.08822300	-1.05781900	-0.50049200
H	-2.41010800	-2.30015700	-1.08251700
H	-2.64806600	-2.20169600	0.66743300
C	-1.40892300	0.45767600	-1.85692700
C	0.05975000	-1.15938100	0.42147700
C	-2.32323100	0.42671400	2.37770400
H	-1.18141000	1.69934900	1.02988000
H	-2.82528400	1.39023100	0.50858800
C	-5.13951500	-2.16242700	-0.61022000
H	-4.09750700	-0.46224700	-1.42292700
H	-4.36701800	-0.37790400	0.31571700
C	-2.12387800	1.80453200	-1.95881000
H	-1.82973400	-0.27664500	-2.55056700
H	-0.36155800	0.58789100	-2.13827500
N	0.24949000	-2.49808800	-0.09172200
C	1.39293300	-0.44577300	0.71032700
C	-2.97821000	1.52812500	3.21179000
H	-3.01747900	-0.42246300	2.30227200
H	-1.43592500	0.05074700	2.89456200
C	-6.54066400	-1.60919200	-0.84780800
H	-5.12713400	-2.76175000	0.30860500
H	-4.86315600	-2.84013700	-1.42673900
C	-1.97609500	2.41903600	-3.35053500



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H	-3.19189400	1.69977800	-1.72411600
H	-1.70424300	2.49943100	-1.22195900
C	0.84698100	-3.54845900	0.72438900
C	0.19434800	-2.87569000	-1.39760700
C	2.53345600	-0.89873500	-0.20389900
C	-3.33568300	1.05247400	4.61614200
H	-3.88015300	1.88722000	2.69948100
H	-2.29618000	2.38572200	3.27446900
H	-6.84721700	-0.94975300	-0.02928000
H	-6.58087600	-1.02899700	-1.77532800
H	-7.27905600	-2.41183000	-0.92423900
C	-2.67148700	3.77204200	-3.46319800
H	-2.37925000	1.72763200	-4.10059300
H	-0.90751600	2.52823400	-3.57825000
C	1.46291600	-4.43434600	-0.35859500
H	1.60101300	-3.14387100	1.40626200
H	0.08149600	-4.07016400	1.31407300
O	0.71856400	-4.11880500	-1.54474700
O	-0.30679400	-2.26655200	-2.32392500
C	3.68783200	-1.46805000	0.34376400
C	2.44312600	-0.77666100	-1.59542800
H	-2.44396000	0.71130500	5.15126800
H	-4.04030400	0.21516800	4.57825700
H	-3.79695000	1.85018900	5.20484000
H	-2.27205300	4.48108700	-2.72958200
H	-2.54161100	4.20982900	-4.45674300
H	-3.74643700	3.67716500	-3.27780300
H	1.36618600	-5.50266100	-0.16474700
H	2.51445000	-4.17996200	-0.53024400
C	4.72913400	-1.89650500	-0.47841100

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H	3.74437700	-1.60623900	1.42102600
C	3.47870500	-1.21113200	-2.41754800
H	1.53446300	-0.37484100	-2.03480700
C	4.62938700	-1.76785100	-1.86158200
H	5.61569100	-2.34067700	-0.03529700
H	3.38265600	-1.12123800	-3.49530500
H	5.43627400	-2.10868700	-2.50290900
B	1.47209700	1.12107500	0.59554500
O	0.81429800	1.86847900	-0.35814900
O	2.31804600	1.87834500	1.36294400
C	1.49492200	3.14637000	-0.42799900
C	0.49043700	4.22949900	-0.77973500
H	0.96581300	5.21523900	-0.75107800
H	0.11382200	4.06582200	-1.79426300
H	-0.35872900	4.23161900	-0.09216800
C	2.54935100	3.01515500	-1.52364600
H	3.07739700	3.95879800	-1.68653400
H	3.28037600	2.23892800	-1.27670200
H	2.05524800	2.72846700	-2.45630000
C	2.11542800	3.26318000	1.00207200
C	1.14950600	3.85320000	2.02605200
H	1.56801300	3.71520700	3.02609400
H	0.99117700	4.92240500	1.85999900
H	0.17925900	3.34713600	1.99293100
C	3.45027700	3.98715700	1.05560400
H	4.20428500	3.47736000	0.45367200
H	3.34478400	5.01539800	0.69511600
H	3.80590900	4.02365400	2.08867900
O	-0.07957000	-1.83950100	3.16543700
H	1.64899800	-2.17267600	3.47362300

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H	-0.71147600	-2.55042800	3.32126300
O	2.62157100	-2.26818200	3.52742700
H	2.92630300	-1.38697200	3.77015200
H	-0.20850200	-1.57341700	2.19972600
H	1.72302900	-0.70178200	1.72806900
TS3R			
P	-1.38883800	-0.31360900	-0.20306400
C	-2.72254800	-1.55107500	-0.30768300
C	-1.91624400	0.91902000	1.04617300
C	-4.07875300	-0.95996400	-0.70263100
H	-2.40030600	-2.29171100	-1.04631000
H	-2.77152800	-2.05016000	0.66728100
C	-1.31080700	0.52372100	-1.84170600
C	0.04096300	-1.18012400	0.47809000
C	-2.51015300	0.33359400	2.33160300
H	-1.03758800	1.53359100	1.27121400
H	-2.63907400	1.58316700	0.56060100
C	-5.18352700	-2.01631100	-0.67389500
H	-4.01395600	-0.53306900	-1.71176400
H	-4.35227800	-0.13681400	-0.02923800
C	-2.01805100	1.87507800	-1.92863200
H	-1.71425200	-0.19328200	-2.56145800
H	-0.25225300	0.64523600	-2.07562900
N	0.21467400	-2.49745400	-0.09953300
C	1.39782800	-0.45186800	0.72194500
C	-2.83709600	1.43807800	3.33732000
H	-3.43205900	-0.21554200	2.09575900
H	-1.80686600	-0.37831600	2.78211200
C	-6.53511500	-1.45241800	-1.09874500
H	-5.25445400	-2.43069000	0.33927300

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H	-4.90233400	-2.84732800	-1.33178400
C	-1.85525500	2.50086600	-3.31322200
H	-3.08794800	1.76854200	-1.70351900
H	-1.59878400	2.55659200	-1.18006300
C	0.76788200	-3.59634600	0.68827000
C	0.21384000	-2.79313600	-1.42564200
C	2.53176000	-0.95964300	-0.16268900
C	-3.44238800	0.87634700	4.61975400
H	-3.52533300	2.16458800	2.88536300
H	-1.91705400	1.98615800	3.57669300
H	-6.84471300	-0.63507100	-0.43937800
H	-6.49313300	-1.05959100	-2.11968100
H	-7.31361600	-2.21921300	-1.06787900
C	-2.55320400	3.85286200	-3.41970600
H	-2.24940400	1.81570000	-4.07357300
H	-0.78453300	2.61438600	-3.52779500
C	1.40420400	-4.43761800	-0.42075400
H	1.49606500	-3.23599000	1.41971600
H	-0.02830600	-4.13062400	1.21914700
O	0.73523900	-4.02303700	-1.62578600
O	-0.24117200	-2.11414900	-2.32716500
C	3.59729400	-1.65718900	0.41798800
C	2.53677900	-0.75467100	-1.54705500
H	-2.75663600	0.16508200	5.09016500
H	-4.37968900	0.34915400	4.41311400
H	-3.65711800	1.66823700	5.34271300
H	-2.16532800	4.55570300	-2.67428000
H	-2.41169400	4.30022800	-4.40717200
H	-3.63001200	3.75246500	-3.24929800
H	1.25383600	-5.51026900	-0.29939100

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H	2.47140300	-4.21971400	-0.53027200
C	4.64280000	-2.13612400	-0.36953800
H	3.57321700	-1.84555400	1.48967800
C	3.57602300	-1.24302600	-2.33496900
H	1.70583900	-0.23334500	-2.01437500
C	4.63504400	-1.93198500	-1.74784600
H	5.46148600	-2.67727100	0.09567100
H	3.55544000	-1.08728900	-3.40918700
H	5.44581700	-2.31165900	-2.36186200
B	1.50610900	1.11430300	0.61304700
O	0.84419900	1.89225200	-0.31362600
O	2.38429100	1.83877300	1.37277800
C	1.54767000	3.16053900	-0.37059500
C	0.55869300	4.27011900	-0.68042100
H	1.05353900	5.24532300	-0.63089000
H	0.16710100	4.14263400	-1.69457600
H	-0.28118600	4.26967300	0.01833500
C	2.57961100	3.03359100	-1.48770500
H	3.12330500	3.97046400	-1.63714900
H	3.29961900	2.23821100	-1.27138400
H	2.06469100	2.78100300	-2.41906400
C	2.19642500	3.23486800	1.04895800
C	1.25838200	3.81426700	2.10424900
H	1.69123300	3.64277600	3.09281800
H	1.11664600	4.89004200	1.96831800
H	0.27850500	3.32696500	2.07543900
C	3.54291600	3.93717800	1.09391500
H	4.27776000	3.43077400	0.46604500
H	3.44638300	4.97528000	0.76017300
H	3.91779200	3.94319600	2.12068500

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O	-0.25962300	-1.81905100	3.00003000
H	1.21081300	-2.17550900	3.32729900
H	-0.79643600	-2.61494200	3.09850100
O	2.20660500	-2.37250600	3.43349400
H	2.54740700	-1.61156800	3.91493700
H	-0.28686600	-1.44596900	1.65889800
H	1.67997900	-0.71990200	1.74768400
M6R			
P	1.41763300	0.26142300	-0.22035700
C	2.77181400	1.47277400	-0.33983000
C	1.90686400	-0.95135700	1.05990300
C	4.12145100	0.84435200	-0.69809800
H	2.47178400	2.19627600	-1.10437600
H	2.81576800	1.99915100	0.62106000
C	1.29623600	-0.59227800	-1.84220800
C	-0.00526000	1.17785500	0.46531000
C	2.46038800	-0.33308400	2.34865500
H	1.02062900	-1.56063100	1.26989200
H	2.64281000	-1.62337700	0.60523800
C	5.23642700	1.88973400	-0.73396000
H	4.05214100	0.35754500	-1.67960000
H	4.38546800	0.06127000	0.02479400
C	1.96647700	-1.96429200	-1.90269900
H	1.71673400	0.10100400	-2.57523300
H	0.23324400	-0.68667500	-2.06716200
N	-0.13018200	2.49765200	-0.11535300
C	-1.38696400	0.48821700	0.69666000
C	2.73450800	-1.40798700	3.40096700
H	3.39708300	0.19764700	2.12899200
H	1.74979200	0.39958500	2.75851100

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C	6.58345800	1.28589100	-1.11598400
H	5.30815100	2.36883800	0.25004700
H	4.96552200	2.67839100	-1.44597800
C	1.75993500	-2.62408200	-3.26524500
H	3.04278500	-1.87807700	-1.70072500
H	1.54422500	-2.61296300	-1.12730600
C	-0.64790200	3.61643700	0.66877100
C	-0.13264000	2.77485700	-1.44488500
C	-2.49454700	1.02485300	-0.20340600
C	3.26947400	-0.80121000	4.69412500
H	3.44389600	-2.14931400	3.00962600
H	1.80158400	-1.94659500	3.61008200
H	6.88312100	0.51068700	-0.40338500
H	6.54088200	0.82763200	-2.10925700
H	7.36917500	2.04568000	-1.13247500
C	2.43336200	-3.98987200	-3.35032000
H	2.14601500	-1.96694900	-4.05388700
H	0.68232600	-2.72561900	-3.44957000
C	-1.25110400	4.47573500	-0.44701200
H	-1.38849400	3.28264500	1.40073900
H	0.16654600	4.12123100	1.19945000
O	-0.61614300	4.01581800	-1.65585700
O	0.29176400	2.06536300	-2.33814400
C	-3.52517200	1.78617000	0.36060800
C	-2.51313200	0.78062100	-1.58112200
H	2.55933900	-0.07166400	5.09534200
H	4.21884100	-0.28335700	4.52153000
H	3.43986400	-1.56584000	5.45713800
H	2.05517600	-4.66443600	-2.57445100
H	2.25803900	-4.46294000	-4.32016800

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H	3.51581300	-3.90218800	-3.21192100
H	-1.04488300	5.54049300	-0.33959200
H	-2.32852300	4.31195300	-0.54657400
C	-4.54905200	2.29062400	-0.43923600
H	-3.48766800	2.00018800	1.42748800
C	-3.53017500	1.29565800	-2.38118900
H	-1.71181100	0.20415900	-2.03515900
C	-4.55400800	2.04901100	-1.81157000
H	-5.34148500	2.88073100	0.01175100
H	-3.52040900	1.10875600	-3.45053600
H	-5.34809700	2.44862000	-2.43468200
B	-1.53466500	-1.07599400	0.61027100
O	-0.87658500	-1.88645900	-0.29147800
O	-2.44403200	-1.76377200	1.36597500
C	-1.61001700	-3.13900300	-0.33597500
C	-0.64442100	-4.27800400	-0.61031300
H	-1.16346600	-5.23967500	-0.54580700
H	-0.23879600	-4.18189000	-1.62245400
H	0.18705300	-4.28294300	0.09843900
C	-2.62240300	-3.00826000	-1.47029600
H	-3.18577300	-3.93491700	-1.61025100
H	-3.32666700	-2.19264500	-1.27877800
H	-2.08860700	-2.78585600	-2.39881300
C	-2.28070700	-3.17013800	1.07446300
C	-1.36908200	-3.74543000	2.15474500
H	-1.81104600	-3.54369900	3.13346200
H	-1.24766700	-4.82652300	2.04356100
H	-0.37923000	-3.27832700	2.12872800
C	-3.64181800	-3.84370100	1.11413500
H	-4.35674900	-3.33633800	0.46445000



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H	-3.56182500	-4.89068000	0.80458100
H	-4.03163700	-3.81946600	2.13502200
O	0.26634700	1.82249400	3.09399300
H	-1.13072600	2.20359700	3.29216400
H	0.80308000	2.61233700	3.23234400
O	-2.15013900	2.44397300	3.32928700
H	-2.54056900	1.74536600	3.86440500
H	0.33603800	1.39737500	1.55351900
H	-1.66034400	0.78361200	1.71709000
TS4R			
P	-1.37991000	0.34215400	-0.28611300
C	-3.11109300	-0.23644400	-0.30707100
C	-1.40535900	1.91123000	0.64049500
C	-4.10604400	0.78307700	-0.87048900
H	-3.13733000	-1.15917400	-0.89033800
H	-3.35932600	-0.48864100	0.73134300
C	-0.75233400	0.61292400	-1.97153300
C	-0.28475200	-0.83130600	0.68762400
C	-2.07611900	1.76728900	2.01508100
H	-0.35861600	2.20553100	0.75663400
H	-1.90780000	2.66859100	0.02866600
C	-5.54455400	0.27813100	-0.75133000
H	-3.87899500	0.97462500	-1.92655900
H	-4.01893700	1.74274000	-0.34568400
C	-1.01027900	1.99918300	-2.56589000
H	-1.16569900	-0.19443300	-2.58504400
H	0.32609200	0.42904900	-1.90493400
N	-0.95252400	-2.11246900	0.79273400
C	1.20920300	-0.93013400	0.31199100
C	-1.68909900	2.91234200	2.95021400

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H	-3.16732000	1.73211200	1.89606200
H	-1.76509200	0.83762700	2.50779100
C	-6.55298500	1.26501300	-1.32969700
H	-5.77024900	0.09106000	0.30576300
H	-5.63033200	-0.68709800	-1.26428500
C	-0.42773900	2.11365100	-3.97440800
H	-2.08465200	2.21801000	-2.59618300
H	-0.55163500	2.76284700	-1.92683400
C	-1.07381600	-2.86828700	2.03324600
C	-1.29214400	-2.85122200	-0.29682700
C	1.61299000	-2.07205900	-0.58031900
C	-2.26923100	2.71378900	4.34580400
H	-2.01460000	3.87139700	2.52684200
H	-0.59519900	2.94382200	3.01682900
H	-6.50024400	2.22897300	-0.81341000
H	-6.36135500	1.44472200	-2.39237900
H	-7.57536300	0.89027500	-1.23377400
C	-0.59112200	3.51504200	-4.55265400
H	-0.91175500	1.37750300	-4.62711200
H	0.63633700	1.84662000	-3.94381000
C	-1.31095200	-4.27996400	1.47272800
H	-0.15402700	-2.78592300	2.62018400
H	-1.92448800	-2.50341300	2.62120700
O	-1.65036600	-4.09415500	0.08807600
O	-1.34604200	-2.46471600	-1.44768300
C	1.68367900	-3.36660100	-0.04312200
C	1.95393300	-1.91280800	-1.92929400
H	-1.88220000	1.78349200	4.77242200
H	-3.36269300	2.65346900	4.31804300
H	-1.99678500	3.53538300	5.01409400

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H	-0.07549400	4.25569500	-3.93232200
H	-0.17871300	3.57970100	-5.56289200
H	-1.64708200	3.79963000	-4.60368400
H	-2.13575200	-4.80392800	1.95635400
H	-0.40896900	-4.89598300	1.52111500
C	2.01165400	-4.46404200	-0.83512600
H	1.50731800	-3.48370500	1.02442500
C	2.29986300	-3.00272000	-2.72231300
H	1.96335800	-0.91494700	-2.36043100
C	2.31145000	-4.28715900	-2.18323500
H	2.04832700	-5.45709600	-0.39556000
H	2.55647600	-2.85002300	-3.76666200
H	2.56816000	-5.13954000	-2.80478100
B	2.03778600	0.34907400	0.21021100
O	1.66997500	1.57573500	0.75328400
O	3.31224800	0.40434700	-0.32645800
C	2.68570000	2.53380800	0.39243100
C	2.83899700	3.54318400	1.51756400
H	3.68109800	4.21474000	1.32080700
H	1.93313200	4.15168500	1.59581900
H	2.99848700	3.04646200	2.47605100
C	2.21752500	3.22654600	-0.88648600
H	2.91677000	4.00496800	-1.20491900
H	2.10578700	2.50369300	-1.70260500
H	1.24661700	3.69662500	-0.70128800
C	3.92324900	1.61421700	0.15885100
C	4.64156600	1.26401300	1.46101500
H	5.35159300	0.45703800	1.26314600
H	5.19056300	2.11963900	1.86469900
H	3.92977800	0.91462800	2.21589400

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C	4.91151100	2.12230500	-0.87700700
H	4.44298600	2.22597300	-1.85762400
H	5.32266600	3.09167200	-0.57686600
H	5.73996800	1.41508000	-0.96985300
O	-0.24995700	-0.27054200	3.86985000
H	0.58187800	-0.76670300	3.52849400
H	-0.67602600	-0.90477900	4.45540300
O	1.60773600	-1.64403200	2.81750400
H	2.50946100	-1.61199900	3.15580200
H	-0.33775000	-0.39351400	1.69359300
H	1.58407600	-1.25567900	1.49581900
<b>M7R</b>			
P	-1.69150200	0.08685700	-0.16774800
C	-3.24186900	0.67630300	0.60915200
C	-1.14967600	1.45311700	-1.25063100
C	-4.21599100	1.34324800	-0.36767600
H	-3.69883600	-0.19504100	1.08256700
H	-2.95497400	1.36784900	1.41106200
C	-2.03168200	-1.34748000	-1.24470000
C	-0.25563000	-0.13905400	0.99575800
C	-0.98485200	2.80627700	-0.54927500
H	-0.20351200	1.14268500	-1.70532300
H	-1.89507700	1.51813900	-2.05334100
C	-5.53830500	1.69562000	0.31466500
H	-4.41648400	0.67194400	-1.21335900
H	-3.77498000	2.25499400	-0.78943000
C	-1.15264200	-1.41794500	-2.50222500
H	-3.09501500	-1.29568800	-1.50885900
H	-1.90101900	-2.23222900	-0.61779700
N	-0.63764900	-0.71763400	2.29928300

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C	0.95778000	-0.66943000	0.29255200
C	-0.87239100	3.94649500	-1.56171000
H	-1.83316300	3.00986800	0.11766100
H	-0.08211200	2.77877100	0.07217500
C	-6.51979500	2.36726100	-0.63986200
H	-5.33612400	2.35602600	1.16685500
H	-5.98385000	0.78287900	0.72729300
C	-1.14610100	-2.82374700	-3.09827300
H	-1.51114300	-0.69470900	-3.24587700
H	-0.12104300	-1.14628700	-2.25732800
C	0.40329800	-0.84854800	3.30989800
C	-1.62612500	-1.62006000	2.52903500
C	1.08925900	-2.06194200	-0.12701500
C	-0.66227100	5.29715700	-0.88562600
H	-1.78212800	3.97669600	-2.17514200
H	-0.04297300	3.73714600	-2.24864300
H	-6.10415500	3.29677300	-1.04212500
H	-6.75405300	1.71334400	-1.48600200
H	-7.45920100	2.61166400	-0.13710300
C	-0.26898300	-2.90851300	-4.34213300
H	-2.17270800	-3.13265100	-3.33493000
H	-0.76719500	-3.51734200	-2.33817800
C	-0.40439600	-1.48847400	4.43785000
H	1.21027100	-1.49128200	2.94005700
H	0.81890500	0.12470000	3.58214700
O	-1.48744600	-2.15007300	3.76461600
O	-2.52449800	-1.95040200	1.77730500
C	0.32194700	-3.13624200	0.38438800
C	2.03818100	-2.42469100	-1.12080400
H	0.24603000	5.29482500	-0.27343500

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H	-1.50220300	5.53962600	-0.22630000
H	-0.56942700	6.10215600	-1.61947700
H	0.75929200	-2.62020000	-4.10096300
H	-0.24496600	-3.92553800	-4.74324500
H	-0.63124400	-2.24310800	-5.13349400
H	-0.82575100	-0.73907700	5.11463000
H	0.15051500	-2.23201800	5.00905100
C	0.49776700	-4.45180800	-0.04144000
H	-0.44010500	-2.95899700	1.13114700
C	2.21257900	-3.73536700	-1.54032500
H	2.64432900	-1.64238100	-1.56443200
C	1.44591800	-4.77419000	-1.00618400
H	-0.12190600	-5.23071900	0.39583800
H	2.95428300	-3.94870700	-2.30637900
H	1.58300700	-5.79844000	-1.33723300
B	2.07071100	0.32688500	0.18076500
O	1.97145100	1.64353800	0.69338500
O	3.34176800	0.14193100	-0.37935700
C	3.11858400	2.37240700	0.24213600
C	3.49041400	3.41190200	1.28751200
H	4.41847600	3.92559800	1.01589800
H	2.69671800	4.16219700	1.35911000
H	3.61530200	2.95675800	2.27187100
C	2.75084000	3.05541500	-1.07538600
H	3.57213800	3.66618800	-1.46197700
H	2.48115100	2.31183300	-1.83285800
H	1.88993100	3.70982600	-0.90889400
C	4.16546600	1.23480300	0.04260200
C	4.83620800	0.82785600	1.35478200
H	5.37916200	-0.10740300	1.19599300

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H	5.54302900	1.58618100	1.70490900
H	4.08701800	0.65757200	2.13455100
C	5.21501000	1.50710100	-1.02344400
H	4.75715500	1.64083100	-2.00548900
H	5.79684200	2.40218700	-0.77928700
H	5.90421200	0.66013000	-1.08382600
H	-0.04537000	0.91382200	1.22601600
TS5R			
P	-1.71969200	0.09653400	-0.14269500
C	-3.57129400	0.04770600	-0.12186200
C	-1.31786100	1.88803800	-0.19728600
C	-4.26762400	0.93223000	-1.15875400
H	-3.83304500	-1.00610600	-0.26170000
H	-3.89353400	0.31902200	0.89101200
C	-1.22843200	-0.62768200	-1.76589800
C	-0.13210100	-0.57697600	1.27416600
C	-1.85417700	2.61669500	1.04032800
H	-0.22338100	1.94514300	-0.21083700
H	-1.68818100	2.35975700	-1.11416200
C	-5.78389500	0.73048600	-1.16312400
H	-3.87352600	0.71816700	-2.16135100
H	-4.04676500	1.98875400	-0.95940600
C	-0.21718100	0.17952300	-2.58151300
H	-2.14261000	-0.79529800	-2.34779400
H	-0.81985300	-1.61526400	-1.52803900
N	-0.84390100	-1.54736900	2.07407000
C	1.05924000	-0.86278800	0.56672100
C	-1.19123100	3.97838100	1.23996800
H	-2.94231500	2.74090600	0.95796400
H	-1.68548500	2.01063000	1.94215300

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C	-6.48649000	1.62035800	-2.18357100
H	-6.17622100	0.93469800	-0.15910000
H	-6.00462900	-0.32291400	-1.37338900
C	0.17936200	-0.53255800	-3.87377700
H	-0.62143000	1.17096100	-2.82434100
H	0.68360300	0.34703000	-1.97717100
C	-0.31831800	-1.90292400	3.38310300
C	-1.63700400	-2.54249000	1.57889200
C	1.36732200	-2.16106100	-0.07581400
C	-1.77307100	4.74917600	2.41999300
H	-1.29280300	4.56970400	0.32069600
H	-0.11724800	3.81254400	1.39184800
H	-6.30206800	2.67925000	-1.97474500
H	-6.12655300	1.41423500	-3.19680400
H	-7.56837400	1.46184300	-2.17526800
C	1.28155800	0.21307400	-4.61918600
H	-0.70367000	-0.64045900	-4.51639900
H	0.51550300	-1.54748900	-3.63036800
C	-1.31679500	-2.98965900	3.79083900
H	0.71057700	-2.27559200	3.30283600
H	-0.33100400	-1.04676700	4.06203400
O	-1.86451900	-3.45967000	2.55223700
O	-2.10813500	-2.64628700	0.46832100
C	1.05085300	-3.41704800	0.47913100
C	2.05153500	-2.18612400	-1.31032900
H	-1.66486400	4.18121100	3.34982500
H	-2.84010700	4.94599600	2.27326700
H	-1.27191500	5.71137300	2.55690200
H	2.18255400	0.29346000	-4.00014900
H	1.55821900	-0.29655700	-5.54633100



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H	0.96608800	1.22984200	-4.87731700
H	-2.13096500	-2.58438300	4.39882500
H	-0.85692300	-3.83202500	4.30732700
C	1.35694500	-4.60910900	-0.17156100
H	0.58165900	-3.48431300	1.45354100
C	2.36859200	-3.37507400	-1.95582200
H	2.34011600	-1.24448300	-1.76570000
C	2.01431900	-4.60170800	-1.39711700
H	1.08532100	-5.55146800	0.29543700
H	2.89119400	-3.33989000	-2.90806700
H	2.25398800	-5.53169800	-1.90272500
B	2.01257600	0.31779400	0.42522700
O	1.78820300	1.57520700	1.00004000
O	3.22766400	0.29994300	-0.24739200
C	2.80216600	2.46656400	0.49945000
C	3.15083200	3.48136800	1.57612200
H	3.99896800	4.09944900	1.26366300
H	2.29855700	4.14419900	1.75297700
H	3.40183700	2.99043300	2.51807100
C	2.23738900	3.17419500	-0.73201700
H	2.95037800	3.89565200	-1.14156800
H	1.98249400	2.45276900	-1.51613200
H	1.32784100	3.71419100	-0.45347500
C	3.95374900	1.47855300	0.13651600
C	4.81241400	1.11026700	1.34560000
H	5.44802800	0.26188700	1.07967400
H	5.45259900	1.94109500	1.65625400
H	4.18595800	0.81351000	2.19232600
C	4.83402500	1.91513300	-1.02324800
H	4.25520700	2.02285800	-1.94273300

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H	5.32629200	2.86769900	-0.80148600
H	5.60942300	1.16388900	-1.19619800
H	-0.10379600	0.37432500	1.80658200
<b>(Z)-<math>\beta</math>-product</b>			
C	1.07337800	-1.04318700	-0.09824900
N	2.44693600	-1.16791500	0.01702100
C	0.32016600	0.07831700	-0.07751500
C	3.41012200	-0.18095500	0.48634100
C	3.05128600	-2.40595800	-0.16092700
C	0.85003700	1.46393900	-0.13691500
C	4.54554500	-1.09922900	0.94884700
H	3.72129800	0.48597600	-0.32205000
H	2.99288600	0.41965200	1.29629300
O	4.33928300	-2.32462300	0.23310000
O	2.54101800	-3.40346800	-0.59569600
C	0.43279900	2.43180800	0.78694400
C	1.72881300	1.85389500	-1.15647500
H	4.48897400	-1.31123500	2.02039800
H	5.53544300	-0.71866600	0.70034600
C	0.91182600	3.73550500	0.71790000
H	-0.27442300	2.15063400	1.56183900
C	2.20679000	3.15994700	-1.22839500
H	2.02360700	1.12284100	-1.90545500
C	1.80496800	4.10378400	-0.28699800
H	0.58396800	4.46868500	1.44848800
H	2.88596000	3.44185200	-2.02729200
H	2.17509500	5.12261700	-0.34244100
B	-1.21333800	-0.15286900	-0.02947500
O	-2.14071500	0.85913600	-0.03890400
O	-1.78718800	-1.40182000	0.03656300

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C	-3.42222200	0.25760600	0.25441200
C	-4.50468100	1.00277100	-0.50737500
H	-5.47441200	0.51250200	-0.37449500
H	-4.58469800	2.02428300	-0.12607200
H	-4.27881600	1.05421300	-1.57381300
C	-3.63862500	0.39187400	1.75993300
H	-4.62196800	0.01949200	2.06030600
H	-2.87203300	-0.15609000	2.31654000
H	-3.57032300	1.44835000	2.03258100
C	-3.20237200	-1.22269500	-0.19642600
C	-3.43797000	-1.42637500	-1.69094200
H	-3.06250200	-2.41248200	-1.97567300
H	-4.50135600	-1.37435900	-1.94074400
H	-2.90284000	-0.67438000	-2.27870300
C	-3.97038700	-2.25637200	0.60916100
H	-3.69101200	-2.22973200	1.66382200
H	-5.04834200	-2.08517300	0.52484200
H	-3.75350300	-3.25631300	0.22407500
H	0.59113600	-2.01475800	-0.17499100
M5S			
P	-1.40298500	0.02636800	-0.23551300
C	-2.80562600	-1.14851900	-0.35613700
C	-1.82658900	1.02193000	1.26612000
C	-4.23141300	-0.60220900	-0.21220700
H	-2.67819000	-1.69326500	-1.29613400
H	-2.59465500	-1.87894200	0.43886200
C	-1.36961900	1.19683000	-1.63216400
C	0.08149500	-0.89539400	-0.31443000
C	-2.21597300	0.17615000	2.48599200
H	-0.93324300	1.61525500	1.47825700

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H	-2.63619000	1.71989200	1.01671600
C	-5.21722700	-1.70763000	0.16917800
H	-4.55258000	-0.15076200	-1.15666800
H	-4.28474800	0.19480300	0.53975600
C	-2.70146500	1.82624400	-2.04401200
H	-0.92545600	0.66582800	-2.48431700
H	-0.65834100	1.97638600	-1.32692200
N	0.28356900	-1.70236400	0.86204500
C	1.37461100	-0.26176400	-0.89368000
C	-2.18619500	0.99176000	3.77833600
H	-3.21927000	-0.24618700	2.34923900
H	-1.54352200	-0.68556200	2.58552100
C	-6.65467300	-1.20512600	0.24944600
H	-4.91745700	-2.13565000	1.13439700
H	-5.14521000	-2.52059900	-0.56331300
C	-2.48714200	2.96749800	-3.03870200
H	-3.33497900	1.06220800	-2.50891200
H	-3.25161000	2.20475100	-1.17194600
C	1.01434600	-1.24830800	2.04035600
C	0.27435900	-3.07492500	0.81792100
C	2.45945500	-1.33050500	-1.04080400
C	-2.61253500	0.17715100	4.99495800
H	-2.84097900	1.86531600	3.66701100
H	-1.17210900	1.38496800	3.92902600
H	-6.75042600	-0.40504100	0.99116800
H	-6.98525400	-0.80507900	-0.71454800
H	-7.34331100	-2.00601500	0.53198500
C	-3.79958800	3.57807600	-3.51814300
H	-1.91483900	2.58915500	-3.89454800
H	-1.86567400	3.74041600	-2.56852700

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C	0.92549700	-2.49121000	2.92264700
H	2.05195400	-0.99970600	1.78507000
H	0.54793300	-0.36620400	2.48844800
O	0.72733200	-3.56879400	2.00234100
O	-0.09585900	-3.80219700	-0.07457400
C	3.61114300	-1.34572200	-0.24751100
C	2.30394900	-2.35704800	-1.98013100
H	-1.95571100	-0.68727800	5.13884300
H	-3.63340300	-0.19993500	4.87684400
H	-2.58074400	0.77535100	5.90962100
H	-4.37669800	3.97921000	-2.67846700
H	-3.62646800	4.39450100	-4.22448900
H	-4.42042300	2.82859500	-4.01944300
H	0.06433500	-2.44805200	3.59960500
H	1.82932300	-2.68901200	3.49988800
C	4.56526100	-2.35507800	-0.37052400
H	3.78687600	-0.54285500	0.46367100
C	3.25307000	-3.36481900	-2.10918100
H	1.42485900	-2.35740500	-2.61462700
C	4.38745900	-3.37336500	-1.29967200
H	5.44936400	-2.33879000	0.26005700
H	3.10622300	-4.14833800	-2.84665800
H	5.12666700	-4.16237400	-1.39812300
B	1.89457600	1.06668500	-0.21543400
O	3.07516600	1.69869600	-0.52345500
O	1.15930100	1.78518700	0.70618900
H	1.13497700	0.04700600	-1.92623400
C	3.25318400	2.77974700	0.41680000
C	3.96369300	3.92983400	-0.27589600
H	4.03156500	4.79658600	0.38942100

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H	4.97890200	3.62468300	-0.54257200
H	3.44740400	4.22613900	-1.19056500
C	4.10670700	2.23839800	1.56169000
H	4.34815000	3.01903500	2.28859400
H	3.59320200	1.42409100	2.08407100
H	5.04072600	1.84679300	1.15032000
C	1.78396800	3.08064300	0.85176300
C	1.06601000	4.03008400	-0.10437600
H	-0.00219000	4.03409000	0.13403100
H	1.44172900	5.05290100	-0.01200700
H	1.18694500	3.70667500	-1.14329500
C	1.61986400	3.54759700	2.28827700
H	1.97172100	2.79436300	2.99607200
H	2.17448300	4.47604000	2.45737700
H	0.56355800	3.74442200	2.49461600
O	0.12047500	-0.54563100	-4.06310100
H	-0.26035100	-1.35553500	-3.66503300
H	-0.21132200	-0.52447700	-4.96643300
O	-0.91693100	-2.50673200	-2.50560400
H	-0.56365500	-2.00555700	-1.70514600
H	-0.70703100	-3.41538800	-2.25385200
TS3S			
P	-1.43341300	0.03687700	-0.24403100
C	-2.79230400	-1.15175800	-0.50180300
C	-1.79073200	0.81849300	1.37929800
C	-4.22530300	-0.62966900	-0.34932700
H	-2.59892400	-1.59441900	-1.48578700
H	-2.58977700	-1.94354700	0.23407300
C	-1.38164800	1.33510900	-1.51454400
C	0.08881900	-0.93055700	-0.43130600

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C	-2.22091900	-0.16196200	2.47923200
H	-0.88568000	1.35882600	1.66571200
H	-2.57779900	1.56528300	1.21262900
C	-5.20852600	-1.77596100	-0.10808300
H	-4.52172500	-0.09239900	-1.25590700
H	-4.31095600	0.09062100	0.47514100
C	-2.69767900	2.04442300	-1.83965900
H	-0.95590200	0.87402900	-2.41828000
H	-0.64164800	2.05614900	-1.14192100
N	0.28281600	-1.77403800	0.72498000
C	1.37818600	-0.20907800	-0.92146300
C	-2.19843200	0.49952700	3.85691500
H	-3.23023500	-0.53915400	2.27518000
H	-1.56800600	-1.04347700	2.48697100
C	-6.65331400	-1.29592600	-0.02463900
H	-4.93312000	-2.29406400	0.81945200
H	-5.10362200	-2.51149300	-0.91436300
C	-2.45262100	3.27293500	-2.71646100
H	-3.36089300	1.35297600	-2.37070000
H	-3.22342500	2.35040100	-0.92478400
C	1.01886200	-1.36796400	1.91248700
C	0.27639200	-3.14707900	0.60998900
C	2.47547600	-1.25203100	-1.14621700
C	-2.67454400	-0.43862300	4.96079700
H	-2.82721200	1.39853000	3.83547400
H	-1.17792300	0.84299000	4.07259700
H	-6.78154700	-0.57332600	0.78832800
H	-6.95878700	-0.80657800	-0.95506400
H	-7.34034800	-2.12693900	0.15625100
C	-3.74758800	3.97311400	-3.11356000

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H	-1.90230400	2.96350500	-3.61319200
H	-1.79970500	3.97278700	-2.17934900
C	0.94885700	-2.65632400	2.73314200
H	2.05191100	-1.09659600	1.66320200
H	0.54904100	-0.51726400	2.41511600
O	0.74265000	-3.68992900	1.76744500
O	-0.09776700	-3.81733200	-0.31810100
C	3.63784400	-1.30389000	-0.37040100
C	2.31431200	-2.21161600	-2.15354300
H	-2.04797500	-1.33517000	5.01273900
H	-3.70377200	-0.76493000	4.78125700
H	-2.64348900	0.04718300	5.93963600
H	-4.30246100	4.30532600	-2.22990100
H	-3.55183700	4.85133300	-3.73460900
H	-4.39858100	3.30089200	-3.68150500
H	0.09916900	-2.64927400	3.42548500
H	1.86365200	-2.87256200	3.28563300
C	4.60529400	-2.28509900	-0.58227500
H	3.81280100	-0.55294100	0.39543000
C	3.27777700	-3.19126800	-2.36724200
H	1.41538300	-2.17886600	-2.76055000
C	4.42739900	-3.23564500	-1.58095200
H	5.49996200	-2.29947200	0.03320600
H	3.12964800	-3.92444400	-3.15438800
H	5.17814200	-4.00177500	-1.74864400
B	1.86577200	1.06663400	-0.13549100
O	3.04126200	1.72811900	-0.38168000
O	1.11574000	1.69954800	0.83502900
H	1.13124400	0.17354600	-1.92766400
C	3.20533600	2.72893600	0.64689700



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C	3.91259800	3.93567800	0.05547600
H	3.97296700	4.74502400	0.79005000
H	4.93043300	3.65784600	-0.22998600
H	3.39915600	4.30304600	-0.83458500
C	4.05411700	2.09805600	1.74838800
H	4.28264900	2.81503400	2.54185300
H	3.54321900	1.23771300	2.19441600
H	4.99481000	1.75075300	1.31333500
C	1.73136900	2.98459500	1.09515600
C	1.01294000	4.00697600	0.21884300
H	-0.05619700	3.98640300	0.45260000
H	1.38334200	5.01970700	0.39995100
H	1.14069400	3.77385600	-0.84321800
C	1.55509900	3.32430300	2.56537300
H	1.90487000	2.51344100	3.20752600
H	2.10622100	4.23549200	2.81817600
H	0.49705900	3.50106800	2.78067900
O	0.24050700	-0.05224100	-4.02405900
H	-0.19316000	-0.86872400	-3.59906100
H	-0.23024800	0.08529200	-4.85204500
O	-0.85466900	-1.89918700	-2.67512100
H	-0.33542200	-1.57876600	-1.48254100
H	-0.70525600	-2.84893400	-2.74220600
M6S			
P	-1.39595200	-0.13751700	-0.44650900
C	-2.71207100	-1.23929900	-1.04788500
C	-1.85898500	0.27787300	1.28565300
C	-4.09728000	-0.58975600	-1.03927700
H	-2.38444600	-1.49702100	-2.05878800
H	-2.68219600	-2.15039300	-0.44069200

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C	-1.40460300	1.41643900	-1.41000100
C	0.20119400	-1.12191100	-0.46747700
C	-2.35183800	-0.86268300	2.18316700
H	-1.00886300	0.80548400	1.72887500
H	-2.66424200	1.01636600	1.19792500
C	-5.17308600	-1.55843300	-1.53146300
H	-4.09421100	0.30134200	-1.68092600
H	-4.35994000	-0.24885000	-0.02783200
C	-2.13694500	2.59518700	-0.77302300
H	-1.82178400	1.12949000	-2.37837200
H	-0.36545300	1.67787100	-1.62960200
N	0.39182200	-1.85916700	0.76188800
C	1.46702800	-0.35698700	-0.89981200
C	-2.80769100	-0.33527100	3.54451000
H	-3.18616000	-1.38974800	1.70433100
H	-1.57049000	-1.61111000	2.34676200
C	-6.55996200	-0.92480800	-1.55009800
H	-5.17605900	-2.44606000	-0.88724400
H	-4.90679800	-1.90575000	-2.53659700
C	-2.13401200	3.79940300	-1.71564600
H	-3.17621200	2.33589000	-0.52976000
H	-1.65168400	2.86677600	0.17420600
C	1.09400800	-1.40810700	1.94713500
C	-0.17678100	-3.09076800	0.94708000
C	2.54178600	-1.36777700	-1.26762100
C	-3.26692700	-1.45692900	4.46994700
H	-3.62013500	0.38780000	3.39999700
H	-1.98175300	0.21757000	4.01101700
H	-6.85491600	-0.59370200	-0.54886400
H	-6.58377600	-0.05155000	-2.20999900

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H	-7.31583300	-1.63105300	-1.90380200
C	-2.71642200	5.04757300	-1.06152900
H	-2.70390100	3.54608000	-2.61733900
H	-1.10790300	3.99150100	-2.05203100
C	1.20868800	-2.73144200	2.71397200
H	2.08041300	-1.00507100	1.70509500
H	0.52652800	-0.64567500	2.49729500
O	0.17888500	-3.56462900	2.16728600
O	-0.91050900	-3.68323400	0.19366600
C	3.67963100	-1.60528900	-0.49384900
C	2.34738100	-2.12111800	-2.43398500
H	-2.46017400	-2.17705600	4.64222300
H	-4.10914700	-2.00385200	4.03475200
H	-3.58491600	-1.06912000	5.44139000
H	-2.13154400	5.33953400	-0.18200600
H	-2.72398200	5.89477200	-1.75248700
H	-3.74634900	4.87627200	-0.73104600
H	1.03744700	-2.62901300	3.78539400
H	2.17508700	-3.21133900	2.53386800
C	4.60211000	-2.58215800	-0.86937300
H	3.87228100	-1.00086200	0.38821500
C	3.26856900	-3.09365500	-2.80705600
H	1.45336600	-1.91319400	-3.02554100
C	4.39770600	-3.33112800	-2.02328900
H	5.48472900	-2.75192300	-0.25973800
H	3.10726600	-3.66905200	-3.71390000
H	5.11595400	-4.09134200	-2.31487900
B	1.87642600	0.85767500	0.00269900
O	3.14004800	1.36296300	0.13993000
O	0.93445300	1.60521600	0.68186500

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H	1.18402100	0.14335800	-1.83894000
C	3.08058500	2.43056600	1.11526300
C	4.06693200	3.51381900	0.71526100
H	3.97753600	4.37983900	1.37871900
H	5.08622300	3.12716100	0.79527200
H	3.90557000	3.83788500	-0.31400400
C	3.46778200	1.82330900	2.46068300
H	3.52023200	2.58403700	3.24446100
H	2.74797900	1.05764800	2.76802100
H	4.45094800	1.35451900	2.36765700
C	1.57811700	2.85273700	1.05013100
C	1.29652100	3.84779700	-0.07198400
H	0.21626400	3.98904100	-0.16062100
H	1.75022600	4.82069600	0.13580100
H	1.67140500	3.47908200	-1.03252400
C	0.98881900	3.33890100	2.36224100
H	1.04179200	2.56955700	3.13586000
H	1.51894300	4.22893800	2.71541100
H	-0.06148300	3.60935200	2.21656600
O	0.76597700	1.38541000	-3.55145700
H	0.20522400	0.49667400	-3.44645200
H	1.59036100	1.09832800	-3.95918500
O	-0.50449800	-0.71311800	-3.08641100
H	-0.02465300	-1.84193000	-1.25908800
H	-1.02274900	-0.97699800	-3.85501800
TS4S			
P	-1.36903100	-0.07913400	-0.37620500
C	-2.67119600	-1.20189100	-0.97147300
C	-1.80617800	0.36491200	1.35047600
C	-4.05996100	-0.55988700	-1.03007500

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H	-2.33564300	-1.50586700	-1.96886100
H	-2.65864000	-2.09255000	-0.33215200
C	-1.37395000	1.40741300	-1.43432800
C	0.19996400	-1.09002700	-0.44484100
C	-2.41739900	-0.75331500	2.20341100
H	-0.90427700	0.78352200	1.80543100
H	-2.52349000	1.19005500	1.27923400
C	-5.12995300	-1.57272400	-1.43765500
H	-4.05012800	0.26611100	-1.75301100
H	-4.33119500	-0.12306900	-0.05874400
C	-2.17544100	2.58733700	-0.88435700
H	-1.75968300	1.06185300	-2.39944300
H	-0.33332500	1.69051900	-1.62203500
N	0.21816000	-1.94313300	0.73841800
C	1.51418300	-0.36311100	-0.70573500
C	-2.62978000	-0.29383600	3.64608800
H	-3.37981700	-1.06395300	1.77838000
H	-1.77989600	-1.64339800	2.19889500
C	-6.51518400	-0.94364700	-1.54030700
H	-5.14416000	-2.39097100	-0.70729800
H	-4.84976000	-2.01977000	-2.39861600
C	-2.23531500	3.72592400	-1.90284500
H	-3.19949600	2.28899000	-0.62203000
H	-1.70562100	2.94536400	0.04154600
C	0.98171200	-1.66094100	1.93858700
C	-0.14008500	-3.26316500	0.66174800
C	2.58932400	-1.35594600	-1.07192200
C	-3.29455700	-1.36711100	4.50176600
H	-3.24122700	0.61704700	3.65110600
H	-1.66056600	-0.01645800	4.08083700

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H	-6.82338800	-0.51122400	-0.58266100
H	-6.52840200	-0.14305100	-2.28682100
H	-7.26722200	-1.68238400	-1.82987900
C	-2.88424400	4.98019800	-1.32775900
H	-2.78998600	3.38483600	-2.78506100
H	-1.21999400	3.95216900	-2.25041700
C	0.69822900	-2.92919300	2.75958100
H	2.04511000	-1.54055200	1.70631500
H	0.62601700	-0.75843100	2.44641300
O	0.18060900	-3.88207900	1.82419300
O	-0.68193300	-3.82435200	-0.25993500
C	3.77896500	-1.50994600	-0.34887400
C	2.40615000	-2.16342700	-2.20626500
H	-2.69682300	-2.28442900	4.52006700
H	-4.28228500	-1.62581900	4.10761400
H	-3.42351400	-1.03114200	5.53400200
H	-2.31397500	5.35896000	-0.47241900
H	-2.93864700	5.77918000	-2.07191700
H	-3.90296400	4.77500400	-0.98226100
H	-0.05768300	-2.75601600	3.53196800
H	1.59362700	-3.34770100	3.21975400
C	4.74297000	-2.43966400	-0.73637000
H	3.96164400	-0.87386700	0.51255900
C	3.36103600	-3.09879500	-2.58819800
H	1.50119300	-2.02986400	-2.79582200
C	4.53629400	-3.24413900	-1.85239200
H	5.65854900	-2.53530100	-0.15958400
H	3.19186100	-3.71222800	-3.46844900
H	5.28405200	-3.97255900	-2.15040500
B	1.87052100	0.86100600	0.13935900

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O	3.12858800	1.41329000	0.25787100
O	0.90254300	1.67372300	0.73031000
H	1.35137700	0.29779800	-1.77524500
C	3.02246900	2.57386900	1.10359100
C	4.01338800	3.62165400	0.62502100
H	3.88513500	4.55871800	1.17657700
H	5.03297100	3.26435400	0.79286900
H	3.89395500	3.81857200	-0.44163200
C	3.35922000	2.12885200	2.52517600
H	3.37260500	2.97209800	3.22174500
H	2.63585200	1.38961000	2.88444600
H	4.34935400	1.66545800	2.52392300
C	1.52180500	2.96545500	0.93442200
C	1.27435100	3.78776200	-0.32893200
H	0.19753600	3.93192400	-0.45250200
H	1.73995900	4.77501900	-0.26299200
H	1.64989400	3.26746800	-1.21753100
C	0.89005100	3.63085200	2.14443600
H	0.92926200	2.98487900	3.02422100
H	1.39911700	4.57166800	2.37701700
H	-0.15936300	3.85992700	1.93368000
O	1.15191200	1.00099500	-2.97457900
H	0.14521600	-0.01473600	-3.30742300
H	1.97144100	0.86042800	-3.46377100
O	-0.59883100	-0.74945700	-3.32860300
H	-0.02141900	-1.74955700	-1.29062900
H	-0.48170900	-1.24047300	-4.14753400
M7S			
P	-1.26270000	-0.02450000	-0.55329500
C	-2.62087400	-1.03135300	-1.23832800

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C	-1.80258200	0.53598200	1.10476100
C	-3.91645500	-0.25929400	-1.50340800
H	-2.24140300	-1.47460100	-2.16649900
H	-2.78089100	-1.86868900	-0.54949600
C	-0.99190400	1.36438000	-1.70464500
C	0.21255900	-1.16227000	-0.50974700
C	-2.65375400	-0.46012800	1.90061600
H	-0.88781800	0.80514000	1.63876500
H	-2.36493700	1.46513400	0.95679600
C	-5.05900600	-1.19462300	-1.89924900
H	-3.75180300	0.47121300	-2.30584400
H	-4.21315100	0.31520800	-0.61500600
C	-1.78669700	2.63471800	-1.39643700
H	-1.23933000	0.97812700	-2.70138100
H	0.08405300	1.55965000	-1.68984100
N	0.02596000	-1.98336100	0.71249100
C	1.56863400	-0.56744500	-0.69111400
C	-2.92464700	0.06060300	3.31246500
H	-3.60944400	-0.63851600	1.39245000
H	-2.14799500	-1.42943700	1.96449100
C	-6.34561000	-0.43742400	-2.20954300
H	-5.23225700	-1.90969300	-1.08594500
H	-4.75300100	-1.78532400	-2.77085900
C	-1.53410900	3.71851600	-2.44356200
H	-2.86223400	2.42268800	-1.34478100
H	-1.49370800	3.00872700	-0.40818000
C	0.87715800	-1.84407800	1.88286800
C	-0.49421700	-3.24636300	0.63927800
C	2.54781900	-1.46028500	-1.30460400
C	-3.80486200	-0.88861900	4.11864200



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H	-3.40070900	1.04710800	3.25057000
H	-1.96740500	0.21115700	3.82780500
H	-6.68059700	0.14075500	-1.34218100
H	-6.20016500	0.26123800	-3.03972600
H	-7.15222800	-1.12120300	-2.48621500
C	-2.24472700	5.02400600	-2.10308000
H	-1.86481400	3.35570400	-3.42428900
H	-0.45400000	3.89179800	-2.52502300
C	0.34039000	-2.99548000	2.73898500
H	1.93082900	-1.96591600	1.61160900
H	0.74707300	-0.86988400	2.36350600
O	-0.26686200	-3.89960300	1.80419900
O	-1.08518100	-3.74294500	-0.29450200
C	3.82002100	-0.98955500	-1.72238000
C	2.30823500	-2.83951400	-1.52471700
H	-3.34146300	-1.87653900	4.20777300
H	-4.77930800	-1.02295800	3.63857000
H	-3.97912400	-0.50860100	5.12867700
H	-1.89692100	5.42040600	-1.14324500
H	-2.06258600	5.78678200	-2.86446600
H	-3.32710300	4.87633200	-2.02948200
H	-0.42775000	-2.65867900	3.44320000
H	1.11917000	-3.53185600	3.28088900
C	4.76082800	-1.82497900	-2.30300500
H	4.05522900	0.05968700	-1.58433900
C	3.25343200	-3.66988200	-2.12268300
H	1.36783100	-3.29159200	-1.22058300
C	4.49294900	-3.17951300	-2.51681800
H	5.71890500	-1.40950900	-2.60622600
H	3.01254000	-4.72003500	-2.26801500

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H	5.23077300	-3.82913300	-2.97654100
B	1.93960500	0.70241500	-0.01051900
O	3.21047100	1.28403900	0.11046500
O	0.99040000	1.52411400	0.65849200
C	3.13715700	2.28010300	1.13454100
C	4.16854000	3.36118200	0.85159400
H	4.06704200	4.19361100	1.55591700
H	5.17335800	2.94408700	0.96144200
H	4.07208900	3.74461300	-0.16580700
C	3.44163600	1.59923600	2.46931000
H	3.48080800	2.31608600	3.29504400
H	2.68669500	0.84004900	2.69801200
H	4.41088400	1.09988000	2.39466600
C	1.65251000	2.74304400	1.03112400
C	1.45562700	3.76100100	-0.09191700
H	0.38690200	3.93275900	-0.24563000
H	1.91826800	4.72200100	0.15086400
H	1.88924400	3.39191500	-1.02707200
C	1.04345000	3.25735700	2.32580700
H	1.05086100	2.48718700	3.10058500
H	1.58920800	4.13158300	2.69536500
H	0.00474700	3.55802200	2.15304900
H	-0.02324000	-1.84830400	-1.33654800
TS5S			
P	-1.33209300	0.50880900	-0.16793100
C	-2.88839500	1.27077400	-0.77991800
C	-1.81098100	-0.86634800	0.95914800
C	-3.78117600	1.92311500	0.27760200
H	-2.59152200	2.00505900	-1.53941000
H	-3.41659900	0.47765100	-1.31893400

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C	-0.47853700	1.78714800	0.83007100
C	0.18040100	-0.09949500	-1.65871200
C	-2.96959300	-1.73227900	0.45540900
H	-0.89939500	-1.46649700	1.06646900
H	-2.05938900	-0.45737900	1.94586600
C	-5.12210400	2.37314400	-0.30348400
H	-3.26706100	2.78914900	0.71357100
H	-3.96354500	1.22064800	1.10307500
C	-0.83907400	1.93103800	2.30949800
H	-0.63045200	2.73534000	0.29703800
H	0.59166900	1.55730700	0.72664500
N	-0.16382000	-1.48332700	-1.85222200
C	1.49125800	0.27003600	-1.23009300
C	-3.17797400	-2.96055800	1.34097900
H	-3.89435100	-1.14076100	0.43248000
H	-2.79547400	-2.05851100	-0.57583200
C	-6.00801800	3.05228800	0.73575600
H	-5.63966900	1.50179800	-0.72313400
H	-4.93860200	3.05716300	-1.14109600
C	-0.03325100	3.04675000	2.97533300
H	-1.91066200	2.12881200	2.43515200
H	-0.63222300	0.98996600	2.83100500
C	0.79408700	-2.57644900	-1.97791500
C	-1.30006800	-1.77876800	-2.55677700
C	2.05488600	1.49811400	-1.82127200
C	-4.32503300	-3.83889300	0.85237500
H	-3.36764900	-2.63684200	2.37215100
H	-2.24828000	-3.54358400	1.36599000
H	-6.22203900	2.37700700	1.57071700
H	-5.52069700	3.94303500	1.14536000

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H	-6.96360500	3.36307200	0.30482500
C	-0.29376200	3.13338700	4.47536600
H	-0.27429700	4.00340100	2.49595700
H	1.03538800	2.87366000	2.79294900
C	-0.17047100	-3.72107600	-2.28460200
H	1.49697600	-2.38157300	-2.79575400
H	1.34022800	-2.73950000	-1.05159400
O	-1.30220300	-3.08678200	-2.90035200
O	-2.19700900	-1.01564300	-2.84142700
C	2.89434100	2.35853200	-1.08144300
C	1.78694200	1.88370700	-3.15167400
H	-4.13893500	-4.19213100	-0.16705800
H	-5.26818700	-3.28322400	0.84301500
H	-4.45961200	-4.71514700	1.49245300
H	-0.01497800	2.19880800	4.97392600
H	0.28060000	3.94173700	4.93585000
H	-1.35341200	3.31677000	4.68133600
H	-0.51017600	-4.21399000	-1.36741400
H	0.23008100	-4.46163700	-2.97622500
C	3.41998000	3.52104000	-1.63149600
H	3.13149500	2.10079300	-0.05404800
C	2.29830800	3.05680200	-3.69633800
H	1.18874200	1.23387800	-3.78513800
C	3.12164400	3.88933100	-2.94256300
H	4.06104900	4.15393700	-1.02354700
H	2.06464200	3.31120000	-4.72668000
H	3.52768800	4.80106300	-3.36889700
B	2.11354600	-0.40336700	-0.03051600
O	3.37133200	-0.15709600	0.51272800
O	1.44350500	-1.38214000	0.72496300

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C	3.64378200	-1.18759100	1.47461100
C	4.51082500	-0.61449100	2.58408000
H	4.65814800	-1.34994500	3.38178900
H	5.49180400	-0.34818000	2.18139300
H	4.06495100	0.28540100	3.01213500
C	4.38832100	-2.30431900	0.74429900
H	4.69326700	-3.10411900	1.42540100
H	3.76702000	-2.73471800	-0.04793900
H	5.28271100	-1.88317300	0.27846300
C	2.20994800	-1.61412000	1.91879600
C	1.63821700	-0.70751200	3.00739300
H	0.57690600	-0.94042100	3.13754400
H	2.14184800	-0.85478500	3.96713900
H	1.72972200	0.34637400	2.72152800
C	2.06976500	-3.07322300	2.32221700
H	2.33909900	-3.74180700	1.50189700
H	2.70650200	-3.30181900	3.18302000
H	1.03275600	-3.27982300	2.60428000
H	-0.24267300	0.49731000	-2.46780400

**(E)- $\beta$ -product**

C	-1.82507200	-0.42351600	-0.21269800
N	-2.40955700	0.83060200	-0.15325900
C	-0.52754900	-0.77382800	-0.07076800
C	-1.84392300	2.03154300	0.44305400
C	-3.79715300	0.92200800	-0.21774100
C	-0.24621600	-2.23871400	-0.02364100
C	-3.02515200	2.99860300	0.31424700
H	-1.56419900	1.83006900	1.48541900
H	-0.97119900	2.38101200	-0.10342300
O	-4.17613600	2.16502500	0.13709200

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O	-4.56543500	0.04902600	-0.52256300
C	0.88711600	-2.77073300	-0.65570400
C	-1.10372200	-3.12852500	0.63856700
H	-2.92689900	3.63930300	-0.56592200
H	-3.17870700	3.61432700	1.20018300
C	1.13840200	-4.13768200	-0.65006900
H	1.57689200	-2.10289300	-1.16398700
C	-0.85755900	-4.49831500	0.64007500
H	-1.96303800	-2.73822600	1.17614300
C	0.26385500	-5.01031300	-0.00575700
H	2.01913900	-4.52380900	-1.15408700
H	-1.53868300	-5.16477600	1.16040200
H	0.46044100	-6.07769000	0.00033900
B	0.71427100	0.17000400	-0.01320200
O	1.86406000	-0.17960800	0.64937700
O	0.83364200	1.37909200	-0.66149900
C	2.73624700	0.97153100	0.64373400
C	4.17712400	0.49862100	0.55317400
H	4.85693300	1.35145700	0.45968400
H	4.43993100	-0.04901900	1.46190400
H	4.32603600	-0.16617400	-0.29948700
C	2.49967500	1.71045300	1.95852800
H	3.17191300	2.56631600	2.06495100
H	1.46685100	2.06590300	2.03090200
H	2.67996300	1.02129000	2.78713100
C	2.22766500	1.76684800	-0.60097100
C	2.86703700	1.30484900	-1.90722700
H	2.32232000	1.74831300	-2.74439200
H	3.91403000	1.61363400	-1.97054800
H	2.81736700	0.21643700	-2.00758800

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C	2.31357400	3.27839400	-0.47447800
H	1.73417700	3.64417600	0.37555300
H	3.35417400	3.59419500	-0.35021100
H	1.92388000	3.74530800	-1.38314600
H	-2.58090500	-1.18902400	-0.37419000
TS6R			
P	-1.48635700	0.39324300	-0.16442400
C	-2.95488400	-0.41349300	-0.92864200
C	-1.88067600	0.62006200	1.60142100
C	-4.29191700	0.30898700	-0.73860400
H	-2.72880300	-0.51944500	-1.99797100
H	-3.00259000	-1.42608800	-0.51093700
C	-1.40648900	2.04384700	-0.96971500
C	-0.00913600	-0.50671000	-0.33508700
C	-2.42447400	-0.65329200	2.26109200
H	-0.95598600	0.96270000	2.08217300
H	-2.60555500	1.43645000	1.68877100
C	-5.46021200	-0.49678800	-1.30863900
H	-4.26503600	1.29112200	-1.22470300
H	-4.47313800	0.49556700	0.32809900
C	-1.05529900	3.19551700	-0.02142200
H	-2.35888200	2.24630100	-1.47249900
H	-0.63881500	1.92781000	-1.74467200
N	0.18142700	-1.15149700	-1.59288000
C	0.79065600	-1.07920500	0.89192000
C	-2.40372100	-0.55808700	3.78592800
H	-3.45241600	-0.83252600	1.92071200
H	-1.84127200	-1.52743600	1.94381400
C	-6.79526400	0.22213800	-1.14549800
H	-5.49975200	-1.47283500	-0.80950300

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H	-5.27302900	-0.69800000	-2.37048300
C	-0.73669400	4.48123200	-0.78522400
H	-1.89863500	3.38424500	0.65572900
H	-0.19950000	2.91374300	0.60344800
C	-0.31367600	-2.48926300	-1.92972300
C	0.61629800	-0.52996800	-2.73680600
C	1.30902800	-2.47694300	0.76837600
C	-3.00342500	-1.79133900	4.45266400
H	-2.95187600	0.33915400	4.09912400
H	-1.36758300	-0.42011700	4.11909000
H	-7.01149100	0.41455100	-0.08962400
H	-6.78797800	1.18589700	-1.66456300
H	-7.61924900	-0.36995100	-1.55248400
C	-0.59575400	5.68615600	0.14032400
H	-1.52790200	4.67475000	-1.52092900
H	0.18732600	4.33562400	-1.35967600
C	0.48256200	-2.75363600	-3.19923900
H	-0.10065200	-3.20870000	-1.13997800
H	-1.39525500	-2.47110600	-2.12126900
O	0.69825800	-1.44443000	-3.74180400
O	0.85447300	0.64037100	-2.92276900
C	0.74437800	-3.50948600	1.52742800
C	2.34965900	-2.80006800	-0.11552900
H	-2.45643800	-2.69649000	4.16884700
H	-4.04883800	-1.92904000	4.15797200
H	-2.97118200	-1.71098400	5.54240400
H	0.17155300	5.51335000	0.90186400
H	-0.32008200	6.58725700	-0.41446900
H	-1.53709400	5.88927300	0.66169800
H	-0.04395300	-3.35344100	-3.94197500



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H	1.45216300	-3.20884100	-2.97066100
C	1.18191900	-4.82542800	1.39791900
H	-0.05374700	-3.27434100	2.22865900
C	2.78166900	-4.11676900	-0.25263100
H	2.81503600	-2.00583100	-0.69050800
C	2.19758400	-5.13645300	0.49737600
H	0.72747900	-5.60781300	1.99869900
H	3.58656900	-4.34674500	-0.94514900
H	2.53927300	-6.16120100	0.38954300
B	1.62489600	0.18237800	0.58028900
O	2.79993000	0.22476600	-0.17730500
O	1.45452400	1.38891300	1.30679900
H	0.21119100	-0.97168300	1.81104100
C	3.29674000	1.57223700	-0.11889000
C	2.73996900	2.35015600	-1.30592300
H	3.15608100	3.36210300	-1.34826100
H	2.98469400	1.82294800	-2.22969300
H	1.64881400	2.40506400	-1.25047600
C	4.81584900	1.52725500	-0.17843700
H	5.24189200	2.52385600	-0.02120500
H	5.22285900	0.84670800	0.57207600
H	5.13235500	1.17527100	-1.16442500
C	2.71329800	2.07660800	1.23907800
C	2.47669800	3.57698900	1.30813800
H	2.00926600	3.83139800	2.26477600
H	3.42406600	4.12176900	1.23692600
H	1.82213300	3.91581100	0.50256400
C	3.54651000	1.62055300	2.43798300
H	3.74342100	0.54530600	2.38494600
H	4.50254000	2.14925600	2.49643500

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H	2.98425800	1.81947100	3.35460500
M8R			
P	-1.39314600	-0.36443300	-0.07365900
C	-2.26225400	-1.74276500	-0.90537100
C	-1.79110200	-0.48414700	1.70049200
C	-3.78179000	-1.72068400	-0.71328000
H	-2.00808300	-1.67195200	-1.97110900
H	-1.83679000	-2.68039000	-0.53058100
C	-2.09452000	1.16807600	-0.79884000
C	0.37105100	-0.41684700	-0.32792000
C	-1.60827200	-1.90679200	2.24496700
H	-1.13531100	0.23585200	2.20269200
H	-2.81978200	-0.14065300	1.85005200
C	-4.46919900	-2.86651200	-1.45629100
H	-4.19200900	-0.76579400	-1.06571300
H	-4.02290900	-1.78836100	0.35562900
C	-2.84337800	2.08719900	0.16588100
H	-2.73451100	0.87370400	-1.63903700
H	-1.22575500	1.67738500	-1.22222700
N	0.78580300	-0.95559400	-1.57875200
C	1.34412300	-0.57329500	0.90959000
C	-1.55412200	-1.92621200	3.77201400
H	-2.43482600	-2.54103000	1.89974800
H	-0.68788900	-2.35441600	1.84688700
C	-5.98230600	-2.85294800	-1.26660300
H	-4.05851200	-3.82065200	-1.10408200
H	-4.22701800	-2.79793200	-2.52368300
C	-3.27731800	3.37736100	-0.52924600
H	-3.72992500	1.58383400	0.57481100
H	-2.18213700	2.32776700	1.00634400

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C	1.03388700	-2.36359600	-1.87281000
C	0.74587000	-0.23257200	-2.74486700
C	2.56858300	-1.39372800	0.73484400
C	-1.42456400	-3.33996100	4.32827100
H	-2.45659400	-1.44764500	4.17195500
H	-0.70554400	-1.31541400	4.10418700
H	-6.24659500	-2.94639100	-0.20834900
H	-6.41584400	-1.91858700	-1.63705300
H	-6.45798500	-3.67767200	-1.80364800
C	-3.93614600	4.35907300	0.43367100
H	-3.96559100	3.13605700	-1.34898100
H	-2.39945100	3.84421400	-0.99401000
C	1.75149100	-2.21844800	-3.21011300
H	1.65612000	-2.83090700	-1.10955700
H	0.09414900	-2.92390700	-1.97161300
O	1.21512300	-1.00597500	-3.75995600
O	0.32426000	0.88556300	-2.91883000
C	2.80110700	-2.49863100	1.56791600
C	3.53467000	-1.09939000	-0.24439600
H	-0.51652200	-3.82568900	3.95609400
H	-2.27790900	-3.95922300	4.03333800
H	-1.37662000	-3.33529400	5.42032900
H	-3.24484700	4.64127900	1.23464100
H	-4.24726900	5.27380600	-0.07808200
H	-4.82349200	3.91825500	0.90018200
H	1.55796000	-3.03034200	-3.91107500
H	2.82998000	-2.09560100	-3.06611100
C	3.93564700	-3.29280800	1.42362000
H	2.07327600	-2.73748900	2.34090400
C	4.66002800	-1.90372500	-0.39840900

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H	3.39623400	-0.22538600	-0.87185900
C	4.86753300	-3.00634100	0.42942300
H	4.08737500	-4.14065900	2.08548400
H	5.39011800	-1.65749400	-1.16459000
H	5.75022400	-3.62648900	0.30856500
B	1.15691200	0.89611400	0.34502400
O	2.19802300	1.61471900	-0.31678800
O	0.28422200	1.84193800	1.01397100
H	0.81344400	-0.82499000	1.82679300
C	1.94223100	3.00759300	-0.14256000
C	1.19990000	3.53549800	-1.36906200
H	1.08531100	4.62427100	-1.33511600
H	1.76349000	3.26626800	-2.26548500
H	0.21440400	3.07375900	-1.45886900
C	3.27637200	3.72927500	0.00103900
H	3.12917000	4.78543600	0.25237600
H	3.89476900	3.26466900	0.77149100
H	3.82208800	3.67991900	-0.94591000
C	1.05529300	3.03571100	1.14755200
C	0.11292000	4.22597900	1.24519200
H	-0.45924500	4.16868100	2.17717800
H	0.66935700	5.16938500	1.24831000
H	-0.59113400	4.23867700	0.40928100
C	1.89350200	2.91969900	2.42325400
H	2.59470000	2.08283000	2.34838700
H	2.45801600	3.83396600	2.63031000
H	1.22348100	2.72907600	3.26689000
<b>TS7R</b>			
P	-1.47199700	-0.14527900	-0.13383900
C	-2.46671300	-1.44818900	-0.92562000

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C	-1.86936100	-0.12518900	1.65515900
C	-3.97835100	-1.19176500	-0.86659600
H	-2.13377300	-1.50456300	-1.96794800
H	-2.20049500	-2.39689300	-0.44461700
C	-1.91782300	1.44111200	-0.94331900
C	0.32881100	-0.46844300	-0.43751900
C	-2.29950200	-1.46842500	2.26211800
H	-0.96407400	0.25393400	2.13987600
H	-2.65661800	0.61936000	1.81121900
C	-4.77331000	-2.41310000	-1.32853100
H	-4.23114100	-0.33371900	-1.50083700
H	-4.28968500	-0.92479700	0.15119300
C	-2.52519600	2.51027700	-0.03339300
H	-2.59713000	1.20361700	-1.76955400
H	-0.98967100	1.80520900	-1.39428500
N	0.48430600	-0.88707300	-1.83841100
C	0.86278100	-1.41227700	0.60795000
C	-2.34963500	-1.38240700	3.78765800
H	-3.28778200	-1.75461300	1.88248400
H	-1.61370800	-2.27130800	1.97324500
C	-6.27672600	-2.15900200	-1.32578600
H	-4.53686600	-3.26062700	-0.67362400
H	-4.44380300	-2.69615800	-2.33561100
C	-2.71424400	3.82873800	-0.78252700
H	-3.49465000	2.17578000	0.35908600
H	-1.86040800	2.67227700	0.82272200
C	0.62963100	-2.26504000	-2.28773400
C	0.78833900	-0.00272500	-2.83626000
C	2.15828300	-1.98932100	0.60793400
C	-2.82432000	-2.68528100	4.42186600

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H	-3.01200600	-0.55925500	4.08345500
H	-1.34979800	-1.12921400	4.16020200
H	-6.62842400	-1.89513000	-0.32317800
H	-6.53763500	-1.33575200	-1.99832600
H	-6.82923200	-3.04421100	-1.65100400
C	-3.27853400	4.92375600	0.11632600
H	-3.37815100	3.66932600	-1.64114900
H	-1.74775500	4.14535200	-1.19325600
C	1.45710800	-2.05194800	-3.55753900
H	1.15007900	-2.86333900	-1.53988000
H	-0.34414700	-2.72148000	-2.50435900
O	1.22075400	-0.68148200	-3.92505200
O	0.68106000	1.20472300	-2.81311100
C	2.50805100	-2.93156100	1.62501900
C	3.17954100	-1.74547600	-0.36080600
H	-2.16035100	-3.51391800	4.15626000
H	-3.83309900	-2.94387000	4.08393600
H	-2.84591700	-2.61130700	5.51223800
H	-2.60863100	5.11879200	0.96027600
H	-3.40867100	5.86113800	-0.43085300
H	-4.25326900	4.63643100	0.52402900
H	1.15419300	-2.68647000	-4.39021000
H	2.52585800	-2.17951400	-3.36138700
C	3.73872800	-3.55899400	1.66675400
H	1.76800000	-3.15794500	2.39074200
C	4.41061000	-2.38766900	-0.30391100
H	3.00798000	-1.01653500	-1.14544100
C	4.71880200	-3.30453700	0.69969000
H	3.94176600	-4.26532000	2.46901800
H	5.15089700	-2.15652500	-1.06745800

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H	5.68376500	-3.79850800	0.73424300
B	1.11180800	0.82431900	-0.00697200
O	2.41531200	1.12533100	-0.29256800
O	0.50486700	1.77117000	0.80913600
H	0.18494100	-1.75085000	1.37910300
C	2.66996200	2.44081900	0.24590200
C	2.45287100	3.43639700	-0.89005200
H	2.70062800	4.45669300	-0.58232000
H	3.09560800	3.15692200	-1.72824000
H	1.41790500	3.40607100	-1.24253800
C	4.10361000	2.48998000	0.74553700
H	4.30212400	3.43478000	1.26230900
H	4.31300400	1.65969000	1.42223700
H	4.78794100	2.41560100	-0.10372500
C	1.58561600	2.55812300	1.36559300
C	1.08166600	3.96665200	1.62496900
H	0.32834200	3.94930000	2.41836300
H	1.90141300	4.61410800	1.95233600
H	0.63026600	4.39952600	0.72968000
C	2.00723700	1.87923500	2.66582400
H	2.35074300	0.85712900	2.47714000
H	2.80377100	2.43454700	3.16862800
H	1.14490300	1.83294800	3.33763700
<b>M9R</b>			
P	-1.69453600	0.15292600	-0.17349100
C	-2.80458300	-1.17096000	-0.76189400
C	-2.07744200	0.54542100	1.56516000
C	-4.23583400	-1.08477100	-0.22524400
H	-2.80061400	-1.09619800	-1.85676900
H	-2.33651000	-2.12764400	-0.50774100

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C	-2.12126300	1.63522200	-1.14097000
C	0.04535800	-0.37967800	-0.53176900
C	-1.75872300	-0.53431700	2.60001000
H	-1.51546500	1.45416600	1.79359600
H	-3.14637100	0.79785000	1.57169400
C	-5.14265000	-2.13398300	-0.86832400
H	-4.65385100	-0.08540900	-0.40821400
H	-4.23162900	-1.22880800	0.86238500
C	-1.56049200	2.95098900	-0.59161200
H	-3.21671100	1.66736600	-1.19582000
H	-1.75257800	1.45691100	-2.15659800
N	0.20196200	-0.39737400	-1.99853700
C	0.27325400	-1.69589800	0.16271700
C	-2.17609900	-0.09305100	4.00183900
H	-2.26591000	-1.47478300	2.34403000
H	-0.68365900	-0.73997100	2.57380000
C	-6.56369300	-2.08461000	-0.31741500
H	-4.71216800	-3.12861000	-0.70181100
H	-5.15788300	-1.97890700	-1.95391300
C	-1.67608300	4.07153600	-1.62247300
H	-2.10109500	3.22782900	0.32223800
H	-0.50782400	2.82122900	-0.32182900
C	0.07641400	-1.56653700	-2.85613100
C	0.67217100	0.68019000	-2.69309000
C	1.41611100	-2.52481400	0.01704800
C	-1.84257400	-1.14333300	5.05619500
H	-3.25254900	0.12091700	4.01539900
H	-1.66850600	0.84972300	4.24306600
H	-6.57292200	-2.26807600	0.76168300
H	-7.02025400	-1.10522900	-0.49328400



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H	-7.19873000	-2.83863300	-0.78948600
C	-1.17642900	5.40500500	-1.07753200
H	-2.72056500	4.16803800	-1.94657900
H	-1.08985300	3.78566200	-2.50296400
C	0.97158600	-1.13688400	-4.02041600
H	0.43902100	-2.46278700	-2.35264100
H	-0.96284100	-1.72018500	-3.17375000
O	0.99881000	0.30062300	-3.95135100
O	0.76882100	1.82350200	-2.29835000
C	1.47493100	-3.76607300	0.72508200
C	2.53719400	-2.26352600	-0.82862500
H	-0.76826400	-1.35189600	5.07321700
H	-2.35948900	-2.08573300	4.84866400
H	-2.13730100	-0.81304800	6.05587900
H	-0.12762800	5.33082900	-0.77219100
H	-1.24905100	6.19547400	-1.82932400
H	-1.75742000	5.71876700	-0.20393000
H	0.58956800	-1.42554300	-4.99927700
H	1.99250600	-1.50955800	-3.89351300
C	2.53422200	-4.64481600	0.60069300
H	0.64823500	-4.01821100	1.38684900
C	3.59388500	-3.15958000	-0.94080000
H	2.58284600	-1.33153400	-1.38045300
C	3.61950600	-4.36267600	-0.23777000
H	2.51730700	-5.57218400	1.16938000
H	4.42198200	-2.90345000	-1.59890500
H	4.45049500	-5.05318100	-0.33280500
B	1.08219300	0.55458900	0.20495700
O	2.41412500	0.60265200	-0.09762800
O	0.75031400	1.32910800	1.30181900

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H	-0.54669500	-2.10897200	0.73916700
C	3.00974600	1.60096400	0.75831000
C	3.05219300	2.90137500	-0.03881000
H	3.55013600	3.69874800	0.52078900
H	3.60404700	2.72613300	-0.96549000
H	2.04395100	3.22486900	-0.31293400
C	4.41082900	1.14572200	1.12953400
H	4.85521000	1.82136300	1.86780100
H	4.40151200	0.13075800	1.53080200
H	5.04364800	1.15174200	0.23809400
C	2.00356400	1.65211500	1.95299100
C	1.86896200	3.00920400	2.62009400
H	1.14114300	2.94820200	3.43457500
H	2.82679000	3.32634200	3.04443800
H	1.52941800	3.76840300	1.91235200
C	2.25748100	0.55670700	2.98493400
H	2.32681400	-0.42398300	2.50277100
H	3.17626600	0.74083800	3.54857400
H	1.42096900	0.53441600	3.69000300
<b>TS8R</b>			
P	1.14721600	-1.14257300	-0.35115900
C	2.87779500	-0.60588000	-0.61741900
C	1.12070000	-2.11632000	1.20475500
C	3.96965300	-1.53225100	-0.07834300
H	2.99686000	-0.48961600	-1.70184100
H	2.94594100	0.40167700	-0.18183000
C	0.76944100	-2.34808300	-1.68591300
C	-0.03117800	0.66518400	-0.37219500
C	1.34336900	-1.29063700	2.47325700
H	0.13585400	-2.58914800	1.24811000

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H	1.87543400	-2.90860500	1.11153700
C	5.36843500	-1.02626800	-0.43220100
H	3.84034700	-2.54553800	-0.48309200
H	3.88555700	-1.61925200	1.01163500
C	-0.48753600	-3.18058800	-1.40427800
H	1.64422900	-2.99262700	-1.84081000
H	0.64241600	-1.76308000	-2.60675900
N	-0.18001000	1.01290200	-1.75000200
C	0.70143800	1.61972200	0.45263000
C	1.33981400	-2.16607300	3.72539200
H	2.29025600	-0.73673800	2.41463400
H	0.54433100	-0.54525000	2.55222200
C	6.46739200	-1.93165200	0.11429700
H	5.49132300	-0.01033600	-0.03828400
H	5.45853500	-0.94921400	-1.52277200
C	-1.07607900	-3.77424000	-2.68194200
H	-0.23719900	-3.98420600	-0.70054400
H	-1.24823300	-2.55492400	-0.92326900
C	0.85581300	1.60464100	-2.59096100
C	-1.04948300	0.29557600	-2.53835400
C	0.75236400	3.04175500	0.31475000
C	1.54480700	-1.35183600	4.99870800
H	2.12369900	-2.92952000	3.64105500
H	0.38542500	-2.70627800	3.77752900
H	6.41555400	-1.99670700	1.20584800
H	6.37481000	-2.94719100	-0.28435500
H	7.46010700	-1.55823600	-0.15066100
C	-2.31428500	-4.61891600	-2.40278200
H	-0.31526300	-4.37837800	-3.19297800
H	-1.33683200	-2.94834400	-3.35397400

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C	0.08576100	1.69919800	-3.90356300
H	1.18014500	2.57610000	-2.22088300
H	1.72075700	0.93397700	-2.67327000
O	-0.85730700	0.61335100	-3.83472000
O	-1.85295200	-0.53122700	-2.16653500
C	1.62259800	3.78946800	1.16039300
C	-0.04642200	3.81993000	-0.57079000
H	0.76338500	-0.59289100	5.10905400
H	2.50824000	-0.83234500	4.98048500
H	1.52395900	-1.98717000	5.88831300
H	-3.09011700	-4.01614300	-1.91899300
H	-2.73630300	-5.02824100	-3.32463100
H	-2.08044500	-5.45828300	-1.73938900
H	0.70121100	1.56336800	-4.79188600
H	-0.47136500	2.63835700	-3.97306300
C	1.70763200	5.16885500	1.10377000
H	2.24271700	3.24393000	1.86880800
C	0.06202200	5.20443700	-0.63076000
H	-0.79736300	3.32268900	-1.17773600
C	0.93919700	5.90445500	0.19507000
H	2.39206000	5.68355100	1.77415100
H	-0.57610500	5.74854000	-1.32359400
H	1.01216600	6.98561000	0.14711800
B	-1.39802800	0.26351300	0.29968600
O	-2.49284100	1.08266000	0.25906800
O	-1.55831000	-0.82261100	1.12847400
H	1.04688700	1.22886100	1.40557900
C	-3.55897600	0.38763600	0.94351400
C	-4.37472600	-0.34771600	-0.11606300
H	-5.24796300	-0.83857500	0.32382600

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H	-4.71932300	0.37803600	-0.85714000
H	-3.76447900	-1.08901200	-0.63784800
C	-4.41892000	1.40943500	1.66802400
H	-5.17978900	0.91093400	2.27750500
H	-3.81609200	2.05451100	2.30963400
H	-4.92953000	2.04006400	0.93549900
C	-2.77162200	-0.58407400	1.88457600
C	-3.45168000	-1.91609800	2.14677100
H	-2.81971300	-2.52849200	2.79685800
H	-4.41152400	-1.76550000	2.65085300
H	-3.62392600	-2.46567500	1.21933100
C	-2.34455600	0.07270900	3.19432200
H	-1.82210600	1.01616000	3.00446600
H	-3.20113600	0.26845200	3.84513500
H	-1.66076100	-0.60018200	3.72112300

**(Z)- $\alpha$ -product**

C	0.40498600	-0.09867900	-0.07715200
N	0.81232900	1.24670900	0.03667000
C	1.24928500	-1.14593200	-0.04208700
C	1.82857400	1.79875700	0.92042900
C	0.07584000	2.24491200	-0.55851300
C	2.72238400	-1.14081500	-0.06475500
C	1.30015900	3.22880000	1.08110600
H	1.86319200	1.24928100	1.86359900
H	2.82264600	1.77737400	0.46344000
O	0.47503600	3.44291400	-0.07267100
O	-0.77889300	2.11119600	-1.39923600
C	3.43830700	-0.24062200	-0.86705600
C	3.43671900	-2.10010900	0.66572800
H	2.08646900	3.98307900	1.08623600

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H	0.67887300	3.33493600	1.97536700
C	4.82823700	-0.28244600	-0.91306400
H	2.89209100	0.47527700	-1.47550000
C	4.82605500	-2.13610900	0.62627900
H	2.89103000	-2.81835100	1.27177800
C	5.52685500	-1.22434200	-0.16081300
H	5.36647900	0.41591500	-1.54641400
H	5.36321400	-2.88054300	1.20565200
H	6.61115500	-1.25547300	-0.19698900
B	-1.14452600	-0.34165400	-0.06854300
O	-2.00156900	0.40512700	0.69221700
O	-1.74462900	-1.38587400	-0.71484600
H	0.78108700	-2.12757500	-0.00601100
C	-3.33857300	-0.00312500	0.31355400
C	-3.79961300	0.94869500	-0.78633700
H	-4.83373100	0.74484800	-1.07905000
H	-3.73580100	1.97378600	-0.41359500
H	-3.15403500	0.87644000	-1.66517700
C	-4.24642600	0.09898400	1.52694900
H	-5.24221900	-0.29193700	1.29470600
H	-3.84218000	-0.45119200	2.37867100
H	-4.35274800	1.14789700	1.81621700
C	-3.09931800	-1.46011900	-0.20409400
C	-4.02397400	-1.89755100	-1.32639100
H	-3.78188800	-2.92142100	-1.62388000
H	-5.06658100	-1.87673500	-0.99347300
H	-3.92027400	-1.25352700	-2.20104500
C	-3.08846700	-2.49455700	0.91799200
H	-2.43273200	-2.17897300	1.73536200
H	-4.09182600	-2.66177600	1.31929800

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H	-2.71164200	-3.44137900	0.52248800
STS1-1			
P	-1.96719800	-0.51881800	-0.32601000
C	-3.35916800	-1.37796800	-1.20480200
C	-2.80031200	0.39377000	1.04380400
C	-4.55857100	-0.51121800	-1.58970600
H	-2.89751500	-1.82752700	-2.09105200
H	-3.67694000	-2.21548800	-0.57179200
C	-1.42091800	0.78448300	-1.52918400
C	0.07777400	-0.95361800	0.58156100
C	-3.32821400	-0.55511400	2.12045900
H	-2.05257600	1.06757000	1.47465600
H	-3.60841200	1.02278800	0.65255500
C	-5.59152900	-1.28097000	-2.41475900
H	-4.21926500	0.36211500	-2.16366800
H	-5.04419000	-0.12015300	-0.68598200
C	-1.85464400	2.22505900	-1.24835900
H	-1.76381900	0.46718800	-2.52174000
H	-0.32663200	0.73137500	-1.54567400
N	0.25715800	-2.32494000	0.54409800
C	0.64872800	0.08560700	0.99025800
C	-3.97804800	0.18921600	3.28636000
H	-4.06032100	-1.24948000	1.68543000
H	-2.50060700	-1.17256400	2.49620100
C	-6.79770500	-0.42387700	-2.78561400
H	-5.92078700	-2.16041100	-1.84747700
H	-5.11182400	-1.66201000	-3.32445300
C	-1.24086900	3.20985300	-2.24227600
H	-2.94936300	2.30844800	-1.27953500
H	-1.54566600	2.51661800	-0.23601200

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C	1.22270200	-2.97369600	1.42526300
C	0.03417800	-3.09598900	-0.57974800
C	0.69610800	1.48871400	1.24296700
C	-4.49352400	-0.75407900	4.36837500
H	-4.80347100	0.80328900	2.90505000
H	-3.24905000	0.88727000	3.71696000
H	-7.30911400	-0.05702900	-1.88961400
H	-6.49315900	0.44791100	-3.37386500
H	-7.52412800	-0.98819000	-3.37697800
C	-1.59159200	4.65648800	-1.91069700
H	-1.57423900	2.96299400	-3.25833300
H	-0.15067300	3.08454700	-2.23356300
C	1.04832800	-4.42419600	0.97633600
H	2.22800500	-2.58632800	1.22924200
H	0.95912300	-2.81501200	2.47219500
O	0.54941300	-4.32760800	-0.36595900
O	-0.51945500	-2.78573300	-1.60600600
C	1.27732300	2.36556700	0.30149000
C	0.17129300	2.04258800	2.42947400
H	-3.67912200	-1.35677400	4.78347400
H	-5.24236100	-1.44291700	3.96387100
H	-4.95628900	-0.20476400	5.19290100
H	-1.22665100	4.91997700	-0.91207500
H	-1.14701400	5.35319100	-2.62721900
H	-2.67560100	4.81244700	-1.92131400
H	0.30776600	-4.95352100	1.58317100
H	1.98092600	-4.98734100	0.95505200
C	1.28286000	3.73770000	0.52282300
H	1.71853700	1.94841200	-0.59944400
C	0.18712300	3.41623000	2.64021100



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H	-0.25521800	1.37823200	3.17586500
C	0.73361300	4.27561100	1.68775100
H	1.72248900	4.39385500	-0.22377200
H	-0.23313300	3.81903100	3.55709400
H	0.74037000	5.34773200	1.85466700
B	2.85747400	-0.96736600	-1.17468000
O	3.24878400	0.31221900	-1.46207200
O	3.74880700	-1.64063700	-0.38140000
H	1.87943600	-1.46585500	-1.62355400
C	4.61571200	0.45151300	-1.00313000
C	4.82245800	1.86329400	-0.48151000
H	5.83569700	1.97865000	-0.08314200
H	4.69695600	2.57638500	-1.30144700
H	4.10429600	2.11320700	0.30143700
C	5.50742700	0.19531400	-2.21581300
H	6.56440700	0.33746800	-1.97427700
H	5.36867000	-0.82016900	-2.59875900
H	5.23521000	0.89712900	-3.00816500
C	4.72262300	-0.67075700	0.08160100
C	4.27165700	-0.20560100	1.46239600
H	4.20051400	-1.07386700	2.12402500
H	4.98735900	0.49774100	1.89747900
H	3.28686800	0.26916200	1.41576200
C	6.08090000	-1.34696300	0.16486800
H	6.35204900	-1.82287800	-0.77904100
H	6.85537000	-0.62002600	0.42950900
H	6.05890700	-2.11644400	0.94130600
STS1-2			
P	-2.02948000	0.42735400	-0.61466900
C	-2.57795600	2.15074900	-0.22686000

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C	-2.81380900	0.08152300	-2.25938300
C	-2.05552400	2.63957800	1.13914400
H	-2.15936700	2.77562400	-1.02587600
H	-3.66837100	2.24608000	-0.28965000
C	-2.88451300	-0.60501700	0.66273100
C	0.68566600	-0.87077300	0.46300200
C	-4.34347700	0.05082200	-2.39405200
H	-2.39557500	0.86192000	-2.90763000
H	-2.38254000	-0.86635000	-2.59811000
C	-1.53082700	4.07381500	1.08357200
H	-1.24431700	1.99283100	1.49898600
H	-2.85260800	2.56988400	1.88919400
C	-4.26992100	-0.15820800	1.13715400
H	-2.19771100	-0.64852000	1.51836100
H	-2.92245100	-1.61848200	0.25161100
N	0.33573500	-2.17459700	0.66198100
C	0.26251100	0.22619300	-0.00716100
C	-4.95949500	-1.31385500	-2.08445600
H	-4.80320800	0.82296600	-1.76321600
H	-4.60874300	0.31679700	-3.42570900
C	-0.97537500	4.54411700	2.42249000
H	-2.33530900	4.74276800	0.75138700
H	-0.74279000	4.12484400	0.32155600
C	-4.92505300	-1.20162800	2.04231200
H	-4.18818000	0.79068400	1.68105400
H	-4.93044700	0.03413500	0.28288900
C	1.16073200	-3.09455600	1.44862100
C	-0.48483200	-2.89103200	-0.19311100
C	0.77813700	1.56571000	-0.28408400
C	-6.48358200	-1.28107500	-2.12253400

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H	-4.62462800	-1.66779700	-1.10329600
H	-4.58121200	-2.04245400	-2.81151400
H	-1.74606600	4.52873200	3.20072600
H	-0.15768500	3.89259000	2.74914200
H	-0.58375700	5.56339900	2.35833700
C	-6.28433600	-0.75065900	2.56691600
H	-4.25523700	-1.42099800	2.88343200
H	-5.03591600	-2.13989200	1.48318700
C	0.32273100	-4.36575400	1.34390500
H	2.15313500	-3.19114900	0.99984200
H	1.26261700	-2.74121200	2.47570900
O	-0.41446500	-4.20356600	0.12269900
O	-1.15883700	-2.47052500	-1.10172800
C	1.54004800	2.22059000	0.69438600
C	0.58254400	2.19657500	-1.51835900
H	-6.84588700	-0.94511200	-3.09998100
H	-6.88001700	-0.58979500	-1.37015200
H	-6.91229900	-2.26798600	-1.92785700
H	-6.97606100	-0.55045800	1.74187000
H	-6.74052700	-1.51126700	3.20660200
H	-6.19324500	0.16917400	3.15378500
H	-0.39105400	-4.45555800	2.16837400
H	0.91488200	-5.27723200	1.26914200
C	2.09718700	3.46907000	0.43745800
H	1.70216100	1.72796900	1.64764200
C	1.14284200	3.44532400	-1.77415000
H	0.00749400	1.68536900	-2.28623900
C	1.90329600	4.08712200	-0.79777700
H	2.68730700	3.95892400	1.20607400
H	0.99100100	3.91417800	-2.74164700

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H	2.33920500	5.06104000	-0.99672500
B	3.67242300	-0.62687800	1.44839800
O	4.02000000	-1.76237500	0.76195200
O	4.22048900	0.51002500	0.92853500
H	3.04185700	-0.64216400	2.45447200
C	5.03402500	-1.38224400	-0.19971400
C	4.82683200	-2.18834700	-1.47070800
H	5.52610000	-1.86735200	-2.24928600
H	5.00913400	-3.24719300	-1.26656700
H	3.80756900	-2.08163500	-1.84626100
C	6.38178400	-1.71972900	0.43298800
H	7.20916000	-1.51688800	-0.25275100
H	6.53915500	-1.14556900	1.35088500
H	6.39661100	-2.78223700	0.68929000
C	4.79781200	0.15846500	-0.35259900
C	3.76679100	0.50082200	-1.42315200
H	2.84383400	-0.06771300	-1.27391100
H	3.52246500	1.56489600	-1.35433100
H	4.15575100	0.29614500	-2.42510900
C	6.05993400	0.98071100	-0.55493200
H	6.75595100	0.86514700	0.27788100
H	6.56556700	0.68893300	-1.48104800
H	5.79166800	2.03791600	-0.63193200
STS1-3			
P	-1.77234500	-0.14592100	0.03917500
C	-3.41125800	0.51850900	-0.56605300
C	-2.03372000	-1.97632300	-0.05998300
C	-4.67991900	0.00314200	0.11469800
H	-3.35983400	1.61319800	-0.46121800
H	-3.46010600	0.31670400	-1.64443000

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C	-1.95346900	0.19862400	1.85751700
C	0.47096400	1.48820600	-0.75702500
C	-2.43190900	-2.44777000	-1.45906900
H	-1.07554700	-2.41978100	0.23270900
H	-2.78642600	-2.28535800	0.67681000
C	-5.95355400	0.55169500	-0.52964900
H	-4.66810200	0.27624500	1.17682100
H	-4.70323700	-1.09398200	0.07545400
C	-0.65895400	0.05546500	2.65541300
H	-2.73400700	-0.45008900	2.27592400
H	-2.31540000	1.23230300	1.94109100
N	-0.33130300	2.51808000	-0.88252200
C	1.48032000	0.71787700	-0.84166800
C	-2.41246500	-3.97049700	-1.58774800
H	-3.43777300	-2.07997000	-1.70680400
H	-1.74759600	-2.01718500	-2.20240900
C	-7.21937200	0.05118100	0.15894800
H	-5.97107600	0.26663900	-1.58939900
H	-5.92707900	1.64866300	-0.50403000
C	-0.83171200	0.48791100	4.10980900
H	-0.30642700	-0.98150400	2.60632700
H	0.12155000	0.66249600	2.18081700
C	-1.09531200	2.81533800	-2.09747200
C	-0.86891200	3.21220800	0.23330100
C	2.81664400	1.35492500	-1.02044200
C	-2.84652300	-4.44665500	-2.97021700
H	-3.06668700	-4.40656700	-0.82201400
H	-1.39907400	-4.33025400	-1.37246800
H	-7.27776600	-1.04153700	0.12413900
H	-7.23683600	0.35057400	1.21181000

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H	-8.12009000	0.44912000	-0.31668900
C	0.46087700	0.36553000	4.91062400
H	-1.61829800	-0.11617600	4.58089900
H	-1.18169300	1.52783600	4.13332600
C	-1.85012400	4.07166100	-1.65245500
H	-0.42512900	2.99400700	-2.93759400
H	-1.75712900	1.97200600	-2.31772900
O	-1.82203000	4.03671400	-0.21302600
O	-0.53560100	3.07773900	1.37243100
C	3.71368600	0.87788800	-1.98272400
C	3.18623400	2.43906200	-0.21218300
H	-2.18948800	-4.04137100	-3.74656300
H	-3.86763100	-4.12108700	-3.19569500
H	-2.81994300	-5.53729500	-3.04663400
H	1.24355000	1.00254800	4.48549100
H	0.32007100	0.66243400	5.95418600
H	0.83151500	-0.66555700	4.90464700
H	-2.89238700	4.08048500	-1.96763900
H	-1.35288600	4.98774400	-1.97788300
C	4.94939400	1.49839300	-2.14447100
H	3.44306700	0.01837300	-2.58246800
C	4.43096100	3.03972500	-0.36759900
H	2.49743000	2.78649700	0.55337500
C	5.31423200	2.57490100	-1.33920000
H	5.63628900	1.12794400	-2.89915400
H	4.70936400	3.87121500	0.27231200
H	6.28515100	3.04410600	-1.46287300
B	1.34209100	-1.14099600	-0.80532200
O	2.63970000	-1.64477400	-1.14074700
O	1.04190000	-1.55601200	0.53422900

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H	0.45611600	-1.30924000	-1.61710300
C	3.07254100	-2.50850100	-0.09406600
C	4.58367100	-2.39296500	0.05205200
H	4.94494300	-2.97438200	0.90739900
H	5.06891600	-2.77933700	-0.84944500
H	4.88665100	-1.35109300	0.17736400
C	2.68970600	-3.93743100	-0.48704100
H	3.05608200	-4.67757400	0.23135400
H	1.60247400	-4.03245500	-0.56824200
H	3.12368600	-4.15981800	-1.46579700
C	2.25746200	-1.99847800	1.13844900
C	2.93353400	-0.81720500	1.83669800
H	2.22318800	-0.36748100	2.53646900
H	3.81653100	-1.13587400	2.40015300
H	3.24248200	-0.05261700	1.11940800
C	1.92954900	-3.07422900	2.16616600
H	1.29186900	-3.85040700	1.73775300
H	2.84336400	-3.54058700	2.55020700
H	1.39999500	-2.62778000	3.01392300
STS1-4			
P	-1.50990600	0.34652200	-0.51066900
C	-2.24782800	0.98691800	1.05630300
C	-2.40359900	1.30760200	-1.82596700
C	-1.61003100	0.31903500	2.27737900
H	-2.06589100	2.06874900	1.08291000
H	-3.33552700	0.84444000	1.05835000
C	-2.16103800	-1.39470200	-0.59149100
C	1.73872800	0.60665700	-0.95761100
C	-3.92426900	1.17607400	-1.99932700
H	-2.15390900	2.34838200	-1.59509200

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H	-1.89574600	1.07796900	-2.77157300
C	-2.00555800	0.98927500	3.59066300
H	-0.51812600	0.33261200	2.16617000
H	-1.88348300	-0.74436700	2.30663000
C	-3.56786000	-1.67446800	-0.05395600
H	-1.43349600	-1.99985900	-0.04252600
H	-2.07380900	-1.69506600	-1.64293500
N	3.07771400	0.68180400	-1.24605800
C	0.85436300	1.36280300	-0.48036500
C	-4.34768800	0.03650400	-2.92691400
H	-4.41425000	1.07095800	-1.02311600
H	-4.30843000	2.11403300	-2.42090600
C	-1.33124200	0.34439600	4.79721400
H	-3.09601000	0.95083100	3.70722100
H	-1.73727900	2.05266700	3.53871200
C	-4.01899500	-3.09845000	-0.38275900
H	-3.57903200	-1.53821400	1.03483500
H	-4.30299800	-0.96933300	-0.45784400
C	3.92936100	1.78526800	-0.81869300
C	3.65260200	0.03092300	-2.33184400
C	0.41764000	2.59758400	0.13986300
C	-5.86139400	-0.14230100	-2.96751100
H	-3.87652000	-0.90220600	-2.61623300
H	-3.96891700	0.24641000	-3.93470000
H	-1.59752200	-0.71481400	4.87718800
H	-0.24029900	0.40652000	4.71373900
H	-1.62140000	0.83256800	5.73193500
C	-5.38585900	-3.43033300	0.20709600
H	-3.26959800	-3.80870400	-0.01177900
H	-4.04640200	-3.22166900	-1.47338700



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C	5.28023900	1.26836400	-1.30772500
H	3.62976800	2.72138300	-1.30655200
H	3.88699900	1.91517500	0.26483700
O	4.95095300	0.42544600	-2.41726400
O	3.13362900	-0.70275000	-3.12360900
C	0.59941500	2.79831800	1.51769400
C	-0.13091000	3.63683600	-0.62855600
H	-6.35827100	0.77876500	-3.29032700
H	-6.25197400	-0.39600300	-1.97546000
H	-6.15426100	-0.93996700	-3.65562400
H	-6.15279700	-2.74518200	-0.16949500
H	-5.69560400	-4.44810900	-0.04603000
H	-5.37342700	-3.34627300	1.29870900
H	5.78114100	0.66757900	-0.54196800
H	5.95195400	2.05263800	-1.65692800
C	0.21328600	3.99465100	2.11325600
H	1.04748000	2.00706400	2.11090500
C	-0.52019200	4.82898300	-0.02763300
H	-0.23570900	3.49891900	-1.70019900
C	-0.35875200	5.00771700	1.34548000
H	0.35952500	4.13600200	3.17973600
H	-0.94343700	5.62383400	-0.63359000
H	-0.66615700	5.93746300	1.81324700
B	1.19033700	-1.47904700	-0.71415700
O	2.42096500	-2.13187300	-0.79589700
O	0.68512200	-1.57672600	0.59469000
H	0.43032000	-1.38381600	-1.63663400
C	2.65449200	-2.80918000	0.44390200
C	4.14337100	-2.76938800	0.75282500
H	4.35390800	-3.20089800	1.73710500

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H	4.68716600	-3.34889300	0.00181400
H	4.52166600	-1.74496500	0.72676400
C	2.19127000	-4.25456600	0.26170700
H	2.40070300	-4.86577300	1.14488800
H	1.11779700	-4.29188200	0.05306800
H	2.71781000	-4.68577000	-0.59352900
C	1.75410400	-2.01521900	1.44304000
C	2.46069400	-0.78618000	2.01683700
H	2.92209700	-0.19001600	1.22443800
H	1.72237500	-0.16590600	2.53427400
H	3.23335700	-1.07231500	2.73713200
C	1.16482700	-2.84143200	2.57654300
H	0.52718100	-3.64101300	2.19461200
H	1.95600500	-3.28395700	3.19080600
H	0.55554200	-2.19812800	3.21957700
SM1			
P	2.09028000	-0.04905900	-0.12297700
C	1.73660000	0.33603600	-1.86696700
C	2.77743000	1.40401200	0.73375900
C	1.22449800	-0.85850300	-2.69027900
H	1.00026200	1.14458900	-1.82241800
H	2.65974500	0.74401500	-2.29640900
C	3.36065900	-1.35375800	-0.06047300
C	0.68031100	-0.70664100	0.81582100
C	3.52423000	2.39024700	-0.16781700
H	1.93096400	1.89878500	1.21548400
H	3.42633400	1.00263800	1.52242400
C	2.31163400	-1.68332200	-3.37989800
H	0.55534500	-0.45963600	-3.45991100
H	0.58386900	-1.50260900	-2.07154400

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C	4.69549900	-0.96345800	-0.70109200
H	2.93537500	-2.24425000	-0.53764400
H	3.50006300	-1.59242100	0.99911600
N	0.83835600	-2.07177600	1.20811200
C	-0.42165200	-0.01212900	1.18005000
C	4.26343200	3.44470400	0.65622800
H	4.24572700	1.87318500	-0.81262900
H	2.79881100	2.87329100	-0.83472700
C	1.71255900	-2.82052300	-4.20188300
H	3.01622400	-2.09696100	-2.64905100
H	2.89907900	-1.02356700	-4.03116100
C	5.65147500	-2.15482700	-0.76359700
H	4.54398800	-0.57238300	-1.71569000
H	5.16020200	-0.15857400	-0.11773900
C	-0.01916300	-3.14356000	0.70769500
C	1.46918100	-2.44204900	2.36735200
C	-1.31276400	-0.66283300	2.18579700
C	4.86054300	4.54255700	-0.21710200
H	5.05422800	2.95225600	1.23548700
H	3.57411600	3.88356700	1.38770500
H	1.14611000	-3.50680600	-3.56346900
H	1.02510000	-2.43386500	-4.96084000
H	2.48752200	-3.39845000	-4.71236400
C	7.00418200	-1.77932600	-1.35844500
H	5.19027400	-2.95187400	-1.36066700
H	5.78562900	-2.56089400	0.24608500
C	-0.11632700	-4.01643400	1.96025900
H	-0.98270800	-2.75260500	0.37295800
H	0.46721200	-3.66439300	-0.12680900
O	1.05921800	-3.67978400	2.72072200

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O	2.29098000	-1.80369500	2.98593400
C	-2.58815000	-1.12015100	1.84476700
C	-0.86773200	-0.80809900	3.50619600
H	4.07593300	5.07479500	-0.76501500
H	5.55644100	4.12634300	-0.95294700
H	5.40646500	5.27596000	0.38203800
H	7.49468800	-1.00497400	-0.76012000
H	7.67335800	-2.64262000	-1.40019600
H	6.89197000	-1.39324300	-2.37675200
H	-0.09457800	-5.08654700	1.75683600
H	-0.99852500	-3.76180000	2.55758200
C	-3.39924300	-1.72364200	2.80291900
H	-2.90732500	-1.03285600	0.81255600
C	-1.68522300	-1.40201200	4.46357600
H	0.12481400	-0.45804800	3.77549800
C	-2.95306800	-1.86437400	4.11527200
H	-4.38541900	-2.08284900	2.52177400
H	-1.32720900	-1.50663100	5.48303900
H	-3.58849500	-2.32961000	4.86235200
B	-1.00305300	1.36527700	0.56266100
O	-0.11230100	2.22870800	-0.17751500
O	-1.74141400	2.17846400	1.47687100
H	-0.90878200	0.51883300	-2.04751300
C	-0.48819200	3.58684100	0.09187700
C	-0.56986600	4.34128500	-1.22924900
H	-0.92710000	5.36587300	-1.07899900
H	0.42504000	4.39492900	-1.68429500
H	-1.23601000	3.83356600	-1.92998700
C	0.59081100	4.21285900	0.97467100
H	0.38301400	5.26637500	1.18483100

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H	0.67354400	3.67878300	1.92668700
H	1.55193000	4.15968200	0.45537300
C	-1.85989100	3.44915600	0.84825500
C	-3.06316600	3.43099200	-0.10087100
H	-3.94879300	3.15790500	0.48123800
H	-3.23689800	4.41609200	-0.54618200
H	-2.95004900	2.69842000	-0.90445400
C	-2.09384500	4.50090200	1.92594400
H	-1.33475600	4.44670800	2.70849600
H	-2.09435500	5.51020400	1.50045900
H	-3.06893500	4.32835500	2.39027200
B	-1.99346300	0.18733000	-1.66866000
O	-2.28512300	-1.17612100	-1.36551900
O	-3.10022500	0.77341100	-2.31655800
H	-1.87935000	0.79951300	-0.28831300
C	-3.52302700	-1.49577600	-2.01468100
C	-4.28917000	-2.51501200	-1.18443400
H	-5.25187800	-2.74855700	-1.65151700
H	-3.71303200	-3.44307300	-1.11572800
H	-4.47812600	-2.15536100	-0.17081200
C	-3.17069000	-2.09433400	-3.37840400
H	-4.05584300	-2.43963300	-3.92097200
H	-2.64419200	-1.35896200	-3.99459800
H	-2.50402600	-2.94779900	-3.22348500
C	-4.21798600	-0.10070200	-2.14019900
C	-4.96387100	0.31893000	-0.87249200
H	-5.29424700	1.35472000	-0.99119200
H	-5.84627400	-0.30309600	-0.69315100
H	-4.31519800	0.27911600	0.00818400
C	-5.13889600	0.03455400	-3.34501300

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H	-4.59345000	-0.10746000	-4.27978700
H	-5.95522300	-0.69416900	-3.29731700
H	-5.57853700	1.03582500	-3.35893600
STS2			
P	1.97312800	-0.24375400	0.15095500
C	1.80588900	-0.17659000	-1.67359500
C	2.91964600	1.20965800	0.74057200
C	1.17029000	-1.43928300	-2.28160100
H	1.19163100	0.70426800	-1.87203400
H	2.80162900	0.01002300	-2.09448700
C	2.99175100	-1.70574400	0.52993600
C	0.45572900	-0.41726700	1.06443100
C	3.78437600	1.90453700	-0.31085000
H	2.19245500	1.91470000	1.15187500
H	3.52288100	0.84373500	1.58114500
C	2.16630600	-2.48464000	-2.78334900
H	0.54127600	-1.12214900	-3.12133800
H	0.45970900	-1.88940200	-1.57738900
C	4.40235400	-1.64912200	-0.06364300
H	2.44370300	-2.58471600	0.17009400
H	3.03830700	-1.77762500	1.62083100
N	0.22769200	-1.70134500	1.63993900
C	-0.57329700	0.52290400	1.08830900
C	4.63967000	3.01128900	0.30550200
H	4.44051100	1.18461000	-0.81631400
H	3.12653200	2.32535300	-1.08247700
C	1.45632800	-3.65040700	-3.46540400
H	2.77769900	-2.86790600	-1.95747200
H	2.86443400	-2.01337600	-3.48766800
C	5.15411900	-2.96141500	0.15890500

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H	4.36755600	-1.43574600	-1.13982700
H	4.96359500	-0.82857900	0.40209200
C	-0.81501000	-2.61589300	1.18525700
C	0.77976100	-2.11909400	2.81755300
C	-1.61860600	0.41028100	2.16784200
C	5.37653200	3.82643900	-0.75176000
H	5.35824700	2.56235700	1.00208000
H	4.00172900	3.67086300	0.90713500
H	0.74610800	-4.12764200	-2.78122400
H	0.89395600	-3.30662200	-4.33939300
H	2.16426500	-4.41318500	-3.80133700
C	6.57507100	-2.91496300	-0.39210700
H	4.59661800	-3.77742300	-0.31836700
H	5.17472600	-3.18620800	1.23191900
C	-1.02858600	-3.44665100	2.45231300
H	-1.70368700	-2.06449700	0.87131400
H	-0.47083600	-3.20989100	0.32971500
O	0.17098800	-3.25790200	3.22245800
O	1.68875100	-1.60434300	3.43406800
C	-2.97525500	0.63948900	1.91223900
C	-1.21732600	0.15406500	3.48549800
H	4.66996800	4.31781400	-1.42957300
H	6.02687400	3.18784200	-1.35836800
H	5.99849400	4.60215700	-0.29747600
H	7.15856400	-2.12557300	0.09246500
H	7.09594800	-3.86225600	-0.22993600
H	6.57221500	-2.71481400	-1.46855300
H	-1.15025200	-4.51339000	2.26429000
H	-1.87417900	-3.07460800	3.03919300
C	-3.90949600	0.57618700	2.94119500

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H	-3.29007400	0.85494000	0.89543600
C	-2.15445300	0.09547700	4.51420300
H	-0.16233800	0.01960500	3.70604100
C	-3.50547800	0.29648300	4.24484800
H	-4.95925200	0.74514900	2.72010500
H	-1.82242100	-0.10642200	5.52793200
H	-4.23695400	0.24301700	5.04526300
B	-0.53834200	1.92674800	0.38980000
O	0.39167100	2.31518300	-0.54671100
O	-1.44617500	2.91044700	0.67501500
H	-1.10854500	0.57586900	-2.08880100
C	0.14712800	3.71323800	-0.84709900
C	0.36797200	3.93045700	-2.33401600
H	0.10468400	4.95475200	-2.61645200
H	1.42388500	3.77438400	-2.57703100
H	-0.22875700	3.23437300	-2.92653900
C	1.14719700	4.52554400	-0.03039500
H	1.04438800	5.59655900	-0.22544000
H	1.01417200	4.35210900	1.04228900
H	2.16161000	4.22580700	-0.30831900
C	-1.33093000	3.90510500	-0.36676900
C	-2.36052200	3.55277800	-1.43653800
H	-3.34840700	3.51227300	-0.97031500
H	-2.38145000	4.30598600	-2.22987200
H	-2.16511200	2.57238900	-1.87876400
C	-1.63127700	5.27036300	0.22936000
H	-1.01031800	5.47441300	1.10344800
H	-1.46902900	6.05847200	-0.51286900
H	-2.67861700	5.30663800	0.53985300
B	-1.95270100	-0.05914000	-1.46360800



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O	-1.84258100	-1.49666300	-1.47380200
O	-3.31715300	0.27951600	-1.75197600
H	-1.58561100	0.33937700	-0.18960600
C	-2.99559600	-1.99780100	-2.14148000
C	-3.29521800	-3.40150600	-1.63391000
H	-4.21766900	-3.79320700	-2.07596300
H	-2.47617300	-4.07292800	-1.91162200
H	-3.39600400	-3.41959900	-0.54610300
C	-2.68709000	-2.04291400	-3.64113200
H	-3.50674700	-2.47982200	-4.22017400
H	-2.48555800	-1.03659100	-4.02124900
H	-1.79170000	-2.65273200	-3.79561000
C	-4.07832100	-0.92548100	-1.79565600
C	-4.71099700	-1.17544200	-0.42553600
H	-5.28044200	-0.28831800	-0.13160100
H	-5.39382000	-2.03119800	-0.44440100
H	-3.94497400	-1.35487400	0.33487800
C	-5.17425200	-0.77106300	-2.84291800
H	-4.76119700	-0.44654000	-3.79995300
H	-5.71449200	-1.71251500	-2.99132300
H	-5.89375500	-0.01582100	-2.51266100
STS3			
P	1.48669100	-0.04905100	-0.09679200
C	3.06674100	0.31279700	0.74793100
C	1.27608900	-1.85776000	-0.00562100
C	4.23239800	-0.61646800	0.40067900
H	3.31527400	1.34889900	0.50321000
H	2.84584300	0.27374000	1.82197700
C	1.57427800	0.36050600	-1.87972900
C	0.17709400	0.79509000	0.71144200

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C	1.20156800	-2.38780200	1.42524800
H	0.35345900	-2.10234500	-0.54130400
H	2.11255200	-2.30721100	-0.55483300
C	5.49718300	-0.23500700	1.17088800
H	4.44095800	-0.56703500	-0.67520500
H	3.97787800	-1.65956000	0.62663900
C	2.18966200	-0.67554500	-2.82342400
H	2.09225200	1.32401100	-1.93151800
H	0.52752300	0.54644400	-2.15868600
N	0.52430100	2.01002000	1.39578700
C	-1.28609800	0.75098100	0.12634300
C	1.04581500	-3.90622700	1.45563700
H	2.10256300	-2.10355400	1.98651300
H	0.34572200	-1.92273900	1.92376100
C	6.67655000	-1.14096200	0.83329900
H	5.28796100	-0.28144300	2.24683900
H	5.75240100	0.80794800	0.94884900
C	2.24201700	-0.16032200	-4.26213300
H	3.20439800	-0.94075600	-2.50056100
H	1.60080600	-1.60064200	-2.79561600
C	-0.03945100	2.36666700	2.69098000
C	1.27586200	3.03022700	0.89717400
C	-1.88206600	2.03567500	-0.30722700
C	0.83656300	-4.44062400	2.86824600
H	1.92791400	-4.37654500	1.00242700
H	0.18995100	-4.18124500	0.82711300
H	6.45088600	-2.18559700	1.07116800
H	6.91966400	-1.08748100	-0.23276900
H	7.57095000	-0.85652600	1.39395800
C	2.82867200	-1.18674800	-5.22564800

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H	2.83574800	0.76116800	-4.29182800
H	1.22893500	0.11385100	-4.58033900
C	0.17956000	3.87985300	2.68711900
H	-1.10242400	2.11305400	2.73686500
H	0.49006800	1.85181800	3.50167500
O	1.25045300	4.08081400	1.75395500
O	1.95184600	3.03602400	-0.11511300
C	-3.22879500	2.34076100	-0.03463400
C	-1.12416600	3.01490800	-0.97036900
H	-0.06292300	-4.00677400	3.31735900
H	1.68429000	-4.18879500	3.51413900
H	0.72434000	-5.52849700	2.87413000
H	2.23248400	-2.10501300	-5.23220400
H	2.85951000	-0.80171100	-6.24844700
H	3.85072900	-1.45581000	-4.93928400
H	0.48176300	4.28626700	3.65205600
H	-0.70461000	4.40934600	2.31872100
C	-3.78834500	3.55377900	-0.41636200
H	-3.83591700	1.60175700	0.47969900
C	-1.68183900	4.23487800	-1.34490300
H	-0.08219000	2.81257400	-1.19922900
C	-3.01726100	4.51567800	-1.06961000
H	-4.83232500	3.75572300	-0.19273900
H	-1.06405400	4.96870000	-1.85503600
H	-3.45156800	5.46836200	-1.35632800
B	-2.07015800	-0.53563000	-0.00382800
O	-1.72021900	-1.77536000	0.55304400
O	-3.30159300	-0.62213300	-0.64961700
C	-2.68181000	-2.74095800	0.09176500
C	-2.90886200	-3.77714400	1.18114900

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H	-3.72848500	-4.45055700	0.90938000
H	-2.00743800	-4.38247400	1.31665500
H	-3.14568900	-3.30220200	2.13524700
C	-2.11726000	-3.40252900	-1.16473400
H	-2.78752000	-4.17707500	-1.54848400
H	-1.95281900	-2.66059300	-1.95301500
H	-1.15872300	-3.87283000	-0.92696600
C	-3.91878800	-1.84404400	-0.22386600
C	-4.74407000	-1.53039000	1.02451500
H	-5.46326400	-0.74344600	0.78154200
H	-5.29696800	-2.40514700	1.37914600
H	-4.10195500	-1.16963400	1.83468800
C	-4.81979100	-2.35878100	-1.33477400
H	-4.28057600	-2.43481300	-2.28071700
H	-5.22984100	-3.34172900	-1.08029900
H	-5.65537800	-1.66797800	-1.47672600
H	-0.89444200	0.43018000	1.31442900
SM2			
P	-1.17550400	-0.13010300	0.16497100
C	-2.92212500	0.31651000	-0.15795500
C	-1.08226800	-1.94954500	-0.06439800
C	-4.00192800	-0.53086000	0.53434500
H	-3.03740500	1.37149500	0.10417400
H	-3.02379400	0.23753900	-1.24744100
C	-0.78263100	0.16153000	1.93730200
C	-0.20732100	0.69828000	-1.03496300
C	-1.83391500	-2.45713500	-1.29873600
H	-0.01665600	-2.17935000	-0.15978600
H	-1.43926400	-2.44109800	0.84913900
C	-5.29816600	-0.54645000	-0.27699100

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H	-4.21072200	-0.12523300	1.52872100
H	-3.66870900	-1.56400400	0.69024500
C	-1.79158000	-0.30550000	2.98873400
H	-0.61496100	1.24096100	2.01197000
H	0.18141700	-0.33975800	2.08660300
N	-0.82623400	1.89643900	-1.53428500
C	1.32541400	0.85622700	-0.94311200
C	-1.39213200	-3.86558100	-1.69024100
H	-2.91632800	-2.45046300	-1.11633300
H	-1.65272400	-1.78724000	-2.14729800
C	-6.41057500	-1.32317900	0.41861200
H	-5.09675200	-0.98607700	-1.26246500
H	-5.61994000	0.48646300	-0.45852000
C	-1.18932000	-0.27191300	4.39427000
H	-2.67262600	0.34541300	2.96467400
H	-2.14464400	-1.32344700	2.77520300
C	-0.99962500	2.14614000	-2.95395400
C	-1.23926200	2.96218800	-0.79158300
C	1.76984400	2.09670400	-0.17336600
C	-2.13256900	-4.38124600	-2.91930200
H	-1.54640900	-4.54773200	-0.84386400
H	-0.31642400	-3.83493000	-1.89538200
H	-6.11388700	-2.36324400	0.59010000
H	-6.64954600	-0.88116400	1.39118200
H	-7.32634000	-1.33143900	-0.17864400
C	-2.19308700	-0.67456100	5.46951900
H	-0.81123600	0.73775300	4.59599100
H	-0.31996800	-0.94099200	4.42644400
C	-1.25321100	3.65814400	-2.95930500
H	-0.10025400	1.87540700	-3.51595800

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H	-1.84245600	1.56800400	-3.35427700
O	-1.63821700	3.96979500	-1.61549400
O	-1.33787800	3.03721700	0.41521600
C	1.90604500	3.31131600	-0.85431700
C	2.00441500	2.08698800	1.20637200
H	-1.94465700	-3.73087300	-3.77965100
H	-3.21434800	-4.40952300	-2.74953600
H	-1.81052100	-5.39133700	-3.18786800
H	-2.56974000	-1.68801500	5.29571300
H	-1.74367700	-0.65190400	6.46614600
H	-3.05317700	0.00268200	5.47573500
H	-2.05743200	3.96477100	-3.62904600
H	-0.34720200	4.22277400	-3.20217600
C	2.23289400	4.48528800	-0.18097900
H	1.75318100	3.32981900	-1.93202000
C	2.34280400	3.25558200	1.88295300
H	1.91751400	1.15348900	1.75551000
C	2.45007000	4.46130800	1.19366100
H	2.32049200	5.41791100	-0.73036600
H	2.52123400	3.22478400	2.95381100
H	2.70510600	5.37372200	1.72340300
B	2.15568200	-0.39748200	-0.46870800
O	1.91888300	-1.11370300	0.68126500
O	3.27213000	-0.83632400	-1.13664200
C	3.08270200	-1.94034400	0.92832100
C	2.62361900	-3.25386600	1.53750400
H	3.47156500	-3.93188900	1.67614000
H	2.17595100	-3.06503300	2.51746600
H	1.87871500	-3.74722000	0.90970000
C	3.96122600	-1.16926800	1.90958700

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H	4.85000400	-1.74234300	2.18740600
H	4.27824600	-0.21143500	1.48536700
H	3.38498100	-0.96619400	2.81682800
C	3.71482400	-2.05931100	-0.49875000
C	3.14258500	-3.21862800	-1.30905800
H	3.49883300	-3.13703900	-2.34017300
H	3.47020600	-4.18254400	-0.90984500
H	2.04959800	-3.18459800	-1.33024300
C	5.23382200	-2.09732400	-0.51679500
H	5.66387800	-1.19687700	-0.07510200
H	5.60237200	-2.97094400	0.03021600
H	5.58402600	-2.17134600	-1.54967400
O	0.70179300	-1.56723000	-2.68033100
H	1.61308400	-1.27871100	-2.81159700
H	0.23666500	-0.78627500	-2.28868000
H	1.66554700	1.02416000	-1.97933100
STS4			
P	-1.22145100	-0.25245600	0.12477300
C	-2.99273300	-0.03491200	-0.29163600
C	-0.95138200	-2.06623900	0.13197800
C	-4.00363100	-0.92594600	0.44342000
H	-3.23349000	1.02024800	-0.13780400
H	-3.04037400	-0.22675900	-1.37131500
C	-0.88209000	0.26653800	1.84936400
C	-0.28540800	0.52710900	-1.16480600
C	-1.48877500	-2.79197100	-1.10486600
H	0.12985700	-2.20893000	0.22508300
H	-1.40736900	-2.46391000	1.04705100
C	-5.32514300	-1.00679000	-0.32241900
H	-4.19600000	-0.52546200	1.44300600

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H	-3.61513800	-1.94099000	0.58786800
C	-1.91036200	-0.10619200	2.91867200
H	-0.74809100	1.35111100	1.80717200
H	0.09242700	-0.18673800	2.07433500
N	-1.02412900	1.59833200	-1.78953800
C	1.21453500	0.88958000	-0.99863400
C	-0.88323400	-4.18750800	-1.24458400
H	-2.58281900	-2.86950900	-1.05755600
H	-1.25883000	-2.21605600	-2.00925700
C	-6.37594600	-1.82623400	0.41888400
H	-5.13941400	-1.44656700	-1.31076200
H	-5.70064300	0.00840800	-0.50013700
C	-1.37030500	0.16195500	4.32413300
H	-2.82036500	0.48624400	2.76750400
H	-2.20199800	-1.16235400	2.84098700
C	-1.14776700	1.71860200	-3.22948800
C	-1.56680100	2.67330400	-1.15233300
C	1.48742200	2.15282900	-0.20644300
C	-1.43671300	-4.94548100	-2.44635900
H	-1.06718600	-4.75910000	-0.32604100
H	0.20376500	-4.07805000	-1.33806000
H	-6.02613600	-2.84963100	0.59012200
H	-6.60137400	-1.38449800	1.39474800
H	-7.31037400	-1.88281900	-0.14594000
C	-2.39775400	-0.13784000	5.41054700
H	-1.05260800	1.20971600	4.38921400
H	-0.47080500	-0.44572600	4.48343300
C	-1.57128100	3.18679900	-3.37147700
H	-0.19322500	1.51773600	-3.72605100
H	-1.89605300	1.01715800	-3.62037600



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O	-2.02800400	3.56743000	-2.06877100
O	-1.71798400	2.83274600	0.04087300
C	1.45584600	3.39423800	-0.85320000
C	1.73761700	2.14291200	1.17035100
H	-1.23938500	-4.40065600	-3.37549300
H	-2.52037900	-5.07989100	-2.36401200
H	-0.98406100	-5.93663200	-2.53876800
H	-2.71524100	-1.18520800	5.37299200
H	-1.99236400	0.05230300	6.40811200
H	-3.28997200	0.48463300	5.28840900
H	-2.38518500	3.33916100	-4.08127900
H	-0.72881500	3.82876100	-3.64730300
C	1.62423700	4.58409000	-0.15082800
H	1.29364700	3.42205700	-1.92961600
C	1.91387500	3.32850800	1.87845800
H	1.79082300	1.19036600	1.68655600
C	1.84823600	4.55575300	1.22266600
H	1.58164300	5.53353000	-0.67636200
H	2.10479700	3.29333600	2.94740500
H	1.97828500	5.48074000	1.77577700
B	2.12672200	-0.37968100	-0.63685000
O	2.01125000	-1.05400400	0.59786200
O	3.45306900	-0.43582900	-1.09055300
C	3.30986200	-1.54931600	0.96662400
C	3.15410900	-2.93937000	1.56664300
H	4.13075900	-3.37810900	1.79642500
H	2.58574900	-2.87266500	2.49925500
H	2.61886500	-3.60902400	0.88997900
C	3.88638100	-0.59438500	2.01086500
H	4.84802200	-0.94889500	2.39389300

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H	4.02108100	0.40733500	1.59344300
H	3.18850700	-0.52473700	2.85136300
C	4.10040900	-1.50398400	-0.38636900
C	3.94913100	-2.78997500	-1.20304900
H	4.34269400	-2.61175700	-2.20859000
H	4.51352900	-3.61509600	-0.75821200
H	2.90145000	-3.08676500	-1.28985900
C	5.57793500	-1.16567500	-0.24568300
H	5.72019500	-0.17863600	0.19740300
H	6.09290700	-1.90957000	0.37114400
H	6.04569400	-1.16339500	-1.23442700
O	1.20837300	-1.52230900	-1.88270600
H	1.72606400	-1.42452600	-2.69376400
H	0.40158800	-0.86599500	-1.92718600
H	1.52714100	1.12606900	-2.03130700
SM3			
P	-1.31763900	-0.26003700	0.06211800
C	-3.07197700	0.17428100	-0.22930100
C	-1.15100300	-2.04665000	-0.24015900
C	-4.11559700	-0.81759100	0.29783400
H	-3.22486300	1.16867100	0.20070100
H	-3.17103700	0.27707600	-1.31757800
C	-0.80260500	0.02453800	1.78133000
C	-0.33910800	0.66279000	-1.23547600
C	-1.60279300	-2.53777800	-1.61601500
H	-0.09196400	-2.27661100	-0.08127400
H	-1.73031300	-2.52822900	0.55912500
C	-5.52740400	-0.38668500	-0.10307000
H	-4.05951100	-0.88977300	1.38845600
H	-3.92460400	-1.82346700	-0.09341600

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C	-1.80547000	-0.43744900	2.84195700
H	-0.60494600	1.09332700	1.87895400
H	0.14409300	-0.52307000	1.85996300
N	-1.00831700	1.91223200	-1.58247600
C	1.20127500	0.78703600	-1.08964100
C	-1.31942800	-4.03155700	-1.76946200
H	-2.67141200	-2.34253700	-1.77727700
H	-1.03712200	-2.00811200	-2.38706500
C	-6.59268600	-1.34613900	0.41656800
H	-5.58597200	-0.32274300	-1.19678200
H	-5.71791600	0.62361600	0.27842400
C	-1.19332800	-0.33363300	4.23967600
H	-2.70772900	0.18479200	2.79706700
H	-2.11749900	-1.47499500	2.66413000
C	-0.92006900	2.44636400	-2.93112000
C	-1.32619700	2.88022600	-0.67349300
C	1.61302100	1.97778300	-0.25736300
C	-1.75528800	-4.56775400	-3.12862100
H	-1.82424900	-4.58787200	-0.96932500
H	-0.24219800	-4.18278500	-1.63442000
H	-6.43477700	-2.35717100	0.02754200
H	-6.57066000	-1.40237800	1.50950900
H	-7.59480300	-1.02644000	0.11895700
C	-2.17265200	-0.74746700	5.33270100
H	-0.85977200	0.69750700	4.40676800
H	-0.29579800	-0.96276300	4.28289700
C	-1.18241600	3.94459900	-2.68596900
H	0.07090700	2.27106500	-3.36107400
H	-1.67119900	1.98751400	-3.58242000
O	-1.55572300	4.04896900	-1.30727300

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O	-1.47299600	2.73856000	0.52135100
C	1.78828500	3.22650500	-0.86963100
C	1.80677100	1.90708900	1.12567200
H	-1.23764100	-4.04325500	-3.93820900
H	-2.83184900	-4.43501800	-3.27999300
H	-1.53390900	-5.63397200	-3.22719300
H	-2.50134300	-1.78277500	5.19508500
H	-1.71794400	-0.67087200	6.32388900
H	-3.06309200	-0.11064000	5.32367400
H	-1.99994400	4.33648800	-3.29196700
H	-0.28878900	4.55267700	-2.84631700
C	2.11529000	4.36356100	-0.13467400
H	1.68189200	3.30193900	-1.95113600
C	2.13891100	3.03708700	1.86820700
H	1.71003300	0.94471800	1.61071700
C	2.28587700	4.27339900	1.24371500
H	2.24065900	5.31732800	-0.63913100
H	2.28686000	2.94969100	2.94102800
H	2.53921200	5.15527000	1.82383600
B	1.92480500	-0.69366000	-0.87680700
O	1.79711900	-1.24214500	0.49788500
O	3.36456400	-0.62908100	-1.11430300
C	3.05936500	-1.73558600	0.93123300
C	2.87241900	-3.13853700	1.50550300
H	3.83030700	-3.58742500	1.79161600
H	2.24608800	-3.08366100	2.40261000
H	2.37682900	-3.79725000	0.78881400
C	3.59613100	-0.82137500	2.03647800
H	4.51352000	-1.21947600	2.48251000
H	3.80036900	0.18063700	1.65264100

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H	2.84361100	-0.73943700	2.82948800
C	3.95224700	-1.67733600	-0.36416100
C	3.90304500	-2.98793700	-1.16700700
H	4.37068400	-2.81172900	-2.14149100
H	4.45311400	-3.79258600	-0.66764400
H	2.87428900	-3.31321500	-1.33313000
C	5.41553000	-1.32974100	-0.10617300
H	5.51476000	-0.33751500	0.33738400
H	5.89114400	-2.06345300	0.55411600
H	5.95885000	-1.32827700	-1.05620100
O	1.24809600	-1.59734500	-1.85575600
H	1.87655400	-1.73929300	-2.57017500
H	-0.48900900	-0.00948600	-2.08842200
H	1.50752200	1.02526700	-2.12112700
STS5			
P	-1.32215900	-0.37436300	0.02988000
C	-2.88533400	-0.93160200	-0.75479000
C	-0.53215100	-1.87587400	0.68613800
C	-3.62311400	-2.07807900	-0.05269100
H	-3.52332200	-0.04880300	-0.83621100
H	-2.61674500	-1.22129400	-1.77892200
C	-1.60346300	0.72970400	1.45158600
C	-0.09567400	0.34340700	-1.19258000
C	-0.25072800	-2.96354100	-0.35808100
H	0.40714300	-1.55678700	1.14648800
H	-1.19479300	-2.24512600	1.47984200
C	-4.91207600	-2.43567200	-0.79404800
H	-3.86920200	-1.79689200	0.97729500
H	-2.98755100	-2.96925600	0.00936800
C	-2.81446300	0.37427100	2.31620200

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H	-1.69885400	1.74185700	1.05231600
H	-0.67928800	0.69426200	2.03944200
N	-0.81785600	1.02823500	-2.28268600
C	1.08604100	1.05565000	-0.57592400
C	0.01270700	-4.31803400	0.29919400
H	-1.08689800	-3.06715300	-1.06248700
H	0.63205700	-2.66690500	-0.93171800
C	-5.66617800	-3.57741800	-0.12061600
H	-4.66801800	-2.70907200	-1.82801500
H	-5.55285100	-1.54759800	-0.85024800
C	-2.93121800	1.33177200	3.50293400
H	-3.73045200	0.43236800	1.71455300
H	-2.73869500	-0.65575900	2.68953100
C	-0.08711400	1.39030600	-3.49215600
C	-1.87079300	1.87704200	-2.10513100
C	0.86763200	2.29384300	0.21543900
C	0.37217100	-5.39312300	-0.72058000
H	-0.87285300	-4.62541000	0.87092400
H	0.82756400	-4.21007800	1.02625800
H	-5.05250800	-4.48308600	-0.07853500
H	-5.94225300	-3.31407100	0.90545300
H	-6.58455200	-3.82114600	-0.66116700
C	-4.14555700	1.02889400	4.37386000
H	-2.98596100	2.35942600	3.12509800
H	-2.01524300	1.27176400	4.10307000
C	-1.18539000	2.12677700	-4.25474900
H	0.76378900	2.03727200	-3.25255500
H	0.28462300	0.50647800	-4.01446600
O	-2.06211600	2.61026700	-3.22473500
O	-2.58110000	1.98849100	-1.12665700

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C	0.17075100	3.40315500	-0.30136700
C	1.35273700	2.42324100	1.53234300
H	1.26998900	-5.11484200	-1.28153000
H	-0.43882400	-5.53563400	-1.44252800
H	0.56185000	-6.35542100	-0.23743400
H	-4.09640100	0.01294400	4.77943300
H	-4.21260600	1.72164500	5.21689900
H	-5.07258100	1.11355100	3.79771600
H	-1.75439100	1.45505300	-4.90475000
H	-0.82522300	2.97953000	-4.82920500
C	-0.09672500	4.53155200	0.46893000
H	-0.15359800	3.39744900	-1.33796800
C	1.10912700	3.55779700	2.29851600
H	1.93210600	1.60498700	1.94952400
C	0.36260100	4.61521200	1.78076900
H	-0.65437100	5.35568100	0.03297800
H	1.49602800	3.61240400	3.31263600
H	0.15892400	5.49558300	2.38226900
B	2.37451600	0.14920300	-0.34750300
O	2.35365800	-1.26556700	-0.21167700
O	3.49899300	0.66330600	0.33394400
C	3.45978700	-1.65127000	0.61140100
C	4.03733700	-2.95961500	0.09067000
H	4.93552800	-3.24453900	0.64914900
H	3.29830300	-3.75909500	0.21132900
H	4.28802300	-2.88714400	-0.96906700
C	2.94022500	-1.84896700	2.03717100
H	3.73151400	-2.17227500	2.72008500
H	2.50488900	-0.92028000	2.42173500
H	2.16347800	-2.61979500	2.03450600

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C	4.41736200	-0.41952200	0.50654300
C	5.33597200	-0.50253800	-0.71604000
H	5.81251800	0.47239900	-0.86039700
H	6.12480600	-1.24755800	-0.57222700
H	4.77058600	-0.75049200	-1.61696800
C	5.25171200	-0.15034300	1.75125600
H	4.61975200	0.06507000	2.61528600
H	5.89467600	-1.00519800	1.98685200
H	5.89288200	0.71872500	1.57810400
O	2.79906400	0.47152800	-2.22080100
H	3.59576200	1.01651100	-2.17386800
H	0.29236100	-0.57516800	-1.65764400
H	1.90858700	1.12635300	-1.68789300
SM4			
P	-1.63307300	-0.48148600	-0.68186500
C	-2.58810800	0.04148600	-2.15455400
C	-0.32165300	-1.55318600	-1.37800600
C	-3.90145900	0.81441600	-1.96448300
H	-1.89237400	0.59175200	-2.79982900
H	-2.78808500	-0.90820100	-2.67086700
C	-2.78596700	-1.38098300	0.39978900
C	-0.97534500	1.00640500	0.12237400
C	-0.44057900	-3.05938300	-1.11153700
H	-0.29031000	-1.34244800	-2.45294500
H	0.61733900	-1.19257800	-0.95485800
C	-4.87621400	0.54931000	-3.11240800
H	-3.69596700	1.88962200	-1.91805900
H	-4.37921200	0.55847400	-1.01104200
C	-3.74621800	-2.33324400	-0.31764400
H	-3.32298000	-0.60694000	0.96068700



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H	-2.14014600	-1.91042300	1.10518200
N	-1.70134600	2.19056300	-0.20677100
C	0.13124000	1.02409000	0.89669800
C	0.94714300	-3.69745100	-1.10978400
H	-0.89256000	-3.23839200	-0.13071000
H	-1.08009000	-3.53544100	-1.86587800
C	-6.14534800	1.38562900	-2.99698600
H	-5.13343600	-0.51790500	-3.12615600
H	-4.37616100	0.75848400	-4.06675600
C	-4.55193400	-3.15510200	0.68864300
H	-4.43633000	-1.76713000	-0.95655600
H	-3.19342700	-3.01438900	-0.97673100
C	-1.21684400	3.23434400	-1.09455900
C	-2.87546900	2.53133400	0.39946100
C	0.59590500	2.32992900	1.42688300
C	0.89504300	-5.20658500	-0.90519800
H	1.51319200	-3.21938400	-0.29965700
H	1.46857600	-3.45548500	-2.04508400
H	-6.66828000	1.17854600	-2.05784000
H	-5.91383000	2.45534300	-3.01571100
H	-6.83582100	1.17733400	-3.81860600
C	-5.53629500	-4.10080800	0.00937700
H	-5.08921100	-2.47313600	1.35867500
H	-3.85812200	-3.72697400	1.31760800
C	-2.13577500	4.39380800	-0.68535800
H	-0.16360000	3.45504000	-0.90370300
H	-1.34139700	2.94482300	-2.14635800
O	-3.23461700	3.77566100	0.00349500
O	-3.53891400	1.85380200	1.15144500
C	1.90128500	2.75203000	1.14355300

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C	-0.22850400	3.14606900	2.21269900
H	0.36470000	-5.70146500	-1.72589300
H	0.37281600	-5.45713900	0.02483200
H	1.89845500	-5.63813500	-0.84939700
H	-5.01486200	-4.80940200	-0.64241700
H	-6.10464400	-4.67864200	0.74299900
H	-6.25246100	-3.54656900	-0.60605400
H	-2.53496000	4.95324000	-1.53151100
H	-1.63476800	5.07557900	0.00744700
C	2.35386600	3.98657600	1.59927500
H	2.54980300	2.11440100	0.54841400
C	0.23865900	4.36867300	2.68829300
H	-1.22837800	2.80431000	2.46996600
C	1.52545800	4.79877000	2.37124600
H	3.36191000	4.30952400	1.35704000
H	-0.40530100	4.98594100	3.30768900
H	1.88509000	5.75644400	2.73483200
B	1.05706400	-0.28416200	1.24472000
O	0.22324700	-1.51224000	1.37784300
O	1.72498100	-0.12184400	2.53502100
H	1.85826600	-0.39983200	0.30112800
C	0.31128400	-1.94278500	2.73169300
C	0.18388600	-3.46030400	2.76562700
H	0.36936500	-3.85684600	3.77017500
H	-0.83043200	-3.75922100	2.47411800
H	0.88757500	-3.92331200	2.06841600
C	-0.80634200	-1.29607400	3.55568600
H	-0.80266700	-1.65117900	4.59138300
H	-0.69500200	-0.20740300	3.55825100
H	-1.78237600	-1.53901200	3.12592800

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C	1.70660200	-1.38757600	3.16307700
C	2.84915700	-2.25014400	2.61252300
H	3.78764600	-1.69828500	2.72300700
H	2.94411600	-3.20237700	3.14510300
H	2.69867900	-2.45612700	1.54773800
C	1.88269400	-1.19703300	4.66372300
H	1.17618700	-0.45932900	5.04920800
H	1.74464800	-2.13937200	5.20587500
H	2.89366100	-0.83234000	4.87018700
B	2.41424100	0.59503900	-1.98783500
O	2.76935300	-0.64838300	-2.43033500
O	3.48009800	1.39623300	-1.68556300
H	1.28705800	0.97390800	-1.94044000
C	4.19398300	-0.78678300	-2.18730100
C	4.79751600	-1.61539000	-3.30818200
H	5.88509800	-1.67486200	-3.19881400
H	4.39677300	-2.63200900	-3.26535900
H	4.56545700	-1.19775800	-4.28956600
C	4.35937600	-1.49907500	-0.84870300
H	5.41343600	-1.70168100	-0.63676200
H	3.93598100	-0.91063900	-0.03047800
H	3.82498400	-2.45300900	-0.88769500
C	4.66858700	0.70412700	-2.14273500
C	4.99454400	1.26695300	-3.52342400
H	5.11943700	2.35000900	-3.44404300
H	5.91889600	0.84054100	-3.92309800
H	4.18296200	1.06776500	-4.22984600
C	5.80210300	0.98563100	-1.17194600
H	5.52181500	0.73490600	-0.14743000
H	6.69395300	0.41246700	-1.44485800

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H	6.05747600	2.04842500	-1.20604500
SM5			
P	-1.71857000	-0.01843300	0.46944200
C	-2.21802000	-1.53484300	1.35485900
C	-0.96012000	1.12248300	1.69000000
C	-3.13664200	-2.53412700	0.63746700
H	-1.29512700	-2.01068900	1.70250400
H	-2.72476800	-1.15104800	2.24954500
C	-3.22610900	0.74967700	-0.20614700
C	-0.64362200	-0.47615000	-0.93822300
C	-0.77216500	0.58332200	3.11004100
H	0.02114300	1.37252600	1.28088900
H	-1.56671100	2.03439300	1.67640400
C	-3.93394400	-3.36055300	1.64752900
H	-2.53855800	-3.21408400	0.02255900
H	-3.82676400	-2.02633300	-0.04700900
C	-4.33139100	0.93265300	0.83689800
H	-3.55090000	0.12495000	-1.04604200
H	-2.89851700	1.71099200	-0.61861100
N	-0.68855800	-1.86217200	-1.23688300
C	0.16766900	0.34895400	-1.62481900
C	0.07459300	1.55818300	3.92854900
H	-1.73921300	0.42124600	3.60391000
H	-0.23682500	-0.37086600	3.07360800
C	-4.78555200	-4.42964400	0.97248900
H	-4.57350800	-2.69204800	2.23823400
H	-3.23907500	-3.82863900	2.35578300
C	-5.50557000	1.73894300	0.28181800
H	-4.69244700	-0.04867500	1.17157600
H	-3.93359500	1.44038800	1.72687600

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C	0.32640300	-2.84766100	-0.86753800
C	-1.60314700	-2.37275100	-2.11569600
C	1.02719300	-0.22617900	-2.70266100
C	0.37764000	1.01011400	5.31740700
H	-0.43525000	2.52850500	4.00025200
H	1.01975800	1.70850300	3.39526000
H	-5.50307400	-3.98146700	0.27798900
H	-4.16182500	-5.12297000	0.39965400
H	-5.34827800	-5.01276400	1.70634700
C	-6.63073400	1.89711800	1.29871900
H	-5.88459600	1.24460100	-0.62066400
H	-5.14511700	2.72619600	-0.03240600
C	0.10671600	-3.86553900	-1.98880200
H	1.32831900	-2.40981200	-0.84273400
H	0.10884200	-3.26549500	0.12374800
O	-1.24833100	-3.63748900	-2.43005600
O	-2.59391400	-1.82220500	-2.54067700
C	2.41434100	-0.26911000	-2.52593400
C	0.45986700	-0.73629600	-3.87541200
H	0.93888300	0.07474300	5.23000700
H	-0.53993700	0.80826800	5.88117500
H	0.98114900	1.71067100	5.90159200
H	-6.27930400	2.41413200	2.19760700
H	-7.46191100	2.47426200	0.88497600
H	-7.02244300	0.92252400	1.60715100
H	0.18605500	-4.90217700	-1.66249100
H	0.77700300	-3.68469000	-2.83486400
C	3.21836000	-0.83516700	-3.51165500
H	2.84424400	0.09364000	-1.59686200
C	1.27264400	-1.28542500	-4.86392700

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H	-0.61883900	-0.70033200	-4.00794000
C	2.65311900	-1.33888300	-4.68152700
H	4.29227900	-0.88528400	-3.35985000
H	0.82534700	-1.67606300	-5.77292200
H	3.28670500	-1.77305300	-5.44896900
B	0.32779400	1.88471000	-1.34876000
O	-0.62926100	2.64383900	-0.72370400
O	1.39933800	2.60770600	-1.77733800
H	1.75044000	0.64106700	0.52690000
C	-0.22599100	4.03303700	-0.85637100
C	-0.57774600	4.76678200	0.42575100
H	-0.22580800	5.80233900	0.38168500
H	-1.66417900	4.78544700	0.55399600
H	-0.13373600	4.28480500	1.29933800
C	-1.00716100	4.59900600	-2.03708800
H	-0.79394400	5.66095200	-2.18576000
H	-0.76700900	4.06093400	-2.95875400
H	-2.07781300	4.48636900	-1.84503900
C	1.30959500	3.90532700	-1.13926700
C	2.14875300	3.82712000	0.13252600
H	3.16643600	3.53262800	-0.13646300
H	2.18837300	4.79266800	0.64486800
H	1.76216300	3.07124500	0.82372900
C	1.86856700	4.95413300	-2.08508700
H	1.38410100	4.91319800	-3.06228700
H	1.73916600	5.95715300	-1.66624500
H	2.93814700	4.78068100	-2.22776900
B	1.84524300	-0.44800100	1.14036800
O	2.27504500	-0.30642500	2.54291400
O	2.86895700	-1.28767000	0.48860300

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H	0.70521500	-0.97419300	1.11281100
C	3.62585000	-0.72181200	2.60815900
C	3.93515200	-1.20488700	4.01899700
H	4.93267900	-1.65517800	4.07847800
H	3.90569900	-0.36073300	4.71591800
H	3.19801900	-1.94012600	4.35061700
C	4.52856400	0.46530300	2.25165900
H	5.59204100	0.23769800	2.38106800
H	4.35564800	0.77428900	1.21594200
H	4.27453500	1.30594600	2.90514100
C	3.68348600	-1.83232600	1.51072500
C	3.05372500	-3.14012800	2.00356800
H	2.91286800	-3.80828200	1.14760400
H	3.68008700	-3.65710600	2.73843300
H	2.07611500	-2.94039700	2.45406700
C	5.07281300	-2.10229800	0.94744600
H	5.47764300	-1.20804500	0.46825500
H	5.76764200	-2.42890400	1.72963200
H	5.01811000	-2.89263900	0.19142000
STS6			
P	0.87474600	0.96038200	-0.73205500
C	0.23533500	2.19682900	-1.92182300
C	0.86799500	1.84152200	0.86486700
C	0.69670000	2.06455000	-3.37752300
H	-0.85252300	2.09827200	-1.82568800
H	0.49532000	3.18608200	-1.52802600
C	2.47088000	0.25676000	-1.28558000
C	-0.37210200	-0.39871800	-0.73026500
C	1.89284100	2.96712000	1.04574900
H	-0.14515100	2.25886400	0.90782200

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H	0.94852300	1.10230100	1.66265800
C	2.01894200	2.78508400	-3.64564800
H	-0.07696300	2.49432500	-4.02391300
H	0.78175200	1.00980500	-3.66321300
C	3.74180200	0.89017100	-0.72669900
H	2.44714900	0.28218400	-2.37983500
H	2.41760500	-0.79944200	-1.00749500
N	-1.07494400	-0.49461900	-1.98878900
C	-0.17141100	-1.55965500	-0.00094000
C	1.48479500	3.87239600	2.20988800
H	2.88570800	2.55343500	1.24519900
H	1.98201200	3.57384200	0.13365800
C	2.53563400	2.53563500	-5.05806500
H	2.77465400	2.46287600	-2.91711500
H	1.87706200	3.86041900	-3.48004500
C	4.98593100	0.28363700	-1.37492900
H	3.74947500	1.97637600	-0.88192800
H	3.76733600	0.72265000	0.35707800
C	-2.52344700	-0.40664600	-2.16081600
C	-0.50755800	-1.20238300	-3.02127900
C	-1.10062300	-2.69879800	-0.29873300
C	2.49076800	4.99226800	2.45223400
H	1.38028500	3.26093300	3.11447000
H	0.49219000	4.29268400	2.00826500
H	2.72977900	1.47019800	-5.21905800
H	1.80213100	2.85502800	-5.80538700
H	3.46483300	3.07985800	-5.24673800
C	6.27360000	0.79271100	-0.73627800
H	4.98044400	0.51531800	-2.44754600
H	4.93640600	-0.80972900	-1.29721900



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C	-2.74511800	-1.51446100	-3.18993600
H	-3.04896800	-0.57221500	-1.21889800
H	-2.80043700	0.57924100	-2.55368700
O	-1.47487500	-1.63561500	-3.85737100
O	0.67346000	-1.38704600	-3.21532900
C	-2.40090400	-2.74149400	0.22278600
C	-0.68578300	-3.73910200	-1.14015200
H	2.59259100	5.62823300	1.56668000
H	3.48092200	4.58820400	2.68676900
H	2.18423700	5.62903100	3.28636600
H	6.31056200	0.53567300	0.32805100
H	7.15601000	0.36019400	-1.21512900
H	6.34879600	1.88207900	-0.81657100
H	-3.50093800	-1.27601900	-3.93791200
H	-2.97500100	-2.47178300	-2.70950100
C	-3.26053300	-3.79068500	-0.09792500
H	-2.74011900	-1.93828100	0.87171800
C	-1.54462800	-4.78827900	-1.46105000
H	0.31695200	-3.70594600	-1.55783600
C	-2.83665000	-4.81694200	-0.94078700
H	-4.26520200	-3.80571600	0.31466500
H	-1.20425800	-5.58113800	-2.12039000
H	-3.50784500	-5.63362900	-1.18883700
B	0.85668600	-1.77042000	1.10916800
O	1.89647700	-0.89674500	1.42556600
O	0.90165700	-2.90571300	1.89207800
H	-1.50355200	-0.05974700	1.73214500
C	2.78820200	-1.59709300	2.31878300
C	3.39101200	-0.59951300	3.29377500
H	3.98834600	-1.11459200	4.05305000

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H	4.05217500	0.08959400	2.75820400
H	2.61747500	-0.01360400	3.79471000
C	3.87921900	-2.23394200	1.46105500
H	4.62077800	-2.75308600	2.07479600
H	3.45112700	-2.94774300	0.75013000
H	4.39293900	-1.44982500	0.89640200
C	1.83411100	-2.65340600	2.95891500
C	1.03418100	-2.08591600	4.12992200
H	0.24654500	-2.79621500	4.39306300
H	1.66402400	-1.92272900	5.00924300
H	0.55616300	-1.13983100	3.85588900
C	2.50344700	-3.95940900	3.35219000
H	2.94270400	-4.45816000	2.48634000
H	3.28737800	-3.78396500	4.09617900
H	1.76171700	-4.63172100	3.79131400
B	-2.21328800	0.74946100	1.14108000
O	-2.19951100	2.12707200	1.53029400
O	-3.56857600	0.36182000	0.91784300
H	-1.43533400	0.58994500	-0.06022600
C	-3.54694400	2.51989200	1.79139200
C	-3.70824000	3.99698100	1.46222100
H	-4.75321600	4.31074200	1.55809300
H	-3.11059500	4.59445300	2.15730000
H	-3.36675200	4.21614200	0.44831900
C	-3.82292600	2.28031400	3.27731700
H	-4.81519800	2.63446500	3.57379700
H	-3.74213500	1.21578500	3.51632900
H	-3.07338700	2.81888200	3.86368800
C	-4.36093500	1.55059900	0.87861100
C	-4.43064800	2.04893400	-0.56579200

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<b>H</b>	<b>-4.84402100</b>	<b>1.25715600</b>	<b>-1.19742000</b>
<b>H</b>	<b>-5.07156100</b>	<b>2.93076300</b>	<b>-0.66078600</b>
<b>H</b>	<b>-3.43075200</b>	<b>2.30133200</b>	<b>-0.93414700</b>
<b>C</b>	<b>-5.75969500</b>	<b>1.22521300</b>	<b>1.38221600</b>
<b>H</b>	<b>-5.72324000</b>	<b>0.73312700</b>	<b>2.35582900</b>
<b>H</b>	<b>-6.36761200</b>	<b>2.13245300</b>	<b>1.46650100</b>
<b>H</b>	<b>-6.25548800</b>	<b>0.54836500</b>	<b>0.68006200</b>

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**Part 14: The geometries (Å) for all the optimized compounds and transition states of PBu<sub>3</sub>-catalyzed hydroboration of propiolonitrile at the M06-2X/6-31G(d,p)/SMD<sub>dichloromethane</sub> level**

**Propiolonitrile**

C	1.04532400	0.00005200	0.00005300
C	-0.38277200	0.00001500	0.00001900
C	-1.07998700	1.21759300	0.00000100
C	-1.07993700	-1.21757200	0.00001100
C	-2.46903500	1.20985700	-0.00001400
H	-0.52837100	2.15181000	0.00002200
C	-2.46900000	-1.20988700	-0.00002000
H	-0.52830800	-2.15178200	0.00002400
C	-3.16235600	-0.00003500	-0.00003000
H	-3.01202100	2.14916600	-0.00001600
H	-3.01192800	-2.14923000	-0.00003300
H	-4.24783800	-0.00003800	-0.00004200
C	2.25735800	0.00001700	0.00008500
C	3.63452500	0.00000500	-0.00000500
N	4.79482100	-0.00002900	-0.00007800

**PBu<sub>3</sub>**

P	-0.41166200	0.17975800	-1.21395600
C	0.82716300	-1.21147800	-1.24658400
C	1.24328900	-1.84128900	0.08125300
H	1.71067800	-0.82400100	-1.77014500
H	0.40207300	-1.97666400	-1.90914800
C	2.31319500	-2.91998900	-0.09731500
H	1.62884500	-1.06902300	0.75992000
H	0.36910900	-2.28293200	0.57578200

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C	2.71866600	-3.56645300	1.22378700
H	1.93924200	-3.68728800	-0.78675600
H	3.19346900	-2.47433800	-0.57807500
H	3.48906300	-4.32952800	1.07962900
H	3.11457900	-2.81973000	1.92035100
H	1.85992100	-4.04605000	1.70536200
C	-1.80615300	-0.60061700	-0.26115200
C	-3.01118300	0.33190200	-0.12427800
H	-1.46514000	-0.92056800	0.73159100
H	-2.09966700	-1.50526200	-0.80992000
C	-4.18761700	-0.32537100	0.59716400
H	-2.71801900	1.23886200	0.42144000
H	-3.33509900	0.66115100	-1.12047600
C	-5.38896200	0.60594000	0.72836500
H	-4.47953800	-1.23171500	0.05173500
H	-3.86242700	-0.65342000	1.59257200
H	-6.22275200	0.11628000	1.23975700
H	-5.12876200	1.50409000	1.29831300
H	-5.74335400	0.92936400	-0.25601200
C	0.30838400	1.29423200	0.09332000
C	1.70507900	1.80160100	-0.26865500
H	0.32723700	0.78248300	1.06437600
H	-0.37407700	2.14719700	0.19503900
C	2.24131500	2.82459500	0.73264500
H	2.40396400	0.95561800	-0.32250700
H	1.68731600	2.25119000	-1.27124000
C	3.64532100	3.30599300	0.37998200
H	1.55549500	3.68000900	0.77485300
H	2.24375900	2.37859300	1.73545600
H	4.01175500	4.04179700	1.10165100

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H	4.35398600	2.47105500	0.36552000
H	3.66227900	3.77206300	-0.61092000
HBpin			
B	0.00000000	0.00000000	1.93323300
O	0.34765700	1.08964900	1.18785800
O	-0.34765700	-1.08964900	1.18785800
H	0.00000000	0.00000000	3.12059000
C	0.00000000	0.78152300	-0.18829400
C	1.02470400	1.41849100	-1.10994700
H	0.83405200	1.12870100	-2.14807800
H	0.95150700	2.50746200	-1.04199300
H	2.04154300	1.12513400	-0.84305000
C	-1.38382000	1.37627000	-0.43370900
H	-1.69658000	1.23851200	-1.47233900
H	-2.13169500	0.91827100	0.22112300
H	-1.35122800	2.44799400	-0.22020200
C	0.00000000	-0.78152300	-0.18829400
C	1.38382000	-1.37627000	-0.43370900
H	1.35122800	-2.44799400	-0.22020200
H	1.69658000	-1.23851200	-1.47233900
H	2.13169500	-0.91827100	0.22112300
C	-1.02470400	-1.41849100	-1.10994700
H	-2.04154300	-1.12513400	-0.84305000
H	-0.83405200	-1.12870100	-2.14807800
H	-0.95150700	-2.50746200	-1.04199300
2H <sub>2</sub> O			
O	1.34866100	-0.04938300	-0.08243600
H	1.69199600	0.85372600	-0.09306500
H	1.68690600	-0.42906900	0.73925700
O	-1.49360600	-0.08199200	-0.04422800

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H	-1.69694600	0.71551800	0.45707400
H	-0.52240000	-0.08917500	-0.08995800
TS1 <sub>CN</sub>			
C	-1.38092200	0.89971700	1.14492900
C	-2.53326100	0.03090700	0.93233900
C	-2.72277700	-0.73780300	-0.22036500
C	-3.51517000	0.01215900	1.93696200
C	-3.87061500	-1.51098600	-0.36697500
H	-1.97389200	-0.72252800	-1.00564200
C	-4.65283500	-0.77130000	1.79036000
H	-3.36802300	0.61314500	2.82840800
C	-4.83496400	-1.53530200	0.63788500
H	-4.00937200	-2.09672400	-1.26997600
H	-5.39873000	-0.78560100	2.57866700
H	-5.72474800	-2.14633700	0.52439600
C	-0.98684000	1.89756200	1.78857900
P	0.46882800	0.06880700	-0.14385800
C	0.86412400	-1.24623200	-1.38833800
C	0.68547300	-2.65541100	-0.82166200
H	1.88646900	-1.10250200	-1.76087200
H	0.18701000	-1.09406400	-2.23802400
C	0.90175400	-3.74023900	-1.87627300
H	1.39024600	-2.81310800	0.00562500
H	-0.32200800	-2.75778100	-0.39497200
C	0.73584900	-5.14571600	-1.30673800
H	0.19307200	-3.58637400	-2.69955300
H	1.90561000	-3.62859500	-2.30478000
H	0.89210300	-5.90963300	-2.07360000
H	1.45372500	-5.32820100	-0.50031700
H	-0.26912000	-5.28447900	-0.89470900

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C	1.70932900	-0.18805900	1.19698200
C	3.17157800	-0.29854700	0.76414800
H	1.40403700	-1.08762100	1.74552600
H	1.58469400	0.65373200	1.88940600
C	4.11003600	-0.47972600	1.95791100
H	3.29728600	-1.14706100	0.07869600
H	3.46580700	0.60109000	0.20914200
C	5.57161900	-0.59353200	1.53575700
H	3.98589000	0.36754600	2.64344500
H	3.81291200	-1.37708400	2.51498300
H	6.22911100	-0.72297100	2.40008500
H	5.72154200	-1.44950600	0.86937400
H	5.89495700	0.30539100	1.00059100
C	1.02078600	1.62139700	-0.96901800
C	0.01698500	2.10526700	-2.01761800
H	2.00509400	1.45906000	-1.42390700
H	1.14887600	2.38010400	-0.18683600
C	0.46288500	3.39850600	-2.69845200
H	-0.12879200	1.32764700	-2.77971700
H	-0.95935600	2.26310600	-1.54023500
C	-0.54039200	3.88329700	-3.74040500
H	0.60848100	4.17175400	-1.93399700
H	1.44056800	3.23858200	-3.16994700
H	-0.20718700	4.80988300	-4.21631500
H	-0.68090900	3.13432200	-4.52690800
H	-1.51714300	4.07333900	-3.28354800
C	-0.10444500	2.85520300	2.21107000
N	0.62431200	3.68605500	2.58955800
M1 <sub>CN</sub>			
C	-0.59638200	-0.68953700	-1.29778800



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C	-2.01876700	-0.34448800	-1.00584800
C	-2.64453600	-0.73391800	0.18491000
C	-2.76047300	0.37758700	-1.94912500
C	-3.96950100	-0.38656400	0.43896500
H	-2.09694500	-1.33630100	0.90601800
C	-4.08398900	0.72597100	-1.69566900
H	-2.28094000	0.66766100	-2.87924700
C	-4.69027700	0.35292500	-0.49671400
H	-4.44133700	-0.70232200	1.36446700
H	-4.64223800	1.29353500	-2.43405100
H	-5.72085900	0.62895200	-0.29687700
C	-0.24046200	-1.29641000	-2.44828700
P	0.65556500	-0.17886300	-0.06008700
C	-0.01847600	0.77240100	1.34141500
C	-0.61741200	2.12245200	0.93341800
H	0.81096300	0.90808800	2.04669400
H	-0.76627100	0.15198800	1.84315700
C	-1.32018000	2.79918800	2.10937200
H	0.17572200	2.77709000	0.55094400
H	-1.33734800	1.98525100	0.11737200
C	-1.92049200	4.14606600	1.72059600
H	-2.11046900	2.13364500	2.47839700
H	-0.60683000	2.92860400	2.93276600
H	-2.42282400	4.61813800	2.56939600
H	-1.14619700	4.83307000	1.36388500
H	-2.65626400	4.02575100	0.91866600
C	1.88104800	0.89141200	-0.88234800
C	2.92492300	1.49024900	0.06440400
H	1.31497300	1.67771700	-1.39505000
H	2.36466600	0.28209000	-1.65256900

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C	3.95594500	2.32000000	-0.70127400
H	2.43473600	2.12535100	0.81268700
H	3.43885500	0.68983800	0.61120500
C	5.00329600	2.93152000	0.22356900
H	4.44384200	1.68363900	-1.44904000
H	3.43774700	3.11270200	-1.25452300
H	5.73410100	3.51984800	-0.33799900
H	4.53706800	3.59192100	0.96207600
H	5.54700700	2.15256800	0.76799200
C	1.51700600	-1.63727300	0.60541900
C	0.56775200	-2.65310800	1.24549800
H	2.25282400	-1.27088900	1.33076100
H	2.06820200	-2.08570800	-0.22909500
C	1.32186000	-3.86660700	1.78814100
H	0.00736000	-2.17855400	2.06201200
H	-0.16752000	-2.98272400	0.50078200
C	0.38400600	-4.88867700	2.42224200
H	1.88269400	-4.33261000	0.96920800
H	2.06208100	-3.53142500	2.52488500
H	0.93611200	-5.75220100	2.80315000
H	-0.16854100	-4.44787900	3.25852500
H	-0.34726000	-5.25239800	1.69332100
C	1.09200300	-1.64142100	-2.73775600
N	2.14686500	-1.99744300	-3.10535100
TS1' <sub>CN</sub>			
C	-1.39669700	1.41208800	2.10301100
C	-2.51279200	1.07150500	1.26927500
C	-2.54186100	1.53411300	-0.06027100
C	-3.53612500	0.21987200	1.71886200
C	-3.55936500	1.13332400	-0.91995500

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H	-1.75978100	2.20523500	-0.40390500
C	-4.53601300	-0.19192400	0.84480600
H	-3.52342500	-0.12902700	2.74649800
C	-4.55251400	0.26001300	-0.47617600
H	-3.57172100	1.49678200	-1.94339000
H	-5.31070800	-0.86648900	1.19670900
H	-5.33945000	-0.06025100	-1.15178600
C	-0.14322300	1.27508300	2.03541100
P	0.88539400	0.06515600	0.22735500
C	-0.03900100	-0.60846200	-1.22350500
C	-1.10722400	-1.63292100	-0.83786900
H	0.68515800	-1.04908300	-1.92164400
H	-0.50296100	0.24614400	-1.72879300
C	-1.93787600	-2.07740800	-2.04124100
H	-0.63087000	-2.51110900	-0.38159100
H	-1.77720600	-1.20593800	-0.07931600
C	-3.00978300	-3.09223900	-1.65841300
H	-2.40870600	-1.19415600	-2.49169900
H	-1.27427100	-2.50310100	-2.80458800
H	-3.60367600	-3.39509200	-2.52551400
H	-2.56116900	-3.99331700	-1.22708500
H	-3.69205900	-2.66981800	-0.91275900
C	1.69962500	-1.39551100	1.00138200
C	2.52037800	-2.29238000	0.07350500
H	0.90644800	-1.97344100	1.49136300
H	2.33121000	-0.99486800	1.80506200
C	3.15550000	-3.46354300	0.82410700
H	1.88059900	-2.68478200	-0.72779600
H	3.30959900	-1.70489700	-0.41205400
C	3.97543500	-4.36506200	-0.09365800

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H	3.79233500	-3.07214700	1.62695900
H	2.36509100	-4.04831600	1.31083100
H	4.42318500	-5.19636500	0.45814500
H	3.35078800	-4.78758100	-0.88762800
H	4.78597500	-3.80433800	-0.57073800
C	2.26897100	1.02973000	-0.51309500
C	1.79397200	2.35647200	-1.11012700
H	2.77354700	0.42163300	-1.27405100
H	2.99073400	1.21439100	0.29282800
C	2.94272200	3.17108300	-1.70339300
H	1.04560400	2.16628600	-1.89113300
H	1.29259400	2.94782400	-0.33222200
C	2.47087400	4.49723900	-2.29137100
H	3.69006100	3.35541000	-0.92182600
H	3.44216600	2.57693400	-2.47874100
H	3.30432500	5.06814600	-2.71018300
H	1.74117300	4.33356400	-3.09130900
H	1.99200200	5.11586100	-1.52536600
C	1.05026000	1.61460400	2.69254100
N	2.07727400	1.85493000	3.17906100
M2 <sub>CN</sub>			
C	0.74761600	0.44913300	-1.10856800
C	1.99366100	-0.18111300	-0.58604700
C	2.50957700	0.14120300	0.67579900
C	2.67878100	-1.11739900	-1.37237800
C	3.67204200	-0.46547400	1.14537500
H	2.00847700	0.89014500	1.28413600
C	3.84111800	-1.72281000	-0.90342700
H	2.28558200	-1.37487900	-2.35177100
C	4.33813500	-1.40355500	0.35921500

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H	4.06123000	-0.19890500	2.12327000
H	4.35645000	-2.44978100	-1.52360400
H	5.24211900	-1.87929200	0.72612000
C	0.52985800	1.09167300	-2.27704900
P	-0.77886400	0.35382200	-0.13220400
C	-0.62168600	-0.67071400	1.36384600
C	-0.33641100	-2.14620600	1.06368100
H	-1.55788400	-0.55864500	1.92397300
H	0.17220600	-0.23905200	1.98120700
C	0.01347600	-2.91930100	2.33424700
H	-1.21340000	-2.59949800	0.58453700
H	0.49428200	-2.23377400	0.35212000
C	0.28468400	-4.39348300	2.05355600
H	0.89782900	-2.45999000	2.79325100
H	-0.80529500	-2.81858500	3.05747800
H	0.53982400	-4.93313300	2.96972100
H	-0.59277300	-4.87705800	1.61193600
H	1.11799000	-4.50818200	1.35261200
C	-2.07407700	-0.38648700	-1.17260900
C	-3.43966000	-0.52072000	-0.49666200
H	-1.69039100	-1.36458500	-1.48677200
H	-2.12513800	0.23946300	-2.06928500
C	-4.45581700	-1.18760200	-1.42427400
H	-3.35052800	-1.11221700	0.42389800
H	-3.81129700	0.46915000	-0.20508400
C	-5.82868600	-1.32261200	-0.77381400
H	-4.53587600	-0.60158000	-2.34764200
H	-4.08075000	-2.17692200	-1.71330400
H	-6.54283800	-1.80198000	-1.44893800
H	-5.77285900	-1.92542500	0.13856300

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H	-6.23114500	-0.34146600	-0.50162000
C	-1.31866700	2.01396700	0.37389300
C	-0.27982300	2.75223700	1.22084700
H	-2.26350200	1.90007900	0.91787500
H	-1.52416100	2.56007800	-0.55383400
C	-0.76377400	4.14581800	1.62011900
H	-0.05393800	2.17277100	2.12567700
H	0.65513400	2.83972800	0.65324900
C	0.26744800	4.89424800	2.45832200
H	-0.99214200	4.71715300	0.71245700
H	-1.70363500	4.05469800	2.17832400
H	-0.09099600	5.88972200	2.73433200
H	0.49144100	4.35026800	3.38185400
H	1.20510900	5.01578200	1.90657800
C	1.61563100	1.25319500	-3.17142600
N	2.40761200	1.46065600	-4.00630400

M3<sub>CN</sub>

C	-0.35816900	-1.06754800	0.10116700
C	-1.51559500	-1.86538300	-0.40419200
C	-2.43445600	-2.44750600	0.47536700
C	-1.70007300	-2.00461100	-1.78416900
C	-3.54220100	-3.12971000	-0.02114300
H	-2.27671800	-2.36467500	1.54751800
C	-2.80757000	-2.68991800	-2.27803400
H	-0.97655300	-1.56402500	-2.46525500
C	-3.73601500	-3.24244300	-1.39760300
H	-4.25249100	-3.57681700	0.66727000
H	-2.94583700	-2.79018500	-3.34993000
H	-4.60269000	-3.77057800	-1.78238900
C	0.90519300	-1.53903000	0.18972700

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P	-0.75593300	0.66251300	0.52849500
C	-2.52180000	0.75973700	0.98450500
C	-3.52906500	0.73813300	-0.17084700
H	-2.61997600	1.69244500	1.55416600
H	-2.71598100	-0.05947900	1.68495300
C	-4.96250100	0.65098200	0.35201300
H	-3.41268100	1.64396800	-0.77882100
H	-3.34359200	-0.11388700	-0.83275500
C	-5.98095500	0.61197700	-0.78226600
H	-5.05806700	-0.25347200	0.96611400
H	-5.16472400	1.50331000	1.01242100
H	-7.00260500	0.54223500	-0.39897900
H	-5.91488400	1.51257300	-1.40140900
H	-5.80424800	-0.25332100	-1.42997300
C	-0.48407500	1.76416500	-0.89073100
C	-0.86958900	3.22206600	-0.61762400
H	-1.05760200	1.34741800	-1.72816300
H	0.58123500	1.67323500	-1.11800600
C	-0.72627200	4.07312100	-1.87964800
H	-1.90226900	3.29004900	-0.25238100
H	-0.22435700	3.62913900	0.16990500
C	-1.06162800	5.53901300	-1.62540900
H	0.29965900	3.98440100	-2.25714900
H	-1.38339500	3.66894300	-2.65936400
H	-0.96193600	6.13300800	-2.53792700
H	-2.08933900	5.64871000	-1.26395100
H	-0.39433800	5.96787100	-0.87093000
C	0.16092200	1.26208700	1.97686500
C	-0.02719600	0.38184600	3.21551800
H	-0.21879700	2.27486800	2.15992200

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H	1.21205800	1.34234900	1.68814100
C	0.84984900	0.86308000	4.37032100
H	-1.07999200	0.39005700	3.52523900
H	0.23267200	-0.65595500	2.97472800
C	0.67876700	0.00351800	5.61833500
H	1.89720000	0.84483300	4.04509600
H	0.60779700	1.90849400	4.59863700
H	1.31673100	0.35503000	6.43389300
H	-0.35789100	0.02332800	5.97060700
H	0.94210800	-1.03869800	5.41136600
C	1.07237600	-2.92887900	-0.16020800
N	1.25543000	-4.04279100	-0.42664400
B	2.31689500	-0.73383500	0.58705400
O	3.44411100	-1.49907700	0.04898900
O	2.35381500	0.57631200	-0.10070500
H	2.33916700	-0.59639700	1.81273600
C	4.28129400	-0.59373500	-0.65053200
C	5.04775200	-1.35367800	-1.72540500
H	5.60605900	-0.66875900	-2.37302900
H	5.76421200	-2.03425600	-1.25471100
H	4.37147900	-1.95087200	-2.34107800
C	5.26486400	0.04510600	0.33558300
H	6.00143500	0.67890300	-0.16894800
H	4.73119000	0.64901200	1.07587300
H	5.79883100	-0.75121300	0.86257300
C	3.25697700	0.44890100	-1.19542200
C	2.51567800	-0.09677300	-2.42177500
H	1.65495300	0.54075800	-2.64844700
H	3.16140400	-0.11623400	-3.30556300
H	2.15393800	-1.11341600	-2.23770600



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C	3.84321200	1.81820900	-1.51107200
H	4.24578200	2.28869400	-0.61130800
H	4.64210400	1.74167700	-2.25659300
H	3.06569800	2.47371800	-1.91876900
M3 <sub>CN'</sub>			
C	0.12359600	0.15316200	-0.42169900
C	0.00535800	1.62312900	-0.19910600
C	-0.07782300	2.15186400	1.09277000
C	0.01401000	2.49269800	-1.29431700
C	-0.14057900	3.52918800	1.28794600
H	-0.10410000	1.47645600	1.94571400
C	-0.04376400	3.86977100	-1.09779800
H	0.07397400	2.08269900	-2.29800700
C	-0.11452500	4.39129600	0.19295900
H	-0.21143700	3.92821300	2.29498600
H	-0.03220300	4.53615800	-1.95464500
H	-0.15670900	5.46516100	0.34506100
C	-0.84060700	-0.54267800	-1.06471000
P	1.66268100	-0.64129500	0.16894300
C	2.74643800	0.55278100	1.00931300
C	3.36969500	1.60943700	0.09191100
H	3.52425000	-0.05216200	1.49169800
H	2.16513100	1.02186000	1.80882900
C	4.13329100	2.65940700	0.89807800
H	4.04804600	1.12475200	-0.62121200
H	2.59081400	2.10820100	-0.49546400
C	4.72923800	3.74105400	0.00346500
H	3.44749600	3.11551100	1.62263700
H	4.92534200	2.16930300	1.47754000
H	5.27297400	4.48720800	0.58922400

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H	5.42609300	3.31104000	-0.72330200
H	3.94122200	4.25892800	-0.55331700
C	2.58080500	-1.32048400	-1.24679500
C	3.92648500	-1.93870800	-0.85464900
H	2.71274400	-0.49229600	-1.95326000
H	1.93619300	-2.06361700	-1.72660900
C	4.65529500	-2.49530300	-2.07785400
H	4.55920700	-1.18587300	-0.36815600
H	3.76889900	-2.74512400	-0.12814100
C	5.99985100	-3.11438000	-1.71049000
H	4.01897700	-3.24423800	-2.56379600
H	4.80178700	-1.68777600	-2.80526100
H	6.50878100	-3.50925000	-2.59388400
H	6.65915300	-2.37369100	-1.24631300
H	5.87076700	-3.93832000	-1.00122200
C	1.27275900	-1.95919500	1.36173100
C	0.35754200	-1.47207500	2.48934800
H	2.23163400	-2.31953300	1.75182600
H	0.81004600	-2.78054200	0.80527000
C	-0.04634900	-2.61035500	3.42491800
H	0.86012000	-0.68313900	3.06405000
H	-0.54699500	-1.02690000	2.05642300
C	-0.99490400	-2.13263100	4.51951200
H	-0.52731600	-3.39968500	2.83482200
H	0.85248500	-3.05285700	3.87113000
H	-1.28589300	-2.95363300	5.18030000
H	-0.52728400	-1.35602500	5.13356900
H	-1.90741900	-1.71090200	4.08457700
C	-0.67107400	-1.95309800	-1.28225800
N	-0.57421400	-3.09440000	-1.47472100

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B	-2.30988200	0.08101600	-1.63454400
O	-3.24427900	-1.05176800	-1.72189800
O	-2.89787100	1.02135100	-0.68256800
H	-2.05630100	0.61673300	-2.71586300
C	-4.43380600	-0.67994200	-1.04569100
C	-5.09935000	-1.92790500	-0.47849000
H	-5.95960200	-1.66762500	0.14824600
H	-5.45646900	-2.56127700	-1.29691500
H	-4.39429100	-2.51340500	0.11628700
C	-5.37613700	0.00260400	-2.04265700
H	-6.35281700	0.22897700	-1.60230700
H	-4.93333900	0.93288400	-2.41142600
H	-5.52935600	-0.66640300	-2.89483000
C	-3.90833000	0.32362700	0.02696400
C	-3.28115200	-0.40782500	1.22192600
H	-2.68907700	0.31055100	1.79947700
H	-4.03888700	-0.84331700	1.88223200
H	-2.61796400	-1.21073200	0.88234700
C	-4.94059000	1.32619800	0.52691300
H	-5.29647100	1.96026100	-0.28815700
H	-5.79942700	0.81858500	0.97979900
H	-4.48913200	1.97347700	1.28595700
TS2S <sub>CN</sub>			
C	-0.70748700	-1.05764100	-0.16149300
C	-1.99698600	-1.71450700	-0.52768500
C	-2.89490400	-2.18280300	0.44225600
C	-2.34038200	-1.87350900	-1.87823700
C	-4.11793800	-2.74031000	0.07599000
H	-2.62311900	-2.11559900	1.49235600
C	-3.55575500	-2.44389500	-2.24826300

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H	-1.64448800	-1.53050400	-2.64082400
C	-4.45610300	-2.86559600	-1.27087700
H	-4.80206900	-3.09023700	0.84346400
H	-3.80410100	-2.55147200	-3.29996000
H	-5.40791900	-3.30242900	-1.55667300
C	0.52463900	-1.62011200	-0.53950000
P	-0.76742000	0.58809300	0.46312100
C	-2.37753800	0.90039400	1.27116500
C	-3.55778100	1.12391700	0.31783900
H	-2.22982900	1.78423700	1.90276000
H	-2.57070900	0.05989200	1.94446200
C	-4.89207700	1.07380500	1.06050000
H	-3.44683600	2.09704100	-0.17720900
H	-3.56704600	0.36587500	-0.47360000
C	-6.07836900	1.25450300	0.11956300
H	-4.97274300	0.10645900	1.57272500
H	-4.90609200	1.84481700	1.84096900
H	-7.02753800	1.22095700	0.66155600
H	-6.02377000	2.21469700	-0.40392000
H	-6.09352400	0.46159300	-0.63588400
C	-0.61625700	1.87352000	-0.82845700
C	-0.61036100	3.30903500	-0.29734000
H	-1.45336200	1.70982000	-1.51867800
H	0.30941200	1.65376300	-1.36827700
C	-0.55618700	4.32990500	-1.43406400
H	-1.50485800	3.49451100	0.31214500
H	0.25695200	3.45507500	0.35897800
C	-0.52799100	5.76636700	-0.92190200
H	0.33242000	4.13445700	-2.04702100
H	-1.42484300	4.18377500	-2.08786100

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H	-0.49005100	6.48317900	-1.74683300
H	-1.41984500	5.98756200	-0.32636800
H	0.34758900	5.93857700	-0.28741000
C	0.50998800	0.91907900	1.72620300
C	0.73381400	-0.23271700	2.70759300
H	0.17967800	1.82192600	2.25440700
H	1.43381700	1.15738800	1.19085000
C	1.69514500	0.16697900	3.82692200
H	-0.22007500	-0.55690400	3.14432100
H	1.13781400	-1.09641500	2.16548500
C	2.04488200	-1.00927200	4.73247300
H	2.61183900	0.57820500	3.38423400
H	1.24642500	0.97590100	4.41659600
H	2.71628100	-0.70618200	5.54070800
H	1.14438300	-1.43649300	5.18593800
H	2.53971300	-1.80320300	4.16327800
C	0.54399800	-3.06534500	-0.64325900
N	0.56524100	-4.22363300	-0.66858500
B	1.90656900	-0.98870200	-0.88901300
O	2.15514500	0.39763400	-0.81117700
O	3.11408700	-1.71592200	-0.87548300
H	1.08737000	-1.35866000	-1.96686400
C	3.55691900	0.56945500	-1.09180600
C	4.04515700	1.81532000	-0.37144500
H	5.12661000	1.93318900	-0.49351400
H	3.55634700	2.69870700	-0.79438200
H	3.81642800	1.77483000	0.69628200
C	3.71722100	0.72667800	-2.60237700
H	4.75648600	0.92789800	-2.87717300
H	3.38484600	-0.17528000	-3.12586000

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H	3.10223200	1.56677900	-2.93830900
C	4.15294300	-0.77400100	-0.56558600
C	4.32684500	-0.76938000	0.95328600
H	4.52454600	-1.79118300	1.28884200
H	5.15835400	-0.13196200	1.26843000
H	3.41031400	-0.41960700	1.44244800
C	5.43890100	-1.20733300	-1.24960900
H	5.28329400	-1.36584200	-2.31864500
H	6.22177900	-0.45408600	-1.11364700
H	5.78977000	-2.14641400	-0.81204700
TS2R <sub>CN</sub>			
C	-0.94713100	-0.67849500	-0.36287300
C	-2.29842000	-1.31606300	-0.29076700
C	-2.80824800	-1.82667600	0.91125100
C	-3.10429500	-1.41588500	-1.43658000
C	-4.07722600	-2.40103000	0.97364500
H	-2.19417600	-1.78105400	1.80638700
C	-4.36656700	-2.00153700	-1.38252800
H	-2.73400200	-1.01767700	-2.37758300
C	-4.86120200	-2.49141600	-0.17413600
H	-4.44746500	-2.78683800	1.91880700
H	-4.96836600	-2.06540300	-2.28423100
H	-5.84828700	-2.94097400	-0.12924700
C	0.12246900	-1.26232100	-1.06196500
P	-0.68571200	0.84280900	0.49285200
C	-2.31855500	1.52769200	0.92099100
C	-3.19338900	1.84609300	-0.30332400
H	-2.14168300	2.41763400	1.53308400
H	-2.80253700	0.78813100	1.56876400
C	-4.67132500	1.56429500	-0.03789500

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H	-3.05365600	2.89629000	-0.58585000
H	-2.87995100	1.24897400	-1.16782500
C	-5.53619600	1.82058300	-1.26646200
H	-4.77213300	0.51534700	0.27181300
H	-5.01570500	2.17692400	0.80463900
H	-6.59022200	1.61056300	-1.06442100
H	-5.45755300	2.86207100	-1.59581100
H	-5.22010700	1.18186100	-2.09854000
C	0.13637900	2.04280400	-0.60320500
C	0.48641900	3.37555900	0.06114500
H	-0.53631900	2.18958100	-1.45621700
H	1.03723600	1.54628500	-0.97708000
C	1.11537200	4.34892900	-0.93618500
H	-0.41428000	3.83090200	0.49397800
H	1.18512800	3.20694900	0.89045300
C	1.50443000	5.67248800	-0.28594700
H	1.99979500	3.87883600	-1.38459200
H	0.40897600	4.52814000	-1.75579000
H	1.94814400	6.35837700	-1.01281800
H	0.63012300	6.16621300	0.15091000
H	2.23367000	5.51509900	0.51554800
C	0.27121700	0.80302900	2.05870900
C	0.16614800	-0.52573000	2.80592100
H	-0.08566900	1.63646300	2.67536200
H	1.31277100	0.99140900	1.78869300
C	1.11587200	-0.57807700	4.00138700
H	-0.86352600	-0.68166200	3.15247600
H	0.40170800	-1.34762600	2.11654200
C	1.01379900	-1.89535700	4.76343900
H	2.14216900	-0.43477700	3.64063900

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H	0.90001500	0.26094400	4.67471200
H	1.70605100	-1.92241200	5.60963100
H	0.00159100	-2.04527600	5.15329100
H	1.24797000	-2.74209200	4.11004100
C	-0.20039900	-2.17925400	-2.13552600
N	-0.45982600	-2.86285500	-3.03459300
B	1.66108900	-1.16508500	-0.82857900
O	2.60540500	-1.47553500	-1.82565000
O	2.24590300	-0.36694200	0.18055700
H	1.03212200	-2.28752400	-0.28867700
C	3.88605100	-1.32565800	-1.19273500
C	4.92776300	-1.02437200	-2.25781700
H	5.89506200	-0.79645000	-1.79852300
H	5.05453600	-1.89857600	-2.90289700
H	4.62565700	-0.18076600	-2.88160100
C	4.22266600	-2.63591400	-0.48034700
H	5.22242200	-2.60917400	-0.03759400
H	3.49660300	-2.85297400	0.30968700
H	4.18749500	-3.45009300	-1.20951400
C	3.62147100	-0.15572500	-0.18894300
C	3.72118300	1.21555400	-0.85568400
H	3.31494400	1.97088200	-0.17399100
H	4.75912300	1.47913600	-1.07964900
H	3.14638000	1.23959000	-1.78704200
C	4.47850900	-0.19067000	1.06697100
H	4.30138300	-1.10161400	1.64236100
H	5.54170900	-0.13721700	0.81059900
H	4.24063100	0.66959000	1.70084900
TS2S <sub>CN'</sub>			
C	0.21146600	0.03628700	-0.24662100



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C	-0.19310400	1.44353200	0.01482000
C	-0.11507700	2.03158400	1.28516300
C	-0.70789500	2.21911300	-1.03576400
C	-0.50009300	3.35502700	1.49141700
H	0.22011400	1.43380700	2.12896400
C	-1.11316800	3.53395100	-0.82942500
H	-0.78028200	1.77458900	-2.02499300
C	-0.99933300	4.11268600	0.43452600
H	-0.42831400	3.78712600	2.48523800
H	-1.50816800	4.11272200	-1.65930500
H	-1.30455700	5.14203000	0.59501400
C	-0.76245400	-0.87808100	-0.67837000
P	1.84289200	-0.51941200	0.14594100
C	2.85366700	0.79990100	0.89060700
C	3.17312600	1.95465000	-0.06499200
H	3.77564300	0.31341500	1.23058000
H	2.33972600	1.16389600	1.78351900
C	3.88426600	3.09641000	0.65952800
H	3.80364000	1.58964100	-0.88562500
H	2.25093800	2.33700700	-0.51811500
C	4.21987900	4.25074700	-0.27889200
H	3.23955500	3.45463000	1.47181200
H	4.79969900	2.71488600	1.12880000
H	4.72402100	5.06283100	0.25223300
H	4.87783700	3.91975100	-1.08906600
H	3.31049800	4.65866300	-0.73220400
C	2.77846000	-1.07844100	-1.32395000
C	4.24140100	-1.44305500	-1.05403000
H	2.70353700	-0.26827100	-2.05879600
H	2.24233300	-1.93787300	-1.73826400

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C	4.93140800	-1.94955600	-2.32113300
H	4.78509100	-0.56879700	-0.67468300
H	4.29949700	-2.21663600	-0.27815100
C	6.39339500	-2.30960700	-2.07727700
H	4.38949300	-2.82477900	-2.69890400
H	4.86165100	-1.17903000	-3.09866200
H	6.87209500	-2.67026100	-2.99185100
H	6.95771900	-1.44042100	-1.72377900
H	6.48204500	-3.09560400	-1.32017000
C	1.78015900	-1.91406600	1.32014600
C	0.95414200	-1.57138600	2.56269200
H	2.80710100	-2.19316400	1.58198200
H	1.33771800	-2.76272600	0.78343700
C	0.81635200	-2.76488700	3.50658500
H	1.42047800	-0.73378000	3.09821800
H	-0.04453100	-1.23475600	2.25209200
C	-0.01854900	-2.42912000	4.73807300
H	0.35562300	-3.59713100	2.96059900
H	1.81419700	-3.10325300	3.81187900
H	-0.11331500	-3.29204600	5.40300500
H	0.43615400	-1.61323600	5.30956200
H	-1.02663500	-2.11374500	4.45005800
C	-0.38194000	-2.09335200	-1.35810500
N	-0.07156300	-3.04940800	-1.93718800
B	-2.31235500	-0.77939100	-0.45863700
O	-2.92073600	0.32883900	0.14799600
O	-3.24085100	-1.51744400	-1.22495000
H	-1.61542800	-1.61495800	0.43324100
C	-4.33545400	0.09704100	0.06550100
C	-5.04496500	1.44109800	0.02469600

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H	-6.11721500	1.30962800	-0.15384500
H	-4.91828900	1.95204400	0.98380800
H	-4.63077900	2.08081600	-0.75740400
C	-4.75773800	-0.69102700	1.30529400
H	-5.84120100	-0.83739900	1.34258000
H	-4.27113600	-1.67138700	1.32915800
H	-4.45239000	-0.13478300	2.19612100
C	-4.45315800	-0.74698400	-1.24318100
C	-4.42514500	0.12760100	-2.49682200
H	-4.28270300	-0.51383000	-3.37097000
H	-5.35803000	0.68506800	-2.62397300
H	-3.59485900	0.83982700	-2.45250800
C	-5.64281600	-1.69278000	-1.28486000
H	-5.59358300	-2.42654700	-0.47774300
H	-6.58234600	-1.13680600	-1.19988900
H	-5.65159500	-2.23203900	-2.23674700

TS2R<sub>CN'</sub>

C	0.12504100	-0.02021500	0.24632500
C	-0.23413600	1.38227900	0.61856200
C	-0.03875200	1.85334800	1.92370400
C	-0.74707700	2.27731100	-0.33252200
C	-0.33159900	3.17295700	2.26786600
H	0.34684100	1.17072000	2.67714200
C	-1.05055300	3.59222600	0.00785400
H	-0.91462700	1.92736900	-1.34681400
C	-0.83960800	4.04671900	1.31000300
H	-0.16965000	3.51334100	3.28627300
H	-1.44771000	4.26585900	-0.74576900
H	-1.07130500	5.07393700	1.57442900
C	-0.86096200	-0.96325400	-0.09205700

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P	1.84030800	-0.42305200	0.09158100
C	2.83790800	1.09260900	0.23970900
C	2.73105200	2.00796100	-0.98557100
H	3.87440200	0.78370800	0.41394500
H	2.49808900	1.61196200	1.14162200
C	3.21611700	3.42308500	-0.67675100
H	3.31616700	1.58257700	-1.81085100
H	1.69141600	2.05979300	-1.32956400
C	3.11308200	4.34296500	-1.88845700
H	2.61320400	3.82639100	0.14677000
H	4.25245300	3.38408300	-0.31870300
H	3.46126200	5.35266200	-1.65396500
H	3.71422000	3.96519400	-2.72203600
H	2.07522300	4.41641100	-2.23035800
C	2.21597000	-1.15836800	-1.53708300
C	3.69524900	-1.49096200	-1.75308100
H	1.85932300	-0.43856500	-2.28364100
H	1.60193300	-2.05996100	-1.64024300
C	3.95546100	-1.98623800	-3.17575900
H	4.31435900	-0.60458500	-1.56148000
H	4.01072100	-2.26053700	-1.03837800
C	5.42094400	-2.34233500	-3.40368100
H	3.32386700	-2.86103600	-3.37190700
H	3.64504600	-1.21046900	-3.88640600
H	5.59145000	-2.69009400	-4.42624200
H	6.06633200	-1.47449300	-3.23236100
H	5.74138900	-3.13644200	-2.72149700
C	2.47745100	-1.58953000	1.34985100
C	2.06878700	-1.22174200	2.77633900
H	3.56898300	-1.59906400	1.24419900

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H	2.11154700	-2.58845300	1.08807900
C	2.64475700	-2.19565700	3.80345600
H	2.40478600	-0.20259200	3.01182000
H	0.97395800	-1.21871800	2.84760800
C	2.22636100	-1.84423100	5.22757800
H	2.31147700	-3.21107200	3.55693500
H	3.73898600	-2.19778700	3.72636200
H	2.64380800	-2.54981900	5.95124900
H	2.56977300	-0.84095400	5.50069400
H	1.13657700	-1.86314200	5.33013400
C	-0.50788500	-2.36368900	-0.02252600
N	-0.20296000	-3.47717500	0.09094800
B	-2.35064800	-0.77907200	-0.52535800
O	-3.28046600	-1.82125200	-0.32768000
O	-3.00572800	0.45298000	-0.70008000
H	-1.42485000	-1.02812200	-1.56379000
C	-4.54686500	-1.30235300	-0.76062400
C	-5.65414100	-2.00642800	0.00680400
H	-6.62634100	-1.55480200	-0.21612400
H	-5.69309500	-3.06003600	-0.28523700
H	-5.48125300	-1.95689200	1.08379500
C	-4.68370400	-1.57032000	-2.25912700
H	-5.66193200	-1.26070400	-2.63838700
H	-3.90727000	-1.04277000	-2.82253200
H	-4.56690900	-2.64313700	-2.43672200
C	-4.39852900	0.21884300	-0.44139200
C	-4.64734100	0.53147900	1.03409300
H	-4.30229700	1.54917600	1.23842700
H	-5.70869700	0.46484800	1.29141700
H	-4.08614600	-0.15542400	1.67515900

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C	-5.22611000	1.13917900	-1.32416000
H	-4.94663400	1.03708900	-2.37483600
H	-6.29365400	0.91921300	-1.21980600
H	-5.06183400	2.17904900	-1.02598800
M4S <sub>CN</sub>			
C	-0.12951300	-0.84272700	-0.42987000
C	0.02052500	-2.26168800	-0.04022800
C	0.12285400	-3.29389200	-0.99763500
C	0.03230100	-2.66154100	1.31162600
C	0.24714900	-4.62898300	-0.62895500
H	0.12797200	-3.04039800	-2.05502300
C	0.18580300	-3.99465200	1.68382700
H	-0.10703400	-1.90760100	2.08063200
C	0.29047700	-4.99225300	0.71710000
H	0.32698700	-5.39033200	-1.40006000
H	0.19399000	-4.25615800	2.73840000
H	0.39259700	-6.03364300	1.00534100
C	-1.08180000	-0.56545100	-1.62558100
P	1.07081900	0.32393000	-0.02438000
C	0.35237500	2.01431000	0.07515500
C	1.14344000	3.14945800	-0.57644500
H	0.21503900	2.20691900	1.14734900
H	-0.65202200	1.96214500	-0.35573900
C	0.39389500	4.47715600	-0.47000200
H	2.13060900	3.24794300	-0.10723000
H	1.31458500	2.92047400	-1.63530400
C	1.16530000	5.63110100	-1.10253600
H	-0.58326600	4.37071200	-0.95758600
H	0.19368400	4.69700500	0.58640400
H	0.61287200	6.57179000	-1.02478300

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H	2.13470000	5.76996100	-0.61243600
H	1.35293700	5.43895800	-2.16392800
C	2.52126200	0.43515500	-1.16473000
C	3.31267700	-0.87350900	-1.20333600
H	3.16257500	1.27333800	-0.86744000
H	2.12506700	0.66871800	-2.15991300
C	4.44828600	-0.83391500	-2.22558700
H	3.73043800	-1.08787500	-0.21020200
H	2.63656900	-1.70515300	-1.44205400
C	5.24287800	-2.13573900	-2.26021000
H	4.02922400	-0.62678800	-3.21790100
H	5.11634700	0.00375900	-1.98891300
H	6.04856100	-2.09340600	-2.99861300
H	5.69290200	-2.34573900	-1.28426200
H	4.59607100	-2.98122600	-2.51654100
C	1.81945800	-0.00615000	1.61073900
C	2.96207000	0.94902200	1.96570900
H	2.16423800	-1.04501500	1.63375800
H	1.00788100	0.08397200	2.34149000
C	3.45073200	0.73200000	3.39802600
H	3.80130400	0.80354900	1.27443100
H	2.63392000	1.99095500	1.85062100
C	4.60237400	1.66309100	3.76339800
H	2.61408000	0.88512800	4.09055000
H	3.76489400	-0.31258000	3.51415000
H	4.93954200	1.49659300	4.79024200
H	5.45870300	1.50577800	3.09950800
H	4.30072500	2.71201900	3.67531800
C	-0.65166100	0.47045900	-2.55534000
N	-0.29926700	1.32140300	-3.25942900

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B	-2.39308700	-0.19278100	-0.83680400
O	-3.19985200	-1.14356200	-0.27015900
O	-2.79471400	1.09348500	-0.57207100
H	-1.23182100	-1.47715100	-2.21102700
C	-4.32117900	-0.44410700	0.32384500
C	-4.70801900	-1.14699400	1.61348100
H	-5.48781500	-0.58457000	2.13665200
H	-5.09984000	-2.14181700	1.38432800
H	-3.84813800	-1.26136700	2.27640000
C	-5.46531500	-0.50255000	-0.68387300
H	-6.37500200	-0.04953600	-0.28030400
H	-5.19860300	0.01258000	-1.61172900
H	-5.67416200	-1.54950200	-0.91915200
C	-3.75337200	1.00102900	0.51346300
C	-2.96485900	1.16481300	1.80983100
H	-2.45704300	2.13348800	1.79355000
H	-3.62194700	1.13395700	2.68314600
H	-2.20714100	0.37932200	1.90875400
C	-4.77539200	2.11343200	0.36405700
H	-5.23612000	2.10265500	-0.62536600
H	-5.56011000	2.01274500	1.12043800
H	-4.28625200	3.08116500	0.50607000
TS3S <sub>CN</sub>			
C	-0.28783100	-0.71554000	-0.52364600
C	-0.29181500	-2.14999300	-0.14309500
C	-0.17626400	-3.18133100	-1.09526400
C	-0.45799800	-2.54428300	1.19823100
C	-0.20336700	-4.52302900	-0.72722200
H	-0.04447600	-2.92667900	-2.14388100
C	-0.46024600	-3.88515400	1.57302600



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H	-0.60455700	-1.77724800	1.95363600
C	-0.33646100	-4.88675700	0.61214800
H	-0.10749600	-5.28900300	-1.49167100
H	-0.58586900	-4.14771900	2.61970500
H	-0.35405600	-5.93308100	0.90014100
C	-1.06625600	-0.36415000	-1.82828000
P	1.03930800	0.29579700	-0.04483500
C	0.54986700	2.06668700	0.04307600
C	1.51832000	3.07657800	-0.57510700
H	0.40776900	2.27660800	1.11120300
H	-0.43761100	2.15286100	-0.41803300
C	0.95495800	4.49547700	-0.50648700
H	2.48745000	3.04134000	-0.06120300
H	1.70272400	2.81782300	-1.62457300
C	1.91203900	5.52711900	-1.09506000
H	0.00067100	4.52160500	-1.04706600
H	0.73065300	4.74757700	0.53771100
H	1.49159300	6.53557500	-1.04719600
H	2.86315900	5.53432900	-0.55234000
H	2.12864300	5.30352200	-2.14470800
C	2.53127000	0.20637500	-1.12318900
C	3.15456900	-1.19102200	-1.13007500
H	3.26014100	0.95777700	-0.79722800
H	2.20938000	0.48652300	-2.13320200
C	4.34436900	-1.28519600	-2.08485000
H	3.48465400	-1.45881800	-0.11719500
H	2.39715800	-1.93179800	-1.41644400
C	4.96812700	-2.67727700	-2.09621100
H	4.01458800	-1.01647600	-3.09587400
H	5.09754800	-0.54176200	-1.79509000

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H	5.81646800	-2.72978900	-2.78441100
H	5.32696000	-2.95388700	-1.09933600
H	4.23636900	-3.43029300	-2.40667800
C	1.63920900	-0.14488800	1.62256000
C	2.87042400	0.65669400	2.05399900
H	1.84961300	-1.21892900	1.64512200
H	0.80389700	0.03889400	2.30806700
C	3.25685600	0.35612900	3.50226700
H	3.71836800	0.42046400	1.39906800
H	2.67783100	1.73277000	1.94794300
C	4.49169800	1.13494900	3.94397800
H	2.41061000	0.59700400	4.15712900
H	3.43736800	-0.72059700	3.60836900
H	4.75367800	0.91108900	4.98177300
H	5.35566000	0.88686600	3.31886400
H	4.32252700	2.21392900	3.86594800
C	-0.54272300	0.71035900	-2.64393900
N	-0.11768700	1.59310900	-3.26493800
B	-2.24317000	0.00892900	-0.86901100
O	-3.16196900	-0.91638500	-0.40268200
O	-2.55694300	1.30562200	-0.48880500
H	-1.24314900	-1.23741900	-2.45769400
C	-4.20465900	-0.17427500	0.26319100
C	-4.67186600	-0.96326800	1.47542400
H	-5.39219800	-0.38208800	2.06016200
H	-5.16314400	-1.88326700	1.14612100
H	-3.83189400	-1.23649700	2.11755500
C	-5.34623300	-0.00675800	-0.73691200
H	-6.21004600	0.48676900	-0.28235500
H	-5.02311600	0.57805600	-1.60349100

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H	-5.65616400	-0.99562300	-1.08554800
C	-3.49853400	1.18015500	0.60020600
C	-2.69473100	1.11820200	1.89718600
H	-2.08118800	2.02068900	1.97550500
H	-3.34917900	1.06912200	2.77189400
H	-2.03154200	0.24666700	1.90293800
C	-4.41242300	2.39341900	0.60045200
H	-4.87490700	2.54371600	-0.37685600
H	-5.20113600	2.27849100	1.35081700
H	-3.83421600	3.28832400	0.84802300
M5S <sub>CN</sub>			
C	-0.39833600	-0.76883100	-0.56990000
C	0.08897900	-2.16337600	-0.30615500
C	0.67068200	-2.93659300	-1.31981700
C	0.00491600	-2.70622100	0.98188800
C	1.18605700	-4.20067400	-1.04672000
H	0.72961900	-2.53347100	-2.32804300
C	0.52666200	-3.96799300	1.25956200
H	-0.47528700	-2.12725300	1.76639700
C	1.12492600	-4.71695800	0.24773000
H	1.64094300	-4.78137600	-1.84373500
H	0.45652600	-4.37070000	2.26553000
H	1.52848700	-5.70150700	0.46263800
C	-1.16231900	-0.57440800	-1.91989500
P	0.81185200	0.47446800	-0.13160500
C	0.20216600	2.18188700	-0.41886600
C	1.21958800	3.13249500	-1.05030500
H	-0.11975400	2.54313600	0.56441200
H	-0.69975200	2.13052600	-1.02752000
C	0.62616500	4.53020400	-1.21954000

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H	2.12836000	3.18961900	-0.43681200
H	1.51700000	2.74864200	-2.03390600
C	1.61782800	5.50567000	-1.84507000
H	-0.27145300	4.45767400	-1.84567100
H	0.29836800	4.90551900	-0.24208300
H	1.17663500	6.49888000	-1.96607400
H	2.51243500	5.60946200	-1.22212600
H	1.93692400	5.15778100	-2.83282700
C	2.37180000	0.17963400	-1.04621000
C	3.27213100	-0.89259000	-0.41182800
H	2.91829300	1.12297600	-1.13718500
H	2.06715000	-0.11351800	-2.05924700
C	4.32479600	-1.39542200	-1.39826500
H	3.76712600	-0.47290400	0.47276800
H	2.68199100	-1.74752500	-0.06444200
C	5.23653200	-2.44554800	-0.77232500
H	3.81437100	-1.82146500	-2.27127800
H	4.91847500	-0.54876900	-1.76448300
H	5.97812700	-2.80909300	-1.48895200
H	5.77400400	-2.03638700	0.08940800
H	4.65370100	-3.30546600	-0.42498800
C	1.19497600	0.36200800	1.64397300
C	2.14913200	1.46155300	2.12488600
H	1.61853300	-0.63004800	1.83398300
H	0.23585200	0.41855800	2.17277100
C	2.53365200	1.26444300	3.59128800
H	3.05984800	1.47040000	1.51155400
H	1.67802400	2.44473200	2.00327500
C	3.46170500	2.36433900	4.09632900
H	1.62173600	1.23647700	4.20006900

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H	3.01707300	0.28656300	3.70578800
H	3.72877200	2.20843000	5.14508200
H	4.38873500	2.39210400	3.51439300
H	2.98594600	3.34688800	4.01338800
C	-0.77733700	0.44817500	-2.83263700
N	-0.46897400	1.31383100	-3.54826800
B	-1.97494600	-0.37542000	-0.49479700
O	-2.89540300	-1.37885700	-0.06521400
O	-2.44953300	0.91438000	-0.08740500
H	-1.36814700	-1.52144700	-2.41266400
C	-4.09289400	-0.69122800	0.30080400
C	-4.82779200	-1.50652700	1.35405900
H	-5.68936500	-0.95482300	1.74480600
H	-5.19335000	-2.43770800	0.91058300
H	-4.16690100	-1.76323700	2.18493900
C	-4.96245800	-0.53355400	-0.94828300
H	-5.93387800	-0.08584200	-0.71724700
H	-4.45822900	0.08826500	-1.69471700
H	-5.13263400	-1.52239300	-1.38396900
C	-3.54261100	0.67998200	0.80509800
C	-2.98730600	0.58421100	2.22738900
H	-2.41760600	1.49301900	2.44595500
H	-3.78220500	0.49009500	2.97364000
H	-2.31882100	-0.27834300	2.32053700
C	-4.52316500	1.83799900	0.70031900
H	-4.81001700	2.01755700	-0.33789700
H	-5.42603500	1.63806000	1.28697700
H	-4.06119200	2.75094500	1.08880400
TS4S <sub>CN</sub>			
C	0.36206500	0.81425500	-0.66223300

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C	-0.32448500	2.14067600	-0.42767000
C	-1.07514200	2.74380500	-1.44223600
C	-0.26459700	2.75842700	0.82634600
C	-1.79064000	3.91224900	-1.19446200
H	-1.09787200	2.28280800	-2.42645300
C	-0.97676100	3.92974200	1.07555600
H	0.34287800	2.31134100	1.60997900
C	-1.75127600	4.50407200	0.06864100
H	-2.37942600	4.36310000	-1.98792100
H	-0.92305500	4.39674100	2.05429100
H	-2.30774200	5.41601800	0.26164600
C	0.95313200	0.56992000	-2.06243700
P	-0.71352200	-0.54516700	-0.10445800
C	-0.00811900	-2.17947800	-0.55109400
C	-1.00143500	-3.17134700	-1.15663100
H	0.43576900	-2.57258900	0.36924600
H	0.81890200	-1.99352700	-1.23891200
C	-0.29739400	-4.46639400	-1.55860100
H	-1.80462600	-3.39299500	-0.44125400
H	-1.46609600	-2.73006200	-2.04581000
C	-1.26419200	-5.48781900	-2.14857800
H	0.48225100	-4.22440200	-2.29124600
H	0.21106000	-4.89267100	-0.68481300
H	-0.74471300	-6.40393200	-2.44312200
H	-2.03923500	-5.75949600	-1.42421400
H	-1.76235400	-5.08435200	-3.03600200
C	-2.38014100	-0.32074600	-0.82249900
C	-3.28998700	0.63985200	-0.03991100
H	-2.85386900	-1.30382600	-0.90185400
H	-2.21725400	0.03674300	-1.84690400

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C	-4.48047900	1.08423200	-0.88783100
H	-3.64896400	0.14168500	0.86929900
H	-2.74139000	1.53057500	0.28454200
C	-5.39237200	2.04321100	-0.13021100
H	-4.10146600	1.57298300	-1.79440900
H	-5.04549400	0.20394900	-1.21821100
H	-6.23735800	2.36204200	-0.74667000
H	-5.79391900	1.57395200	0.77397700
H	-4.84028800	2.93895800	0.17460400
C	-0.86806100	-0.49786500	1.70611600
C	-1.67962200	-1.67222200	2.26590500
H	-1.32875700	0.45849200	1.97643300
H	0.15424000	-0.50269100	2.10294700
C	-1.89570800	-1.53342900	3.77265100
H	-2.65483200	-1.73263700	1.76519400
H	-1.15992600	-2.61581800	2.05909900
C	-2.67255800	-2.70995900	4.35412800
H	-0.92086000	-1.44786000	4.26797000
H	-2.43147600	-0.59722200	3.97156500
H	-2.82564000	-2.59193400	5.43030500
H	-3.65678500	-2.80043900	3.88311100
H	-2.13739300	-3.65122400	4.19233000
C	0.33647800	-0.29161300	-2.97467000
N	-0.16485200	-1.07791600	-3.69007200
B	1.83781400	0.57171600	-0.20828600
O	2.31816300	-0.62165900	0.33641600
O	2.77102600	1.59489200	-0.11854500
H	1.40857600	1.45805400	-2.48987000
C	3.62798900	-0.34029200	0.87466300
C	4.52732200	-1.54270800	0.64093800

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H	5.55345400	-1.32110600	0.95145200
H	4.16870200	-2.39102500	1.23127400
H	4.53263600	-1.83442300	-0.41102300
C	3.45266400	-0.08690900	2.37023200
H	4.41408200	0.06748000	2.86841500
H	2.82349500	0.79186900	2.54481200
H	2.96737200	-0.95715000	2.82174400
C	4.04323300	0.94758600	0.09232900
C	4.63471200	0.63366800	-1.28054000
H	4.71938100	1.56555700	-1.84681000
H	5.62942500	0.18724400	-1.19618200
H	3.98556300	-0.04675400	-1.84014400
C	4.95332800	1.89086200	0.86020900
H	4.47440000	2.25154600	1.77270800
H	5.88940300	1.38965000	1.12668500
H	5.19569500	2.75514600	0.23536800

M6S<sub>CN</sub>

C	-0.28664600	-0.45464000	-0.94428400
C	0.49291300	-1.76227200	-1.03915300
C	1.24283300	-2.09040200	-2.17248000
C	0.54096200	-2.63108700	0.06075400
C	2.04964700	-3.22801800	-2.18932000
H	1.20189100	-1.45701800	-3.05121800
C	1.34094400	-3.76927900	0.04583500
H	-0.05195600	-2.41011400	0.94654600
C	2.11027100	-4.06642500	-1.07887000
H	2.63100000	-3.45867200	-3.07710400
H	1.36042500	-4.42573000	0.91037000
H	2.73971900	-4.95075200	-1.09338500
C	-0.57991300	0.20983400	-2.26352200



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P	0.78401800	0.72745700	0.05801100
C	0.01184700	2.38564400	0.00192400
C	0.52516200	3.32893000	-1.09078300
H	0.15124500	2.84017200	0.98850300
H	-1.06003000	2.20614500	-0.12428200
C	-0.35141500	4.57772800	-1.18666100
H	1.55967000	3.62452800	-0.87766900
H	0.52647300	2.81427600	-2.05796100
C	0.15376200	5.55536500	-2.24266000
H	-1.37448000	4.26561800	-1.42688400
H	-0.38956600	5.07178800	-0.20740300
H	-0.48641600	6.43975400	-2.30556400
H	1.17046800	5.89236000	-2.01409400
H	0.17166700	5.08398300	-3.23066500
C	2.43675400	0.77701300	-0.71766500
C	3.41297200	-0.30369500	-0.23078500
H	2.86212000	1.77246800	-0.55432800
H	2.25441200	0.68168300	-1.79620000
C	4.61650000	-0.42560400	-1.16386200
H	3.75543100	-0.05846500	0.78252300
H	2.91955300	-1.27984600	-0.16925500
C	5.59357900	-1.49868300	-0.69577700
H	4.25544000	-0.66902500	-2.17132800
H	5.12500300	0.54368000	-1.23756400
H	6.44532300	-1.58813500	-1.37563500
H	5.98217000	-1.26940500	0.30193900
H	5.09793700	-2.47429600	-0.64555100
C	1.01721200	0.25769000	1.80908400
C	1.81858400	1.26702500	2.64062700
H	1.52129300	-0.71555400	1.80384600

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H	0.01737100	0.10803000	2.23309900
C	2.19116900	0.69211200	4.00742300
H	2.73475000	1.55816500	2.11016000
H	1.23173500	2.18121300	2.78336700
C	2.94553200	1.69832000	4.87033200
H	1.27746800	0.36982300	4.52184900
H	2.80221700	-0.20721600	3.86160000
H	3.21222200	1.26977700	5.84030000
H	3.87021000	2.01910900	4.37949100
H	2.33799200	2.59052900	5.05319100
C	-1.64182100	1.08810200	-2.38630300
N	-2.56661300	1.81669300	-2.48311200
B	-1.66942400	-0.66441200	-0.19121300
O	-2.17773800	0.23969500	0.70314000
O	-2.47636900	-1.74428600	-0.39346100
H	0.20386600	0.28817600	-3.00815200
C	-3.38361700	-0.34322900	1.26703400
C	-4.41314200	0.75778800	1.44868000
H	-5.36711400	0.33647200	1.78037000
H	-4.06648600	1.46131000	2.21070100
H	-4.57092500	1.30646400	0.51813500
C	-2.98764000	-0.94155400	2.61286200
H	-3.85402000	-1.36307700	3.12971100
H	-2.23788600	-1.72988800	2.48973600
H	-2.56281900	-0.15298000	3.24037600
C	-3.76340900	-1.42391500	0.19860900
C	-4.63823100	-0.87630700	-0.92476800
H	-4.71151300	-1.63345400	-1.71000300
H	-5.64634000	-0.65177500	-0.56547700
H	-4.20623000	0.02863700	-1.36344800

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C	-4.36677600	-2.69451100	0.77172000
H	-3.68144800	-3.18916800	1.46260900
H	-5.29839800	-2.46760800	1.29937300
H	-4.59564300	-3.38745700	-0.04231600
TS5S <sub>CN</sub>			
C	0.69512600	0.91276400	-0.97016900
C	0.06909900	2.22721800	-0.57757000
C	-0.59748600	3.04417200	-1.49514600
C	0.10594800	2.63158600	0.76613500
C	-1.23793900	4.21129900	-1.07605400
H	-0.62221900	2.77979400	-2.54675500
C	-0.51872200	3.80003500	1.18420500
H	0.62223700	2.00988000	1.49560800
C	-1.20566900	4.59231300	0.26235000
H	-1.75967700	4.82539800	-1.80415100
H	-0.47352800	4.09218400	2.22879900
H	-1.70245500	5.50203800	0.58500100
C	0.77750100	0.58493100	-2.35164200
P	-0.83254400	-0.44815300	-0.09640600
C	-0.39880000	-2.12225900	-0.72291800
C	-1.50827900	-2.91862500	-1.41157800
H	-0.00376900	-2.66860700	0.14193800
H	0.44058100	-1.98606800	-1.41281900
C	-1.03215800	-4.31626600	-1.80654900
H	-2.38532400	-3.00397300	-0.75669600
H	-1.83714600	-2.38245600	-2.31072600
C	-2.11392500	-5.11673200	-2.52505800
H	-0.14757700	-4.22379200	-2.44864100
H	-0.70835700	-4.85292200	-0.90586900
H	-1.75804200	-6.11388600	-2.79906100

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H	-2.99801900	-5.23897300	-1.89042700
H	-2.43024600	-4.61011000	-3.44274400
C	-2.36814700	0.10447300	-0.93892700
C	-3.14984400	1.17438400	-0.16614600
H	-3.01444500	-0.75333000	-1.15053300
H	-2.03861200	0.49976800	-1.91096000
C	-4.19243200	1.86217500	-1.04613700
H	-3.64703300	0.71242800	0.69677900
H	-2.47263800	1.93773000	0.23476800
C	-4.96679600	2.93417200	-0.28664400
H	-3.68253900	2.31500200	-1.90642400
H	-4.88371400	1.11221700	-1.45079800
H	-5.70246800	3.42846800	-0.92737200
H	-5.50024000	2.50342100	0.56723800
H	-4.28507300	3.70067300	0.09814600
C	-1.27996600	-0.66922400	1.67651400
C	-2.35190600	-1.72757500	1.95474800
H	-1.59610600	0.31313000	2.04859500
H	-0.34800400	-0.92158500	2.19787600
C	-2.72321900	-1.79299500	3.43661900
H	-3.25222300	-1.51164500	1.36415100
H	-1.98923800	-2.71017400	1.62641300
C	-3.77655600	-2.85860600	3.72361100
H	-1.81931400	-1.99497400	4.02458400
H	-3.09090400	-0.81015500	3.75678600
H	-4.03184400	-2.89207600	4.78648600
H	-4.69641100	-2.66002000	3.16383700
H	-3.41784500	-3.85151900	3.43328200
C	1.71795700	-0.34053900	-2.82848600
N	2.51961100	-1.09962200	-3.21989200

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B	1.96956700	0.48293300	-0.14165200
O	2.21028600	-0.81086200	0.23248500
O	2.95885400	1.35002400	0.22558700
H	0.07272100	0.96911300	-3.07922000
C	3.40569000	-0.80412100	1.05545700
C	4.21086000	-2.05523000	0.75162100
H	5.16859800	-2.03014500	1.28064600
H	3.65736100	-2.93659200	1.08728500
H	4.39795600	-2.15400700	-0.31933300
C	2.93663900	-0.80247200	2.50680400
H	3.78280400	-0.84925600	3.19773600
H	2.35180600	0.09558500	2.73143900
H	2.30517700	-1.67945900	2.67493500
C	4.09262200	0.53599400	0.63115700
C	4.98034100	0.38472800	-0.60049800
H	5.27000900	1.37969000	-0.94861600
H	5.88777700	-0.17918200	-0.36797300
H	4.44743900	-0.12117000	-1.41221000
C	4.83729900	1.24999900	1.74497400
H	4.17253800	1.50828200	2.57154100
H	5.64540300	0.61785200	2.12600700
H	5.27909700	2.17150900	1.35644300

**(E)- $\beta$ -product<sub>CN</sub>**

C	-0.98817200	1.00368500	-0.05756000
C	-2.22833600	0.19303800	-0.05244900
C	-3.40759500	0.65144100	0.55294400
C	-2.23699600	-1.06382800	-0.67392500
C	-4.56599300	-0.11683700	0.51843500
H	-3.41035700	1.60241100	1.07724100
C	-3.39933300	-1.82689300	-0.71690100

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H	-1.32735900	-1.44001900	-1.13228100
C	-4.56732200	-1.35561600	-0.12134200
H	-5.46754900	0.24827900	1.00012600
H	-3.39101600	-2.79267300	-1.21205700
H	-5.47203900	-1.95482100	-0.14595300
C	-1.06605200	2.35031200	-0.06877000
C	0.07379600	3.21894300	-0.03082300
N	0.95168100	3.97396000	0.00711500
B	0.40657200	0.26630300	-0.02313200
O	1.55161200	0.80378000	-0.53057500
O	0.57416200	-0.96664400	0.53829100
H	-2.01960900	2.87162500	-0.10442400
C	2.55937800	-0.24367800	-0.48958800
C	3.90751700	0.38518800	-0.18744300
H	4.66733700	-0.39212100	-0.06018800
H	4.20786200	1.02400100	-1.02228500
H	3.87036600	0.99517900	0.71680500
C	2.56555700	-0.89427600	-1.86911200
H	3.34504000	-1.65731100	-1.94260100
H	1.59943000	-1.35781200	-2.09215500
H	2.75995200	-0.12533300	-2.62113900
C	2.00916500	-1.18665500	0.62903500
C	2.42767900	-0.75394900	2.03060500
H	1.85032500	-1.32356500	2.76336600
H	3.49049900	-0.94450100	2.20138500
H	2.23272200	0.31114000	2.18951400
C	2.29374900	-2.66224800	0.41558600
H	1.85625200	-3.02380700	-0.51682300
H	3.37341900	-2.83917400	0.39088200
H	1.87166200	-3.23957300	1.24256300

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**M4R<sub>CN</sub>**

C	0.13247100	0.53711800	-0.74494800
C	0.46933400	1.97006500	-0.56967200
C	0.36418500	2.59944000	0.68544000
C	0.91835500	2.76770600	-1.64150600
C	0.75132400	3.92449200	0.87612500
H	-0.03777600	2.03219600	1.52046000
C	1.27723100	4.09970400	-1.46185700
H	1.01433800	2.32074100	-2.62863400
C	1.21178900	4.68514400	-0.19675800
H	0.66923500	4.36997100	1.86384800
H	1.62908500	4.67942600	-2.31070500
H	1.50219600	5.72127100	-0.05404700
C	-0.78753700	0.20375100	-1.94971600
P	1.17893200	-0.66471800	-0.09589200
C	2.07088800	-0.05883200	1.37935900
C	3.21469000	0.92072000	1.08493600
H	2.45567500	-0.94869100	1.89260700
H	1.33075600	0.39344800	2.04511700
C	3.67874200	1.63676400	2.35216800
H	4.05821600	0.37941600	0.63837100
H	2.90034100	1.67242000	0.35219400
C	4.79020900	2.64177000	2.06926100
H	2.81914200	2.15454500	2.79699700
H	4.01512600	0.89668300	3.08923000
H	5.11564500	3.14750100	2.98270500
H	5.66342900	2.14995600	1.62801400
H	4.44574900	3.40674800	1.36504300
C	2.53394800	-1.25461100	-1.20733600
C	3.52214100	-2.26860300	-0.62331500

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H	3.05845800	-0.34219400	-1.52080100
H	2.05811600	-1.66641500	-2.10382700
C	4.69195000	-2.53053100	-1.57336300
H	3.91750400	-1.91280300	0.33684300
H	3.00906500	-3.21598800	-0.41953600
C	5.67142200	-3.56067300	-1.01953800
H	4.30028300	-2.87061000	-2.53984200
H	5.21473800	-1.58489700	-1.76411800
H	6.50378900	-3.73140100	-1.70808900
H	6.08996200	-3.22866200	-0.06356600
H	5.17450500	-4.52150700	-0.84981600
C	0.27502300	-2.17711900	0.39799800
C	-0.49429600	-2.03331000	1.71130600
H	0.99792400	-2.99800800	0.46653400
H	-0.41522500	-2.41855900	-0.41901600
C	-1.36146700	-3.26135200	1.98585600
H	0.21054600	-1.89010900	2.54045100
H	-1.13099300	-1.13999000	1.66747900
C	-1.99332700	-3.23715300	3.37420900
H	-2.13796700	-3.31580800	1.21318200
H	-0.75073700	-4.16694500	1.87989700
H	-2.65964500	-4.09139700	3.52536000
H	-1.22326300	-3.27111600	4.15208900
H	-2.57833800	-2.32496500	3.53109100
C	-0.49452800	-1.00955300	-2.69889200
N	-0.27867200	-1.99670900	-3.26688900
B	-2.16393200	0.14780000	-1.19115300
O	-2.68657700	-0.97339700	-0.59071800
O	-2.93428200	1.26908900	-1.02307900
H	-0.78233000	1.03195800	-2.66621800



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C	-4.01330400	-0.60769200	-0.12866400
C	-4.30604200	-1.32529400	1.17607100
H	-5.25398600	-0.97416400	1.59669900
H	-4.38946500	-2.40183500	1.00093400
H	-3.51200000	-1.15171500	1.90483300
C	-4.99350300	-1.04242600	-1.21410400
H	-6.02863700	-0.86278700	-0.91089700
H	-4.80432200	-0.50914900	-2.15078200
H	-4.86563100	-2.11282300	-1.39584000
C	-3.90310400	0.94591100	0.00321700
C	-3.29791500	1.38762400	1.33286300
H	-3.05955500	2.45296700	1.27300800
H	-3.99250800	1.23032300	2.16260600
H	-2.37090400	0.84105100	1.53835400
C	-5.19059000	1.70062800	-0.27665700
H	-5.54881600	1.51691400	-1.29137700
H	-5.96928800	1.40187100	0.43215100
H	-5.01770700	2.77419100	-0.16113300

TS3R<sub>CN</sub>

C	0.05083500	0.52036600	-0.74939500
C	0.46858200	1.93977300	-0.59617000
C	0.31174100	2.60960600	0.63009600
C	1.05876500	2.66329300	-1.64951600
C	0.77563800	3.91059900	0.81543700
H	-0.18545500	2.09218300	1.44585200
C	1.50213300	3.97092200	-1.47602200
H	1.19574800	2.17746700	-2.61331200
C	1.37610900	4.59951700	-0.23670200
H	0.65006200	4.39330200	1.78072100
H	1.96399700	4.49640900	-2.30708600

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H	1.72973500	5.61644100	-0.09815800
C	-0.76448800	0.20563600	-2.03933100
P	1.10768300	-0.68857900	-0.09589000
C	1.94375200	-0.08853600	1.41383100
C	3.11707300	0.86992100	1.17127800
H	2.28816500	-0.98032700	1.95150100
H	1.17783900	0.38189800	2.03796200
C	3.53985500	1.57170300	2.46077600
H	3.96877300	0.31382400	0.75966600
H	2.84919300	1.63022800	0.42898900
C	4.68898400	2.54773300	2.23225500
H	2.67410600	2.11043400	2.86697900
H	3.82299800	0.82188400	3.21023300
H	4.98308200	3.04506900	3.16078100
H	5.56939400	2.03337100	1.83307000
H	4.39883600	3.32123700	1.51308100
C	2.48937300	-1.21903600	-1.19582900
C	3.45505600	-2.26331800	-0.62691000
H	3.02428900	-0.29271100	-1.44424600
H	2.04308800	-1.58471300	-2.12641200
C	4.68344800	-2.44252300	-1.52014000
H	3.78481700	-1.97608000	0.38008500
H	2.94195700	-3.22691800	-0.52653000
C	5.63679900	-3.50881300	-0.98994500
H	4.35492300	-2.70654400	-2.53280900
H	5.20755600	-1.48209200	-1.60273000
H	6.51135800	-3.61991300	-1.63706000
H	5.99258100	-3.25208500	0.01342900
H	5.13954500	-4.48232600	-0.92814400
C	0.20447000	-2.21124200	0.35521300

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C	-0.57467800	-2.09495100	1.66612700
H	0.93138300	-3.02924800	0.41383200
H	-0.47893800	-2.43758900	-0.47103300
C	-1.45135000	-3.32471100	1.89920500
H	0.12393500	-1.97911700	2.50453100
H	-1.20606500	-1.19794400	1.63808100
C	-2.09013200	-3.33733600	3.28446700
H	-2.22398300	-3.34992400	1.12127800
H	-0.84628900	-4.23104600	1.76920500
H	-2.76206200	-4.19172400	3.40704300
H	-1.32429700	-3.39871500	4.06486200
H	-2.67073700	-2.42672600	3.46484700
C	-0.49629100	-1.02873500	-2.74772500
N	-0.30281900	-2.03809200	-3.28511300
B	-2.05509100	0.20618200	-1.15868200
O	-2.62984600	-0.91626800	-0.58084600
O	-2.80952600	1.34830800	-0.97919800
H	-0.72326600	1.03608500	-2.74809400
C	-3.95010400	-0.51421300	-0.14419600
C	-4.30999800	-1.25449300	1.13151500
H	-5.25854500	-0.88175500	1.53209600
H	-4.42510300	-2.32274500	0.92520900
H	-3.53537800	-1.12932400	1.89040500
C	-4.91975100	-0.88036600	-1.26534200
H	-5.95586300	-0.67319100	-0.98309900
H	-4.68738600	-0.32588200	-2.17977300
H	-4.82486100	-1.94868100	-1.47758400
C	-3.78966700	1.03015400	0.03179400
C	-3.19162600	1.41036500	1.38409200
H	-2.91283800	2.46739000	1.35942900

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H	-3.90660500	1.25652500	2.19727200
H	-2.29093700	0.82203200	1.58945000
C	-5.05082700	1.83370700	-0.23621600
H	-5.40168400	1.69434800	-1.26060200
H	-5.84781400	1.53773700	0.45336900
H	-4.84655900	2.89742000	-0.08456600

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C	0.06977800	-0.47675000	-0.76406700
C	-0.54567000	-1.84583700	-0.68357900
C	-0.28980500	-2.65583200	0.42905800
C	-1.43209100	-2.31116300	-1.66258200
C	-0.94254500	-3.87641600	0.58582700
H	0.42584100	-2.31338500	1.17177600
C	-2.07790700	-3.53640700	-1.51450500
H	-1.62438000	-1.69800100	-2.53998000
C	-1.84418600	-4.31720800	-0.38283200
H	-0.74035400	-4.48881800	1.45958100
H	-2.76890500	-3.87897400	-2.27880500
H	-2.35110700	-5.26972100	-0.26282500
C	0.71713100	-0.15040100	-2.15010600
P	-0.99559500	0.76139200	-0.02222600
C	-1.78288100	0.09313500	1.48427600
C	-3.01269800	-0.79680400	1.26715000
H	-2.04949000	0.96066800	2.09970200
H	-0.99826300	-0.45011800	2.02422900
C	-3.41348400	-1.50697800	2.55936200
H	-3.85003000	-0.18528200	0.90773400
H	-2.81940000	-1.55160100	0.49817300
C	-4.62909700	-2.40616400	2.36197500
H	-2.56297800	-2.10711500	2.90723000

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H	-3.61508200	-0.76394200	3.34098800
H	-4.90151700	-2.91951100	3.28826800
H	-5.49744900	-1.82743400	2.03045500
H	-4.42478000	-3.16785900	1.60181000
C	-2.33354600	1.24286500	-1.16357300
C	-3.27802500	2.32267500	-0.62454000
H	-2.88136000	0.31658200	-1.38021200
H	-1.86680800	1.57213400	-2.09768400
C	-4.50795500	2.48378000	-1.51793900
H	-3.60382000	2.07707500	0.39478700
H	-2.74593400	3.27896200	-0.56559800
C	-5.43871700	3.58699200	-1.02514600
H	-4.18092400	2.70086600	-2.54197700
H	-5.04792500	1.52957400	-1.55704000
H	-6.31547700	3.68560200	-1.67102700
H	-5.79165400	3.37753500	-0.00994200
H	-4.92466600	4.55340300	-1.00716200
C	-0.05997800	2.23698800	0.48699100
C	0.68713200	2.04283300	1.81156400
H	-0.77351400	3.06527200	0.56106900
H	0.64435700	2.46642800	-0.31796900
C	1.70961500	3.15501100	2.03026700
H	-0.02737200	2.02615600	2.64344800
H	1.21458000	1.08229700	1.80076600
C	2.39804600	3.04614500	3.38682600
H	2.44891900	3.09592700	1.22308300
H	1.21619600	4.13120800	1.94089900
H	3.17735400	3.80479300	3.50278400
H	1.67939000	3.17560500	4.20303000
H	2.86540500	2.06327100	3.51239200

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C	0.64763600	1.16634200	-2.67803100
N	0.62275500	2.26307100	-3.07018900
B	1.69268100	-0.37256500	-0.83573000
O	2.41268300	0.73675000	-0.28456300
O	2.49608900	-1.55045100	-0.75707300
H	0.60179400	-0.93631000	-2.89132300
C	3.78612700	0.33530300	-0.28536500
C	4.53388700	1.10449700	0.79212900
H	5.54815400	0.71000100	0.91647700
H	4.61405800	2.15973200	0.51263100
H	4.01292800	1.04239300	1.75080300
C	4.37686200	0.64317700	-1.66286300
H	5.45288800	0.44730700	-1.69859500
H	3.88614300	0.04673700	-2.43840400
H	4.20811200	1.70064200	-1.88669500
C	3.67267500	-1.19978500	-0.02528300
C	3.43004100	-1.51318900	1.45256100
H	3.14108100	-2.56431000	1.54644500
H	4.32458600	-1.34611400	2.06066500
H	2.61793500	-0.89394300	1.84986400
C	4.84475500	-2.01744500	-0.54787200
H	4.93897500	-1.92157500	-1.63158100
H	5.78294900	-1.69726500	-0.08228000
H	4.69199400	-3.07502300	-0.31176900
TS4R <sub>CN</sub>			
C	-0.21368500	-0.65343100	0.96415600
C	0.43023300	-2.01863100	0.82466600
C	0.09236700	-2.85423200	-0.24541300
C	1.39942900	-2.44928100	1.73688300
C	0.73756400	-4.07682500	-0.42307000

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H	-0.68235600	-2.54185400	-0.94129400
C	2.05013700	-3.66678000	1.55796900
H	1.63813700	-1.81716400	2.58912000
C	1.72597900	-4.48151700	0.47244700
H	0.46632200	-4.71372700	-1.25985300
H	2.80831400	-3.98346200	2.26778500
H	2.23077800	-5.43268100	0.33468300
C	-0.71651100	-0.25778500	2.36035100
P	0.86375100	0.60934000	0.21359800
C	1.13759000	0.11931900	-1.52779500
C	2.31000600	-0.85144600	-1.74372900
H	1.28651500	1.02608400	-2.12143600
H	0.19326900	-0.32855300	-1.86091100
C	2.21943400	-1.53254700	-3.10811700
H	3.25628000	-0.30215700	-1.66766900
H	2.33114500	-1.62437700	-0.96793600
C	3.38341500	-2.48861300	-3.34563500
H	1.27140000	-2.08309100	-3.16353900
H	2.18751400	-0.77144000	-3.89748400
H	3.30411200	-2.98006500	-4.31918700
H	4.34070700	-1.95824800	-3.31334500
H	3.40662900	-3.26732700	-2.57572500
C	2.49481700	0.68165800	1.02122300
C	3.38993000	1.78597100	0.44334600
H	2.96126800	-0.30152900	0.89754700
H	2.32379100	0.84230600	2.09106900
C	4.81728700	1.67893000	0.97997900
H	3.41308400	1.73118500	-0.65314400
H	2.98002100	2.76944000	0.70107600
C	5.71459700	2.79610600	0.45787100

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H	4.78974500	1.70257100	2.07597900
H	5.23212300	0.70350200	0.69739100
H	6.73292800	2.70127400	0.84464400
H	5.76782900	2.77731600	-0.63570600
H	5.33199700	3.77722900	0.75701700
C	0.10030600	2.27415400	0.34674400
C	-0.17305800	2.97206600	-0.98576700
H	0.76335000	2.87180300	0.98019600
H	-0.83470400	2.13538700	0.89302300
C	-0.91316600	4.29109100	-0.76954000
H	0.76830000	3.16674800	-1.51561700
H	-0.78062500	2.31770600	-1.62210200
C	-1.21564300	5.00378200	-2.08366500
H	-1.84758600	4.08859400	-0.23153600
H	-0.31411400	4.94068700	-0.11971000
H	-1.74609200	5.94478900	-1.91382200
H	-0.29336900	5.23242000	-2.62788300
H	-1.83938800	4.37893500	-2.73168200
C	-0.14246300	0.77314300	3.09587900
N	0.33245100	1.68995200	3.66148600
B	-1.69794100	-0.48776200	0.49224100
O	-2.19652300	0.59253800	-0.22738100
O	-2.63943500	-1.49647600	0.63033100
H	-1.17149400	-1.06952600	2.91684900
C	-3.63547000	0.45078200	-0.21496900
C	-4.19786700	1.08782000	-1.47358100
H	-5.27603000	0.91223600	-1.54335600
H	-4.03058300	2.16888800	-1.44347000
H	-3.71795200	0.69117800	-2.37066100
C	-4.15370800	1.16746800	1.02925500



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H	-5.24539400	1.13544400	1.08292400
H	-3.74012400	0.72077100	1.93876100
H	-3.84077800	2.21492800	0.99085800
C	-3.80077000	-1.10029500	-0.12889800
C	-3.69641900	-1.77631900	-1.49438100
H	-3.59816400	-2.85539200	-1.34661900
H	-4.58432100	-1.58941700	-2.10521800
H	-2.81643100	-1.42035100	-2.04044200
C	-5.05059900	-1.56470000	0.59983800
H	-5.05685300	-1.21887500	1.63522500
H	-5.94925000	-1.19319900	0.09697800
H	-5.08838400	-2.65778300	0.60276800

**M6R<sub>CN</sub>**

C	0.34055400	-0.63453300	-1.07900700
C	-0.11630000	-2.08238700	-0.91359100
C	0.38264900	-2.87555000	0.12566700
C	-1.06885800	-2.63131900	-1.77821100
C	-0.07837800	-4.17751800	0.31468300
H	1.14099800	-2.47366800	0.79468600
C	-1.53943900	-3.92706700	-1.58574600
H	-1.43448700	-2.02949200	-2.60676800
C	-1.04854900	-4.70373400	-0.53530600
H	0.32217000	-4.77950700	1.12494800
H	-2.28653300	-4.33509000	-2.25984900
H	-1.41116000	-5.71653500	-0.38988200
C	0.62344000	-0.15040800	-2.49700800
P	-0.87244900	0.45970500	-0.23942200
C	-0.90743500	0.01688800	1.53809600
C	-1.88418500	-1.11314700	1.89970200
H	-1.15280500	0.91931200	2.10675600

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H	0.12193000	-0.25231800	1.80168400
C	-1.57301400	-1.69292800	3.27847400
H	-2.91096200	-0.72823400	1.88507300
H	-1.84125100	-1.92228300	1.16267100
C	-2.54358800	-2.80543300	3.66068900
H	-0.54678700	-2.08254100	3.27317000
H	-1.60072900	-0.89276300	4.02839200
H	-2.30601400	-3.22287400	4.64299700
H	-3.57321300	-2.43463400	3.69295600
H	-2.50485900	-3.62016300	2.92967800
C	-2.56855500	0.24369000	-0.86872100
C	-3.54321300	1.25827100	-0.25603600
H	-2.87778600	-0.78197000	-0.64259100
H	-2.53334100	0.35420400	-1.95707600
C	-4.98166700	0.97383400	-0.68789000
H	-3.48477300	1.23687900	0.84041900
H	-3.26539600	2.27272000	-0.56763200
C	-5.96570800	1.99274900	-0.12272000
H	-5.03167200	0.97348900	-1.78327700
H	-5.25956700	-0.03560500	-0.36051900
H	-6.98949400	1.77320700	-0.43780100
H	-5.94454000	1.99320100	0.97211900
H	-5.71975300	3.00406200	-0.46221100
C	-0.39871500	2.20983500	-0.50844500
C	-0.40582300	3.08370700	0.74506400
H	-1.08428100	2.59562900	-1.27075400
H	0.59833800	2.18559400	-0.95505400
C	-0.03799200	4.52937400	0.41367800
H	-1.39397200	3.06331100	1.22321200
H	0.31318300	2.68092000	1.46926100

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C	-0.00460400	5.41331600	1.65627500
H	0.94038000	4.54552000	-0.08204700
H	-0.75978700	4.92763100	-0.30970000
H	0.25740100	6.44467000	1.40463200
H	-0.97989100	5.42703100	2.15389200
H	0.73278400	5.04583500	2.37766300
C	-0.27451600	0.58971900	-3.24109400
N	-1.04118000	1.27276300	-3.82575600
B	1.76188100	-0.31885000	-0.46318500
O	2.03008700	0.74015300	0.37727100
O	2.87423400	-1.06539900	-0.75235000
H	1.40709700	-0.68399500	-3.02223800
C	3.47397500	0.90018400	0.37916000
C	3.90611900	1.44524300	1.72785100
H	4.99808200	1.48662600	1.78823000
H	3.51926600	2.46075300	1.85358400
H	3.53138600	0.82908000	2.54753500
C	3.80635000	1.88493600	-0.73742700
H	4.88068400	2.08013300	-0.79025500
H	3.46513200	1.50666900	-1.70684100
H	3.29365900	2.83048900	-0.53870600
C	3.95324400	-0.55370500	0.06970100
C	4.01524300	-1.43135200	1.31656200
H	4.13138700	-2.47392200	1.00837200
H	4.86222800	-1.16022700	1.95288600
H	3.09570200	-1.34507300	1.90521500
C	5.25128900	-0.64007900	-0.71313700
H	5.16037500	-0.15487000	-1.68670600
H	6.06501300	-0.16592700	-0.15546200
H	5.51293200	-1.68949400	-0.87404700

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**TS5R<sub>CN</sub>**

C	0.35800500	-0.92099900	-1.26433300
C	-0.27516500	-2.19861000	-0.76739600
C	0.40171000	-2.97947900	0.17864600
C	-1.54907100	-2.62018300	-1.17558700
C	-0.17585500	-4.12736900	0.71698900
H	1.40097200	-2.69906300	0.50024000
C	-2.12831300	-3.76594300	-0.63790200
H	-2.10103800	-2.04610500	-1.91093400
C	-1.44931400	-4.52194800	0.31647300
H	0.37313600	-4.71099400	1.44966100
H	-3.11883200	-4.06641300	-0.96572400
H	-1.90592400	-5.41219300	0.73732500
C	0.34152800	-0.57512400	-2.64313100
P	-0.89133600	0.58767300	-0.15063900
C	-1.10424000	0.60831800	1.68160000
C	-1.89706800	-0.61434000	2.15689700
H	-1.59247700	1.53579700	2.00429600
H	-0.09383600	0.59844400	2.10608100
C	-1.91242000	-0.74584400	3.67888300
H	-2.92989200	-0.55057200	1.78983900
H	-1.46983900	-1.52901900	1.72448500
C	-2.69074900	-1.97591900	4.13582900
H	-0.87930100	-0.80364200	4.04326500
H	-2.34887500	0.15956100	4.11889000
H	-2.68038600	-2.07734100	5.22470000
H	-3.73570100	-1.91997100	3.81348100
H	-2.26010200	-2.88751400	3.70732100
C	-2.59922700	0.55428600	-0.83003300
C	-3.51091500	1.67764100	-0.32828000

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H	-3.03910300	-0.41840700	-0.58640300
H	-2.49609700	0.59333400	-1.92270200
C	-4.88157400	1.64889400	-1.00552200
H	-3.64409800	1.58363000	0.75758500
H	-3.04306300	2.65541900	-0.50273800
C	-5.80431900	2.75070100	-0.49381000
H	-4.74752400	1.74839200	-2.08951200
H	-5.34406900	0.66840200	-0.83771700
H	-6.77833300	2.71848200	-0.99004100
H	-5.97347700	2.65131600	0.58351300
H	-5.36974100	3.73978000	-0.67271200
C	-0.21903700	2.21687500	-0.70107400
C	0.21351500	3.16571700	0.41613600
H	-0.96820700	2.69792200	-1.33978600
H	0.63896900	1.98591300	-1.34675300
C	0.79815600	4.46634300	-0.13427700
H	-0.64014200	3.40390300	1.06289400
H	0.95874000	2.66381700	1.04632500
C	1.33965300	5.36727700	0.97128900
H	1.59899200	4.23096400	-0.84685100
H	0.02454300	4.99575100	-0.70409800
H	1.74314300	6.30026800	0.56804500
H	0.55296800	5.62398100	1.68850900
H	2.14171100	4.86595900	1.52454100
C	-0.66228500	-0.92075500	-3.55942200
N	-1.48666700	-1.19970800	-4.34247300
B	1.76324400	-0.57026900	-0.61582600
O	1.94891200	0.34459600	0.38943100
O	2.92981700	-1.13434900	-1.04502600
H	1.08899600	0.11524700	-3.02127700

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C	3.37733800	0.60553300	0.46638600
C	3.75046500	0.87976300	1.91204800
H	4.83481500	0.99164200	2.00833700
H	3.28248400	1.81301800	2.23965600
H	3.41898200	0.07684800	2.57297400
C	3.64530800	1.83392200	-0.39692600
H	4.70144400	2.11492400	-0.36610300
H	3.36112200	1.65515700	-1.43940400
H	3.05508900	2.67138200	-0.01419000
C	3.97907600	-0.70478800	-0.13664700
C	4.15459800	-1.80816700	0.90174300
H	4.34634400	-2.75260200	0.38555400
H	4.99982700	-1.59482600	1.56190700
H	3.25685300	-1.92377800	1.51641500
C	5.25971300	-0.51179500	-0.92918000
H	5.10598100	0.15207100	-1.78188400
H	6.04204100	-0.09181900	-0.28941500
H	5.60645900	-1.47887800	-1.30322700

**(Z)- $\beta$ -product<sub>CN</sub>**

C	0.88469400	0.81046500	0.01393000
C	1.97053600	-0.19542300	0.01277900
C	1.84681200	-1.34603600	0.80470800
C	3.12176100	-0.03310000	-0.77005000
C	2.86689000	-2.29069400	0.84103800
H	0.95001100	-1.48989200	1.39890400
C	4.13433000	-0.98704000	-0.74262200
H	3.21404400	0.83084600	-1.42110500
C	4.01333300	-2.11368900	0.06812700
H	2.76421400	-3.16951000	1.46976200
H	5.01675800	-0.85125900	-1.35982900

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H	4.80543500	-2.85559100	0.09079000
C	1.09625200	2.14238400	0.03631300
C	2.38701900	2.76297000	0.12128100
N	3.40973900	3.30135500	0.20272300
B	-0.62628200	0.36128400	-0.01474100
O	-1.64685100	1.26976800	-0.03519300
O	-1.04239600	-0.93718200	-0.03074900
H	0.25775100	2.83309100	0.02361700
C	-2.87395200	0.52134100	0.17903200
C	-3.99101500	1.16857700	-0.61959700
H	-4.90367400	0.56897000	-0.54804000
H	-4.20227900	2.16171700	-0.21395400
H	-3.72124800	1.27559600	-1.67176100
C	-3.17267900	0.58894700	1.67345100
H	-4.11954500	0.09607600	1.90938000
H	-2.37683000	0.11680100	2.25756600
H	-3.24325700	1.63795500	1.97241900
C	-2.47207700	-0.91256900	-0.29901100
C	-2.63552700	-1.10727100	-1.80302500
H	-2.15104900	-2.04331600	-2.09248700
H	-3.69152700	-1.16184100	-2.08077200
H	-2.16761400	-0.29003300	-2.36025800
C	-3.13437700	-2.04645700	0.46258100
H	-2.89198400	-2.01069100	1.52623200
H	-4.22130100	-1.99530200	0.34614400
H	-2.79269100	-3.00463500	0.06195900
M7S <sub>CN</sub>			
P	-1.24158800	0.31124600	0.59000500
C	-2.75344200	-0.37352900	1.36807800
C	-0.26804300	0.83726100	2.06549800

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C	-3.82077000	-0.87439600	0.39985700
H	-2.44667400	-1.15521600	2.07126900
H	-3.14879800	0.44483000	1.98153000
C	-1.74323000	1.86563000	-0.23462600
C	-0.48528500	-0.72298900	-0.59961900
C	0.62494900	-0.27452700	2.61987700
H	0.34798900	1.68868800	1.76050700
H	-0.98080400	1.18265100	2.82494000
C	-5.07744400	-1.35264400	1.12554200
H	-3.41872400	-1.69525100	-0.20772200
H	-4.08914500	-0.06425000	-0.29334900
C	-2.72549000	2.72464900	0.56481900
H	-2.16070700	1.60372500	-1.21371400
H	-0.82124800	2.43125000	-0.41718600
C	0.35378200	0.04777400	-1.64897800
C	1.35163800	0.15352300	3.89362800
H	0.03463600	-1.17747200	2.82541500
H	1.35932900	-0.55014600	1.85196500
C	-6.14645000	-1.84703100	0.15654000
H	-5.47592300	-0.53245000	1.73539600
H	-4.80365900	-2.15568400	1.82103600
C	-2.95216400	4.07910900	-0.10672400
H	-3.68703800	2.20433400	0.65640900
H	-2.35079200	2.88289300	1.58480400
C	2.31782000	-0.91703000	4.39111700
H	0.61385700	0.38204000	4.67292600
H	1.89707100	1.08572000	3.69959400
H	-6.44972100	-1.05022900	-0.53080300
H	-5.77258300	-2.68222000	-0.44475700
H	-7.03938500	-2.18893800	0.68699500



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C	-3.96532200	4.93547600	0.64587200
H	-3.29221000	3.91463900	-1.13654400
H	-1.99451800	4.60900500	-0.17665300
H	3.07719400	-1.14049700	3.63342700
H	1.78836200	-1.85004400	4.61067900
H	2.83438500	-0.60109800	5.30190000
H	-3.63132100	5.12778300	1.67081700
H	-4.11271000	5.90129300	0.15482200
H	-4.93773800	4.43523400	0.70040100
B	1.79950000	0.47943700	-1.15875000
O	2.97626800	0.18676200	-1.78682100
O	1.95788400	1.21974300	-0.01866700
H	-0.16682000	0.97681300	-1.91908500
C	4.04210200	0.55860900	-0.87008400
C	5.22937000	1.05892800	-1.67244900
H	6.00900600	1.43233800	-1.00121900
H	5.64768500	0.23590600	-2.25804200
H	4.94106000	1.85817400	-2.35762900
C	4.40988900	-0.70005300	-0.08984500
H	5.25793300	-0.51709700	0.57583200
H	3.56469100	-1.05913500	0.50693600
H	4.68679500	-1.48663700	-0.79749500
C	3.34774600	1.64211500	0.01794000
C	3.39881800	3.03755900	-0.59564500
H	2.72816300	3.69442700	-0.03514200
H	4.40904900	3.45296400	-0.54990100
H	3.07285300	3.02139500	-1.64010000
C	3.81248500	1.67348400	1.46263900
H	3.62020900	0.72232300	1.96477300
H	4.88467500	1.88812100	1.51165900

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H	3.28295100	2.46502300	2.00109700
O	-1.57629000	1.59377000	-3.73898800
H	-2.01944300	0.77126100	-3.44843300
H	-0.93195100	1.28704800	-4.38920500
O	-2.59505700	-0.72671600	-2.65657200
H	-2.00079900	-0.86627300	-1.87537900
H	-3.49445800	-0.74613300	-2.30726100
C	0.00179400	-2.05957200	-0.21610500
C	-0.76335700	-2.94721500	0.57776600
C	1.24638200	-2.56012900	-0.66267200
C	-0.29826000	-4.20338200	0.94291100
H	-1.75770400	-2.65826100	0.89741100
C	1.70495600	-3.82638700	-0.30507000
H	1.88673200	-1.95907000	-1.29952500
C	0.94784000	-4.65997100	0.51146200
H	-0.92759700	-4.84037100	1.55855300
H	2.67354500	-4.15549300	-0.67227200
H	1.30797000	-5.64426500	0.79189000
C	0.41475400	-0.66750000	-2.92857300
N	0.46615800	-1.20798200	-3.95125600
TS6S <sub>CN</sub>			
P	1.08964100	-0.19128600	0.46271300
C	2.88327600	0.10854700	0.61220500
C	0.35434100	0.47975500	2.00205900
C	3.73952700	-0.72754100	-0.34283500
H	3.02838200	1.18155500	0.43077000
H	3.16024500	-0.07791100	1.65694100
C	0.84485400	-1.99318300	0.39256200
C	0.48717800	0.57551100	-1.05067300
C	0.95481200	1.80720000	2.48410400

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H	-0.71633500	0.58402000	1.80587000
H	0.46895200	-0.28815400	2.77663200
C	5.19328300	-0.25693600	-0.35762000
H	3.32824000	-0.67234000	-1.35483000
H	3.70014300	-1.78381500	-0.04791200
C	1.41559900	-2.76555700	1.58550100
H	1.29659200	-2.31210700	-0.55786100
H	-0.23354100	-2.16640400	0.31627900
C	-0.65565100	-0.21062900	-1.75410500
C	0.09603100	2.43453600	3.58168800
H	1.97040300	1.64218300	2.86316700
H	1.03819700	2.51934200	1.65508500
C	6.05604200	-1.10045300	-1.29096800
H	5.60087500	-0.28816700	0.66075000
H	5.22367600	0.79385500	-0.67326700
C	1.30448500	-4.27457400	1.36491700
H	2.46850700	-2.50268900	1.74938400
H	0.87622700	-2.49467600	2.50136300
C	0.66613000	3.76337300	4.06625800
H	0.00536200	1.73371900	4.42114400
H	-0.91780300	2.58780600	3.18985600
H	6.06648900	-2.14836300	-0.97397000
H	5.66749100	-1.06801200	-2.31434500
H	7.09012800	-0.74515600	-1.31160200
C	1.82948100	-5.07395100	2.55286300
H	1.85936800	-4.54335700	0.45789900
H	0.25461800	-4.53227400	1.17616300
H	0.73160500	4.47896100	3.23968300
H	1.67318300	3.63333600	4.47599000
H	0.04106100	4.20680200	4.84635600

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H	1.26854900	-4.83790900	3.46316200
H	1.74554300	-6.14990200	2.37688900
H	2.88366400	-4.84666000	2.74234000
B	-2.01165000	-0.52567600	-0.99062000
O	-3.17589100	-0.85558200	-1.61709800
O	-2.10104900	-0.55506300	0.37543200
H	-0.22721400	-1.18989900	-2.03284000
C	-4.20915200	-0.90531700	-0.59477900
C	-5.19802900	-2.00147800	-0.94795200
H	-5.93552200	-2.11765200	-0.14781400
H	-5.72854800	-1.73233800	-1.86512800
H	-4.69664200	-2.95780300	-1.10729000
C	-4.89238700	0.45806800	-0.60060300
H	-5.72284100	0.48784900	0.10973700
H	-4.18663300	1.25668800	-0.35023800
H	-5.28366700	0.65101800	-1.60263700
C	-3.37857100	-1.16886300	0.70419500
C	-3.10014700	-2.64841800	0.94866800
H	-2.36108000	-2.74133000	1.75018600
H	-4.00759000	-3.17600200	1.25420800
H	-2.70113600	-3.13003600	0.04991600
C	-3.92525600	-0.50973900	1.95751200
H	-3.96643200	0.57636900	1.85192200
H	-4.93142700	-0.88185300	2.17315500
H	-3.28254900	-0.75133900	2.80888900
O	1.76170300	-2.18058000	-2.72863200
H	1.95807500	-1.20461800	-2.95009000
H	1.32233100	-2.53467300	-3.51058500
O	2.09545800	0.32798100	-3.07807600
H	1.42858100	0.48372200	-1.96042800

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H	3.00389300	0.63675600	-2.97212700
C	0.23212300	2.04539000	-0.81835100
C	1.26103900	2.95593700	-1.09405000
C	-0.96911900	2.54495400	-0.29327000
C	1.11604900	4.31327800	-0.81365700
H	2.17834500	2.58227400	-1.54140400
C	-1.12187800	3.90233700	-0.02279700
H	-1.78396800	1.86282500	-0.06343000
C	-0.07478900	4.79035000	-0.27024700
H	1.92997600	4.99915000	-1.02872600
H	-2.05778500	4.26716600	0.39027600
H	-0.19225500	5.84726500	-0.05184900
C	-0.97196400	0.43396300	-3.03179200
N	-1.26967000	0.94386500	-4.02703400

M8S<sub>CN</sub>

P	1.10167000	-0.23951900	0.39703600
C	2.91633800	-0.39832100	0.45001800
C	0.65052800	0.91350600	1.74039500
C	3.50869200	-1.46493800	-0.47265100
H	3.32786700	0.59118600	0.21771600
H	3.16817100	-0.60828900	1.49775300
C	0.37611900	-1.87423700	0.69205000
C	0.57854200	0.38447900	-1.27182400
C	1.65527300	2.04268000	2.00361800
H	-0.33553200	1.30894500	1.48252400
H	0.52092300	0.30117100	2.64130100
C	5.03086000	-1.52217900	-0.34891000
H	3.22911200	-1.26459500	-1.51258100
H	3.08373400	-2.44680500	-0.22762000
C	0.90405400	-2.59827800	1.93230900

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H	0.57912200	-2.44623800	-0.22064500
H	-0.70552600	-1.72113700	0.75935600
C	-0.82942300	-0.02507600	-1.67220700
C	1.05506700	3.10178900	2.92718900
H	2.56742800	1.63446900	2.45487600
H	1.95264800	2.52472600	1.06494000
C	5.63898100	-2.58372500	-1.25985400
H	5.30242500	-1.72549500	0.69445300
H	5.44822100	-0.53775200	-0.59433500
C	0.22364400	-3.95782400	2.09733800
H	1.98905900	-2.74180900	1.85229000
H	0.72762600	-1.99372700	2.83087300
C	2.03017800	4.24199600	3.19983600
H	0.74755900	2.63368000	3.87067800
H	0.14359400	3.49724200	2.46094600
H	5.25383700	-3.57859100	-1.01285700
H	5.39683900	-2.38348900	-2.30863200
H	6.72805600	-2.61359000	-1.16649500
C	0.73753200	-4.71794300	3.31536200
H	0.38598700	-4.55053700	1.18877800
H	-0.85999500	-3.80716300	2.17925700
H	2.31938500	4.73414500	2.26506100
H	2.94275400	3.87341300	3.67970100
H	1.58818700	4.99774800	3.85499000
H	0.56197000	-4.14981200	4.23475600
H	0.23916000	-5.68558600	3.41933400
H	1.81408500	-4.90169100	3.23708700
B	-2.07978400	0.05915200	-0.85541700
O	-3.34362700	-0.31136800	-1.31269700
O	-2.13078700	0.43788300	0.49256500

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H	-1.32701200	-2.16048600	-1.50421100
C	-4.29414200	0.07152500	-0.30322400
C	-5.45123200	-0.91398400	-0.31145900
H	-6.13733800	-0.71000100	0.51695100
H	-6.00858500	-0.81624900	-1.24742900
H	-5.09644900	-1.94347700	-0.23132100
C	-4.78866300	1.47551300	-0.64599700
H	-5.56861000	1.80834000	0.04488900
H	-3.96565700	2.19696900	-0.62079000
H	-5.20230300	1.46493600	-1.65790800
C	-3.42587600	0.04492600	0.99317000
C	-3.28515900	-1.36361700	1.56897400
H	-2.50376800	-1.35519700	2.33613500
H	-4.21613300	-1.70437000	2.03089500
H	-3.00173300	-2.07816900	0.78772600
C	-3.85362000	1.02230500	2.07438900
H	-3.80587600	2.05332800	1.71796900
H	-4.87582100	0.80931000	2.40291800
H	-3.19093300	0.92710900	2.93998000
O	-1.42463200	-3.08722900	-1.79668200
H	0.33896000	-2.82453700	-2.42987100
H	-1.97663500	-3.00076900	-2.58700900
O	1.27432200	-2.55196000	-2.46116000
H	1.28655500	-0.13772200	-1.92905700
H	1.77224800	-3.36542900	-2.31193900
C	0.90369700	1.87192000	-1.30299200
C	2.16981000	2.30354600	-1.70918700
C	-0.02461300	2.81983300	-0.85990700
C	2.51354200	3.65354200	-1.65271200
H	2.89004000	1.57343700	-2.07317800

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C	0.31960600	4.16714700	-0.79506600
H	-1.01490500	2.49169100	-0.55463400
C	1.59171700	4.58788400	-1.18568600
H	3.49896300	3.97407700	-1.97679100
H	-0.40697100	4.89235600	-0.44083200
H	1.85693100	5.63947400	-1.13730300
C	-0.97672600	-0.36202100	-3.02857800
N	-1.11976700	-0.68561600	-4.14567200

**M9S<sub>CN</sub>**

P	-1.13063100	0.41850700	0.16110500
C	-2.95124400	0.48858200	0.17067800
C	-0.61990100	-0.45337700	1.68077900
C	-3.56301500	1.31994900	-0.95978700
H	-3.31165300	-0.54618900	0.13353200
H	-3.23930400	0.89210500	1.14974100
C	-0.49138200	2.11721200	0.18373200
C	-0.54942700	-0.43994500	-1.38666200
C	-1.54228300	-1.59500800	2.12486600
H	0.39668700	-0.81013400	1.49176200
H	-0.54971000	0.30973600	2.46581800
C	-5.08717500	1.36995500	-0.85273100
H	-3.28492400	0.89692900	-1.93277400
H	-3.16348600	2.34170900	-0.93530100
C	-1.12783500	3.01730900	1.24561900
H	-0.63439100	2.52121100	-0.82528900
H	0.58807000	2.02468200	0.34104700
C	0.79802600	0.05010500	-1.88270000
C	-0.89306700	-2.41882100	3.23618800
H	-2.49799600	-1.18874100	2.47721700
H	-1.76909200	-2.25948600	1.28281600



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C	-5.71600100	2.18734700	-1.97632300
H	-5.36468200	1.79600700	0.11923400
H	-5.48142400	0.34649500	-0.87012200
C	-0.47723200	4.40083000	1.25820600
H	-2.20313200	3.12373600	1.05508400
H	-1.02585700	2.56143700	2.23879700
C	-1.78313400	-3.57175000	3.68766400
H	-0.65893100	-1.76663200	4.08689800
H	0.06357400	-2.81117900	2.86816700
H	-5.35097500	3.21938400	-1.96118400
H	-5.47078700	1.76142400	-2.95451400
H	-6.80530700	2.21514400	-1.88575700
C	-1.10071000	5.32169800	2.30183200
H	-0.56994500	4.84856300	0.26147500
H	0.59676200	4.28940200	1.45192300
H	-1.99683400	-4.24470300	2.85035000
H	-2.73962900	-3.20320900	4.07272900
H	-1.30677300	-4.15861900	4.47782900
H	-0.99645700	4.90176200	3.30764700
H	-0.62409100	6.30572500	2.29856900
H	-2.16881500	5.46585100	2.10910700
B	2.04843400	0.19104300	-1.07926300
O	3.28152000	0.63278100	-1.55830200
O	2.12846900	-0.08866200	0.29522600
C	4.25977800	0.35099400	-0.54327100
C	5.36242400	1.39497800	-0.60916600
H	6.07010700	1.26065900	0.21534400
H	5.91098600	1.28888600	-1.54943600
H	4.95597600	2.40728500	-0.56389200
C	4.82838000	-1.03846000	-0.82796400

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H	5.63060700	-1.29842300	-0.13131800
H	4.04575000	-1.80139700	-0.76321500
H	5.23247800	-1.05064600	-1.84372500
C	3.40467600	0.38828900	0.76214300
C	3.20169300	1.80834700	1.28826900
H	2.42139500	1.79246800	2.05649000
H	4.11674100	2.20670700	1.73603600
H	2.88643300	2.48069100	0.48351800
C	3.89315600	-0.52344900	1.87576000
H	3.88905100	-1.56938900	1.56188100
H	4.90847100	-0.25056500	2.18082900
H	3.23825800	-0.42421000	2.74701100
H	-1.31722800	-0.13384600	-2.10897300
C	-0.73082400	-1.93413500	-1.15194000
C	-1.95271500	-2.54382600	-1.45351000
C	0.28257400	-2.70140500	-0.56833100
C	-2.17037200	-3.88856900	-1.15741400
H	-2.73945000	-1.95844500	-1.92557900
C	0.06295500	-4.04213300	-0.26332200
H	1.23705000	-2.23564400	-0.33936900
C	-1.16531300	-4.63888200	-0.55114500
H	-3.12251500	-4.34883900	-1.40309500
H	0.85400300	-4.62524500	0.19880600
H	-1.33219400	-5.68525700	-0.31498800
C	0.83951500	0.38289000	-3.24243600
N	0.86446800	0.66781000	-4.38013900
TS7S <sub>CN</sub>			
P	1.52771800	-0.19507000	-0.04143400
C	3.29274700	-0.01234700	0.47188500
C	0.54666700	0.41095000	1.39258400

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C	4.25798000	-0.64798400	-0.52993400
H	3.48863600	1.06374300	0.55383800
H	3.42493800	-0.44499200	1.47282800
C	1.21893800	-2.01060700	-0.07873800
C	0.22554900	0.65314200	-1.84911300
C	0.98685900	1.78150200	1.91985400
H	-0.48767600	0.47041200	1.02972700
H	0.56544400	-0.33102500	2.19993200
C	5.72013900	-0.45191800	-0.13079500
H	4.09058300	-0.21686000	-1.52637400
H	4.05009500	-1.72265200	-0.61833600
C	1.74787400	-2.81120200	1.11284200
H	1.64368300	-2.39364300	-1.01470200
H	0.13090500	-2.12943900	-0.16534300
C	-0.88791100	-0.21238700	-1.91505000
C	-0.07849600	2.40473200	2.82107000
H	1.92795300	1.68182200	2.47552300
H	1.18506400	2.46841900	1.08704800
C	6.68493100	-1.08563400	-1.12811200
H	5.87965700	-0.88252800	0.86569700
H	5.92731900	0.62179200	-0.04283700
C	1.34142600	-4.28337600	1.03656300
H	2.84296700	-2.74094800	1.15039800
H	1.37544900	-2.38434300	2.05278600
C	0.33042600	3.78057600	3.33601500
H	-0.28291500	1.73214500	3.66433300
H	-1.01353900	2.48479600	2.25013200
H	6.51069500	-2.16350300	-1.21012500
H	6.55778800	-0.65157200	-2.12526500
H	7.72586700	-0.93635000	-0.82783000

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C	1.88674700	-5.09798800	2.20543600
H	1.69853000	-4.70590000	0.08937000
H	0.24658900	-4.35142900	1.01341200
H	0.50960600	4.46594400	2.50025100
H	1.25313900	3.72248400	3.92299200
H	-0.44425600	4.21941200	3.97126800
H	1.52329800	-4.70469500	3.16068600
H	1.58314700	-6.14647700	2.13799300
H	2.98112900	-5.06693300	2.22764600
B	-2.14442400	-0.38029500	-1.04093900
O	-2.97139500	-1.46973400	-1.22437600
O	-2.57817600	0.41756400	0.00306600
C	-4.14162700	-1.27188400	-0.40252700
C	-4.63117000	-2.62184200	0.09318400
H	-5.45537300	-2.49269200	0.80181400
H	-4.99683300	-3.21135000	-0.75204900
H	-3.83057600	-3.18143700	0.58082000
C	-5.20013100	-0.60729000	-1.27891400
H	-6.14407100	-0.48368600	-0.74082200
H	-4.86234500	0.37397700	-1.62637600
H	-5.37909900	-1.23796500	-2.15366700
C	-3.59950200	-0.32438600	0.71222400
C	-2.90131100	-1.07745400	1.84244300
H	-2.38842700	-0.35734800	2.48660800
H	-3.61967900	-1.63391300	2.45071400
H	-2.15794100	-1.77961600	1.44903300
C	-4.61574400	0.65382500	1.27450800
H	-5.01315400	1.30829600	0.49648500
H	-5.44618200	0.11406600	1.74022600
H	-4.14145900	1.27577000	2.03918300

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H	0.99188500	0.45660300	-2.59704600
C	0.24180100	2.08467300	-1.43382800
C	1.43172000	2.80228200	-1.63850900
C	-0.85074400	2.74562400	-0.86859800
C	1.53980700	4.13311300	-1.25996600
H	2.28337400	2.29352300	-2.08615400
C	-0.73823300	4.08103800	-0.47690100
H	-1.78729600	2.22317500	-0.72235800
C	0.45261700	4.77666600	-0.66327700
H	2.46871400	4.66964800	-1.42621000
H	-1.59254700	4.57792200	-0.02660200
H	0.53342700	5.81506700	-0.35683500
C	-0.68943200	-1.30671100	-2.80745000
N	-0.51216600	-2.19335900	-3.54235600
<i>(E)</i> - $\alpha$ -product <sub>CN</sub>			
C	-1.71776300	1.73018300	0.00238100
C	-0.36777400	1.82083200	-0.04374100
B	0.71477600	0.68113900	-0.01406000
O	2.00162200	0.94194200	-0.38904500
O	0.51803600	-0.58920300	0.44132700
C	2.69965500	-0.33268300	-0.39377300
C	4.13537900	-0.10857100	0.04525300
H	4.65603800	-1.06661600	0.13830800
H	4.65706800	0.49271100	-0.70414700
H	4.18425600	0.41418600	1.00207200
C	2.65025800	-0.85185100	-1.82716800
H	3.20907500	-1.78601700	-1.92848900
H	1.61863600	-1.02409900	-2.15007400
H	3.09746000	-0.10559000	-2.48878300
C	1.83689900	-1.18300900	0.59424400

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C	2.23668600	-0.98893300	2.05332700
H	1.47436100	-1.44328600	2.69140200
H	3.19713400	-1.46598300	2.26596100
H	2.30925100	0.07340700	2.30543000
C	1.74870200	-2.66001400	0.25458400
H	1.30806500	-2.81797300	-0.73168300
H	2.74488900	-3.11262800	0.27339300
H	1.12734900	-3.16901500	0.99632100
H	-2.28491400	2.65482000	0.10744900
C	-2.53863000	0.51770200	-0.07563800
C	-3.78080300	0.51422400	0.57594700
C	-2.15638200	-0.60785900	-0.81797600
C	-4.59832700	-0.60934900	0.53274000
H	-4.09377800	1.39659400	1.12751000
C	-2.98166500	-1.72470100	-0.87234900
H	-1.22226200	-0.59647800	-1.36887800
C	-4.19827800	-1.73204200	-0.19030700
H	-5.55046500	-0.60584900	1.05332800
H	-2.68026800	-2.58875400	-1.45586800
H	-4.84007200	-2.60638400	-0.23485600
C	0.17923200	3.15213800	-0.02805500
N	0.63913000	4.21613500	-0.01473700
STS1 <sub>CN-1</sub>			
C	-2.63380900	-1.98543800	0.13871600
C	-4.01919500	-2.23245400	-0.11298100
C	-4.84010400	-1.18126400	-0.55085500
C	-4.55870400	-3.51229600	0.08451800
C	-6.19019800	-1.41267600	-0.78307000
H	-4.41077500	-0.19615800	-0.70422000
C	-5.91053100	-3.73101400	-0.15107800

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H	-3.91535600	-4.31798000	0.42197800
C	-6.72561700	-2.68490400	-0.58295300
H	-6.82482000	-0.59926000	-1.11980100
H	-6.32944900	-4.71999100	0.00234000
H	-7.78084000	-2.86200600	-0.76486100
C	-1.46397700	-1.75321400	0.35805100
P	-0.30263900	1.01340000	0.69766700
C	-0.20293600	1.53946700	-1.07255300
C	-0.41386200	3.02468400	-1.37736900
H	-0.94142600	0.94019300	-1.61993700
H	0.78097300	1.20636300	-1.42752500
C	-0.16236000	3.34422100	-2.85120500
H	-1.44104200	3.31088800	-1.11620900
H	0.24677900	3.64087800	-0.75623800
C	-0.41475900	4.81274900	-3.17835200
H	0.87265800	3.07981500	-3.10209200
H	-0.80494400	2.70841100	-3.47311800
H	-0.22220600	5.02664900	-4.23343900
H	-1.45255000	5.08866200	-2.96412300
H	0.23248700	5.46323800	-2.58084700
C	1.30702100	1.40742200	1.48179400
C	2.09633700	2.62571200	1.00044700
H	1.92413600	0.50763800	1.34206700
H	1.10630200	1.47862400	2.55853100
C	3.47698700	2.67072100	1.65702500
H	2.22343200	2.57815000	-0.08972500
H	1.54990300	3.55366700	1.21255500
C	4.36641400	3.76762800	1.08157900
H	3.35743700	2.81199600	2.73840000
H	3.95512100	1.69093200	1.52581800

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H	5.34212600	3.79282600	1.57518300
H	4.53649700	3.60851100	0.01105500
H	3.90456800	4.75342800	1.20186200
C	-1.56288900	2.12454800	1.45811100
C	-2.97004400	1.78805800	0.95715300
H	-1.31096900	3.17271100	1.25348000
H	-1.50230100	1.97825300	2.54251700
C	-4.03968700	2.72892700	1.50759000
H	-2.99355900	1.82422000	-0.14181200
H	-3.21403500	0.75460500	1.23745500
C	-5.43861400	2.35071200	1.02966300
H	-4.00401600	2.71206900	2.60384800
H	-3.80585100	3.75682600	1.20306400
H	-6.19600000	3.03341500	1.42509600
H	-5.50024500	2.38067800	-0.06398000
H	-5.70019100	1.33675400	1.35102200
C	-0.12925200	-1.42673300	0.61431400
N	0.99056400	-1.76343300	0.74875400
B	2.51823800	-2.28303000	1.06597800
O	2.86156000	-3.17634000	-0.01530700
O	3.45512800	-1.18472400	1.03574600
H	2.36973600	-2.76470100	2.17535600
C	4.09345900	-2.73120500	-0.57501500
C	4.11190200	-3.05191000	-2.06345500
H	5.00235800	-2.63277500	-2.54447400
H	4.12866400	-4.13679000	-2.20678600
H	3.22389900	-2.65812400	-2.56286100
C	5.23448300	-3.46835300	0.13143400
H	6.20973400	-3.23880400	-0.30933800
H	5.25934500	-3.20873900	1.19423300



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H	5.06198900	-4.54517500	0.04576600
C	4.09131300	-1.20687200	-0.24092400
C	3.24953900	-0.39756000	-1.23207500
H	3.11310000	0.61219300	-0.82810800
H	3.73840200	-0.31162300	-2.20772400
H	2.26393500	-0.85193700	-1.37613300
C	5.47560800	-0.58458100	-0.12050100
H	6.03256200	-1.02319600	0.71014200
H	6.04809900	-0.72744800	-1.04349300
H	5.38812200	0.49254700	0.05733700

STS1<sub>CN</sub>-2

C	-2.84251000	-1.95441600	-0.01662700
C	-4.24384400	-1.94284300	0.25621400
C	-4.82315800	-0.79483300	0.81899300
C	-5.03936500	-3.05465500	-0.05797400
C	-6.19102300	-0.76169400	1.05852000
H	-4.19363100	0.05616800	1.06086500
C	-6.40587000	-3.00975400	0.18847700
H	-4.58054100	-3.93571600	-0.49407800
C	-6.98151300	-1.86706000	0.74356000
H	-6.64027000	0.12637600	1.49124700
H	-7.02357800	-3.86779600	-0.05518100
H	-8.04999300	-1.83819900	0.93224100
C	-1.65582600	-1.92588700	-0.26739700
P	-0.09698700	0.67805100	-0.02572900
C	0.86825300	1.75268100	-1.18869800
C	0.68942000	3.26835300	-1.07183200
H	0.60637000	1.43012000	-2.20379400
H	1.91366900	1.45613400	-1.04188100
C	1.62155300	4.02264800	-2.02070800

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H	-0.34952300	3.54015200	-1.30095100
H	0.87592900	3.60085900	-0.04405500
C	1.43101800	5.53436700	-1.94377000
H	2.66114300	3.76552400	-1.78112200
H	1.44561200	3.67768900	-3.04737300
H	2.10454100	6.05911400	-2.62752300
H	0.40464400	5.81312300	-2.20518800
H	1.62778200	5.90328700	-0.93155500
C	0.82366500	0.67346100	1.57473900
C	1.40150600	1.98945000	2.09409600
H	1.62716000	-0.05568400	1.43009600
H	0.12980500	0.24418800	2.31007500
C	2.08128900	1.81450100	3.45293300
H	2.13627800	2.37489000	1.37477200
H	0.61276800	2.74909200	2.17689400
C	2.70657600	3.10813000	3.96505200
H	1.34617000	1.44320200	4.17799700
H	2.85213000	1.03760400	3.36752800
H	3.18830700	2.96415300	4.93647200
H	3.46445500	3.47930600	3.26711700
H	1.94989400	3.89141600	4.08015400
C	-1.62680900	1.64161100	0.36189100
C	-2.61079400	1.68895500	-0.80954900
H	-1.36196800	2.65736600	0.68264700
H	-2.09567300	1.14943400	1.22484100
C	-3.81732600	2.58084700	-0.51894500
H	-2.10507500	2.05210200	-1.71474900
H	-2.95346900	0.67063800	-1.03737700
C	-4.87440900	2.50887100	-1.61613300
H	-4.26250100	2.28724800	0.44105300

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H	-3.47422100	3.61579300	-0.39339500
H	-5.72000700	3.16947300	-1.40381500
H	-4.45552800	2.80145500	-2.58479000
H	-5.26176300	1.48891300	-1.71503800
C	-0.31132700	-1.83746100	-0.60004300
N	0.71460400	-2.28150400	-0.96974200
B	2.22119700	-1.83993300	-1.55891100
O	2.69945900	-0.82400900	-0.64549600
O	3.12906200	-2.94182200	-1.51016200
H	1.90914600	-1.48527200	-2.68065500
C	4.00614400	-1.22187200	-0.21917700
C	4.26600400	-0.70565100	1.18883200
H	5.25882800	-1.01221500	1.53582800
H	4.23116900	0.38977300	1.19089500
H	3.52353600	-1.07362000	1.90052200
C	5.02262100	-0.61289800	-1.18790200
H	6.05347400	-0.81682300	-0.88240400
H	4.87292700	-1.00479300	-2.19855900
H	4.88052800	0.47174900	-1.21557900
C	3.93644200	-2.77507500	-0.34521400
C	3.22409000	-3.41615400	0.84891500
H	2.96819700	-4.44840800	0.59232300
H	3.85609900	-3.42866900	1.74268000
H	2.29789400	-2.88332300	1.08689400
C	5.27919800	-3.45273900	-0.57647100
H	5.72606600	-3.12422400	-1.51734000
H	5.97422000	-3.23313500	0.24095600
H	5.14340300	-4.53766700	-0.62440600
STS2 <sub>CN</sub> -1			
C	1.69911000	-2.20998000	-0.95539100

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C	2.99881200	-2.35771100	-0.39254700
C	4.15681400	-2.24166800	-1.18996900
C	3.15526000	-2.63598600	0.98217300
C	5.41798500	-2.35526700	-0.61881900
H	4.05253500	-2.04945900	-2.25365700
C	4.42408500	-2.74572700	1.53859900
H	2.27202900	-2.75681800	1.60235100
C	5.56421000	-2.60096700	0.74781200
H	6.29690700	-2.24911300	-1.24831800
H	4.52148800	-2.94909500	2.60088600
H	6.55260600	-2.68771600	1.18692700
C	0.72030600	-1.46507700	-1.25901400
P	0.95898800	0.68172600	-0.70058700
C	0.05474000	2.27021000	-0.98520000
C	0.58094500	3.46891000	-0.19199600
H	-1.00129900	2.08535400	-0.75406700
H	0.11190800	2.46342800	-2.06307400
C	-0.16090900	4.75928400	-0.54445800
H	0.47722200	3.27657800	0.88348100
H	1.65383300	3.60205800	-0.38650600
C	0.34772800	5.95646000	0.25272300
H	-0.05270200	4.95385900	-1.61846500
H	-1.23294900	4.61700800	-0.35959900
H	-0.19154100	6.87041000	-0.01174400
H	0.22277900	5.79242600	1.32805300
H	1.41235400	6.12877000	0.06348200
C	2.69586700	1.00192900	-1.25266200
C	3.76071900	1.12004400	-0.16004300
H	2.66737300	1.91622900	-1.85783000
H	2.95583200	0.18158000	-1.92942200

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C	5.15152900	1.33939200	-0.75405800
H	3.51796600	1.94930300	0.51673500
H	3.77298700	0.20538500	0.44814400
C	6.23788600	1.37074800	0.31578800
H	5.36164100	0.53461500	-1.46997500
H	5.15867600	2.27615000	-1.32575300
H	7.22675200	1.53628100	-0.12138600
H	6.05324600	2.17039600	1.04094500
H	6.26531200	0.42247300	0.86351000
C	0.98315100	0.48073900	1.12438200
C	-0.43612600	0.35365600	1.68441700
H	1.51643400	1.31331200	1.59611500
H	1.55834800	-0.42991500	1.32547100
C	-0.44688200	-0.10965100	3.14039600
H	-0.94819000	1.32271400	1.60591100
H	-1.02486000	-0.35377300	1.08316400
C	-1.86444100	-0.21693600	3.69444000
H	0.04937600	-1.08619600	3.20303000
H	0.14730900	0.58216400	3.75060300
H	-1.87045000	-0.62136400	4.71077900
H	-2.34866900	0.76557400	3.72365600
H	-2.47158100	-0.87139000	3.05944100
C	-0.56175300	-1.64494000	-1.82031600
N	-1.62458700	-1.76506400	-2.27112300
B	-3.75747700	-2.32116200	-0.28716600
O	-3.42649500	-1.30167100	0.56595300
O	-4.85297800	-2.05467700	-1.05655900
H	-3.18323300	-3.35911800	-0.31235500
C	-4.51363000	-0.34159200	0.51591000
C	-3.94285900	1.06002800	0.64272000

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H	-4.73154500	1.80601800	0.50132700
H	-3.52073900	1.19443200	1.64274600
H	-3.15473100	1.23562700	-0.09308200
C	-5.42831900	-0.65163300	1.69757800
H	-6.25633700	0.06014200	1.75594800
H	-5.83951300	-1.66279500	1.62202200
H	-4.84842600	-0.58370000	2.62231400
C	-5.17506100	-0.65319000	-0.86744600
C	-4.53410500	0.11294500	-2.02091700
H	-4.89680800	-0.30398800	-2.96437500
H	-4.79947200	1.17336000	-1.98492700
H	-3.44543000	0.01556300	-2.00325200
C	-6.68538100	-0.49079100	-0.89999200
H	-7.17580100	-1.15425800	-0.18523400
H	-6.96250700	0.54291400	-0.67034100
H	-7.05574300	-0.72864500	-1.90099500

STS2<sub>CN-2</sub>

C	-0.50354600	-1.72228300	-1.69337700
C	-1.38746300	-2.61204400	-1.01926100
C	-0.91736100	-3.46037200	0.00525100
C	-2.75449500	-2.66779800	-1.36380200
C	-1.79504000	-4.29623900	0.68390700
H	0.13656900	-3.44158900	0.26860100
C	-3.61977100	-3.51096000	-0.67654200
H	-3.12475900	-2.03742800	-2.16697800
C	-3.15163100	-4.32583600	0.35433100
H	-1.41586100	-4.93053100	1.48020800
H	-4.67038200	-3.53068800	-0.95040400
H	-3.83161400	-4.98103000	0.88877800
C	0.04012100	-0.58630100	-1.80101100

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P	-0.56513800	0.89863700	-0.21671500
C	-0.10567800	2.59399500	0.37228500
C	-1.03471200	3.19111900	1.43175900
H	-0.04816000	3.24795100	-0.50564600
H	0.91368300	2.49493100	0.76270800
C	-0.51602700	4.52932600	1.96098200
H	-2.03662300	3.33694600	1.00833700
H	-1.14557600	2.48914900	2.26969400
C	-1.44716700	5.14068100	3.00353200
H	0.48144800	4.38222800	2.39295300
H	-0.39209000	5.22296600	1.12021500
H	-1.06206600	6.09531200	3.37302100
H	-2.44169600	5.32084900	2.58234700
H	-1.56565600	4.47189000	3.86246200
C	-0.39244000	-0.17846500	1.27730800
C	-1.67553200	-0.64403900	1.96679400
H	0.24809000	0.36746900	1.98063200
H	0.17928700	-1.04937000	0.94333600
C	-1.37017500	-1.55751400	3.15360800
H	-2.26135500	0.21780700	2.31135700
H	-2.30559800	-1.19044800	1.25182900
C	-2.63549800	-2.12233900	3.79064700
H	-0.73073300	-2.38162100	2.81058600
H	-0.78821800	-1.00150900	3.89980300
H	-2.40327000	-2.76616700	4.64389400
H	-3.28978100	-1.31863300	4.14475200
H	-3.19965400	-2.71593600	3.06299500
C	-2.36638000	1.00299200	-0.57434700
C	-2.65829600	1.91529800	-1.76684800
H	-2.90924700	1.34145700	0.31560300

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H	-2.70176300	-0.01826300	-0.78714400
C	-4.14395300	1.94189000	-2.12402900
H	-2.32083000	2.93713600	-1.54624700
H	-2.08074300	1.57734800	-2.63804400
C	-4.44103900	2.85188000	-3.31166700
H	-4.47616800	0.91981800	-2.34594300
H	-4.71773700	2.27214900	-1.24905600
H	-5.50726300	2.85704200	-3.55505400
H	-4.14059300	3.88318400	-3.09918100
H	-3.89503700	2.52330300	-4.20201200
C	0.96473500	0.04560500	-2.65705400
N	1.73564200	0.58942100	-3.33392800
B	3.13435300	1.38452600	-0.70565800
O	2.49257000	0.47365900	0.09333300
O	4.42957100	1.05687000	-0.97503600
H	2.62090200	2.38429800	-1.08889900
C	3.50624100	-0.45033600	0.57546900
C	2.91235700	-1.84604100	0.66637500
H	3.70039900	-2.57912600	0.86610700
H	2.19341200	-1.89120700	1.48970700
H	2.40222700	-2.11862900	-0.26097700
C	3.92314800	0.04560400	1.95657700
H	4.64622400	-0.63139800	2.41957400
H	4.36382300	1.04553900	1.90064400
H	3.03705900	0.09472900	2.59561500
C	4.63475200	-0.29851700	-0.49734100
C	4.44869800	-1.22411800	-1.69577200
H	5.14019000	-0.91963400	-2.48583600
H	4.66117500	-2.26301800	-1.42929200
H	3.43117700	-1.16188300	-2.09111500



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C	6.04743100	-0.41708200	0.04850500
H	6.25368400	0.34713100	0.80009500
H	6.19956700	-1.40380100	0.49695400
H	6.76454700	-0.29971400	-0.76852200
STS3 <sub>CN-1</sub>			
P	-1.73741800	-0.41008700	-0.99231500
C	-2.87098500	-1.87669500	-0.96616200
C	-0.94700900	-0.55010200	-2.65350900
C	-3.53766100	-2.09451000	0.39294700
H	-3.63238400	-1.69181700	-1.73431200
H	-2.31923300	-2.77508300	-1.27362100
C	-0.52417600	-0.77935700	0.35265200
C	-0.62748000	2.40379000	-1.02787200
C	0.13857100	-1.60949300	-2.87966800
H	-1.80041700	-0.72528200	-3.31997100
H	-0.55639300	0.44063200	-2.91367700
C	-4.54162100	-3.24677000	0.36952600
H	-4.04693000	-1.17347200	0.70837600
H	-2.77420000	-2.30054400	1.15488200
C	0.06360400	-2.18877000	0.47865200
H	-1.07951500	-0.53652300	1.26982600
H	0.27952800	-0.03681700	0.28917600
C	-1.74422600	1.96874600	-0.67094000
C	1.54236600	-1.11141200	-2.53508100
H	-0.08873900	-2.52340800	-2.31552100
H	0.12986100	-1.89821300	-3.93821500
C	-5.20664700	-3.46607600	1.72481800
H	-4.02704400	-4.16347400	0.05508900
H	-5.30562300	-3.04262300	-0.39096000
C	0.65561200	-2.42528000	1.86883400

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H	-0.70056600	-2.95254900	0.28224900
H	0.85057800	-2.33617000	-0.27049500
C	-3.00080900	2.35078300	-0.03735000
C	2.59539800	-2.20062900	-2.71225500
H	1.56606400	-0.72355000	-1.50636500
H	1.77803200	-0.25569700	-3.18024800
H	-4.46152300	-3.69573600	2.49361300
H	-5.74798700	-2.56943300	2.04422200
H	-5.92003900	-4.29436400	1.69170400
C	1.30463000	-3.80014400	1.99257300
H	-0.13870800	-2.32128300	2.61951200
H	1.38704200	-1.63470100	2.07521100
C	-2.99411300	3.50429900	0.76426700
C	-4.19910100	1.65362100	-0.22045800
H	2.56034800	-2.61067200	-3.72746900
H	2.42857200	-3.02998400	-2.01447800
H	3.60640500	-1.81683500	-2.54418600
H	2.08903000	-3.93305700	1.23893400
H	1.75803000	-3.94511200	2.97773800
H	0.56728800	-4.59623900	1.84297800
C	-4.16299900	3.93646400	1.37831900
H	-2.06339000	4.04536400	0.90091400
C	-5.36925000	2.09823400	0.38745700
H	-4.21067900	0.76710700	-0.84615200
C	-5.35428000	3.23535400	1.19218500
H	-4.14333500	4.82241200	2.00494000
H	-6.29441500	1.55254100	0.23179200
H	-6.26638100	3.57448600	1.67288700
B	2.56732200	1.78866900	1.00934600
O	2.55002600	0.43724100	1.23538100

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O	3.79327700	2.26524000	0.64899600
H	1.61033400	2.47665100	1.15632400
C	3.93645000	0.00324000	1.25514900
C	4.02706400	-1.39695300	0.67569000
H	5.07379200	-1.67933300	0.52262600
H	3.58071400	-2.11509100	1.36944100
H	3.50126200	-1.46150700	-0.27945400
C	4.37545500	0.00740800	2.71653400
H	5.39567800	-0.37138000	2.82365400
H	4.32886600	1.01523100	3.14010500
H	3.70435500	-0.63879800	3.28935200
C	4.63746800	1.10927100	0.40449900
C	4.58341300	0.82138400	-1.09284400
H	3.56905800	0.55894100	-1.40823000
H	4.88191500	1.72096200	-1.63772700
H	5.26532100	0.00851900	-1.35958100
C	6.05608500	1.43888800	0.83489800
H	6.08852000	1.80393400	1.86319800
H	6.69323600	0.55252300	0.75434100
H	6.46536800	2.21377000	0.18089500
C	0.63707500	2.38337100	-1.55051400
N	1.72279100	2.41026000	-1.98348900
STS3 <sub>CN</sub> -2			
P	2.06234200	0.65157500	0.06370200
C	1.96484100	0.87116100	1.89383800
C	3.28095800	1.95487900	-0.45325200
C	1.00076600	-0.10375700	2.57626000
H	2.97927200	0.75079300	2.29207200
H	1.65837200	1.90432200	2.10037500
C	0.39286400	1.16078100	-0.53197300

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C	0.97780000	-2.25062000	0.02025800
C	2.99425300	3.43021900	-0.13267200
H	4.21655400	1.62977300	0.01813900
H	3.42993100	1.83691000	-1.53370200
C	0.71274900	0.27357800	4.02782600
H	1.41391600	-1.11835000	2.53794800
H	0.04887500	-0.14028100	2.02853800
C	-0.32713300	2.27359100	0.23940800
H	-0.23267600	0.25685000	-0.53233800
H	0.52133800	1.43689800	-1.58648100
C	2.07744300	-1.73001300	-0.27513800
C	2.18747000	4.13786200	-1.22284700
H	2.48411900	3.52588300	0.83381700
H	3.95120100	3.95427800	-0.01698600
C	-0.23574800	-0.71969200	4.69237400
H	0.27700100	1.28059600	4.05666900
H	1.65585200	0.32552800	4.58663400
C	-1.53386700	2.80208600	-0.53669100
H	-0.65888300	1.88451900	1.21034100
H	0.35026300	3.10723000	0.45982600
C	3.44130800	-2.08428600	-0.66123100
C	1.75132400	5.53758200	-0.80392500
H	1.30485400	3.54299900	-1.48458400
H	2.79909300	4.19175600	-2.13191600
H	-1.18040200	-0.78154000	4.14106500
H	0.20072200	-1.72375400	4.71083600
H	-0.46383300	-0.43298300	5.72290800
C	-2.40116600	3.73908100	0.29743900
H	-2.13153200	1.95218800	-0.88573700
H	-1.17595600	3.32245200	-1.43553000

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C	3.95915500	-3.29777900	-0.18250800
C	4.22311100	-1.29550600	-1.51094000
H	2.61579800	6.15572600	-0.53891500
H	1.09463900	5.49474200	0.07243600
H	1.20790000	6.04592200	-1.60540300
H	-1.82166400	4.59251900	0.66638500
H	-3.24064800	4.13173000	-0.28403400
H	-2.81180900	3.21562000	1.16788100
C	5.24048300	-3.70140100	-0.53958200
H	3.34756900	-3.91029000	0.47205900
C	5.49943700	-1.71115700	-1.87684000
H	3.82140400	-0.36552000	-1.89851100
C	6.01439700	-2.90998600	-1.38748600
H	5.63517300	-4.63617900	-0.15433100
H	6.09276100	-1.09572300	-2.54546600
H	7.01435400	-3.22691500	-1.66625900
B	-3.08040000	-0.24228600	0.48439900
O	-2.88468400	-0.38093700	-0.86340900
O	-4.32768300	-0.61404300	0.89749800
H	-2.27401700	0.23275900	1.21837900
C	-4.17728000	-0.68046700	-1.44732300
C	-3.98207300	-1.65052900	-2.59955700
H	-4.94991400	-1.96453100	-3.00291500
H	-3.42125700	-1.15992900	-3.39996700
H	-3.42680200	-2.53542000	-2.28276700
C	-4.74390500	0.64441200	-1.95163500
H	-5.70563300	0.50347300	-2.45270100
H	-4.87757900	1.35275400	-1.12739100
H	-4.04124300	1.07908300	-2.66812100
C	-4.97218800	-1.26122000	-0.23045300

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C	-4.77862900	-2.76351900	-0.05031300
H	-3.71725600	-3.02529700	-0.05169000
H	-5.20175400	-3.05830200	0.91396200
H	-5.28869900	-3.32489800	-0.83816400
C	-6.45077000	-0.91175500	-0.21424200
H	-6.60862000	0.16797900	-0.18375000
H	-6.94668900	-1.31592700	-1.10242000
H	-6.92027400	-1.35385200	0.66886600
C	-0.30566200	-2.36653100	0.47236200
N	-1.38823400	-2.51857500	0.88767800

SM1<sub>CN</sub>

C	0.71744000	-0.20244800	-0.36548700
C	0.07723300	0.96157200	0.31040200
C	-0.59363800	1.92062600	-0.46009500
C	0.09983800	1.10759200	1.70347100
C	-1.22109600	3.00433700	0.14825300
H	-0.61573700	1.81474600	-1.54113800
C	-0.53134500	2.19033500	2.31099500
H	0.59018300	0.35441600	2.31551400
C	-1.18856700	3.14406600	1.53494000
H	-1.73670800	3.73863600	-0.46268400
H	-0.51563900	2.28471000	3.39233300
H	-1.67716200	3.98932700	2.00925500
C	0.16345700	-1.06536300	-1.24195400
P	2.47617200	-0.56764400	-0.07377900
C	3.30719300	0.69671400	0.93261900
C	3.37205600	2.06747800	0.24968500
H	4.31341900	0.31604900	1.14637700
H	2.77949700	0.76226600	1.88913900
C	3.87582400	3.14456800	1.20918400

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H	4.03282700	2.01204900	-0.62443200
H	2.37949200	2.35434700	-0.11996100
C	3.97080200	4.51131300	0.53954100
H	3.19457700	3.19743400	2.06748600
H	4.85657600	2.84941900	1.60220700
H	4.32749600	5.27265100	1.23859300
H	4.66119600	4.48531200	-0.30978800
H	2.99233700	4.83002500	0.16571400
C	3.30397000	-0.63804500	-1.69030200
C	4.80894600	-0.90327400	-1.61339700
H	3.09433500	0.31703500	-2.18662000
H	2.78390100	-1.41692700	-2.25786200
C	5.43429600	-0.96319300	-3.00737500
H	5.30075400	-0.11319500	-1.03153600
H	4.99750200	-1.84936800	-1.09148800
C	6.93550900	-1.22685100	-2.95333000
H	4.93759700	-1.74897100	-3.58886100
H	5.23958200	-0.01775400	-3.52792500
H	7.36751900	-1.26766900	-3.95691000
H	7.45251100	-0.43796600	-2.39727100
H	7.14816500	-2.17955300	-2.45753300
C	2.64394900	-2.18169900	0.74209200
C	1.93444100	-2.25230000	2.09628100
H	3.71619200	-2.38386000	0.84532700
H	2.22627200	-2.91585900	0.04350200
C	2.09405800	-3.62691700	2.74519000
H	2.33499300	-1.48343200	2.76993500
H	0.86727100	-2.03660500	1.95900200
C	1.38149600	-3.71205200	4.09093900
H	1.69846000	-4.39031500	2.06468700

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H	3.16172700	-3.84294900	2.87340800
H	1.50238300	-4.70049000	4.54245000
H	1.77917900	-2.97160800	4.79272400
H	0.30919900	-3.52321300	3.97762300
C	-1.18977700	-0.92197800	-1.54415600
N	-2.30968500	-0.95074500	-1.87007800
B	-3.86682300	-0.44586000	-2.10312600
O	-4.72203900	-1.46500000	-1.53811800
O	-4.06680500	0.76200000	-1.34612900
H	-3.90820700	-0.28155300	-3.30973400
C	-5.55725500	-0.83566100	-0.56954900
C	-5.87247400	-1.82792100	0.54181700
H	-6.43356700	-1.34617000	1.35005200
H	-6.48408400	-2.64454100	0.14539100
H	-4.95931400	-2.25975900	0.95708600
C	-6.85294400	-0.40283900	-1.26155900
H	-7.58051200	0.00924800	-0.55487400
H	-6.64454800	0.34885000	-2.02908100
H	-7.30028500	-1.27468700	-1.74806000
C	-4.69994600	0.39014400	-0.12465400
C	-3.63845600	0.00307600	0.91230600
H	-2.90773500	0.81483500	0.99001000
H	-4.08426100	-0.15681700	1.89972200
H	-3.11040700	-0.90853600	0.62032800
C	-5.49886800	1.57992200	0.39000300
H	-6.15748900	1.97767200	-0.38516900
H	-6.10407300	1.30201700	1.25972400
H	-4.81217700	2.37669700	0.69499200
STS4 <sub>CN</sub>			
C	0.78325600	0.36153600	0.11945700



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C	0.53869800	1.72370600	-0.40629100
C	-0.76530200	2.08594500	-0.80055100
C	1.54462000	2.69569200	-0.53735100
C	-1.03820200	3.35107300	-1.30378200
H	-1.57003900	1.36233100	-0.70133200
C	1.26802500	3.96106800	-1.05028300
H	2.55645900	2.48458100	-0.21055000
C	-0.02396700	4.30009400	-1.44009700
H	-2.05533300	3.59631100	-1.59649300
H	2.07174300	4.68667600	-1.13420900
H	-0.23968900	5.28655100	-1.83762300
C	-0.24996000	-0.46301700	0.43837100
P	2.40059300	-0.35858300	0.35022500
C	3.59816300	0.06320400	-0.95937700
C	3.05741800	-0.19534400	-2.36699800
H	4.48540200	-0.54935800	-0.75824100
H	3.90753200	1.10526000	-0.84285300
C	4.10149600	0.11691700	-3.43798700
H	2.74330900	-1.24347400	-2.45766000
H	2.16405800	0.41876400	-2.53346900
C	3.57359300	-0.13523600	-4.84651000
H	4.41264200	1.16415100	-3.33884500
H	4.99499800	-0.49403100	-3.25905800
H	4.33003700	0.09411700	-5.60210500
H	3.27933800	-1.18222400	-4.97259900
H	2.69499700	0.48494300	-5.05081100
C	2.19237100	-2.17055300	0.32675000
C	3.49857900	-2.96774900	0.29093300
H	1.56788700	-2.40651300	-0.54128900
H	1.60648400	-2.42187600	1.21745300

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C	3.23041000	-4.46961400	0.39530400
H	4.03521100	-2.76485800	-0.64406700
H	4.15893600	-2.66254900	1.11240200
C	4.51493000	-5.28950100	0.33160600
H	2.70214600	-4.67529800	1.33390200
H	2.55556400	-4.76980200	-0.41533700
H	4.30689000	-6.36012300	0.40912900
H	5.04306100	-5.11801700	-0.61204900
H	5.19310700	-5.01974800	1.14781300
C	3.16644000	0.03899500	1.95902800
C	3.36148800	1.53049200	2.23455200
H	4.12505300	-0.49257300	1.99881400
H	2.50762800	-0.40788400	2.71375700
C	3.97108700	1.77188400	3.61506900
H	4.01376400	1.96946600	1.46826600
H	2.39552200	2.04579100	2.16612600
C	4.17434100	3.25590300	3.90267800
H	3.31590900	1.33110100	4.37609900
H	4.93012200	1.24362900	3.68325900
H	4.60556700	3.41334900	4.89511500
H	4.84843400	3.70863200	3.16817000
H	3.22301800	3.79585700	3.85988300
C	-1.30897900	-1.07068300	0.72260500
N	-2.36417900	-1.78388400	0.86518900
B	-3.65918100	-1.32319600	0.34718700
O	-4.86937000	-1.80600000	0.87279300
O	-3.83603300	-0.06282200	-0.26093100
H	-2.97312800	-2.25040200	-0.45562400
C	-5.90133600	-1.03864900	0.23478000
C	-7.10819500	-0.97605500	1.15694200

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H	-7.87150000	-0.30567500	0.74875500
H	-7.54800500	-1.97285600	1.25583900
H	-6.82753300	-0.62611200	2.15240100
C	-6.26918500	-1.73714000	-1.07426400
H	-7.10476500	-1.24177500	-1.57711400
H	-5.41421900	-1.76122300	-1.75775800
H	-6.55968800	-2.76798500	-0.85282900
C	-5.19230500	0.33465000	-0.00469000
C	-5.18448400	1.20970100	1.24814400
H	-4.48959600	2.04001100	1.09250400
H	-6.17536500	1.62160100	1.46177400
H	-4.84687800	0.63785500	2.11800500
C	-5.71484900	1.12118900	-1.19614500
H	-5.58283800	0.56572800	-2.12691000
H	-6.77752800	1.35364600	-1.07132600
H	-5.16813100	2.06545000	-1.28119400
STS5 <sub>CN</sub>			
C	-1.52833200	-0.80842900	-1.09251200
C	-2.96473300	-1.21628200	-1.18735400
C	-3.28322400	-2.57884200	-1.11124700
C	-4.00142800	-0.29827100	-1.39301400
C	-4.60200500	-3.00888300	-1.22111800
H	-2.48006500	-3.29558900	-0.96763400
C	-5.32151800	-0.72806000	-1.50724000
H	-3.77440900	0.75856600	-1.49503100
C	-5.62691600	-2.08408200	-1.41526700
H	-4.82941300	-4.06839400	-1.15520000
H	-6.10977500	-0.00090600	-1.67664200
H	-6.65591200	-2.41888100	-1.50037700
C	-0.60314100	-1.41383700	-1.84958500

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P	-1.06739200	0.40079500	0.22048100
C	-2.47107100	1.35365200	0.90456900
C	-2.80530100	2.65045600	0.15931600
H	-2.20230800	1.57407100	1.94467400
H	-3.33472300	0.68157400	0.93747200
C	-4.16037100	3.20539700	0.59502000
H	-2.02126400	3.39265600	0.35435000
H	-2.81290400	2.49134700	-0.92631200
C	-4.48804300	4.52891400	-0.08779300
H	-4.93611500	2.46335600	0.36615100
H	-4.16366500	3.33449000	1.68431500
H	-5.46439400	4.90731100	0.22681200
H	-3.73909000	5.29010400	0.15339200
H	-4.50741900	4.41287300	-1.17630400
C	0.13654500	1.60254900	-0.41952800
C	0.88858900	2.36317600	0.67418400
H	-0.43569100	2.28725300	-1.05598100
H	0.85296400	1.08703200	-1.06047200
C	1.79255100	3.43006300	0.05862000
H	0.18544500	2.82738800	1.37910500
H	1.50350900	1.65761400	1.24833400
C	2.55362800	4.22808500	1.11177300
H	2.49131200	2.92844100	-0.62144900
H	1.18297700	4.10836200	-0.55155300
H	3.21838100	4.96310600	0.64906600
H	1.86400100	4.76737500	1.76978200
H	3.16602200	3.57180500	1.73888500
C	-0.39325700	-0.52362900	1.64239400
C	-1.38853100	-1.54593900	2.20104300
H	-0.12225900	0.21770900	2.40433800

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H	0.52295400	-1.02259800	1.31296000
C	-0.79224600	-2.31175300	3.38175100
H	-2.31070600	-1.04416000	2.52066600
H	-1.66784500	-2.25438700	1.41143100
C	-1.76193700	-3.34650700	3.94316400
H	0.13261300	-2.80384900	3.05687700
H	-0.50955100	-1.60004300	4.16710300
H	-1.32148500	-3.88843600	4.78451500
H	-2.68282000	-2.87025200	4.29516800
H	-2.03668400	-4.07954300	3.17791200
C	0.78036100	-1.27658400	-1.89690000
N	1.82087800	-1.32438400	-2.56750800
B	2.54148200	-0.95044300	-1.25214600
O	3.11364200	0.35699400	-1.12336800
O	3.45315500	-1.92606500	-0.75890000
H	1.39647100	-0.99032200	-0.48599600
C	4.43690300	0.17990600	-0.59956400
C	4.77123700	1.33355700	0.33392200
H	5.73019200	1.16165100	0.83480100
H	4.84919700	2.26603000	-0.23465400
H	3.99658700	1.46024400	1.09450500
C	5.40657100	0.15676800	-1.78113500
H	6.44935000	0.10730200	-1.45260500
H	5.19996400	-0.69909100	-2.43070900
H	5.27128300	1.07176800	-2.36486100
C	4.33901300	-1.21187300	0.10675700
C	3.69799700	-1.10766900	1.49320400
H	3.41659500	-2.11098800	1.82753600
H	4.38652000	-0.67791700	2.22696100
H	2.79471300	-0.48896300	1.46361200

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C	5.65322700	-1.97224300	0.19586600
H	6.04293200	-2.20027900	-0.79835600
H	6.40235400	-1.39256000	0.74528000
H	5.49770600	-2.91656700	0.72638900
STS6 <sub>CN</sub>			
C	-0.60654100	-0.40213000	0.09836800
C	-0.74575700	-1.88376000	0.10450600
C	-0.20106500	-2.63364300	-0.94477300
C	-1.40863900	-2.54632100	1.14441300
C	-0.33286500	-4.01933200	-0.95978100
H	0.31810500	-2.12008600	-1.74830100
C	-1.54155900	-3.93207800	1.12493000
H	-1.79851500	-1.97500200	1.98320100
C	-1.00986900	-4.67087000	0.06960200
H	0.09084600	-4.58997100	-1.78014500
H	-2.05291600	-4.43471000	1.93981600
H	-1.11703400	-5.75078700	0.05321400
C	0.57995100	0.19858100	-0.04385300
P	-2.06243400	0.67610800	0.21288800
C	-3.60122700	-0.29225200	0.22887500
C	-3.87072300	-1.03889800	-1.08214400
H	-4.40469800	0.42203100	0.44679500
H	-3.55477500	-0.98688600	1.07226500
C	-5.06015300	-1.98836700	-0.94518600
H	-4.06450500	-0.31536100	-1.88375200
H	-2.98584300	-1.61522400	-1.37925100
C	-5.34571700	-2.73887600	-2.24159400
H	-4.84928200	-2.70384200	-0.14074900
H	-5.94549100	-1.41871200	-0.63700900
H	-6.19638600	-3.41658400	-2.12959400

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H	-5.57453500	-2.04369800	-3.05583400
H	-4.47838000	-3.33477500	-2.54396500
C	-2.10815800	1.76044900	-1.24506400
C	-3.34730900	2.65757800	-1.31070600
H	-2.04698200	1.10379400	-2.12077800
H	-1.18597400	2.34973500	-1.21064200
C	-3.31754500	3.54703500	-2.55389300
H	-4.25719600	2.04412200	-1.32693000
H	-3.40063000	3.28763700	-0.41451900
C	-4.54118000	4.45327200	-2.64081200
H	-2.40384000	4.15271700	-2.53908800
H	-3.25864300	2.91214300	-3.44622100
H	-4.50728000	5.08049400	-3.53572600
H	-5.46357200	3.86447600	-2.67835600
H	-4.60146200	5.11411000	-1.77001200
C	-1.97420200	1.67848100	1.72252800
C	-1.92832000	0.84041800	3.00281100
H	-2.84458700	2.34493300	1.71277200
H	-1.07388000	2.29520100	1.62025200
C	-1.84476700	1.72452400	4.24684700
H	-2.82065700	0.20410900	3.06728400
H	-1.05742200	0.17372800	2.97119400
C	-1.79313100	0.90350300	5.53107600
H	-0.95369300	2.35898400	4.17340500
H	-2.70997500	2.39831600	4.26852300
H	-1.73147700	1.54828100	6.41194400
H	-2.68689700	0.27932400	5.63376700
H	-0.92071600	0.24233000	5.53694500
C	1.08343100	1.51421800	-0.08666800
N	2.29823100	1.73514400	-0.17500200

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B	3.28779800	0.48433100	-0.25579700
O	4.02170600	0.39103100	-1.46480200
O	4.17346800	0.29904000	0.83472000
H	2.09708800	-0.38588800	-0.16264200
C	5.32925100	-0.09341000	-1.14524100
C	6.33228400	0.48355000	-2.13376000
H	7.35625300	0.21697500	-1.85051500
H	6.14079200	0.07935200	-3.13254000
H	6.25419300	1.57147200	-2.18678100
C	5.30641900	-1.61956800	-1.25088800
H	6.29861400	-2.05503000	-1.09692500
H	4.61619100	-2.04628900	-0.51668600
H	4.95852300	-1.89779600	-2.24995400
C	5.50851500	0.39397700	0.32422100
C	5.93442600	1.86141900	0.39903100
H	5.83521200	2.20434700	1.43298400
H	6.97374300	2.00206000	0.08628200
H	5.28992800	2.48307900	-0.23031100
C	6.43217400	-0.46520400	1.17411700
H	6.05571700	-1.48689900	1.25818900
H	7.43997200	-0.49514900	0.74610500
H	6.50423100	-0.04469500	2.18183900



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