

Supporting Information

Conformationally Locked Pyramidalicity Explains the Diastereoselectivity in the Methylation of *trans*-Fused Butyrolactones

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1. Computational details

The DFT calculations were carried out with the *Gaussian 16* suite of programs (Revision A.03).¹ The reported calculations were performed with dispersion-corrected ω B97X-D exchange-correlation functional.² The SMD implicit solvation model was used to model the global solvation effects.³ The applied solvent was tetrahydrofuran (THF) relying on the literature precedents. The ultrafine integration was applied to enhance the accuracy of the numerical integration in all the DFT calculations. The reported Gibbs free energies were obtained from ω B97X-D/Def2TZVPP electronic energies and all the additional terms computed at the ω B97X-D/Def2SVP level according to the following formula: $G = E_0' + (G_0 - E_0) + (G_{\text{sol}} - E_0)$. Herein, E_0' and E_0 are electronic energies obtained with the Def2TZVPP and the Def2SVP basis sets,⁴ G_0 and G_{sol} denote gas-phase and solution-phase Gibbs free energies obtained from ω B97X-D/Def2SVP calculations ($T = 298.15$ K). Harmonic vibrational frequency calculations were carried out to confirm the nature of the obtained structures. No imaginary frequencies were found for all the minima reported. For the transition states, only one imaginary frequency was found.

In the case of the annulated-rings, a conformational analysis was performed. We applied Monte Carlo sampling using the standard OPLS_2005 force field, which was carried out with *MacroModel* software.⁵ The most important parameters from a practical standpoint were the followings: Solvent: none, Optimization method: PRCG, Maximum iteration of optimization: 15 000, Convergence threshold of optimization: 0.05, Steps per rotatable bond: 300 Maximum number of steps: 10 000, CSearch method: Mixed torsional/Low-mode sampling, Torsional sampling option: Extended, Energy window: 10 kcal/mol.

Molecular structures were visualized using *CYLView* and the unimportant H atoms were omitted for clarity.⁶

The relevance of using molecular models that neglect the effect of the Li^+ counterion was examined and justified in our previous work,⁷ but other literature precedence support this view as well.^{8,9}

2. Energy Decomposition by Activation Strain Model

To gain insight into the origin of stereoselectivity, the activation-strain model was employed. In the framework of this model, the activation energy can be divided into distortion energy (ΔE_{dis}), which is required for deformation of the ground state intermediates into the geometries of TS structures, and interaction energy (ΔE_{int}), which quantitatively describes the interactions between the distorted reactants (Figure S1). The use of this theoretical approach was justified by the fact that the inclusion of thermal correction did not change the relative energy difference as well as the earliness of the TSs. The electronic energies of each fragment were calculated at the ω B97X-D/Def2TZVPP level of theory and can be found in Table S2. The difference of the total distortion energies was found to be 3.0 kcal/mol in favour of the **syn-TS**, whereas the interaction was slightly more favourable in the **anti-TS** by 0.9 kcal/mol. On the whole, the reduced distortion of the **anti-TS** overruled the favorable interaction energy presented by the **anti-TS**, resulting in an activation energy difference of 2.1 kcal/mol. Thereafter, the distortion energies were further partitioned with respect to the reactants. We found that the enolate fragment in the **anti-TS** presented a greater distortion compared to **syn-TS** ($\Delta\Delta E_{\text{dis}}(\text{en}) = 1.9$ kcal/mol). Thus, the preference of the **syn-TS** could be ascribed to the reduced distortion of the enolate fragment.

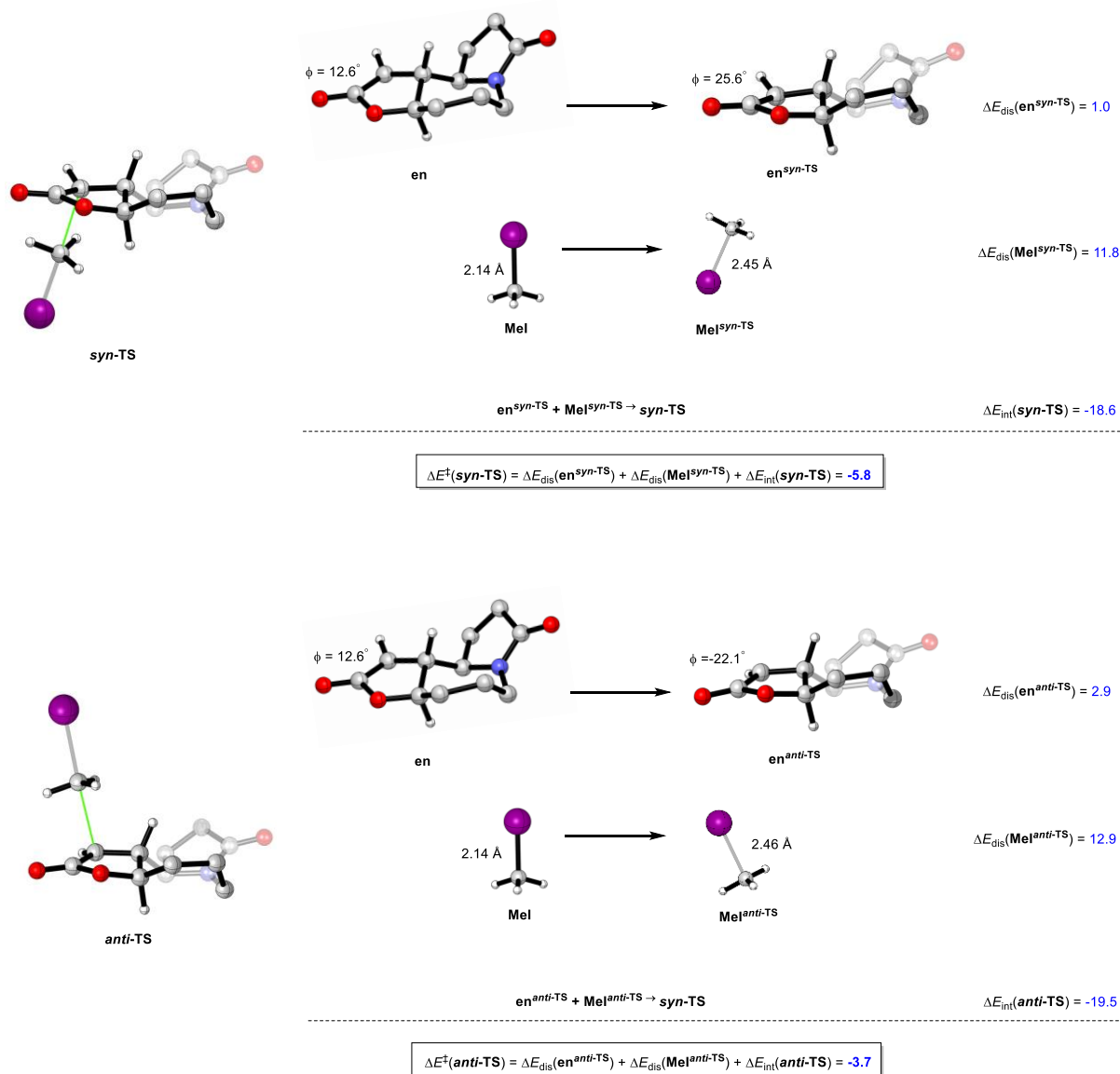


Figure S1: Energy Decomposition scheme for the *syn* and *anti* pathways. Energies are given in kcal/mol.

3. Results obtained for model enolates **en_{but}**, **en_{hep}** and **en_{hex}**

The optimized structures of the ground state enolates **en_{but}**, **en_{hep}** and **en_{hex}**, as well as the identified transition states are compiled in Figures S2-4. In addition to the most stable transition states, other TS conformers are presented too.

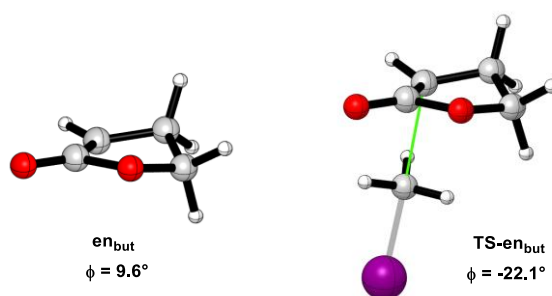


Figure S2: Structure of the ground state enolate of the monocyclic butyrolactone (**en_{but}**) and the located methylation transition state. Only a single methylation transition state could be located for this system. Alternative facial attack of the MeI leads to spontaneous ring flipping of the enolate.

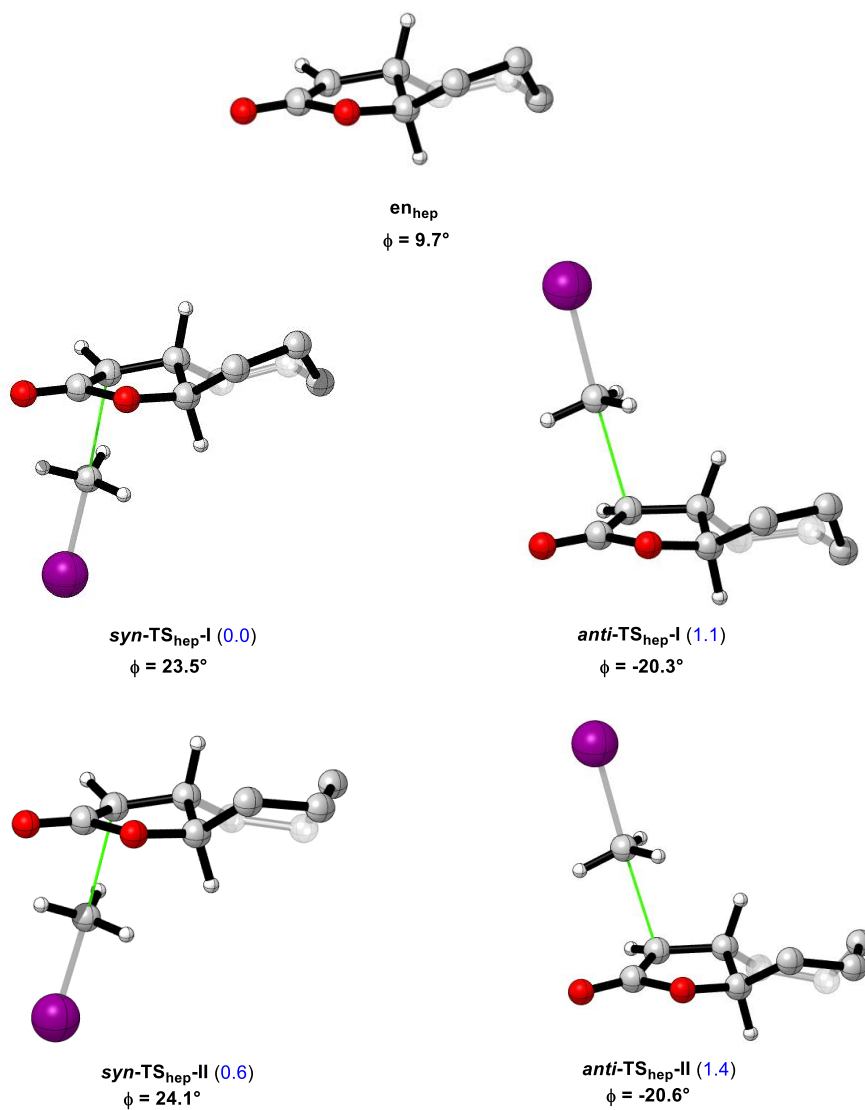


Figure S3: Structure of the ground state enolate of *trans*-cycloheptane-fused butyrolactone (en_{hep}) and the diastereomeric transition states of its methylation reaction. The boat-like conformation of the fused-cycloheptane was found to be high-energy conformation. Relative stabilities are given in parenthesis (in kcal/mol) with respect to *syn-TS_{hep-I}*.

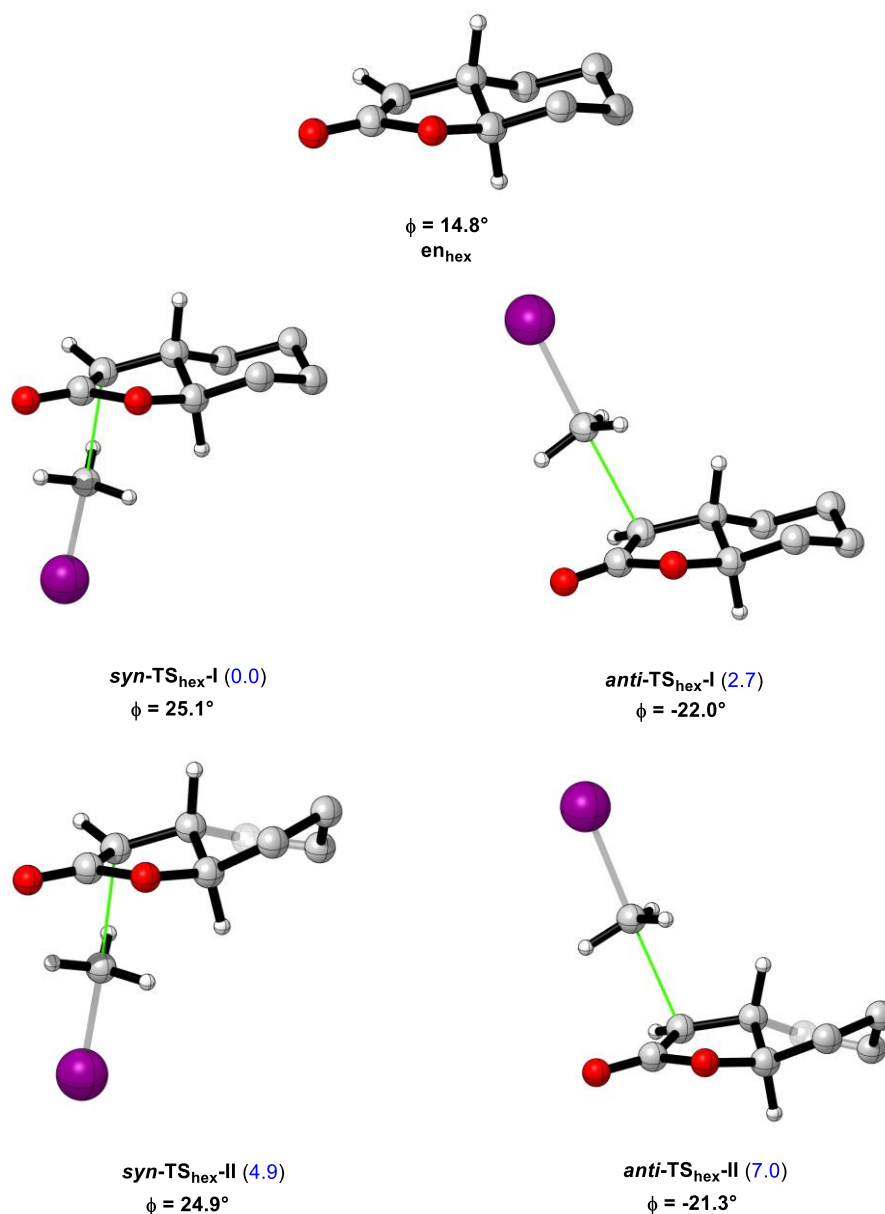


Figure S4: Structure of the ground state enolate of *trans*-cyclohexane-fused butyrolactone (en_{hex}) and the diastereomeric transition states of its methylation reaction. The fused-chair conformation was found to be more favorable than twist-boat conformation. Relative stabilities are given in parenthesis (in kcal/mol) with respect to *syn*-TS_{hex}-I.

4. $\Delta E(\phi)$ potential energy curves

In the main text, we present the $\Delta E(\phi)$ potential curve for enolate en . The potential energy surface of en was mapped in a set of constrained geometry optimizations initiated from the ground state (energetically most stable) structure ($\phi_0 = 12.6^\circ$). The ϕ dihedral angle was varied by 5 degrees in both directions ($\phi_0 + 5^\circ$, $\phi_0 + 10^\circ$, ... $\phi_0 + 35^\circ$; $\phi_0 - 5^\circ$, $\phi_0 - 10^\circ$, ... $\phi_0 - 45^\circ$), and for each fixed ϕ_i value, the geometry of the enolate was optimized. The variation of the computed electronic energy as a function of ϕ defines the $E(\phi)$ potential energy curve, which is depicted in Figure S5. The reference state for the relative energies is the ground state en ($\phi_0 = 12.6^\circ$). A few representative enolate structures, namely those corresponding to $\phi = 12.6^\circ$ (ground state), $\phi = 22.6^\circ$ and $\phi = -22.4^\circ$ are illustrated in Figure S6. The latter two dihedral angles are very close to those measured in the *syn*-TS and *anti*-TS transition states identified computationally for the methylation of en with MeI ($\phi = 25.6^\circ$ and $\phi = -22.1^\circ$, respectively; see $\text{en}^{\text{syn-TS}}$ and $\text{en}^{\text{anti-TS}}$ in Figure S1).

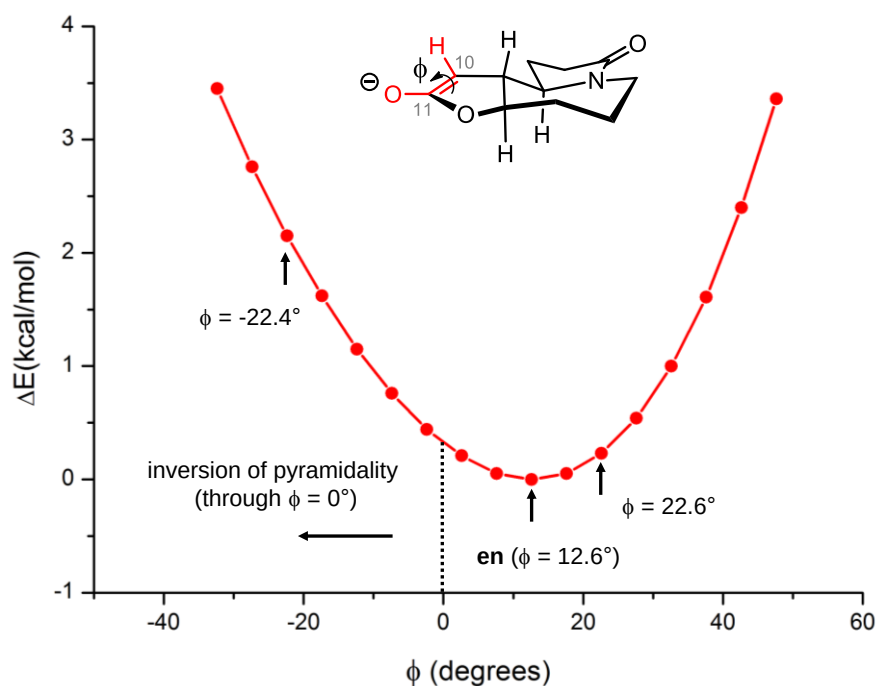


Figure S5: $\Delta E(\phi)$ potential energy curve derived for enolate **en**. The energies of two representative enolate structures are highlighted by arrows.

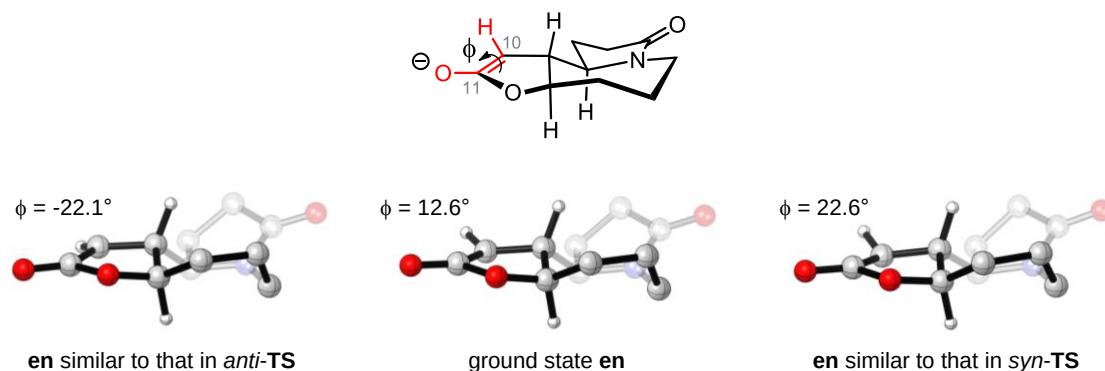


Figure S6: Representative enolate structure from the $\Delta E(\phi)$ potential energy curve derived for enolate **en**.

We computed analogous $\Delta E(\phi)$ curves for the model enolates **en_{but}**, **en_{hep}** and **en_{hex}** as well, which are all depicted in Figure S7. For simplicity, we have uniformly chosen $\phi = 25^\circ$ and $\phi = -22^\circ$ values to represent the dihedral angles measured in the *syn* and *anti* methylation transition states. The optimized data are listed in Table S1 and they justify the above choice.

We point out that all curves, including that obtained for the monocyclic butyrolactone enolate **en_{but}** as well, reflect a general tendency that the energy penalty of reaching the dihedral angle $\phi = -22^\circ$ characteristic of the *anti*-**TS** transition state is significantly larger than the energy change accompanied by the $\phi = 25^\circ$ pyramidalization at *syn*-**TS**. However, the computed energy difference (illustrated by color arrows in Figure S7), varies in the series. The smallest $\Delta\Delta E$ is found for **en_{hep}** (1.1 kcal/mol) followed by **en** (1.8 kcal/mol), and **en_{hex}** (2.4 kcal/mol). These results reflect the same trend as the computed stereoselectivities ($\Delta\Delta G$ values are 1.1, 1.5 and 2.7 kcal/mol, respectively), and they also correlate well with the inherent pyramidalty of the ground state enolates ($\phi = 9.7^\circ$, 12.6° and 14.8° , respectively).

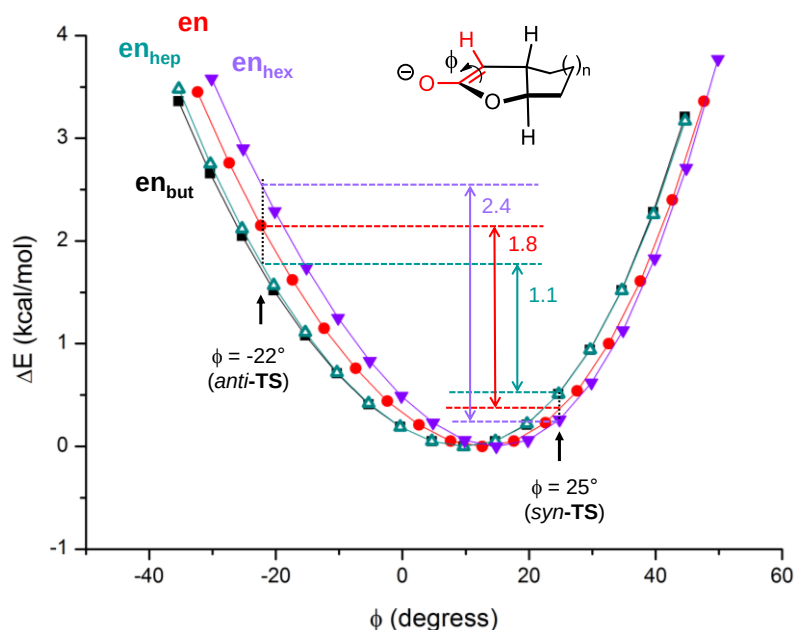


Figure S7: $\Delta E(\phi)$ potential energy curves derived for enolates **en_{but}** (black) and **en** (red). Dihedral angles measured in the optimized structures of **en** and the two transition states (*syn*-TS and *anti*-TS) are marked by arrows.

Table S1. Computed ϕ values (in degrees) in various enolates and the corresponding methylation transition states.

enolates	$\phi(\text{syn-TS})$	$\phi(\text{enolate})$	$\phi(\text{anti-TS})$	$\Delta\Delta G^a$
en	25.6	12.6	-22.1	1.5
en_{but}	22.0	9.6	-22.0	-
en_{hep}	23.5	9.7	-20.3	1.1
en_{hex}	25.1	14.8	-22.0	2.7

^a Computed stereoselectivity in kcal/mol.

It is interesting to note that $\Delta E(\phi)$ potential energy curves computed for the monocyclic **en_{but}** and the enolate involving a *trans*-fused cycloheptane (**en_{hep}**) hardly differ, suggesting that this type of ring fusion does not alter either the internal ring strain of the 5-membered cyclic enolate unit ($\phi = 9.6^\circ$ and 9.7° in **en_{but}** and **en_{hep}**, respectively), nor the torsional strain induced in the two methylation pathways. On the other hand, *trans*-fusion with a more constrained cyclohexane ring has a notable effect: the pyramidity of the ground state enolate **en_{hex}** increases to $\phi = 14.8^\circ$, and the torsional strain on the *anti* methylation pathway is more enhanced as well. These effects lead to higher stereoselectivity for **en_{hex}**. The pyramidity of the C₁₀ carbon atom in enolate **en** is somewhat between those in **en_{hep}** and **en_{hex}**, and this is also valid for the torsional effects, which implies that the inclusion of the cyclic amide unit in the *trans*-fused system imposes additional structural restraint in the enolate. These results indicate that the degree of the pyramidity represented by dihedral angle ϕ is also a good measure of the ring strain induced in the 5-membered enolate ring.

5. Results obtained for selected literature precedents of *syn* selective methylations

We examined 8 different methylation reactions reported previously for *trans*-fused butyrolactones. The optimized structures of the ground state enolates, as well as the identified transition states are compiled in Figures S8-15. In addition to the most stable transition states, other TS conformers are presented too. We note that all literature examples report *syn* selectivities, however, information regarding the diastereoselectivity is quite diverse. The relevant information is compiled in Table S2. The correlation between the experimental and computed diastereoselectivities is very reasonable.

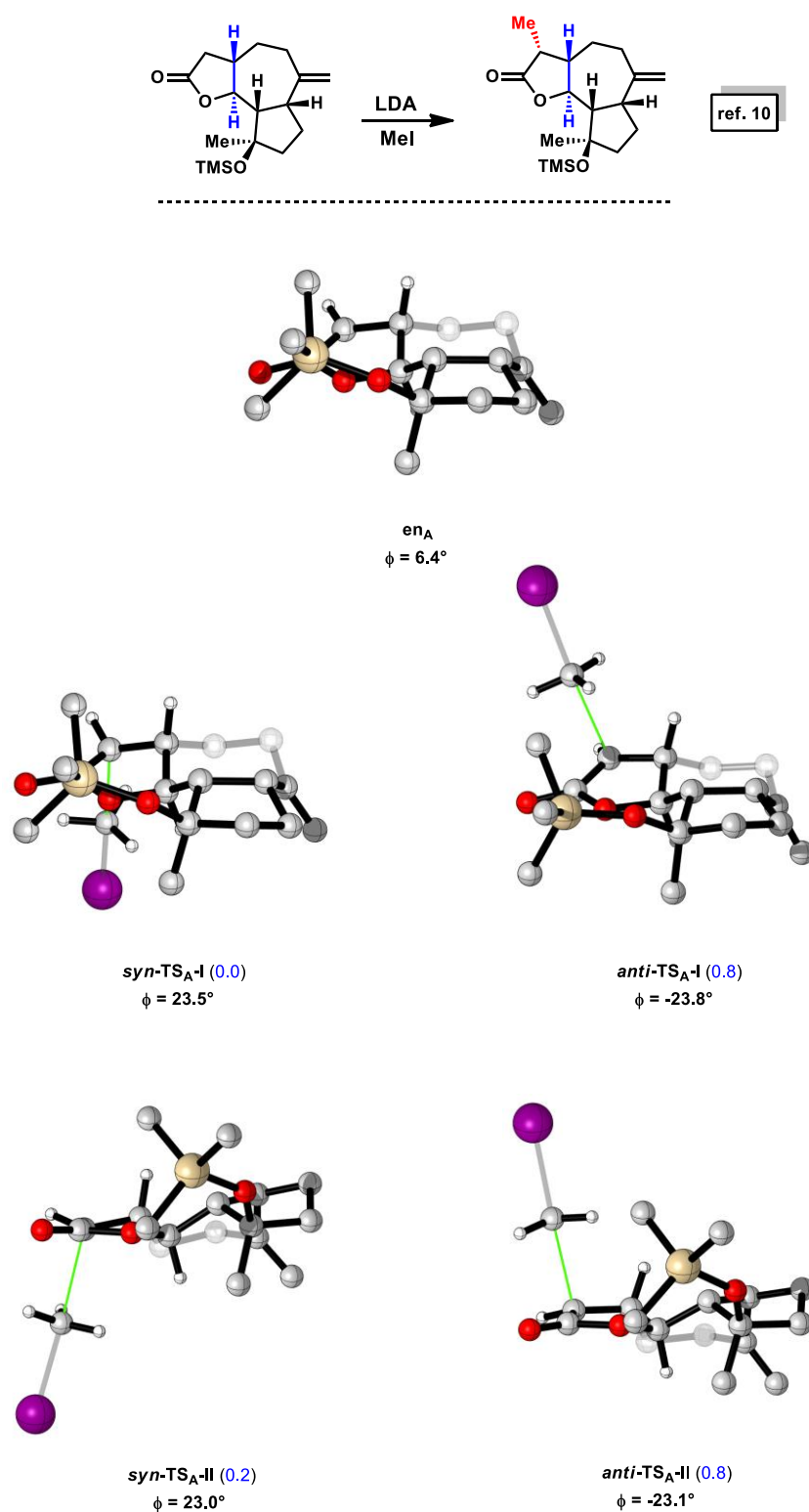


Figure S8: Structure of the ground state enolate of en_A and the diastereomeric transition states of its methylation reaction within 1.1 kcal/mol energy window of *syn*-TS conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn-TS_A-I*.

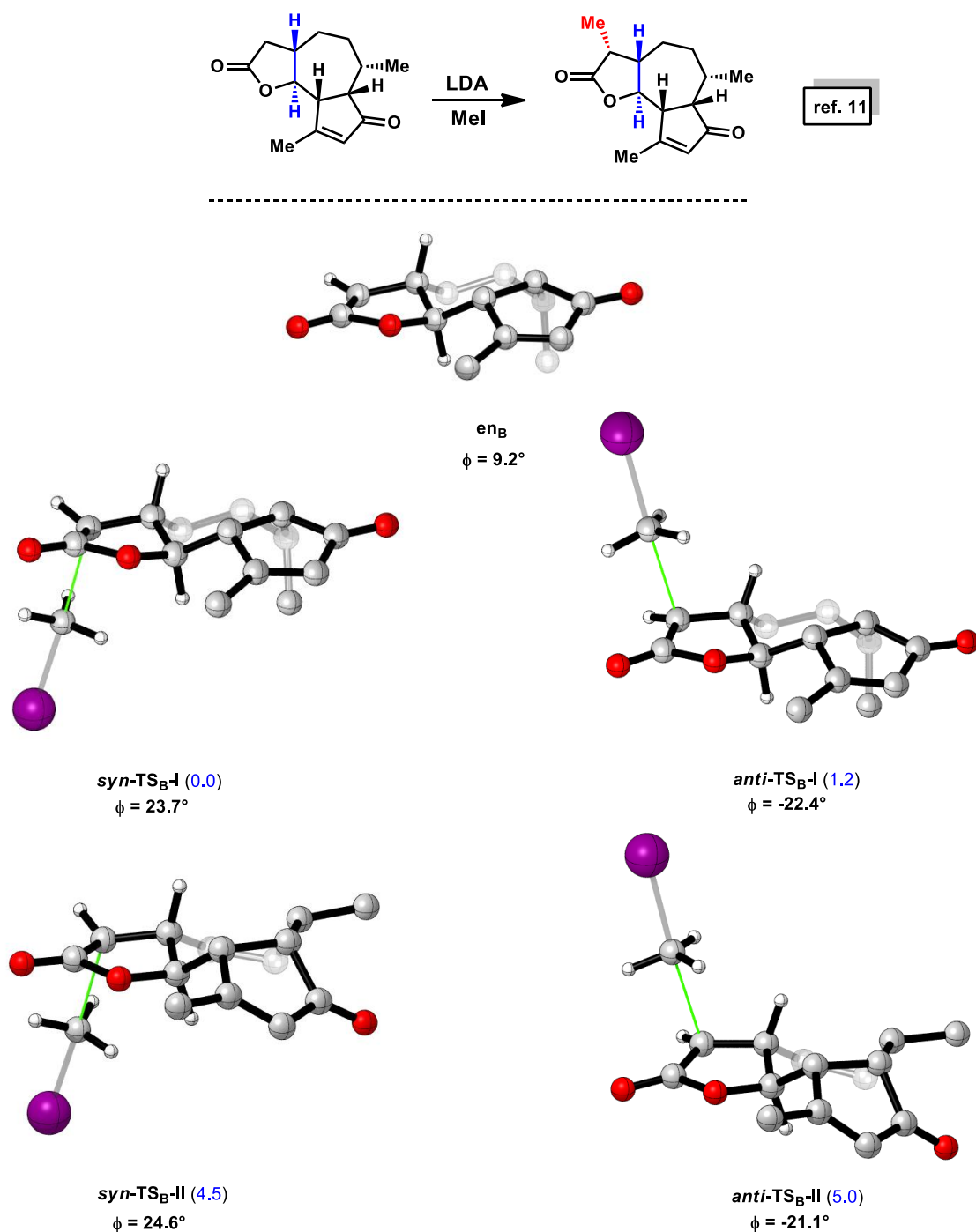


Figure S9: Structure of the ground state enolate of en_B and the diastereomeric transition states of its methylation reaction within 4.5 kcal/mol energy window of *syn*-TS conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn*-TS_{B-I}.

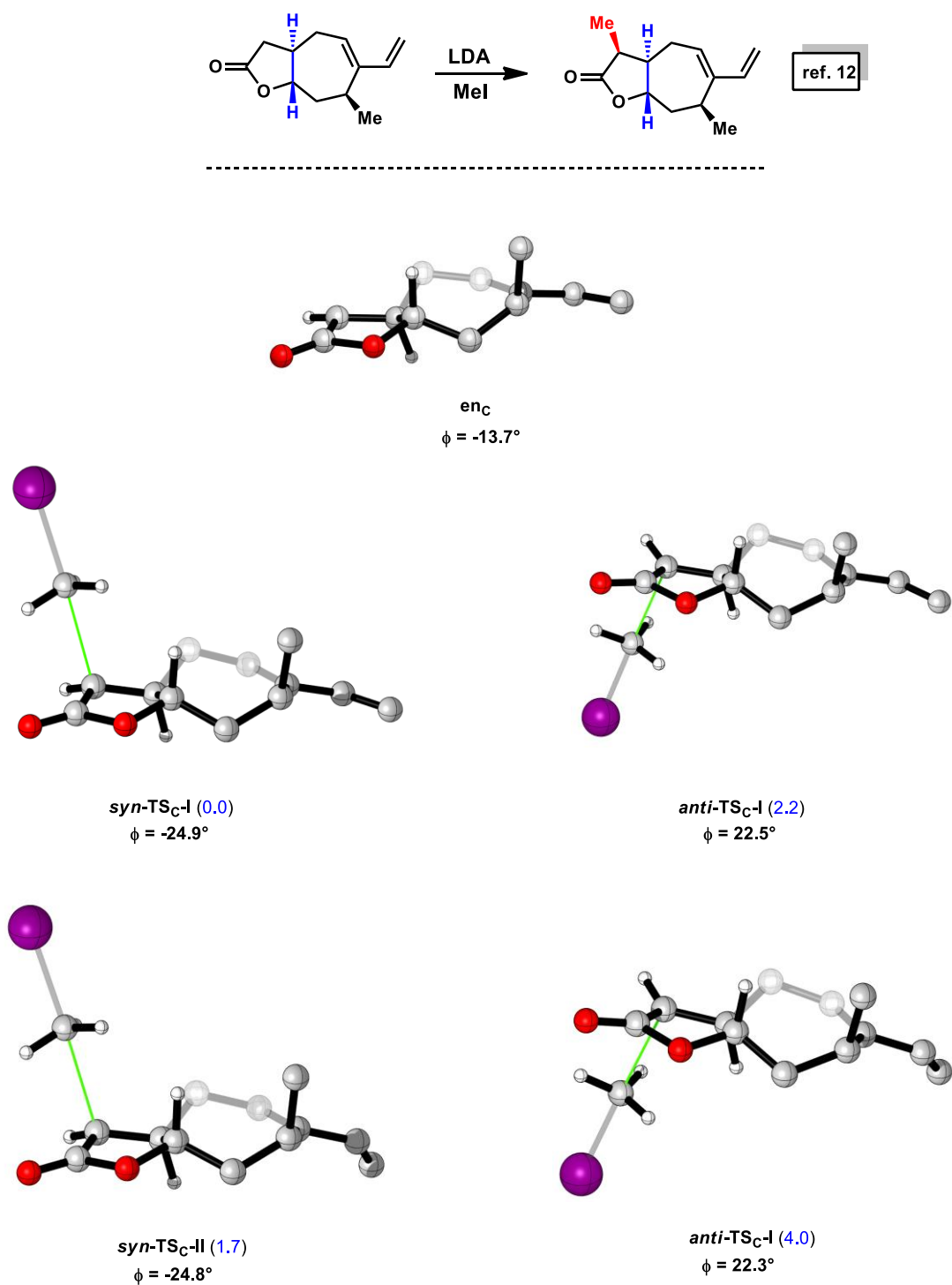


Figure S10: Structure of the ground state enolate of **enc** and the diastereomeric transition states of its methylation reaction within 1.8 kcal/mol energy window of *syn*-TS conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn*-TS_{C-I}.

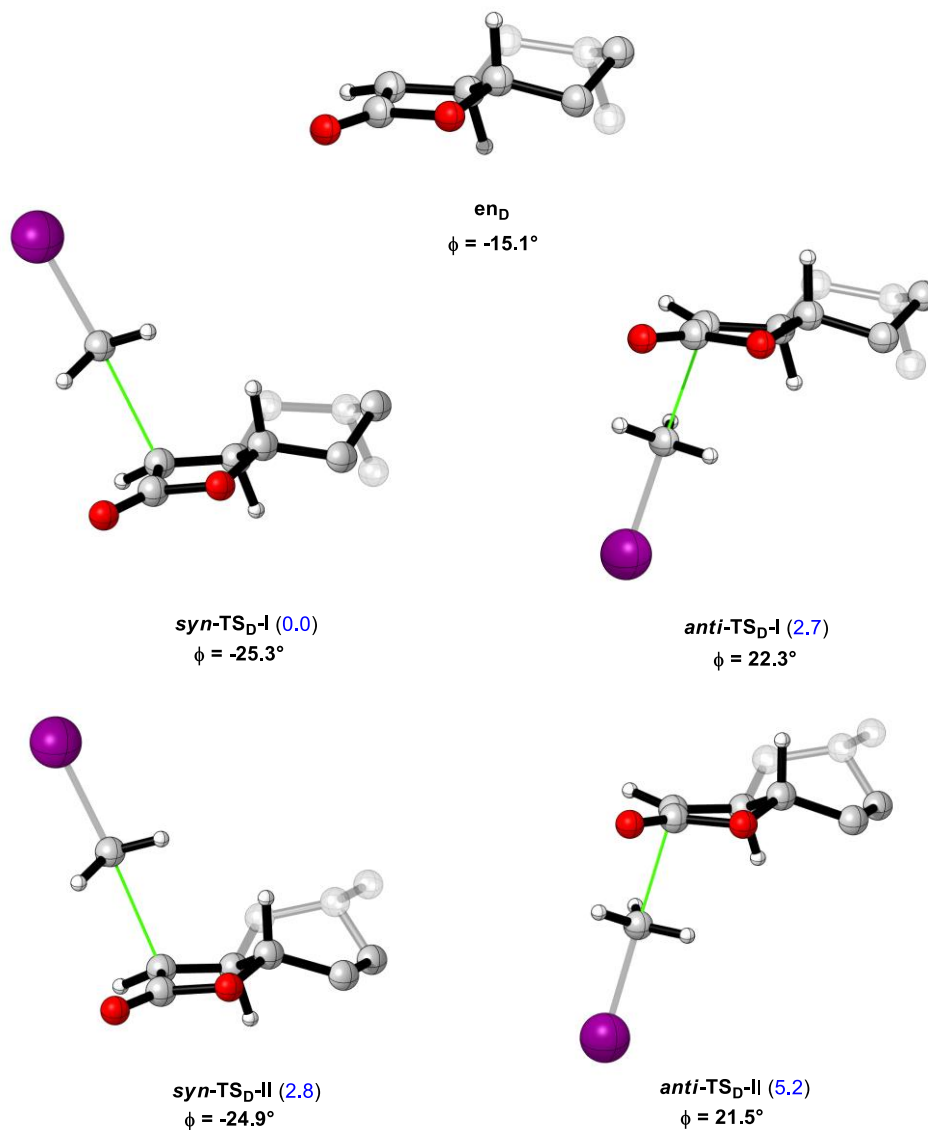
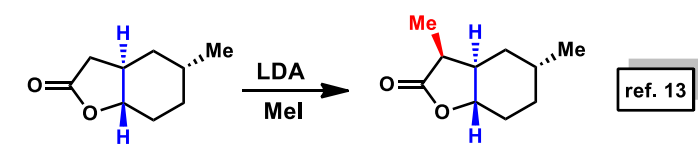


Figure S11: Structure of the ground state enolate of **en_D** and the diastereomeric transition states of its methylation reaction. The fused-chair conformation was found to be more favorable than twist-boat conformation. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn*-TS_{D-I}.

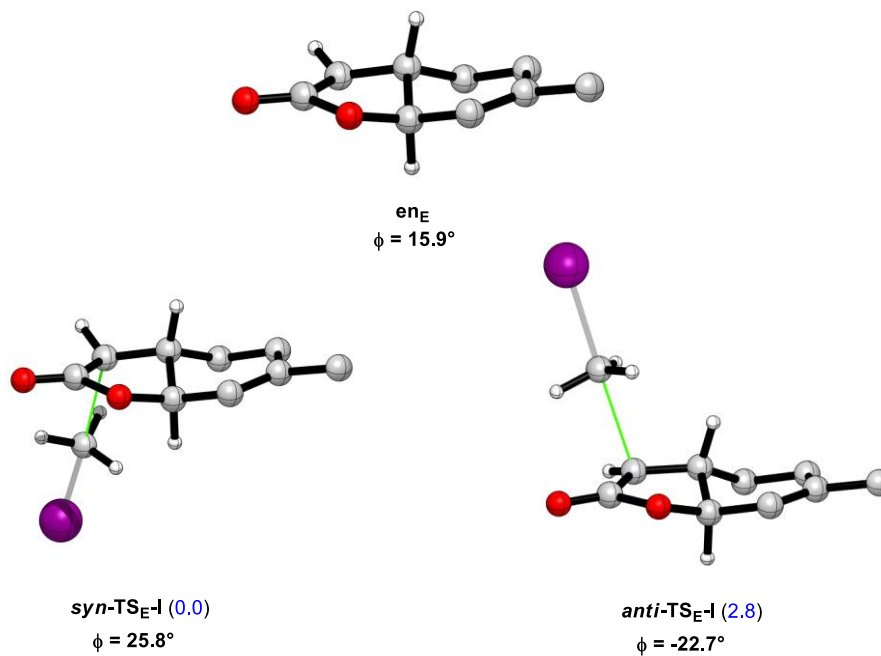
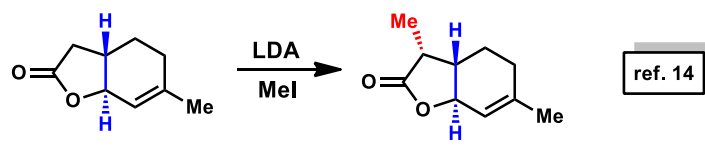


Figure S12: Structure of the ground state enolate of **en_E** and the diastereomeric transition states of its methylation reaction. The conformational analysis revealed no further conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn*-TS_{E-I}.

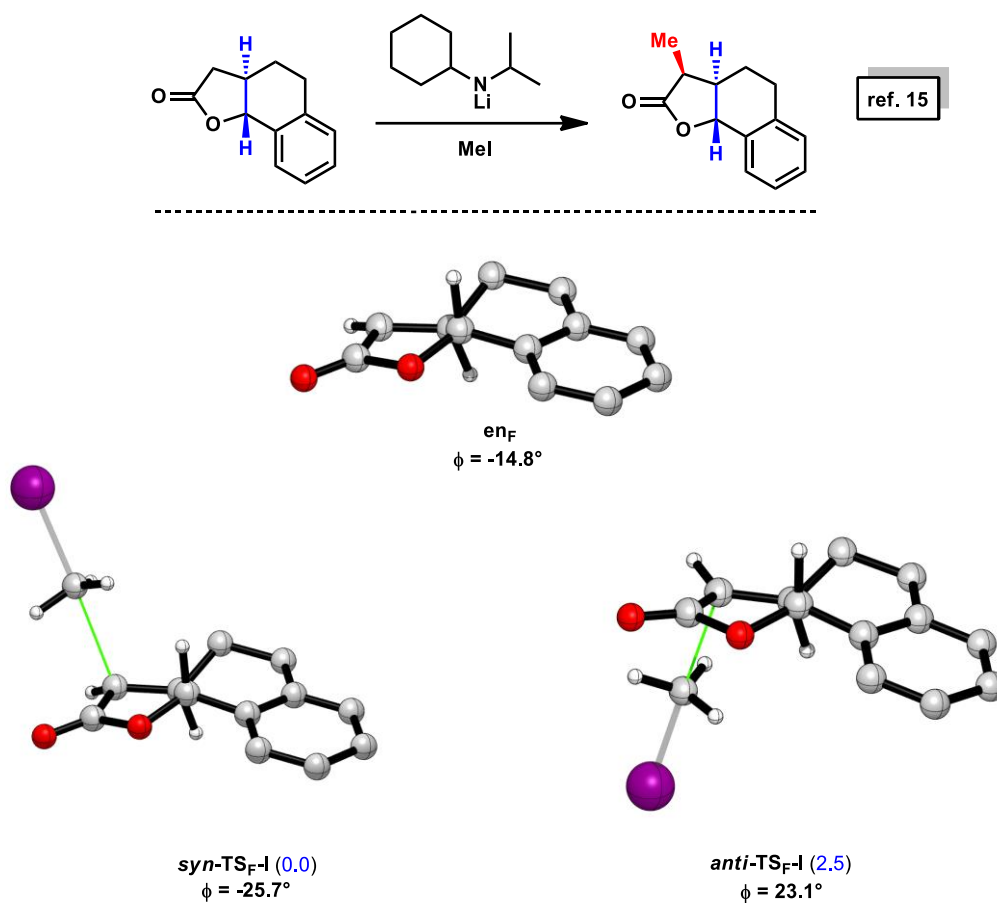


Figure S13: Structure of the ground state enolate of en_F and the diastereomeric transition states of its methylation reaction. The conformational analysis revealed no further conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn-TS_{F-I}*.

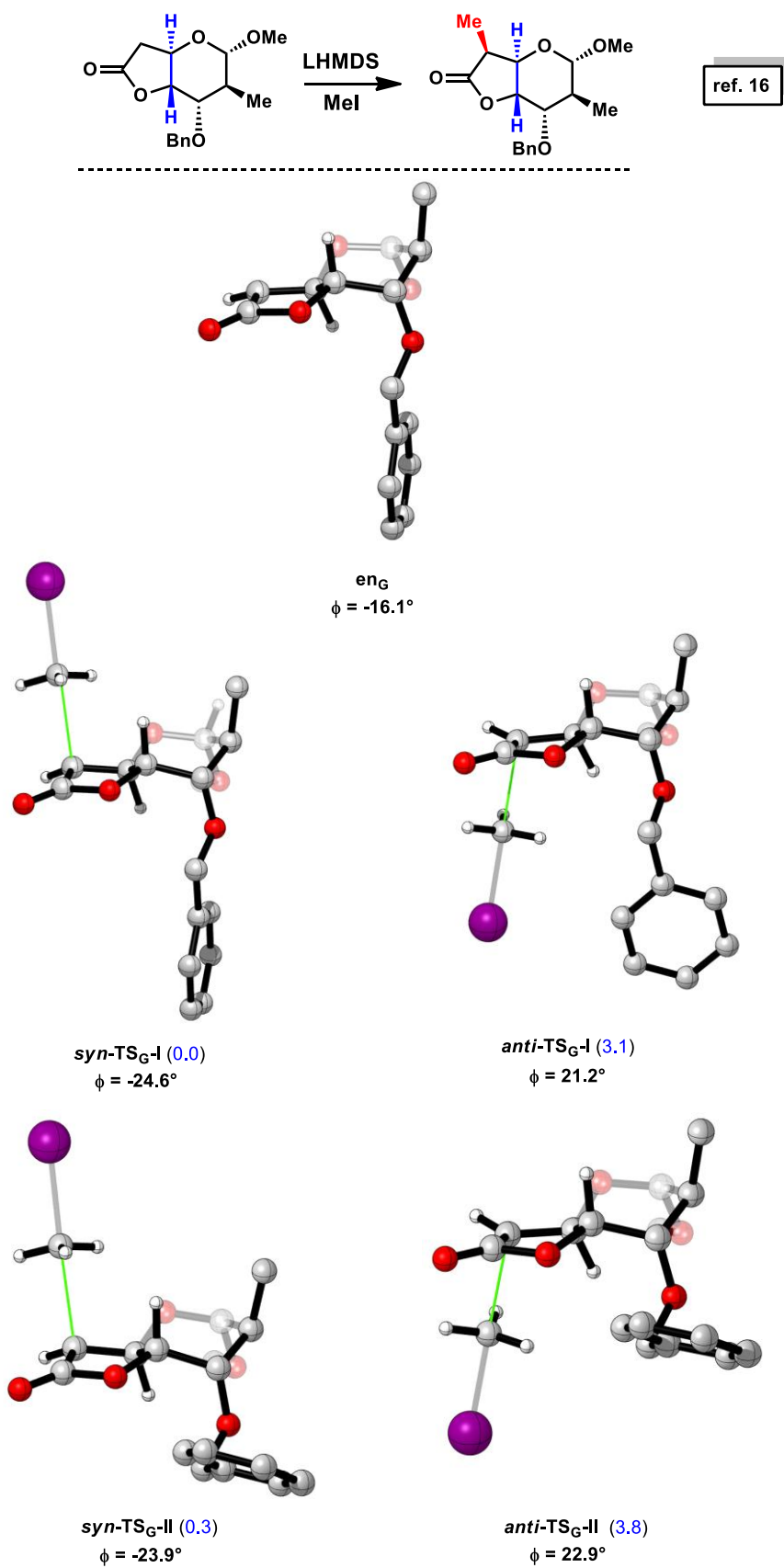


Figure S14: Structure of the ground state enolate of **en_G** and the diastereomeric transition states of its methylation reaction within 1.0 kcal/mol energy window of *syn*-TS conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn*-TS_G-I.

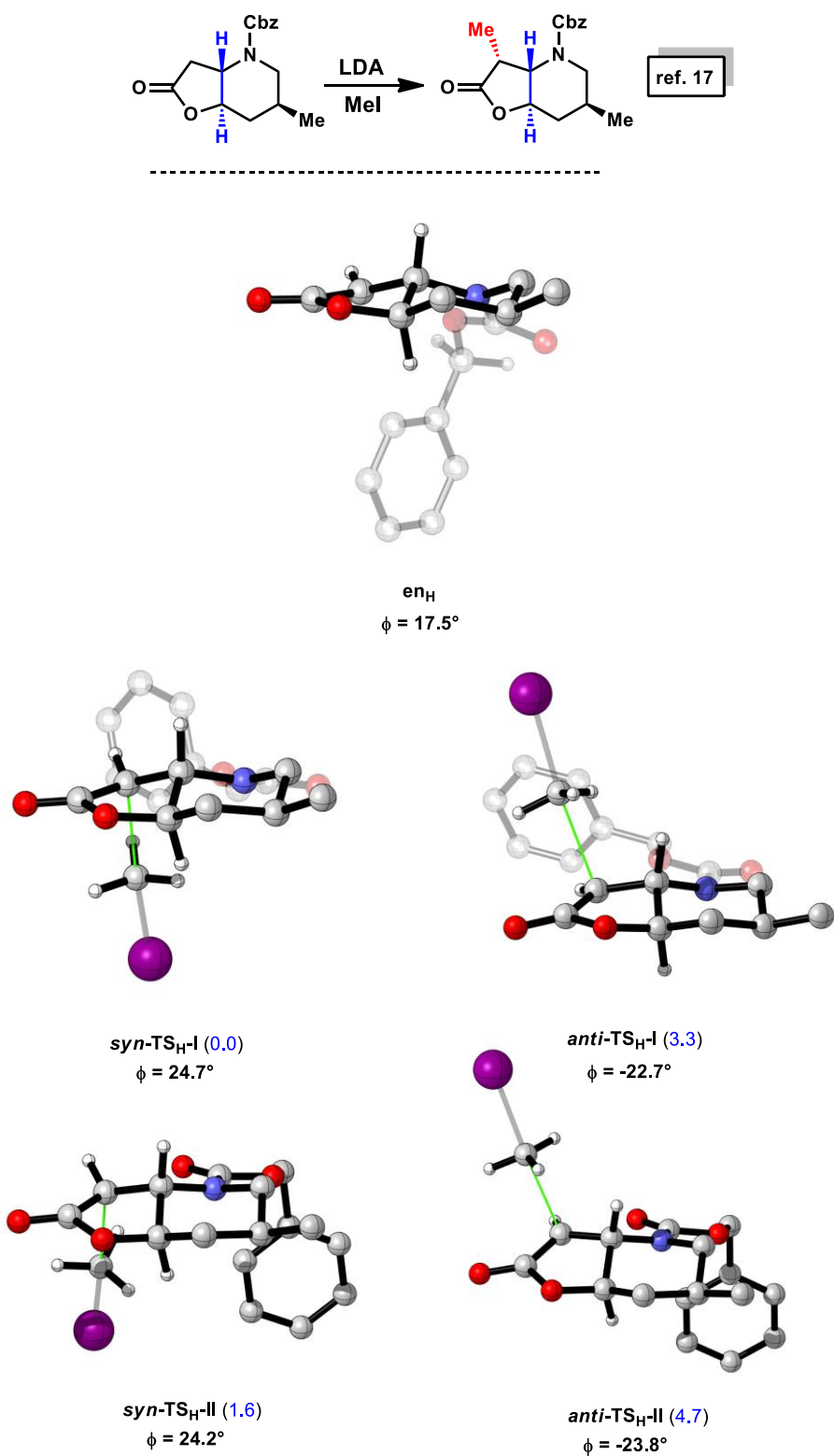


Figure S15: Structure of the ground state enolate of en_H and the diastereomeric transition states of its methylation reaction within 3.1 kcal/mol energy window of *syn*-TS conformations. Relative stability is given in parenthesis (in kcal/mol) with respect to *syn*-TS_{H-I}.

Table S2 Summary of the reported selectivities and the DFT-calculated free energy differences ($\Delta\Delta G^\ddagger$) along with the calculated selectivities. The reported selectivity is given as it was in the cited reference and we converted that into percentage for comparison (given in parenthesis).

Compound	Reported selectivity	DFT-calculated $\Delta\Delta G^\ddagger$ (kcal/mol)	Calculated selectivity %
A	8:1 (<i>syn:anti</i>) (= 88% <i>syn</i>)	0.8	79.4
B	*	1.2	88.3
C	>20:1 (<i>syn:anti</i>) (>95% <i>syn</i>)	2.2	97.6
D	exclusively <i>syn</i> (= 100% <i>syn</i>)	2.7	99.0
E	*	2.8	99.1
F	*	2.5	98.6
G	exclusively <i>syn</i> (= 100% <i>syn</i>)	3.1	99.5
H	only <i>syn</i> detected (= 100% <i>syn</i>)	3.3	99.6

*The authors reported only one diastereomer without commenting on the observed selectivity.

6. Computed energy components of the reported structures.

Table S3 Summary of energy data (given in Hartree) computed for optimized structures at the ω B97X-D/Def2SVP level of theory.

Structure	E_0^1	G_0	E_0	G_{sol} (THF)	G
<i>syn</i> -TS	-1045.8479	-1044.7773	-1045.0113	-1045.0787	-1045.6812
<i>anti</i> -TS	-1045.8443	-1044.7737	-1045.0076	-1045.0760	-1045.6788
en	-708.1372	-707.1493	-707.3541	-707.4334	-708.0118
MeI	-337.7013	-337.6326	-337.6436	-337.6453	-337.6921
MeI in <i>syn</i> -TS	-337.6826	-	-	-	-
en in <i>syn</i> -TS	-708.1356	-	-	-	-
MeI in <i>anti</i> -TS	-337.6807	-	-	-	-
en in <i>anti</i> -TS	-708.1326	-	-	-	-
<i>syn</i> -TS _{hep-I}	-839.0106	-838.1989	-838.4017	-838.4674	-838.8737
<i>syn</i> -TS _{hep-II}	-839.0097	-838.1980	-838.4009	-838.4666	-838.8727
<i>anti</i> -TS _{hep-I}	-839.0085	-838.1966	-838.3992	-838.4652	-838.8719
<i>anti</i> -TS _{hep-II}	-839.0079	-838.1962	-838.3986	-838.4647	-838.8715
<i>syn</i> -TS _{hex-I}	-799.6943	-798.9511	-799.1262	-799.1912	-799.5843
<i>syn</i> -TS _{hex-II}	-799.6865	-798.9433	-799.1183	-799.1834	-799.5766
<i>anti</i> -TS _{hex-I}	-799.6895	-798.9456	-799.1212	-799.1871	-799.5799
<i>anti</i> -TS _{hex-II}	-799.6824	-798.9388	-799.1140	-799.1798	-799.5731
<i>syn</i> -TS _{A-I}	-1517.1325	-1515.6051	-1515.9986	-1516.0594	-1516.7999
<i>syn</i> -TS _{A-II}	-1517.1317	-1515.6028	-1515.9963	-1516.0577	-1516.7995
<i>anti</i> -TS _{A-I}	-1517.1303	-1515.6030	-1515.9966	-1516.0585	-1516.7986
<i>anti</i> -TS _{A-II}	-1517.1299	-1515.6011	-1515.9946	-1516.0568	-1516.7987
<i>syn</i> -TS _{B-I}	-1107.1986	-1106.0249	-1106.3003	-1106.3661	-1106.9890
<i>syn</i> -TS _{B-II}	-1107.1911	-1106.0187	-1106.2941	-1106.3602	-1106.9818
<i>anti</i> -TS _{B-I}	-1107.1957	-1106.0223	-1106.2972	-1106.3634	-1106.9870
<i>anti</i> -TS _{B-II}	-1107.1908	-1106.0181	-1106.2933	-1106.3587	-1106.9811
<i>syn</i> -TS _{C-I}	-954.4958	-953.5272	-953.7631	-953.8288	-954.3257
<i>syn</i> -TS _{C-II}	-954.4923	-953.5242	-953.7596	-953.8255	-954.3229
<i>anti</i> -TS _{C-I}	-954.4916	-953.5223	-953.7585	-953.8253	-954.3221
<i>anti</i> -TS _{C-II}	-954.4881	-953.5193	-953.7550	-953.8220	-954.3194
<i>syn</i> -TS _{D-I}	-839.0109	-838.1997	-838.4013	-838.4662	-838.8742
<i>syn</i> -TS _{D-II}	-839.0061	-838.1950	-838.3963	-838.4613	-838.8697
<i>anti</i> -TS _{D-I}	-839.0062	-838.1942	-838.3963	-838.4622	-838.8700
<i>anti</i> -TS _{D-II}	-839.0018	-838.1901	-838.3918	-838.4576	-838.8659
<i>syn</i> -TS _{E-I}	-837.7739	-836.9875	-837.1643	-837.2302	-837.6631
<i>anti</i> -TS _{E-I}	-837.7688	-836.9817	-837.1589	-837.2258	-837.6586
<i>syn</i> -TS _{F-I}	-952.1137	-951.1933	-951.3889	-951.4560	-951.9852
<i>anti</i> -TS _{F-I}	-952.1086	-951.1878	-951.3836	-951.4519	-951.9812
<i>syn</i> -TS _{G-I}	-1335.0375	-1333.5693	-1333.8819	-1333.9507	-1334.7937
<i>syn</i> -TS _{G-II}	-1335.0387	-1333.5686	-1333.8822	-1333.9504	-1334.7932
<i>anti</i> -TS _{G-I}	-1335.0316	-1333.5601	-1333.8732	-1333.9435	-1334.7888
<i>anti</i> -TS _{G-II}	-1335.0317	-1333.5605	-1333.8739	-1333.9433	-1334.7877
<i>syn</i> -TS _{H-I}	-1314.0162	-1312.5846	-1312.8888	-1312.9589	-1313.7822
<i>syn</i> -TS _{H-II}	-1314.0138	-1312.5825	-1312.8878	-1312.9590	-1313.7797
<i>anti</i> -TS _{H-I}	-1314.0097	-1312.5769	-1312.8809	-1312.9522	-1313.7770
<i>anti</i> -TS _{H-II}	-1314.0034	-1312.5740	-1312.8764	-1312.9502	-1313.7748

7. Cartesian coordinates of the reported structures

Cartesian coordinates of the optimized geometries are given below in standard XYZ format (units are in Å). The first line indicates the total number of atoms, the second line shows the molecule name (as used in the main text and here in the Supporting Information).

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syn-TS

C	-0.83009700	-0.58208100	-0.06967000
C	-1.20931500	0.85863500	0.30470300
C	0.66496300	-0.87334400	-0.29515900
N	-1.19156600	1.76284700	-0.82432100
C	0.04411300	2.27424300	-1.41415700
C	-2.28915700	1.90334600	-1.61951900
C	0.95179500	1.14749900	-1.92851700
C	-0.48029000	3.22571100	-2.50476700
C	1.50818500	0.31120000	-0.75588000
C	2.23437500	1.56798000	-2.58372000
O	2.78037000	-0.14354500	-1.14940500
C	3.24924000	0.63983300	-2.21966800
O	4.37950100	0.45424100	-2.62451100
C	-1.86228900	2.67861000	-2.85795600
O	-3.39682700	1.45604700	-1.38688100
H	-1.21016400	-1.25282300	0.71803000
H	-1.40878300	-0.82884700	-0.97381400
H	-2.23966800	0.86677100	0.68795800
H	-0.55067000	1.25729900	1.09359300
H	1.12021800	-1.26440600	0.62945300
H	0.77759900	-1.66921500	-1.04829100
H	0.60465900	2.83887300	-0.65063500
H	0.31830400	0.50106700	-2.58158100
H	-0.57002800	4.24251300	-2.09366300
H	0.20993800	3.27281700	-3.35660700
H	1.64325800	1.00365600	0.10265700
H	-1.82910500	1.96002200	-3.69322400
H	-2.61191700	3.44005800	-3.11275000
C	3.27453000	3.57282600	-1.51700500
I	4.29159000	5.60017500	-0.59714700
H	4.12065500	3.17965500	-2.07436900
H	3.02878400	3.08627600	-0.57849400
H	2.47165100	4.05497600	-2.06331000
H	2.25765000	1.97147400	-3.59822000

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anti-TS

C	-0.60994300	-0.38011200	-0.10922200
C	0.26625200	-0.51707300	-1.36525600
C	-2.09798300	-0.75426000	-0.25256900
N	0.07582900	0.55713400	-2.31766700
C	-1.09489700	0.66002500	-3.18901800
C	0.77700900	1.72029300	-2.18621100
C	-2.40157600	0.70700600	-2.39078200
C	-0.79074100	1.93499400	-3.99992400
C	-2.65106600	-0.63340200	-1.66454400
C	-3.67251200	0.83249500	-3.17613600
O	-4.04191800	-0.84548600	-1.66190800
C	-4.60209200	-0.15338400	-2.75780400

O	-5.73224700	-0.42886300	-3.10842500
C	0.13532200	2.75154800	-3.10129600
O	1.72159900	1.89671700	-1.44037800
H	-0.15995900	-0.99295200	0.68853700
H	-0.50815600	0.66376600	0.22664700
H	1.32261700	-0.47211000	-1.06436200
H	0.09990600	-1.48142400	-1.87194900
H	-2.26699000	-1.79030900	0.08332400
H	-2.70894300	-0.11691500	0.40618600
H	-1.13865600	-0.21962100	-3.85551900
H	-2.27416900	1.52220900	-1.63785000
H	-0.26997800	1.66462400	-4.93117800
H	-1.71260000	2.46233000	-4.27612300
H	-2.19184000	-1.43052100	-2.28919000
H	-0.41911600	3.45300800	-2.45675500
H	0.90339100	3.33191000	-3.63015400
C	-4.82570400	2.65682200	-2.06088300
I	-5.88967100	4.57946200	-0.94942600
H	-4.55292100	2.10693700	-1.16486600
H	-4.05042400	3.22121100	-2.56784000
H	-5.68586800	2.30939900	-2.62626700
H	-3.74785500	1.29205900	-4.16124600

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en

C	-3.58459100	1.05886900	-0.16105800
C	-3.24088900	-0.43365700	-0.03704200
C	-5.07158600	1.41754700	-0.33509100
N	-3.27028100	-1.13158700	-1.30393100
C	-4.51747300	-1.49507000	-1.98468200
C	-2.17099900	-1.15316700	-2.10486200
C	-5.39924200	-0.27803600	-2.29883400
C	-3.99883000	-2.25173200	-3.22107700
C	-5.94038400	0.34821500	-0.99296100
C	-6.69065400	-0.56398300	-2.99071000
O	-7.20076300	0.87766700	-1.28002700
C	-7.71592400	0.21995000	-2.45348600
O	-8.87791400	0.45268600	-2.75316700
C	-2.60695200	-1.67344500	-3.46764800
O	-1.05061700	-0.78885300	-1.79121100
H	-3.18943300	1.57562900	0.72969000
H	-2.99635100	1.44021200	-1.01092100
H	-2.21390300	-0.53260700	0.34377200
H	-3.91730700	-0.94351600	0.66826200
H	-5.52241000	1.65451400	0.64340500
H	-5.16359200	2.33371400	-0.94009000
H	-5.10959800	-2.16912000	-1.34174100
H	-4.73566200	0.45751800	-2.82563000
H	-3.92183900	-3.32640400	-2.99278000
H	-4.68782300	-2.13980500	-4.06736800
H	-6.06793700	-0.49150200	-0.27123400
H	-2.62994300	-0.80704300	-4.14894800
H	-1.86809100	-2.38345000	-3.86483800
H	-6.77708900	-0.98870000	-3.99185300

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MeI

C	-1.24571600	0.09054800	-0.01360000
H	-0.86954000	-0.93784300	0.00686200
H	-0.86951200	0.62251900	-0.89393600
H	-2.34066500	0.10249000	0.00700500
I	-0.53201500	1.09995400	1.73466100

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MeI in *syn*-TS

C	4.27255600	3.96369300	-1.43131200
I	5.28961600	5.99104200	-0.51145400
H	5.11868100	3.57052200	-1.98867600
H	4.02681000	3.47714300	-0.49280100
H	3.46967700	4.44584300	-1.97761700

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en in *syn*-TS

C	-0.45936200	-0.77332500	-0.00982400
C	-0.83858000	0.66739100	0.36454900
C	1.03569800	-1.06458800	-0.23531300
N	-0.82083100	1.57160300	-0.76447500
C	0.41484800	2.08299900	-1.35431100
C	-1.91842200	1.71210200	-1.55967300
C	1.32253000	0.95625500	-1.86867100
C	-0.10955500	3.03446700	-2.44492100
C	1.87892000	0.11995600	-0.69603400
C	2.60511000	1.37673600	-2.52387400
O	3.15110500	-0.33478900	-1.08955900
C	3.61997500	0.44858900	-2.15982200
O	4.75023600	0.26299700	-2.56466500
C	-1.49155400	2.48736600	-2.79811000
O	-3.02609200	1.26480300	-1.32703500
H	-0.83942900	-1.44406700	0.77787600
H	-1.03804800	-1.02009100	-0.91396800
H	-1.86893300	0.67552700	0.74780400
H	-0.17993500	1.06605500	1.15343900
H	1.49095300	-1.45565000	0.68929900
H	1.14833400	-1.86045900	-0.98844500
H	0.97539400	2.64762900	-0.59078900
H	0.68903900	0.30982300	-2.52173500
H	-0.19929300	4.05126900	-2.03381700
H	0.58067300	3.08157300	-3.29676100
H	2.01399300	0.81241200	0.16250300
H	-1.45837000	1.76877800	-3.63337800
H	-2.24118200	3.24881400	-3.05290400
H	2.62838500	1.78023000	-3.53837400

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MeI in *anti*-TS

C	-6.58921800	2.99864900	-1.98273100
I	-7.65318500	4.92128900	-0.87127400
H	-6.31643500	2.44876400	-1.08671400
H	-5.81393800	3.56303800	-2.48968800
H	-7.44938200	2.65122600	-2.54811500

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en in *anti*-TS

C	-0.36753400	-0.58958700	0.00000000
C	0.50866100	-0.72654800	-1.25603400
C	-1.85557400	-0.96373500	-0.14334700
N	0.31823800	0.34765900	-2.20844500
C	-0.85248800	0.45055000	-3.07979600
C	1.01941800	1.51081800	-2.07698900
C	-2.15916700	0.49753100	-2.28156000
C	-0.54833200	1.72551900	-3.89070200
C	-2.40865700	-0.84287700	-1.55532200
C	-3.43010300	0.62302000	-3.06691400
O	-3.79950900	-1.05496100	-1.55268600
C	-4.35968300	-0.36285900	-2.64858200
O	-5.48983800	-0.63833800	-2.99920300
C	0.37773100	2.54207300	-2.99207400
O	1.96400800	1.68724200	-1.33115600
H	0.08245000	-1.20242700	0.79775900
H	-0.26574700	0.45429100	0.33586900
H	1.56502600	-0.68158500	-0.95514000
H	0.34231500	-1.69089900	-1.76272700
H	-2.02458100	-1.99978400	0.19254600
H	-2.46653400	-0.32639000	0.51540800
H	-0.89624700	-0.42909600	-3.74629700
H	-2.03176000	1.31273400	-1.52862800
H	-0.02756900	1.45514900	-4.82195600
H	-1.47019100	2.25285500	-4.16690100
H	-1.94943100	-1.63999600	-2.17996800
H	-0.17670700	3.24353300	-2.34753300
H	1.14580000	3.12243500	-3.52093200
H	-3.50544600	1.08258400	-4.05202400

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en_{but}

C	1.55559000	1.39722700	-1.90842200
C	2.13717400	0.63359800	-0.70647000
C	2.83223200	1.76174000	-2.60310900
O	3.36384700	0.10135700	-1.11214100
C	3.85684900	0.90190300	-2.20952900
O	5.01210500	0.69287600	-2.56748900
H	0.86739200	0.73721600	-2.49586000
H	2.28763400	1.34474700	0.13721400
H	2.90155400	2.36218500	-3.51113900
H	0.92911700	2.24399600	-1.55940900
H	1.48293500	-0.18149000	-0.34150500

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TS-en_{but}

C	-0.69716200	-0.08087800	-0.24397900
C	-1.17143800	-1.06712900	0.83711900
C	-2.01513900	0.25221900	-0.88040200
O	-2.36922900	-1.63722300	0.37479000
C	-2.92636700	-0.79854200	-0.61732800
O	-4.04113600	-1.06320000	-1.03491900
H	-0.16081900	0.77187000	0.21489400
H	-0.44537400	-1.87023800	1.05180300
C	-3.23471100	2.01728700	0.55611100
I	-4.34264800	3.73730900	1.79339000
H	-2.77091400	1.45879800	1.36479600

H	-2.56931600	2.61688500	-0.05746700
H	-4.07098800	1.53406000	0.05520900
H	-2.10195700	0.80947100	-1.81458600
H	0.02897500	-0.57021000	-0.93208200
H	-1.35871200	-0.52532800	1.78739100

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en_{hep}

C	0.84651000	0.22683100	0.06520100
C	0.39884300	1.61974600	0.53781000
C	2.35403300	0.01960500	-0.14674900
C	1.52844400	3.13074200	-1.26137000
C	2.44663100	2.02992000	-1.80747400
C	3.11924100	1.23449000	-0.66724900
C	3.66779500	2.48820900	-2.53962700
O	4.37990000	0.83425300	-1.12214500
C	4.77051900	1.70214100	-2.20757500
O	5.92225100	1.59488600	-2.61174700
H	0.48943900	-0.52899500	0.78590500
H	0.31266200	0.01189600	-0.87672200
H	-0.57828900	1.51629300	1.04205500
H	1.09476600	2.00428600	1.30454600
H	2.82650200	-0.30656200	0.79610900
H	2.51461800	-0.79918100	-0.86682600
H	2.11931500	3.74136600	-0.55438000
H	1.79614700	1.33989200	-2.40748900
H	3.25728400	1.95108100	0.17494600
H	3.65142600	3.11763100	-3.43073900
H	1.25688400	3.81089800	-2.08789700
C	0.23867000	2.64997900	-0.58951500
H	-0.30553100	3.52620800	-0.19276300
H	-0.42474700	2.20673400	-1.35604800

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syn-TS_{hep}-I

C	0.85367800	0.22746600	0.04943500
C	0.38637400	1.61123600	0.52847300
C	2.36559600	0.03375800	-0.14024500
C	1.52555400	3.15279100	-1.23263100
C	2.45867900	2.06538000	-1.77552800
C	3.12632100	1.25646500	-0.64431700
C	3.68269200	2.53810100	-2.50738500
O	4.39179100	0.85657500	-1.11677500
C	4.75837500	1.66285700	-2.21380700
O	5.87497400	1.53003400	-2.68156000
H	0.49580100	-0.53898900	0.75699600
H	0.33603000	0.01436800	-0.90174600
H	-0.59574200	1.49349000	1.01752400
H	1.06609200	1.99656600	1.30916100
H	2.82709600	-0.29129000	0.80736300
H	2.54332900	-0.78048300	-0.86098800
H	2.08758500	3.75919000	-0.50088300
H	1.83769200	1.37768900	-2.39881200
H	3.28056200	1.95566500	0.20532900
C	4.79041900	4.55483000	-1.42533000
I	5.85531200	6.54158600	-0.52510500
H	5.60274000	4.14887300	-2.02373400

H	4.56575900	4.04351400	-0.49391500
H	3.96301800	5.03196800	-1.93952500
H	3.62548400	2.98883900	-3.50043100
H	1.26563300	3.84151600	-2.05469200
C	0.23058000	2.64895300	-0.59188800
H	-0.32767100	3.51579000	-0.19751600
H	-0.41319000	2.20638300	-1.37482100

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***syn*-TS_{hep}-II**

C	1.00929000	0.21044300	0.39395400
C	0.02545300	1.16359300	-0.29902500
C	2.34018800	-0.03904800	-0.31567000
C	1.45306200	3.08868500	-1.36198600
C	2.46558100	2.03694200	-1.83226800
C	3.11064800	1.21922800	-0.69418200
C	3.69636800	2.54381200	-2.53201600
O	4.39819600	0.86076900	-1.13874400
C	4.77754000	1.68302400	-2.21990700
O	5.90956100	1.57500400	-2.65671100
H	1.20957800	0.60973400	1.40536700
H	0.51369700	-0.76318300	0.54993200
H	-0.15762000	0.83135100	-1.33599200
H	-0.94358600	1.07793600	0.22194200
H	2.98412400	-0.65928400	0.32912300
H	2.17522900	-0.61934500	-1.24014300
H	2.00078000	3.96948600	-0.99124000
H	1.90291900	1.31985800	-2.47397600
H	3.21381100	1.86829500	0.20369100
C	4.78140400	4.55365300	-1.41118400
I	5.83817500	6.52180700	-0.45968900
H	5.62634000	4.10763100	-1.93128500
H	4.45833200	4.07293800	-0.49246300
H	4.02026200	5.04893600	-2.00469500
H	3.65512900	2.99880700	-3.52389300
H	0.89602200	3.43536700	-2.24954600
C	0.45641000	2.63832200	-0.27767100
H	0.88570000	2.84128300	0.71927200
H	-0.44092400	3.27664800	-0.34091900

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***anti*-TS_{hep}-I**

C	-3.50336500	0.62129700	0.58383200
C	-2.47795900	0.25016300	-0.50188000
C	-4.93689600	0.09961500	0.39039300
C	-3.71175200	1.06681400	-2.65703600
C	-5.05904900	1.22654100	-1.94846700
C	-5.37734900	0.00121200	-1.06276200
C	-6.28369200	1.26011400	-2.81444400
O	-6.76524000	-0.22206000	-1.13848200
C	-7.24809500	0.33972300	-2.34427300
O	-8.36143100	0.02660900	-2.72596600
H	-3.13502100	0.26616600	1.56048200
H	-3.52206700	1.72185800	0.65902000
H	-1.47077900	0.31127700	-0.05520300
H	-2.60593900	-0.80361400	-0.80669600
H	-5.04686200	-0.89571700	0.85270000

H	-5.64563900	0.76111500	0.91432800
H	-3.71102600	0.09688000	-3.18700400
H	-4.97656000	2.13560000	-1.30504300
H	-4.86864800	-0.87252600	-1.52435200
C	-7.55531700	3.18788900	-1.90537400
I	-8.69828100	5.15041400	-1.02529500
H	-7.28929600	2.71640200	-0.96330500
H	-6.76878300	3.70284100	-2.44710300
H	-8.37198600	2.74273600	-2.46817500
H	-6.29851100	1.63138900	-3.83913900
C	-2.49033700	1.16401600	-1.73733600
H	-1.58197700	0.96473900	-2.33265400
H	-2.39440200	2.20668300	-1.38235700
H	-3.62019300	1.83928800	-3.43989000

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***anti*-TS_{hep-II}**

C	-3.90610700	-0.32501300	0.93722100
C	-2.95124600	0.51257600	0.07175500
C	-5.40640300	-0.15428000	0.68688100
C	-3.98840900	0.62022000	-2.33610500
C	-5.34485200	0.86006900	-1.66813500
C	-5.80567300	-0.31087300	-0.77209600
C	-6.53391900	1.01535800	-2.57060700
O	-7.20530200	-0.39313700	-0.89549300
C	-7.59797300	0.20384800	-2.11852400
O	-8.72704000	-0.00166900	-2.52671600
H	-3.63964700	-1.38897300	0.79562800
H	-3.70465700	-0.10530700	1.99952100
H	-3.20698500	1.58311300	0.15114900
H	-1.94145600	0.41112300	0.50508200
H	-5.96051600	-0.89321000	1.28844800
H	-5.74058300	0.84071600	1.02822200
H	-4.12434000	-0.08402900	-3.17453700
H	-5.21374300	1.75284900	-1.01405000
H	-5.36587200	-1.25575500	-1.16397500
C	-7.63431100	3.07660300	-1.71511100
I	-8.59676000	5.14947800	-0.88606500
H	-7.44084600	2.58930600	-0.76337200
H	-6.78500800	3.50068700	-2.24074100
H	-8.47440300	2.70586400	-2.29718600
H	-6.48043300	1.36943400	-3.60000100
C	-2.88162200	0.08632800	-1.40466300
H	-2.88396100	-1.01779500	-1.42819600
H	-1.90187900	0.38261500	-1.81607100
H	-3.66105200	1.57163100	-2.78945500

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en_{hex}

C	-0.99599100	1.34431600	-1.10840800
C	-2.46595500	1.15447300	-0.69734000
C	-3.12944100	2.83697200	-2.46019500
C	-3.32448400	1.41973700	-1.92215000
C	-4.34057500	2.90864200	-3.33628100
O	-4.69767600	1.25556400	-1.76204800
C	-5.32644500	2.07857800	-2.78359900
O	-6.52558600	1.91005100	-2.96225900

H	-0.72203500	0.52649100	-1.79970900
H	-0.33199600	1.24114800	-0.23245400
H	-2.62804000	0.13424700	-0.31016500
H	-2.74140900	1.85749700	0.10777700
H	-3.19220600	3.53679700	-1.58410200
H	-2.97115700	0.72988300	-2.72672800
H	-4.61920900	3.77323700	-3.94227300
C	-1.69515100	2.97027700	-2.96985800
H	-1.53279000	2.25537700	-3.79739300
H	-1.50551600	3.97731000	-3.38044500
C	-0.72481700	2.68679900	-1.81024400
H	-0.82490300	3.49849800	-1.06655700
H	0.32356000	2.71303000	-2.15687100

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***syn*-TS_{hex}-I**

C	-1.19934200	0.80277800	0.47008000
C	0.00233000	-0.05410700	0.03675400
C	-0.73106700	2.48293000	-1.41448700
C	0.38652700	1.54958700	-1.87175200
C	0.99340400	0.86715800	-0.64762000
C	1.65344300	2.01209900	-2.53049400
O	2.18383000	0.27789700	-1.09389100
C	2.65873200	1.06455200	-2.17797300
O	3.78033200	0.84852900	-2.59652800
H	-0.86899800	1.47926700	1.27876600
H	-1.98728400	0.16578100	0.90578000
H	0.45673200	-0.55046400	0.90968700
H	-0.31217700	-0.84554900	-0.66491900
H	-0.31787800	3.26478000	-0.75253700
H	-0.11386100	0.75414900	-2.47751800
H	1.25113200	1.67025700	0.08003300
C	2.68914900	4.09087300	-1.45018900
I	3.67284700	6.11276700	-0.57635700
H	3.54687200	3.63849900	-1.94229500
H	2.36139700	3.63116300	-0.52252000
H	1.91880900	4.52420700	-2.07965400
H	1.67231800	2.41562900	-3.54577500
H	-1.19283600	3.00445900	-2.26945800
C	-1.78923800	1.65289000	-0.66862800
H	-2.58354900	2.30374400	-0.26536100
H	-2.27931400	0.97923600	-1.39486600

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***syn*-TS_{hex}-II**

C	-1.34850400	0.05307300	0.13881200
C	0.06359700	-0.56656300	0.01410400
C	-0.71352300	2.16626100	-1.18189300
C	0.23551200	1.14827900	-1.82906300
C	0.98095100	0.40141500	-0.72423600
C	1.40392700	1.55378300	-2.67921600
O	2.09380000	-0.19422300	-1.33410100
C	2.42207200	0.57880900	-2.47795700
O	3.46509500	0.33612400	-3.05585600
H	-1.84402800	-0.30267500	1.05686700
H	-1.97645800	-0.29322000	-0.69896000
H	0.47777000	-0.80709900	1.00698400

H	0.02253500	-1.50957000	-0.55392600
H	-0.16545100	3.09558800	-0.95783900
H	-0.40573200	0.40333000	-2.35780600
H	1.34630000	1.16462900	-0.00226300
C	2.72632600	3.54535600	-1.77432400
I	3.97723500	5.48600400	-1.05737900
H	3.47739700	3.02367600	-2.36314400
H	2.48260700	3.12165000	-0.80456500
H	1.92343800	4.04361300	-2.30758400
H	1.28651800	1.96774600	-3.68332700
H	-1.51322400	2.43735800	-1.89100100
C	-1.32235500	1.59073400	0.12252300
H	-0.73298400	1.93665900	0.98871000
H	-2.34162500	1.97990000	0.28023800

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***anti*-TS_{hex}-I**

C	-0.34187000	-0.70361600	-0.29740200
C	0.61235400	0.28939500	-0.98531200
C	-0.49805000	-0.25750000	-3.17736700
C	-0.12020700	0.84451200	-2.18960800
C	-0.72900200	0.57464300	-4.40510800
O	0.54691900	1.81959000	-2.94543100
C	-0.08484100	1.82622700	-4.22548100
O	0.06561000	2.79916600	-4.94084700
H	-1.17304200	-0.12935900	0.15038500
H	0.16819500	-1.20790200	0.54028100
H	0.90312400	1.09063500	-0.28663700
H	1.53756000	-0.21484600	-1.31212400
H	0.40353600	-0.90512800	-3.30708000
H	-1.07304200	1.28789400	-1.81762900
C	1.01770900	-0.19202700	-5.97328700
I	2.71112900	-1.04726200	-7.52233500
H	1.63343800	-0.15034200	-5.07912300
H	0.31851400	-1.01631200	-6.06510900
H	0.79336800	0.74899300	-6.46929900
H	-1.50845400	0.42048300	-5.14956900
C	-1.54277600	-1.15914800	-2.53007000
H	-2.44893100	-0.57346900	-2.29029300
H	-1.85674900	-1.96738400	-3.21151200
C	-0.93275900	-1.75893000	-1.25059100
H	-0.12869600	-2.45602600	-1.54663300
H	-1.68005900	-2.36220000	-0.70745300

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***anti*-TS_{hex}-II**

C	-1.17794500	1.99409800	-0.69217100
C	-2.55668800	1.30307900	-0.54528300
C	-3.11337000	2.89315900	-2.41445300
C	-3.34808400	1.50068900	-1.83012600
C	-4.37161800	3.05554800	-3.21469900
O	-4.73751800	1.34909100	-1.71305500
C	-5.31934700	2.09433400	-2.78002600
O	-6.47291700	1.85966100	-3.08888400
H	-0.41327300	1.45235400	-0.11215200
H	-1.22765300	3.00548600	-0.25684200
H	-2.44170800	0.22965600	-0.32247500

H	-3.12208400	1.74656100	0.28974200
H	-3.08913700	3.61346100	-1.56262100
H	-2.98540500	0.76657900	-2.58419500
C	-5.57099400	4.87661700	-2.04854500
I	-6.66740100	6.74363100	-0.91088000
H	-5.25848200	4.31886000	-1.17008100
H	-4.81656300	5.45411100	-2.57224500
H	-6.42114400	4.49163300	-2.60612100
H	-4.45581500	3.55898700	-4.17673700
C	-1.71424000	2.92468300	-3.03769300
H	-1.74884600	2.49300000	-4.05220900
H	-1.37239900	3.96677700	-3.14921500
C	-0.72168200	2.11806400	-2.15774300
H	0.28263100	2.57130500	-2.19127400
H	-0.60485600	1.10178400	-2.57108400

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en_A

C	3.83137200	9.28644400	-4.21125200
C	2.51673400	8.53002000	-4.29535200
C	4.10832800	10.36431500	-5.32277500
C	1.81172000	8.33729900	-6.75992500
C	2.76847700	9.39437200	-7.30715200
C	2.97272700	10.55994800	-6.31670000
C	2.33066500	10.15292700	-8.52162500
O	3.21437300	11.70214100	-7.09330300
C	2.67555000	11.49178800	-8.42208700
O	2.64735600	12.47987600	-9.15117000
H	4.60623100	8.50966200	-4.33702300
H	4.98962600	10.04280500	-5.89834700
H	0.83650100	8.80978400	-6.54967700
H	3.75102500	8.87486600	-7.44705000
H	2.02196800	10.70564900	-5.75973900
H	2.00621800	9.69652500	-9.45636600
C	2.32833900	7.62686900	-5.49971000
H	1.63206800	6.81656000	-5.22851500
H	3.29452600	7.14731200	-5.73951500
C	1.56654900	8.58905300	-3.35433900
H	1.64408000	9.22553200	-2.47086800
H	0.65326000	7.99381200	-3.45053700
C	4.56991300	11.65485000	-4.57470200
C	4.12505800	9.99786200	-2.87809700
H	4.49322700	9.30180400	-2.10858900
H	3.21400200	10.46539200	-2.47530500
C	5.11898700	11.08509800	-3.25509400
H	6.11030900	10.65323900	-3.46915600
H	5.25040700	11.86293600	-2.48666200
H	1.63040100	7.57761600	-7.53983600
C	3.42743300	12.64003500	-4.30645500
H	3.80791700	13.47867900	-3.70265100
H	3.03483800	13.02206100	-5.25705400
H	2.59731400	12.16220700	-3.76375100
O	5.61987400	12.32100900	-5.22449800
Si	5.97668800	12.91611500	-6.75658600
C	6.24092500	11.55232400	-8.02147500
C	7.67749500	13.67983900	-6.42524900
C	4.85015200	14.28075900	-7.36772200

H	5.30188700	11.04235200	-8.27813700
H	6.65261100	11.98735500	-8.94756700
H	6.96445100	10.81068400	-7.64406000
H	7.60334000	14.49806700	-5.69051000
H	8.37733000	12.92910100	-6.02399200
H	8.11119200	14.09303900	-7.35139100
H	4.45698900	14.86359600	-6.51883600
H	5.42496900	14.96942600	-8.01059400
H	4.00619600	13.86864300	-7.94646400

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***syn*-TS_A-I**

C	3.82359600	9.28806200	-4.21284000
C	2.52855800	8.50088800	-4.28985400
C	4.08332500	10.35805600	-5.33816900
C	1.77293800	8.29706700	-6.72050700
C	2.67718000	9.38665300	-7.28766000
C	2.92334500	10.55107900	-6.30610200
C	2.16720100	10.14377200	-8.48392900
O	3.16701400	11.68205900	-7.11640300
C	2.65896000	11.46659200	-8.41534400
O	2.69026300	12.40141400	-9.19687500
H	4.61963200	8.53071200	-4.32375900
H	4.94802300	10.03007400	-5.93496800
H	0.79308200	8.72817900	-6.45728300
H	3.66119000	8.90493400	-7.49896900
H	1.99202100	10.72850800	-5.73051200
C	-0.21157200	10.74568000	-8.24794200
I	-2.62349500	11.26674800	-8.12183200
H	0.06811200	11.46436400	-9.01317000
H	0.03049100	10.98148200	-7.21673400
H	-0.32376800	9.70288600	-8.52116900
H	2.05734200	9.67221400	-9.46206400
C	2.35749300	7.59161000	-5.49077400
H	1.70276000	6.75079000	-5.21249300
H	3.33672600	7.15685500	-5.75996300
C	1.57492200	8.55023800	-3.35274300
H	1.63709400	9.19664400	-2.47558400
H	0.67417700	7.93607700	-3.44466900
C	4.56963100	11.65228500	-4.60109500
C	4.09227200	10.02128900	-2.88868900
H	4.44106300	9.33710700	-2.10037200
H	3.17525700	10.50070500	-2.51422600
C	5.09947800	11.09218700	-3.26968000
H	6.08789400	10.64689000	-3.46820700
H	5.23212100	11.87969400	-2.51209600
H	1.58442400	7.54705300	-7.50717300
C	3.44905600	12.66624600	-4.34922000
H	3.84704200	13.50028300	-3.75123100
H	3.06432700	13.05602600	-5.29937100
H	2.60720300	12.21428900	-3.80306200
O	5.64171500	12.28329900	-5.24919500
Si	6.02648200	12.93371600	-6.74708000
C	6.27100400	11.59920400	-8.04643600
C	7.72112500	13.68543900	-6.39052500
C	4.88778800	14.29922600	-7.33162000
H	5.32326400	11.11128600	-8.31071900

H	6.68601700	12.04530600	-8.96526400
H	6.97989400	10.83496900	-7.68806500
H	7.64415400	14.48339500	-5.63460000
H	8.41795200	12.92342900	-6.00648000
H	8.15900300	14.12235400	-7.30327900
H	4.54683700	14.91404100	-6.48322200
H	5.43734400	14.95843600	-8.02477900
H	4.01241200	13.89101600	-7.86031000

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***syn*-TS_A-II**

C	2.63296600	7.16889700	1.70833700
C	1.42462900	6.25177800	1.59114100
C	2.50010600	8.52148900	0.95583300
C	1.03086200	6.11289800	-0.96039100
C	1.88351600	7.34405500	-1.27609200
C	1.61708600	8.48729200	-0.27766700
C	1.59480300	8.05192900	-2.57319400
O	1.78558400	9.69458600	-0.98839500
C	1.74932300	9.44532900	-2.37809300
O	1.80967100	10.40494000	-3.12434300
H	3.46608200	6.61096500	1.25217500
H	3.51051700	8.78052900	0.60775100
H	-0.02809200	6.41691700	-0.92251600
H	2.95330600	7.03715200	-1.20328900
H	0.55678800	8.40877600	0.03181500
C	-0.82977900	8.16889800	-3.05783200
I	-3.22171500	8.20631600	-3.65326200
H	-0.47823400	8.94245400	-3.73494700
H	-0.94305900	8.42955800	-2.01040100
H	-0.65118800	7.12978000	-3.30884000
H	1.87576700	7.62299300	-3.53683500
C	1.39144900	5.38742500	0.34508300
H	0.67965900	4.56075000	0.49816100
H	2.38901300	4.92640400	0.22708700
C	0.45999800	6.15857900	2.51357000
H	0.46189800	6.75649200	3.42750600
H	-0.37945800	5.47018600	2.37854800
C	2.13237700	9.62027600	2.01661200
C	3.03434700	7.61173100	3.12362800
H	4.11394000	7.83271600	3.12081100
H	2.85995800	6.83145400	3.88024500
C	2.25905200	8.90160400	3.38254600
H	2.75284900	9.57129900	4.09990400
H	1.25663200	8.67707300	3.77684300
H	1.11482500	5.39220400	-1.79123900
C	0.73284900	10.21393800	1.85579000
H	0.56751900	10.95711000	2.65123500
H	0.61469700	10.70086900	0.87941400
H	-0.03518200	9.43112300	1.94682200
O	3.09235200	10.65957700	2.00358800
Si	3.65558600	11.77781600	0.88498700
C	4.79432800	10.99676800	-0.38628500
C	4.67141600	12.93208500	1.97420500
C	2.31104900	12.75212800	0.01919700
H	5.33991100	11.78313700	-0.93371300
H	5.53575000	10.33296200	0.08687700

H	4.20656400	10.42266300	-1.11710700
H	5.46033800	12.37572800	2.50490000
H	5.15315000	13.72057800	1.37305900
H	4.03514600	13.41880600	2.73037100
H	1.84004100	12.13254500	-0.75955900
H	1.54055300	13.10666400	0.72169100
H	2.75789600	13.63400600	-0.46979200

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***anti*-TS_A-I**

C	0.78581000	1.44520400	-3.12409900
C	1.56049400	1.58143800	-4.42909000
C	-0.75128800	1.14187400	-3.26033300
C	0.06504800	2.79553100	-6.13505800
C	-1.22724900	2.56304200	-5.35968800
C	-1.25698900	1.17390300	-4.68731200
C	-2.51138700	2.53250800	-6.14027300
O	-2.59672200	0.73649700	-4.73102300
C	-3.27128800	1.39899300	-5.77957500
O	-4.35968500	0.96422100	-6.11675400
H	0.86553600	2.43411900	-2.64317400
H	-1.31034800	1.90663400	-2.69769300
H	0.18533300	2.00132500	-6.89243800
H	-1.25515100	3.34101700	-4.56083400
H	-0.65113200	0.47916200	-5.30301900
C	-3.91317300	4.04815700	-4.91583400
I	-5.26294400	5.68608900	-3.62534000
H	-3.54664500	3.49951400	-4.05440500
H	-3.26056200	4.77996200	-5.37948800
H	-4.73039200	3.61792900	-5.48790600
H	-2.65466600	3.03175100	-7.09800100
C	1.30841700	2.84416300	-5.23441100
H	2.19372800	3.05415100	-5.85545200
H	1.20131800	3.69454700	-4.53816300
C	2.44223600	0.68094800	-4.87909300
H	2.97824300	0.85210800	-5.81751700
H	2.66252200	-0.25206100	-4.35731300
C	-1.00428500	-0.18519400	-2.48619500
C	1.31756700	0.39500300	-2.12319400
C	0.08100500	-0.11648100	-1.39912500
H	-0.26563300	0.60701900	-0.64410600
H	0.22583400	-1.08350700	-0.89293100
H	-0.00700000	3.74871900	-6.68558900
H	1.80078400	-0.44150200	-2.64699400
H	2.07592700	0.82097000	-1.44934900
O	-2.24604900	-0.21799400	-1.84478600
C	-4.31809300	-1.62904000	-3.48851400
C	-4.72144200	1.27822100	-2.52815400
C	-4.52302200	-0.99993200	-0.51121100
H	-4.15766300	-1.20031300	-4.48900400
H	-3.73635400	-2.55814000	-3.38069900
H	-5.38696800	-1.88571500	-3.39554200
H	-4.14406800	2.12406800	-2.12312000
H	-4.84647800	1.42382500	-3.61061700
H	-5.71935900	1.31141200	-2.06139700
H	-4.28456600	-0.28831300	0.29552700
H	-5.61701500	-1.13565300	-0.53218300

H	-4.06111000	-1.96712900	-0.25533100
C	-0.82347400	-1.42159900	-3.37140800
H	-0.91435000	-2.33034000	-2.75646300
H	-1.59272700	-1.44609900	-4.15423800
H	0.16116200	-1.42557200	-3.86369500
Si	-3.88846800	-0.36251500	-2.17222600

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***anti*-TS_A-II**

C	3.23952500	4.18931800	-2.25470200
C	4.10965200	3.35441800	-1.32391100
C	1.76370300	3.71502800	-2.35763900
C	3.77343700	0.94381300	-2.23938400
C	2.52170300	1.33523700	-3.02539500
C	1.59491200	2.22236500	-2.16557000
C	1.57802000	0.23232700	-3.41459300
O	0.26840400	1.84194900	-2.45340600
C	0.26321500	0.53309500	-2.99148800
O	-0.80584500	-0.04203100	-3.07535300
H	3.69760200	4.08922400	-3.25112400
H	1.42911000	3.95326900	-3.37836600
H	3.46062000	0.47255700	-1.29144000
H	2.86711200	1.91259300	-3.91431500
H	1.79828000	1.97377200	-1.10552600
C	1.08206800	0.72152100	-5.72914900
I	0.66865100	1.26485700	-8.11144300
H	1.10893100	1.75038400	-5.38469800
H	2.02600300	0.20980900	-5.88274500
H	0.18118400	0.13918700	-5.55564800
H	1.88964700	-0.79614400	-3.59549100
C	4.72798200	2.11517400	-1.94727700
H	5.54468100	1.75680700	-1.30037700
H	5.19508300	2.42284900	-2.90035100
C	4.37432900	3.68334100	-0.05403400
H	5.02051700	3.05413800	0.56540900
H	3.96491500	4.57991200	0.41658300
C	0.90711400	4.62758100	-1.41132700
C	3.08686800	5.67943000	-1.91477300
C	1.86849600	5.77228400	-0.99692700
H	1.33919200	6.73153600	-1.07577600
H	2.16484100	5.64695200	0.05564200
H	4.33426500	0.17587100	-2.79826400
H	4.00047900	6.11391700	-1.48079200
H	2.87863100	6.22168000	-2.85091600
O	-0.16356000	5.21549300	-2.12080200
C	-2.55754700	3.44378700	-2.04734400
C	-1.01713700	3.94949500	-4.65237000
C	-2.46080200	6.26208600	-3.25687700
H	-2.74830500	3.77512200	-1.01424500
H	-3.53015000	3.33748100	-2.55644100
H	-2.07200700	2.45564700	-2.03148400
H	-0.57050300	2.95551200	-4.51217500
H	-1.90759200	3.82578200	-5.28966800
H	-0.30285700	4.58863900	-5.19493000
H	-1.84843400	7.00378500	-3.79375900
H	-3.37035400	6.07583600	-3.85100600
H	-2.76348900	6.70540100	-2.29486200

C	0.36951500	3.91379300	-0.16996600
H	-0.19786700	4.63551200	0.43813200
H	-0.28810400	3.07893900	-0.44369800
H	1.19686700	3.51872100	0.43917600
Si	-1.49481900	4.66727600	-2.98990700

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enb

C	-0.89421500	-0.25507900	0.86477700
C	-1.36569600	1.21676200	0.97295300
C	0.58538000	-0.59572100	0.55440400
C	-0.00566200	2.36658600	-0.94873400
C	0.91447100	1.19220500	-1.28405200
C	1.48158600	0.49629900	-0.03400100
C	2.19800100	1.51751900	-1.98176400
O	2.70529200	-0.06940600	-0.41033700
C	3.22341300	0.68522600	-1.54489000
O	4.37949900	0.45416400	-1.86795500
H	-1.54817800	-0.72393500	0.11134300
H	0.61046600	-1.39344100	-0.21127100
H	0.53066000	3.05442100	-0.27095200
H	0.28294600	0.45020600	-1.84088500
H	1.67473600	1.28044200	0.72918100
H	2.26531700	2.08623600	-2.90967500
C	-1.36399600	1.97262800	-0.36558000
H	-1.97486600	2.88402800	-0.23164200
H	-1.90154300	1.35385600	-1.10680200
C	1.09882100	-1.22792600	1.83217500
C	-1.17172400	-0.95443900	2.20153000
C	0.10913300	-1.43874500	2.72480700
H	-2.42659100	1.10854800	1.26109300
C	-0.70267000	2.00679000	2.10511600
H	-1.12163500	3.02505200	2.14936900
H	-0.88387000	1.52950700	3.08033300
H	0.38371600	2.10253700	1.97525100
H	0.20988000	-1.92092100	3.69890700
O	-2.26526000	-1.04695600	2.72209800
H	-0.18335500	2.94306200	-1.87297700
C	2.52896300	-1.60701200	2.00150400
H	2.83493800	-2.28193200	1.18801400
H	3.17268900	-0.72493200	1.87199500
H	2.71097100	-2.08229800	2.97619600

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syn-TS_B-I

C	-0.88812400	-0.25648300	0.84011700
C	-1.36193900	1.21250200	0.97216700
C	0.59780400	-0.58682300	0.55198300
C	0.00170400	2.39742500	-0.91995700
C	0.92237200	1.22706200	-1.26288500
C	1.48949400	0.51106000	-0.02520300
C	2.20551100	1.55343800	-1.97529700
O	2.71470800	-0.05954100	-0.42664700
C	3.19210100	0.61781500	-1.57822300
O	4.30353100	0.34199500	-1.98351700
H	-1.52799600	-0.71236900	0.06732700
H	0.63617200	-1.38607700	-0.21142500

H	0.52032400	3.07756900	-0.22297300
H	0.30768800	0.49132300	-1.83591200
H	1.70204900	1.27326100	0.75073400
C	3.33753600	3.54989200	-0.99478500
I	4.44593700	5.56693600	-0.14892400
H	4.17260900	3.09843900	-1.52362500
H	3.06128800	3.12191500	-0.03659200
H	2.56160100	4.04275900	-1.56964500
H	2.21392000	1.91997000	-3.00369400
C	-1.35836500	1.98919900	-0.35413900
H	-1.96877800	2.89788500	-0.20933400
H	-1.89047900	1.38243200	-1.10876000
C	1.10031100	-1.21288200	1.83954300
C	-1.18281100	-0.98184300	2.15955800
C	0.09574600	-1.45138800	2.70589300
H	-2.42351900	1.09763200	1.25359900
C	-0.70317600	1.98500300	2.11854200
H	-1.12315200	3.00133800	2.17904900
H	-0.88524700	1.49177800	3.08527800
H	0.38380700	2.08819700	1.99791800
H	0.18366500	-1.93890000	3.67819700
O	-2.28464300	-1.09897800	2.65279800
H	-0.16703600	2.98628800	-1.83725200
C	2.53597600	-1.55583000	2.04080200
H	2.89363600	-2.18928100	1.21557000
H	3.15628100	-0.64916400	1.98243600
H	2.70008100	-2.06028300	3.00323800

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***syn*-TS_B-II**

C	-0.93021800	-0.48338700	0.68279100
C	-1.71566600	0.58761700	-0.09406700
C	0.55298300	-0.78054700	0.34297000
C	-0.02458400	2.35487800	-0.94830900
C	0.94085400	1.21017500	-1.28023100
C	1.41287100	0.44584600	-0.02922300
C	2.26208700	1.58113000	-1.89838400
O	2.72684900	0.01388800	-0.28961000
C	3.25653200	0.70046400	-1.41239100
O	4.41163100	0.48074300	-1.71848900
H	-1.45636000	-1.44228100	0.51131000
H	0.64667000	-1.48181800	-0.50298700
H	0.55109800	3.21063800	-0.56328300
H	0.38980800	0.49334000	-1.92821500
H	1.43119000	1.13776700	0.83832600
C	3.32154800	3.59647100	-0.91781400
I	4.40144300	5.64406100	-0.07264800
H	4.19670900	3.11244100	-1.34324500
H	2.95235600	3.22799400	0.03409500
H	2.61729500	4.08488700	-1.58163900
H	2.33325600	1.93098400	-2.92990900
C	-1.12741400	2.00167700	0.06060300
H	-0.75377200	2.11495300	1.09172800
H	-1.93877300	2.74220700	-0.03041200
C	1.07510900	-1.40523600	1.62340000
C	-0.92130700	-0.38521400	2.21746900
C	0.27151800	-1.12302700	2.66661600

H	-1.64873900	0.30894500	-1.16015300
C	-3.20221100	0.54974500	0.27763600
H	-3.61505500	-0.46707300	0.17241500
H	-3.35285100	0.86546300	1.31821700
H	-3.77740200	1.21553400	-0.38501500
H	0.45151300	-1.37714700	3.71230400
O	-1.75271000	0.14524700	2.92292900
H	-0.48471200	2.69747400	-1.89130900
C	2.35143300	-2.17182200	1.65972300
H	2.28924200	-3.02980800	0.97053700
H	3.16703600	-1.53835400	1.28147800
H	2.57978200	-2.53827000	2.67025200

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***anti*-TS_B-I**

C	-0.45191800	-0.08517400	-0.25270400
C	0.47455300	-0.06013700	-1.49624300
C	-1.95610500	-0.43765800	-0.38145600
C	-1.07723500	1.02718500	-3.31179100
C	-2.36189400	0.98713100	-2.48824400
C	-2.57379500	-0.36082300	-1.77336300
C	-3.66148100	1.10862200	-3.23205100
O	-3.96753500	-0.55523700	-1.69269400
C	-4.57679300	0.13100600	-2.78117600
O	-5.71841100	-0.15902500	-3.07778500
H	-0.34355400	0.90308000	0.22268700
H	-2.54081500	0.28525700	0.21787100
H	-1.05198700	0.15542200	-3.98969400
H	-2.25946400	1.78125500	-1.70974500
H	-2.15753400	-1.16346100	-2.41395500
C	-4.80780500	2.90350600	-2.06299800
I	-5.86587100	4.79149300	-0.87826500
H	-4.50369500	2.34410600	-1.18327200
H	-4.05551200	3.48780600	-2.58171600
H	-5.68215200	2.55722400	-2.60698400
H	-3.75649400	1.56658900	-4.21625700
C	0.19700700	1.09896400	-2.46796400
H	1.06698400	1.18108800	-3.14333700
H	0.17710000	2.03604200	-1.88380300
C	-2.09258200	-1.77436700	0.32169400
C	0.09355400	-1.12471500	0.73535700
C	-0.95622000	-2.12591500	0.95584000
H	-0.81007600	-3.01353000	1.57359600
H	-1.10614600	1.91452600	-3.96641400
O	1.21152600	-1.11159200	1.20554100
H	1.46143600	0.15383000	-1.04970400
C	0.62464500	-1.41114900	-2.20264500
H	-0.31796400	-1.78219800	-2.62723600
H	1.34661000	-1.32379800	-3.03020100
H	1.00412100	-2.17901400	-1.51172400
C	-3.37574500	-2.53102900	0.33257900
H	-4.18952300	-1.88729500	0.69896200
H	-3.67272600	-2.79443400	-0.69299900
H	-3.30614600	-3.43652100	0.95154200

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***anti*-TS_B-II**

C	-0.48280200	-0.00385800	-0.16738200
C	0.26198000	0.93150800	-1.14001400
C	-2.01372300	-0.22544300	-0.28577400
C	-1.04958300	0.95526000	-3.38181300
C	-2.33451000	0.97868300	-2.54781400
C	-2.51736500	-0.31966300	-1.73646100
C	-3.63854200	1.04961100	-3.28825600
O	-3.88720300	-0.63523100	-1.75949300
C	-4.50639900	0.02254500	-2.86201400
O	-5.62368800	-0.33132600	-3.18151900
H	-0.33631600	0.42251200	0.84344000
H	-2.58854300	0.57967000	0.20161600
H	-1.20628000	0.30688100	-4.26022800
H	-2.23558500	1.82381900	-1.83182700
H	-1.96285000	-1.14342500	-2.23341400
C	-4.86404100	2.74658100	-2.02417300
I	-5.96697100	4.52540600	-0.73755600
H	-4.52609300	2.15164600	-1.18102100
H	-4.13739300	3.37530300	-2.52755100
H	-5.72795500	2.38887000	-2.57758700
H	-3.75530400	1.51950700	-4.26454300
C	0.19544400	0.48086200	-2.61236700
H	0.27297500	-0.61838800	-2.64353900
H	1.09435100	0.84461800	-3.13678600
C	-2.22162400	-1.54879100	0.42318100
C	0.05447400	-1.43534000	-0.00338800
C	-1.06678200	-2.23548100	0.51877200
H	-0.94249700	-3.24800200	0.90587900
H	-0.87545300	1.97127400	-3.77599000
O	1.18387300	-1.82395700	-0.21544700
H	-0.23527200	1.91368300	-1.06518400
C	1.71138000	1.13756100	-0.68474800
H	2.28668500	0.20719600	-0.77907800
H	2.19364600	1.92038800	-1.29120400
H	1.75713800	1.45517700	0.36973800
C	-3.57180500	-1.98841700	0.87022900
H	-3.98497300	-1.25520200	1.58192800
H	-4.25129800	-1.99318100	0.00502000
H	-3.54457500	-2.97749500	1.34837000

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enc

C	1.95421600	6.35663000	5.17468900
C	2.12345100	5.06407100	5.96637800
C	1.98789100	6.25192200	3.63911200
C	4.08073600	3.97484400	4.65902300
C	3.57672700	4.26797000	3.24312800
C	3.29240100	5.75817800	3.04104100
C	4.51454100	4.05291100	2.09685400
O	3.33510600	5.97506500	1.66036400
C	4.23495500	4.99221300	1.09812300
O	4.56506500	5.14934200	-0.06981800
H	1.78181600	7.25585500	3.22978600
H	4.49174000	2.95313800	4.69088400
H	4.98774900	3.09756900	1.86193200
C	3.04679600	4.10082200	5.74489500
H	3.04076400	3.28005100	6.47512900

H	4.93882200	4.64311100	4.86730800
H	1.16917200	5.59768500	3.29692700
H	0.94088400	6.72395700	5.40182900
H	4.13829900	6.31098900	3.51020600
H	2.61159000	3.70905400	3.14221400
C	2.92867600	7.41370100	5.71986000
H	2.78812400	8.37793000	5.20538500
H	2.76913000	7.56955500	6.79849900
H	3.97452900	7.10561700	5.57661900
C	1.28028100	4.89029000	7.16558900
H	1.44520000	3.94468400	7.69745400
C	0.37461400	5.73232200	7.68325300
H	-0.17171700	5.46948500	8.59271000
H	0.14427000	6.70230800	7.23532000

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syn-TSc-I

C	2.51526700	5.04179800	1.16231800
C	2.83139700	4.28062400	2.44538300
C	1.03991600	5.39706100	0.90371000
C	0.96264400	2.48892100	2.37111400
C	-0.19033800	3.41695700	1.98488400
C	0.11071600	4.21519300	0.71570800
C	-1.50140700	2.80480200	1.58155200
O	-1.14097500	4.62073800	0.21547400
C	-2.11454600	3.69627600	0.65785800
O	-3.23673100	3.77150400	0.19474200
H	0.99707000	6.01525200	-0.00866700
H	0.60907200	1.77494800	3.13110000
C	-1.24897500	0.82268300	0.01446900
I	-1.09404300	-1.14842100	-1.38904500
H	-0.46549100	1.41997300	-0.44184400
H	-1.02769000	0.36268900	0.97159100
H	-2.27451900	1.12668900	-0.18023900
H	-2.14093200	2.28493000	2.29890300
C	2.18098600	3.19016100	2.90906000
H	2.60749000	2.74297700	3.81614500
H	1.23774900	1.87264400	1.49442200
H	0.65987000	6.02187900	1.72842500
H	3.01553000	6.01816000	1.25257900
C	4.03279600	4.69143100	3.19938800
H	4.21439000	4.10663600	4.10959500
C	4.91653200	5.65401100	2.90338600
H	4.83226900	6.28452400	2.01468000
H	5.77356500	5.83936000	3.55552600
C	3.17407400	4.32591500	-0.02806500
H	3.00052200	4.87967800	-0.96441500
H	4.26060900	4.24006400	0.12686300
H	2.77747200	3.30867200	-0.15972700
H	0.56330900	3.51607300	-0.01948100
H	-0.30789500	4.13779700	2.82730800

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syn-TSc-II

C	2.48440500	5.04367300	1.17372600
C	2.76249600	4.31373400	2.48898200
C	1.01666800	5.39744100	0.87767500

C	0.93354600	2.49759600	2.38178300
C	-0.21584700	3.41904700	1.96935800
C	0.09467800	4.20783800	0.69557500
C	-1.52062000	2.79913500	1.55660200
O	-1.15323000	4.60392400	0.17877800
C	-2.12788900	3.67895100	0.61882500
O	-3.24518000	3.74549300	0.14228300
H	0.98988000	5.99784400	-0.04716600
H	0.56757900	1.78729100	3.13969000
C	-1.24029000	0.80617700	0.00244700
I	-1.05921800	-1.17029900	-1.38798500
H	-0.45295300	1.40465900	-0.44560000
H	-1.03031800	0.35344400	0.96561300
H	-2.26411900	1.10615400	-0.20717100
H	-2.16477900	2.27978800	2.27016300
C	2.13779000	3.20874000	2.94306600
H	2.56863500	2.76216500	3.84718600
H	1.22660600	1.87388000	1.51620100
H	0.62024700	6.03598500	1.68382500
H	3.00002800	6.01627600	1.25282200
C	3.92130900	4.85198900	3.23725000
H	4.74060900	5.24495500	2.61872600
C	4.04277100	4.93376700	4.56662300
H	3.23600400	4.61092100	5.23149600
H	4.94843600	5.33333500	5.03050000
C	3.15996300	4.28834600	0.01788200
H	4.24390400	4.19741200	0.19136600
H	2.75942800	3.26990900	-0.08774400
H	3.00900200	4.81402300	-0.93840600
H	0.55690100	3.50345400	-0.02859700
H	-0.34594400	4.14785400	2.80322400

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***anti*-TS_C-I**

C	1.93309900	6.34370500	5.15714100
C	2.13141800	5.05908000	5.95677900
C	1.96233000	6.24534000	3.62125000
C	4.03530000	3.90574800	4.61224300
C	3.50049100	4.23487000	3.22212600
C	3.26396500	5.73605900	3.04059400
C	4.37114500	3.95818000	2.02984600
O	3.35092900	5.97600700	1.65571200
C	4.27906200	5.04373500	1.12382400
O	4.76418200	5.26281700	0.02989600
H	1.76968700	7.25255700	3.21584700
H	4.38291700	2.86058400	4.62782500
C	2.98427200	2.51287500	0.61157500
I	1.59511400	0.99548800	-0.72836200
H	3.70405800	2.79312200	-0.15304000
H	2.21485300	3.23643400	0.86583400
H	3.27207600	1.79301400	1.37020000
H	5.20713700	3.25967100	2.01611000
C	3.03958400	4.08352300	5.72794800
H	3.05671100	3.28456800	6.48038100
H	4.93591700	4.51967200	4.80787500
H	1.13871600	5.60053000	3.27406100
H	0.91371500	6.69027600	5.38703500

H	4.10922900	6.26771800	3.52944200
H	2.51698500	3.71556200	3.14376700
C	2.88901000	7.42135400	5.69635200
H	2.72080300	8.38393000	5.18773800
H	2.73724300	7.56969600	6.77650100
H	3.94097400	7.13832900	5.54460900
C	1.32882300	4.91244500	7.18952400
H	1.51091100	3.97946300	7.73674600
C	0.44009300	5.76633900	7.71466700
H	-0.07732100	5.52409400	8.64614800
H	0.19277200	6.72541600	7.25270700

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anti-TSc-II

C	1.93114600	6.32384200	5.13272500
C	2.08446800	5.00781000	5.89973300
C	1.98378000	6.25968400	3.59666600
C	4.01777100	3.87745000	4.59845600
C	3.50503800	4.22992200	3.20534300
C	3.28797600	5.73592500	3.03244600
C	4.38712900	3.95410200	2.02095900
O	3.39647100	5.98676700	1.65108600
C	4.32019700	5.04753800	1.12302100
O	4.82165500	5.27036800	0.03703700
H	1.81774200	7.27787100	3.20698600
H	4.35799600	2.82946000	4.60228800
C	2.99537100	2.54212400	0.56953000
I	1.60019300	1.06048600	-0.80158500
H	3.72744400	2.82167700	-0.18363600
H	2.23394300	3.27378100	0.82471000
H	3.26577000	1.81051700	1.32334700
H	5.21310200	3.24368900	2.01028700
C	3.00275700	4.04019600	5.70126100
H	3.01259400	3.24702500	6.45857700
H	4.92129300	4.47926300	4.81701000
H	1.15581600	5.63612800	3.22233000
H	0.91752700	6.69154100	5.36788400
H	4.13291400	6.25337500	3.53687100
H	2.51633100	3.72340600	3.10938200
C	2.91032100	7.35775800	5.71331900
H	2.74901400	7.48802300	6.79524100
H	3.95470800	7.04352600	5.57304600
H	2.78058600	8.33824000	5.22808100
C	1.16763600	4.89961400	7.05912500
H	0.93923200	5.84513400	7.57099900
C	0.57495000	3.78609600	7.50268200
H	-0.08005200	3.80200600	8.37774300
H	0.71687800	2.82645500	6.99675300

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end

C	-3.20005300	-4.60629200	-5.53026800
C	-2.17003700	-3.59424500	-4.99835900
C	-2.87768400	-4.17024000	-2.64908100
C	-2.70142000	-3.05915100	-3.68067600
C	-3.01829400	-3.31295100	-1.42793400
O	-1.94280500	-2.07365000	-3.05542900

C	-2.28942900	-2.13419900	-1.64281300
O	-1.90481500	-1.20623800	-0.94363700
H	-1.92698300	-4.76153000	-2.63358200
H	-3.72339100	-2.65334400	-3.87974900
H	-3.17091500	-3.69367700	-0.41593700
C	-3.96455200	-5.12301900	-3.14261800
H	-4.91568300	-4.56504000	-3.21537300
H	-4.13794100	-5.94481800	-2.42502900
C	-3.59477300	-5.71363600	-4.52508800
H	-4.49585300	-6.20786800	-4.93362100
H	-1.18468400	-4.06548600	-4.84168200
H	-4.11364700	-4.04602200	-5.79739500
H	-2.84142200	-5.07216500	-6.46555200
H	-2.02631400	-2.78199800	-5.73070400
C	-2.51199300	-6.79370200	-4.42757900
H	-2.81123400	-7.58881000	-3.72549400
H	-2.32854800	-7.26076000	-5.41002800
H	-1.55682000	-6.38255300	-4.06879700

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***syn*-TS_D-I**

C	9.61117800	0.45028400	0.15982900
C	9.11394800	0.79334300	1.57528100
C	7.45396000	-0.83630600	-0.32613100
C	7.02991500	-0.54012000	1.10915900
C	7.59948700	0.81323300	1.52273400
C	5.60340500	-0.32624000	1.53059000
O	6.93476300	1.15651900	2.70723100
C	5.64667200	0.55725900	2.64907300
O	4.82332200	0.88313500	3.48307800
H	9.45268300	0.04830100	2.31480500
H	7.51441500	-1.31095400	1.75313200
H	7.30942600	1.54484400	0.73403300
C	4.23925900	1.14011700	-0.06730100
I	2.84063900	2.40887500	-1.56884600
H	3.69159700	1.24588100	0.86616900
H	5.16260900	1.70467800	-0.15661600
H	4.20604000	0.17579300	-0.56371600
H	4.87303500	-1.13864900	1.55655600
H	7.05610900	-1.80628700	-0.67065700
C	8.99675600	-0.83293900	-0.44622100
H	7.02812200	-0.06775600	-0.99479700
H	9.24850200	-0.82916900	-1.52191000
H	9.51536400	1.76984900	1.89138500
H	9.35793300	1.29782500	-0.50094800
H	10.71182900	0.37025400	0.14726700
C	9.63080900	-2.09484100	0.14803400
H	9.19993300	-3.00249500	-0.30392800
H	10.71835500	-2.11139900	-0.03175000
H	9.47327500	-2.16277600	1.23487700

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***syn*-TS_D-II**

C	9.64028200	-0.17735900	0.36762600
C	9.10658500	0.70763100	1.51760600
C	7.30648800	-0.71734400	-0.52577900
C	6.97694200	-0.51524000	0.95810000

C	7.58881300	0.80363400	1.42385700
C	5.57609200	-0.32385600	1.46194300
O	6.94378300	1.13246900	2.62413000
C	5.65890600	0.52975200	2.59916500
O	4.86430600	0.83376400	3.46885900
H	9.36827100	0.27006700	2.49400600
H	7.49447900	-1.33267400	1.51433200
H	7.32691800	1.57413900	0.66601600
C	4.15382600	1.23039300	0.01572600
I	2.70294300	2.60148700	-1.34787700
H	3.67945100	1.33500600	0.98880600
H	5.09025400	1.75981400	-0.13259000
H	4.03718400	0.28460100	-0.50301400
H	4.84261700	-1.13310600	1.48548300
H	7.24682900	-1.79000700	-0.78090200
C	8.72155600	-0.17830700	-0.86893800
H	6.55832900	-0.20508200	-1.15296900
H	8.61266500	0.87443600	-1.18571500
H	9.55939800	1.71192500	1.48316200
H	10.65262800	0.14627200	0.07258200
H	9.74483700	-1.21960200	0.71615800
C	9.34723000	-0.93880600	-2.03431400
H	10.30911500	-0.49690500	-2.34240900
H	9.53414300	-1.99038800	-1.75692400
H	8.67923200	-0.94081200	-2.91042500

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***anti*-TS_D-I**

C	-3.16472800	-4.59347600	-5.69816000
C	-2.16948400	-3.53482100	-5.18716400
C	-2.66252600	-4.28922500	-2.84268000
C	-2.64970300	-3.11351200	-3.81425300
C	-2.70062000	-3.53806500	-1.54208700
O	-1.93168900	-2.09688300	-3.16771400
C	-2.25222800	-2.21307000	-1.78047700
O	-2.04831600	-1.25620000	-1.05678700
H	-1.68376900	-4.81153500	-2.95026500
H	-3.70523300	-2.77225400	-3.92739200
C	-0.57170200	-4.15246400	-0.44952700
I	1.50960000	-4.86216800	0.62564600
H	-0.18181800	-3.99309300	-1.45101300
H	-1.13777300	-5.05989600	-0.26813500
H	-0.78211200	-3.27003000	0.14956000
H	-3.27280400	-3.81153100	-0.65700400
C	-3.72379900	-5.28562000	-3.29215100
H	-4.71527000	-4.79867200	-3.26745500
H	-3.78014000	-6.15171700	-2.61061100
C	-3.41554600	-5.77433500	-4.72922500
H	-4.31091000	-6.30452500	-5.10091100
H	-1.14593600	-3.93977900	-5.11941800
H	-4.12905000	-4.08693700	-5.87992500
H	-2.83794500	-4.98892600	-6.67515100
H	-2.13592900	-2.68052100	-5.88254600
C	-2.26292000	-6.78334300	-4.76344600
H	-2.46026600	-7.63083200	-4.08805400
H	-2.12357200	-7.18646700	-5.77987000
H	-1.30917100	-6.33236900	-4.45173000

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anti-TS_D-II

C	-2.57645200	-5.12736800	-5.40032700
C	-2.03392100	-3.70370200	-5.12497600
C	-2.71487200	-4.32104600	-2.78755100
C	-2.61820900	-3.19580900	-3.81539500
C	-2.70441600	-3.51849600	-1.52020500
O	-1.90742300	-2.15656100	-3.19713800
C	-2.23203200	-2.21280300	-1.80979700
O	-2.00995300	-1.23347200	-1.12254500
H	-1.78585600	-4.93244500	-2.87612800
H	-3.65413100	-2.83632300	-4.00523800
C	-0.56520600	-4.14105300	-0.45303100
I	1.52174700	-4.86391600	0.60130600
H	-0.19462900	-4.02456600	-1.46767000
H	-1.14895900	-5.02754000	-0.22888700
H	-0.74162600	-3.23441900	0.12029700
H	-3.26898000	-3.74415900	-0.61670500
C	-3.86826800	-5.24418800	-3.18673900
H	-4.82494800	-4.83728600	-2.81627800
H	-3.74255700	-6.23375000	-2.71398700
C	-3.93888200	-5.40406800	-4.73200000
H	-4.64140300	-4.64317900	-5.11660400
H	-0.93599900	-3.72136600	-5.03817200
H	-2.66355900	-5.30101300	-6.48591700
H	-1.85647300	-5.87769500	-5.03136500
H	-2.28114600	-3.01881200	-5.95233000
C	-4.48894000	-6.77038100	-5.13147000
H	-5.46051800	-6.96410500	-4.64895600
H	-4.62976100	-6.85233500	-6.22180700
H	-3.79872600	-7.57304300	-4.82088400

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en_E

C	1.73457700	7.60643100	-1.65668700
C	2.90839300	6.98558300	-1.84750100
C	0.58635500	5.30620300	-1.30083400
C	1.97587300	4.91305300	-0.81327600
C	2.97782200	5.48974300	-1.80715900
C	2.51294200	3.51685200	-0.76162400
O	4.20753000	4.91800100	-1.48683900
C	3.89786800	3.58555000	-0.98766400
O	4.83959600	2.81541200	-0.85946000
H	3.81318500	7.55645300	-2.08715900
H	2.11760000	5.46329700	0.15351600
H	2.66895200	5.11338100	-2.81294000
H	2.09713700	2.71447600	-0.14845400
H	-0.20941300	4.87319400	-0.67146900
C	0.46541100	6.84561800	-1.29840400
H	0.43503400	4.90484400	-2.31896500
H	0.15673100	7.19025500	-0.29150200
H	-0.34930300	7.17287800	-1.97193300
C	1.58745500	9.10164200	-1.73401300
H	2.54651300	9.59384500	-1.95471600
H	0.86385800	9.39494000	-2.51595300
H	1.20234400	9.51249700	-0.78328800

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***syn*-TS_E-I**

C	1.73623900	7.60093600	-1.65224100
C	2.90754500	6.98033400	-1.85690800
C	0.57372000	5.30324400	-1.31818000
C	1.96440900	4.90590600	-0.84346800
C	2.96687000	5.48528900	-1.83377100
C	2.49572300	3.50330700	-0.78378100
O	4.19914500	4.90001300	-1.50826900
C	3.90613400	3.60971600	-0.98589700
O	4.82753500	2.83369900	-0.82237900
H	3.81335300	7.54712400	-2.09782800
H	2.12164800	5.43675100	0.12624400
H	2.67584200	5.12350900	-2.84665100
C	1.87883500	2.04652100	-2.78735700
I	1.24114900	0.54759700	-4.57345700
H	2.75798100	1.53843900	-2.39873600
H	2.05188000	2.95024700	-3.36388900
H	0.97078500	2.00910800	-2.19471600
H	2.15165400	2.78019500	-0.04009200
H	-0.21643500	4.86770100	-0.68544700
C	0.46359900	6.84268400	-1.30147500
H	0.40889000	4.91540700	-2.33837000
H	0.15586100	7.18024200	-0.29265100
H	-0.34728300	7.17863700	-1.97327700
C	1.59464100	9.09685600	-1.71521900
H	2.55534300	9.58827600	-1.92789900
H	0.87490000	9.39705500	-2.49693200
H	1.20712900	9.49726500	-0.76183500

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***anti*-TS_E-I**

C	-2.59760000	-4.78894800	5.39553100
C	-2.20147300	-3.57376000	4.98805200
C	-2.80105000	-4.19716900	2.65329900
C	-2.66934800	-3.06294600	3.66230000
C	-2.84725900	-3.39234100	1.38679500
O	-1.88729400	-2.08403100	3.02906200
C	-2.27798000	-2.11819400	1.65450700
O	-2.02715900	-1.15344000	0.95742400
H	-1.85537800	-4.78733800	2.70735700
H	-3.68876500	-2.63550400	3.80900500
C	-0.85612600	-4.13140100	0.14207700
I	1.08798700	-4.96011700	-1.10703700
H	-0.39033500	-4.06871900	1.12163400
H	-1.50841900	-4.97557800	-0.05380100
H	-1.01583600	-3.20145900	-0.39772600
H	-3.48397000	-3.57734700	0.52332100
C	-3.88769000	-5.13126700	3.16014400
H	-4.83444500	-4.57321400	3.26879900
H	-4.08558900	-5.95528900	2.45565800
C	-3.43981200	-5.70979700	4.52154300
H	-2.84223900	-6.62604600	4.35268100
H	-4.31727400	-6.04611400	5.10383700
H	-1.58676000	-2.93341500	5.62950000
C	-2.21080700	-5.35681700	6.73326800

H	-1.57571200	-4.66188700	7.30175900
H	-3.10220500	-5.58565100	7.34356400
H	-1.65977900	-6.30607700	6.61394100

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en_F

C	-2.01116400	2.00659000	1.55537400
C	-0.93068100	1.01252800	1.96827000
C	-0.43433000	0.34780700	0.68858400
C	0.39855800	1.39965200	2.53362100
O	0.74813500	-0.30574500	1.00733700
C	1.35774300	0.48344600	2.07741100
O	2.51511300	0.21598700	2.36070100
H	-1.57369600	2.73392500	0.84891200
H	-1.45357100	0.23023400	2.57875000
H	-0.20274600	1.18209800	-0.01728300
H	0.54207000	1.92309300	3.48057100
H	-2.38164000	2.58973300	2.41477500
C	-3.18978900	1.24915100	0.90817600
H	-3.79216100	1.92938800	0.28128100
H	-3.87161800	0.90464000	1.70665200
C	-2.82298200	0.01313300	0.09110300
C	-3.82718300	-0.70240600	-0.56920700
C	-1.50370900	-0.47886400	0.03815700
C	-3.54613400	-1.88199700	-1.25851400
H	-4.85689000	-0.33073600	-0.53135900
C	-1.22646700	-1.66863400	-0.63660900
C	-2.24057000	-2.37214900	-1.28424600
H	-4.34944900	-2.42251000	-1.76688900
H	-0.19490800	-2.02760500	-0.63119300
H	-2.01315200	-3.30383000	-1.80978500

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syn-TS_F-I

C	-2.01415400	2.02645400	1.54088000
C	-0.92684700	1.03797200	1.94253400
C	-0.43214800	0.37329900	0.66319800
C	0.40178300	1.42775000	2.52128900
O	0.75962200	-0.27846800	0.99295800
C	1.34220000	0.45300300	2.06941900
O	2.47745200	0.17828600	2.39933300
H	-1.59557400	2.75810100	0.82903400
H	-1.42605200	0.25232100	2.55935800
H	-0.19482700	1.19109600	-0.05458800
C	1.39176300	3.50162500	1.48407500
I	2.35746800	5.57188700	0.64169800
H	2.27388300	3.04694200	1.92702300
H	1.04128400	3.08792900	0.54372700
H	0.64888600	3.93144600	2.14709700
H	0.50601100	1.78307700	3.54910800
H	-2.37969400	2.60494600	2.40420800
C	-3.18973600	1.25711400	0.90340300
H	-3.79365000	1.93117000	0.27301700
H	-3.86850700	0.91733900	1.70589500
C	-2.81978200	0.01679100	0.09449700
C	-3.82599500	-0.71268200	-0.54759300
C	-1.49864100	-0.46569300	0.02561300

C	-3.54221500	-1.89340100	-1.23220100
H	-4.85799300	-0.35016600	-0.49958300
C	-1.21631700	-1.65515100	-0.64678500
C	-2.23289200	-2.37182500	-1.27469000
H	-4.34692600	-2.44443300	-1.72602300
H	-0.18242300	-2.00656800	-0.65902000
H	-2.00391800	-3.30340400	-1.79867100

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anti-TS_F-I

C	-0.22049400	1.10878500	3.42911300
C	0.17234700	2.23986900	2.48528000
C	-0.33241100	1.88638700	4.70829200
O	0.93536600	3.13776500	3.23888900
C	0.36945000	3.11227100	4.55492300
O	0.60949600	4.03735300	5.30386200
H	0.63528800	0.39337600	3.47041500
H	-0.77168400	2.75387000	2.19055400
C	1.39507000	0.92727800	6.13443900
I	3.08448500	-0.13970200	7.58635400
H	2.00246700	0.99113300	5.23602500
H	0.66248500	0.13030600	6.19903500
H	1.24968200	1.83514200	6.71356300
H	-1.09127100	1.74868000	5.47680500
C	-1.36178500	0.35355600	2.76529000
H	-2.20141200	1.04716300	2.58462900
H	-1.75126100	-0.45090100	3.40937100
C	-0.85693200	-0.25331500	1.43653800
H	-0.43276100	-1.25167200	1.64223900
H	-1.70272700	-0.42900300	0.75052600
C	0.22552800	0.53314400	0.69928400
C	0.73064200	0.04156000	-0.50869800
C	0.78635700	1.71325200	1.22516700
C	1.76759300	0.68984900	-1.17834300
H	0.30858200	-0.87794700	-0.92711500
C	1.83393500	2.35392700	0.56415800
C	2.32769400	1.84597700	-0.63590800
H	2.14565100	0.28410800	-2.12036300
H	2.25583300	3.25340200	1.01739900
H	3.15103900	2.35097500	-1.14753900

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eng

C	3.93357400	3.31433400	0.45609900
C	4.27428200	1.97085100	-0.17257200
C	2.47582600	3.14361400	0.61874300
O	3.19978100	1.62631000	-0.98820000
C	2.02490900	2.25420800	-0.36844400
O	0.94039200	1.92515800	-0.81502100
H	4.22745600	4.16051100	-0.20247300
H	4.30790000	1.26257000	0.68097600
H	1.80565900	3.91586000	0.99796100
C	6.12515500	3.48488600	1.30241600
H	6.65426500	3.43908000	2.27881700
C	5.67871000	1.98280700	-0.75601300
H	5.93184200	0.98070100	-1.16363200
C	6.63043200	2.31315900	0.41937400

H	7.56982100	2.65931500	-0.03742900
O	4.78070800	3.44051800	1.63209900
O	6.49925800	4.69045100	0.66941800
C	6.12723200	5.83547400	1.37512300
H	6.50385500	6.70425800	0.81599700
H	5.03311300	5.91977800	1.48298900
H	6.57011000	5.84978400	2.39262700
C	6.92391200	1.09314300	1.29319700
H	7.73730300	1.30895600	2.00378000
H	6.04116800	0.79657600	1.87914400
H	7.23188300	0.23105100	0.68173700
O	5.92880400	2.96235100	-1.73421600
C	5.12459600	2.98487400	-2.87785200
H	5.50331800	2.26899500	-3.63823600
H	4.09040300	2.68312900	-2.64031200
C	5.13209200	4.38057000	-3.45208900
C	5.60752600	5.45499100	-2.69340800
C	4.63908900	4.62330800	-4.73872800
C	5.58327600	6.74755400	-3.21774700
H	5.99213300	5.24995000	-1.69090500
C	4.61412500	5.91504900	-5.26003700
H	4.26405000	3.78773200	-5.33749500
C	5.08834800	6.98485300	-4.49954300
H	5.95410800	7.58020800	-2.61387400
H	4.22115500	6.08828200	-6.26539700
H	5.06918100	7.99960300	-4.90554600

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***syn*-TS_G-I**

C	3.92935000	3.27504600	0.54995600
C	4.27127600	1.96921900	-0.14915800
C	2.47163100	3.06830400	0.76102900
O	3.17377700	1.68258700	-0.97236400
C	2.03014900	2.27513700	-0.34468300
O	0.94156100	2.02881200	-0.81156300
H	4.16212300	4.13932200	-0.10564300
H	4.32256200	1.19748200	0.64197300
C	2.37482900	1.57357000	2.72208100
I	2.39014500	0.18335600	4.76445300
H	1.43799700	2.09307400	2.89480600
H	2.36544600	0.75986000	2.00380900
H	3.30583300	2.09853400	2.90831900
H	1.81480200	3.88185100	1.07549500
C	6.13285700	3.46606700	1.34318900
H	6.67181800	3.39890400	2.31046600
C	5.66268600	2.03562700	-0.75697500
H	5.93004100	1.06373400	-1.22189100
C	6.62361200	2.31995600	0.42343500
H	7.56098300	2.67604500	-0.02913200
O	4.78561700	3.39107800	1.69705400
O	6.45942400	4.68828000	0.73573100
C	6.13639600	5.80858100	1.50716300
H	6.47856500	6.69627700	0.95718700
H	5.05150300	5.88874100	1.68660800
H	6.64316800	5.78275900	2.49276400
C	6.91198800	1.07146800	1.25903200
H	7.74441000	1.25534400	1.95526500

H	6.04178900	0.77125500	1.86180600
H	7.19219900	0.22108800	0.61921700
O	5.85892900	3.07291400	-1.68117900
C	5.14061800	3.02936600	-2.87988700
H	5.59976300	2.30450800	-3.58508700
H	4.10232200	2.69887900	-2.70940000
C	5.14106300	4.40686800	-3.49649100
C	5.58266400	5.51202800	-2.76297300
C	4.67541500	4.59845300	-4.80179900
C	5.55354700	6.78625800	-3.33055200
H	5.94641500	5.34771600	-1.74583900
C	4.64571500	5.87153000	-5.36613600
H	4.32636100	3.73842300	-5.38119900
C	5.08647700	6.97273400	-4.63064200
H	5.89880100	7.64369400	-2.74694300
H	4.27514700	6.00571500	-6.38561800
H	5.06322700	7.97275400	-5.07088400

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***syn*-TS_G-II**

C	3.82904000	3.24712400	0.81562200
C	4.22525900	2.11850300	-0.12155000
C	2.39543600	2.91068300	1.02758700
O	3.10560400	1.88971500	-0.93571500
C	1.95785400	2.29419300	-0.18577700
O	0.86890900	2.06606500	-0.66387900
H	3.98759200	4.22992700	0.32687000
H	4.37943400	1.22651500	0.51470200
C	2.45562400	1.09192000	2.68235900
I	2.60307500	-0.63764200	4.44701800
H	1.49100500	1.50413400	2.95900200
H	2.48342500	0.41726800	1.83253500
H	3.35592700	1.63519000	2.94989700
H	1.70373000	3.60917900	1.50288600
C	6.04529200	3.46085000	1.55786000
H	6.63500500	3.23189700	2.46953900
C	5.56701800	2.41079900	-0.77102600
H	5.88848600	1.55034400	-1.38995100
C	6.57275300	2.58365000	0.39378300
H	7.42988800	3.12912500	-0.02779500
O	4.72510800	3.20385200	1.93593500
O	6.24951800	4.80346100	1.21681700
C	5.89845400	5.70270400	2.22613500
H	6.15486900	6.71148200	1.87367600
H	4.82148300	5.66352000	2.46074800
H	6.45566600	5.50154600	3.16380300
C	7.05370200	1.23633600	0.93686300
H	7.89596900	1.37529400	1.63181200
H	6.25877600	0.71062400	1.48729600
H	7.39499200	0.57948400	0.12275300
O	5.61364400	3.58836100	-1.54371100
C	4.80142400	3.62275000	-2.69548900
H	3.73432000	3.56948000	-2.43319800
H	4.99807500	4.60592900	-3.15027300
C	5.13174800	2.53153300	-3.69257800
C	6.34928900	2.55898900	-4.38285400
C	4.25706000	1.46119200	-3.90311600

C	6.68095500	1.54861700	-5.28222700
H	7.04417800	3.38437700	-4.20347600
C	4.58637400	0.44926000	-4.80628000
H	3.33338600	1.41414500	-3.32023600
C	5.79515400	0.49132600	-5.49909800
H	7.63337300	1.58375600	-5.81755400
H	3.89582700	-0.38359900	-4.95942000
H	6.05240000	-0.30345800	-6.20399200

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***anti*-TS_G-I**

C	-0.10917000	4.63337900	7.08665800
C	-1.61558400	4.79925100	6.96272500
C	0.25649900	5.95110800	7.67974700
O	-1.85208900	6.16561900	6.75778300
C	-0.82566800	6.85061100	7.48773700
O	-0.98371300	8.02910800	7.72921300
H	0.34298200	4.47179900	6.08802000
H	-2.02826400	4.52324900	7.95367600
C	1.51253100	7.01202800	5.89992100
I	2.81981300	8.09171000	4.07447800
H	0.80997000	6.49588200	5.25267400
H	2.33750700	6.43808100	6.30853600
H	1.19715800	7.92910000	6.38991900
H	1.05112600	6.12833300	8.40033000
C	-0.30723800	2.31479400	7.08467700
H	-0.24705600	1.47298400	7.80659400
C	-1.75962800	2.39422600	6.53473000
C	-2.15407000	3.78462200	5.96912700
H	-3.26142200	3.84596800	5.90548100
H	-1.78764700	1.70352100	5.67942900
O	0.11156800	3.42435300	7.82368300
O	0.53537000	2.03884500	6.00279800
O	-1.60679400	3.89528900	4.68114000
C	1.88158800	1.89265200	6.34543800
H	2.02475400	1.09625100	7.10449000
H	2.42401800	1.61367400	5.43201900
H	2.31088800	2.82481500	6.74860600
C	-2.74906700	1.91237100	7.59713000
H	-3.78523900	1.96963400	7.23056000
H	-2.54825500	0.86516200	7.87132900
H	-2.68172600	2.51342300	8.51675900
C	-2.04874100	5.00550800	3.93252000
H	-3.13356300	4.90004000	3.71722400
H	-1.91704400	5.94069400	4.49801300
C	-1.26469500	5.04762000	2.64804700
C	-1.44089800	4.05252300	1.67928400
C	-0.31100300	6.04255400	2.42522400
C	-0.68498500	4.05837100	0.51029800
H	-2.17315300	3.26010300	1.85616600
C	0.45487200	6.04922500	1.25905200
H	-0.14355100	6.82120900	3.17401300
C	0.26669100	5.05882600	0.29801500
H	-0.83190900	3.27497300	-0.23797500
H	1.21150400	6.82579900	1.12671500
H	0.86732800	5.05891500	-0.61520300

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anti-TS_G-II

C	-0.16568500	4.63614300	7.12774300
C	-1.66285600	4.79448900	6.92378100
C	0.16392000	5.95340200	7.74498300
O	-1.88991400	6.16271900	6.70567100
C	-0.90615500	6.85243400	7.49065400
O	-1.08490700	8.02935700	7.72111200
H	0.34120100	4.48127200	6.15400800
H	-2.12445600	4.52294600	7.89390400
C	1.59532200	6.95611700	6.10094500
I	3.16247800	7.92545000	4.41390100
H	0.88866900	6.56138900	5.37777400
H	2.32132800	6.27576400	6.53192100
H	1.35660400	7.88808700	6.60509800
H	0.89669100	6.11959900	8.53077200
C	-0.35397500	2.31639700	7.11359100
H	-0.31905900	1.47433400	7.83653300
C	-1.78094900	2.38752800	6.50239100
C	-2.16092900	3.77315800	5.91673800
H	-3.26371900	3.82659900	5.82479800
H	-1.77073600	1.69595400	5.64742300
O	0.02417800	3.42824900	7.87214900
O	0.54023100	2.04904100	6.07102200
O	-1.57679400	3.86167100	4.63911900
C	1.86902000	1.90662900	6.47851500
H	2.27519500	2.83941000	6.90374600
H	1.97780400	1.10938400	7.24218500
H	2.45680600	1.63083600	5.59252300
C	-2.81270700	1.90204900	7.52193500
H	-2.61664100	0.85754600	7.80962400
H	-2.79087000	2.50747500	8.44098200
H	-3.83123600	1.95082200	7.10835900
C	-1.82752600	5.04349200	3.91017700
H	-1.41593500	5.92439500	4.42504600
H	-1.28422700	4.91312900	2.96246100
C	-3.29922100	5.26417900	3.62930800
C	-4.01443100	6.26755500	4.29039300
C	-3.97572400	4.42543800	2.73575000
C	-5.37712400	6.44143600	4.04370800
H	-3.49471700	6.88558200	5.02736700
C	-5.33618600	4.59556200	2.49035600
H	-3.42221300	3.62827400	2.23146800
C	-6.04005700	5.60962500	3.14285800
H	-5.92462500	7.22869800	4.56764500
H	-5.85125500	3.93708600	1.78603700
H	-7.10741900	5.74680000	2.95112500

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en_H

C	6.49402600	-4.75962800	1.97472900
C	7.11865300	-6.15927400	2.08239200
C	4.82005000	-7.15955300	1.72167100
C	6.28044700	-7.10376400	1.24692400
C	4.40408400	-8.39762600	1.00814100
O	6.71114700	-8.42466900	1.20055200
C	5.54470000	-9.21911700	0.89963300

O	5.72765600	-10.39267800	0.62559400
H	6.60303100	-4.42759500	0.92691300
H	8.16509600	-6.14188300	1.73446800
H	7.12685300	-6.49822800	3.13390700
H	4.80691000	-7.27009500	2.83645000
H	6.23374400	-6.69191500	0.21376800
H	3.41910900	-8.85176700	1.10854800
C	4.98530700	-4.79574300	2.27135200
H	4.53411300	-3.81902600	2.05732400
H	4.85071900	-5.00751600	3.35205200
N	4.26144700	-5.80227700	1.51353800
C	3.21077500	-5.40328600	0.76130700
O	2.92907700	-4.24478800	0.50858000
O	2.44811100	-6.43551600	0.33960100
C	1.63678000	-6.20106500	-0.78477000
H	1.19493300	-5.19374400	-0.73664600
H	0.82761100	-6.94522200	-0.71993400
C	2.39560000	-6.38186700	-2.08183500
C	3.53995500	-7.18608500	-2.12297100
C	1.94084300	-5.76983500	-3.25392400
C	4.21208900	-7.36985800	-3.33144000
H	3.90753100	-7.66043000	-1.19721200
C	2.61147500	-5.96306400	-4.46074300
H	1.05613300	-5.12623000	-3.22062800
C	3.75222400	-6.76548700	-4.50153200
H	5.10628200	-7.99788500	-3.34955500
H	2.24852500	-5.47641500	-5.37009300
H	4.28439200	-6.91426100	-5.44493500
C	7.18807800	-3.74356900	2.87611700
H	8.26431200	-3.68571700	2.65022000
H	6.76011400	-2.73537900	2.75502000
H	7.08623100	-4.02683300	3.93734100

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***syn*-TS_H-I**

C	6.39569600	-4.69730400	2.99961000
C	7.43224000	-5.75242000	2.58583500
C	5.76322800	-6.64822900	0.90705300
C	7.17500400	-6.09239800	1.13541500
C	5.96588400	-7.21822600	-0.46096200
O	8.03611900	-7.03224800	0.56556900
C	7.32854100	-7.64072800	-0.50589000
O	7.94525100	-8.36130100	-1.26282800
H	6.60084500	-3.78437200	2.41276400
H	8.45498100	-5.36730800	2.72926800
H	7.32952800	-6.65989700	3.20705600
H	5.57408000	-7.44935500	1.66439300
H	7.22884700	-5.14868800	0.55211700
C	5.95940400	-5.44589500	-2.26259800
I	5.71187300	-3.76323000	-3.99019400
H	5.86184400	-4.80139900	-1.39530100
H	5.10985600	-6.07152400	-2.51230500
H	6.94728700	-5.83121700	-2.50304600
H	5.22059900	-7.85481100	-0.93661000
C	4.97000500	-5.14398300	2.64408000
H	4.25833800	-4.32906400	2.82308800
H	4.69315600	-5.98522900	3.31415700

N	4.81652800	-5.57514400	1.26181900
C	3.68338900	-5.19566700	0.61247900
O	2.92490800	-4.32352900	0.99248200
O	3.47307000	-5.89803500	-0.51253700
C	2.53006800	-5.37151200	-1.43032400
H	2.96361900	-4.49492300	-1.94012400
H	1.63443700	-5.03660300	-0.88417900
C	2.19508400	-6.44994300	-2.42564600
C	1.62046100	-7.65061700	-1.99142500
C	2.46315000	-6.27965100	-3.78535500
C	1.31065100	-8.65719400	-2.90075200
H	1.43055600	-7.79656300	-0.92507000
C	2.14988300	-7.28724500	-4.69930600
H	2.94813300	-5.36112900	-4.12870200
C	1.57216600	-8.47589200	-4.26062600
H	0.86851200	-9.59228600	-2.54818900
H	2.37639400	-7.14329700	-5.75820800
H	1.33502700	-9.26828300	-4.97483600
C	6.48599500	-4.34677900	4.48130300
H	7.49503600	-3.99152500	4.74123900
H	5.76677300	-3.55840800	4.75441500
H	6.27198200	-5.22910400	5.10734800

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***syn*-TS_H-II**

C	2.76706200	-4.76823600	-0.49956500
C	2.99645900	-4.82824900	-2.01683100
C	5.36264000	-5.58248100	-1.55825900
C	4.03968000	-5.89308800	-2.26655500
C	6.24080300	-6.54868300	-2.28151700
O	4.38282000	-6.12099800	-3.59995300
C	5.70347100	-6.65142000	-3.59778600
O	6.14073700	-7.10635100	-4.63467900
H	2.32516400	-5.73339700	-0.19452400
H	2.05455400	-5.05969200	-2.54019700
H	3.35534100	-3.85412000	-2.39367600
H	5.64020800	-4.52078400	-1.77801600
H	3.66874100	-6.83868500	-1.81712000
C	5.98946900	-8.93355000	-1.57059300
I	5.94958800	-11.25444200	-0.82854300
H	6.33754100	-9.08441600	-2.58950500
H	4.93474700	-8.71057300	-1.43719200
H	6.67795500	-8.52458900	-0.83724900
H	7.32315500	-6.54914400	-2.16316800
C	4.08858800	-4.62355200	0.27213400
H	3.89721100	-4.70893600	1.34622800
H	4.48985700	-3.60538700	0.08486700
N	5.10071900	-5.60323300	-0.10905000
C	5.95965400	-6.13798200	0.79374200
O	6.97400200	-6.75604500	0.55581700
O	5.54515300	-5.90320200	2.07216700
C	6.25126600	-6.56852400	3.10863800
H	6.26976100	-5.87060100	3.95800200
H	7.28025500	-6.76023900	2.77307500
C	5.57018700	-7.85695300	3.50257500
C	5.59106300	-8.95954900	2.63863600
C	4.88668000	-7.96231700	4.71721700

C	4.93390900	-10.13844700	2.98112400
H	6.12407200	-8.89717300	1.68647700
C	4.23650700	-9.14568000	5.06830500
H	4.86023100	-7.10496500	5.39662900
C	4.25707200	-10.23442000	4.19797300
H	4.95958100	-10.97595000	2.27951700
H	3.70694500	-9.21393700	6.02211700
H	3.74326100	-11.16080600	4.46668500
C	1.80469900	-3.65297500	-0.10330800
H	0.83857000	-3.76653300	-0.61843600
H	1.61261300	-3.64982000	0.98148400
H	2.21339400	-2.66566400	-0.37602600

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***anti*-TS_{H-I}**

C	-7.04015300	-3.60177500	-8.51146300
C	-6.41318600	-2.21994800	-8.27147300
C	-4.15407600	-3.34360600	-8.12449600
C	-5.00860600	-2.28259700	-8.82184200
C	-2.80085400	-2.89055100	-8.59061500
O	-4.25532200	-1.10704900	-8.74977200
C	-2.89425800	-1.51360300	-8.91702700
O	-2.07584100	-0.67603200	-9.23888800
H	-7.11478500	-3.74351300	-9.60443600
H	-7.00480800	-1.43451100	-8.76915900
H	-6.38920300	-1.98616800	-7.19249100
H	-4.26943600	-3.20419400	-7.01844800
H	-5.07761500	-2.60531400	-9.88344300
C	-1.57839300	-2.73673700	-6.45698100
I	-0.40985600	-2.87210900	-4.33028700
H	-2.39179700	-2.07450100	-6.17134700
H	-1.80371500	-3.79102100	-6.57005900
H	-0.78803600	-2.31075200	-7.06913900
H	-1.98140900	-3.51927700	-8.91522500
C	-6.14927800	-4.72841800	-7.97030400
H	-6.18284200	-4.69031400	-6.86050700
H	-6.54493500	-5.70567200	-8.27229100
N	-4.75477200	-4.65654600	-8.40068100
C	-4.08557500	-5.84311600	-8.42077400
O	-4.60838000	-6.94020500	-8.46456500
O	-2.75107200	-5.68830400	-8.37620300
C	-1.97426800	-6.87331500	-8.41871200
H	-2.16332100	-7.41333900	-9.35984600
H	-2.27906900	-7.53980300	-7.59568800
C	-0.52728900	-6.47753300	-8.29753900
C	0.34720500	-6.61072500	-9.37835500
C	-0.04759300	-5.92627500	-7.10418100
C	1.67724600	-6.20369600	-9.27061100
H	-0.02121500	-7.02660800	-10.32018300
C	1.27360300	-5.50228500	-6.99690000
H	-0.71672000	-5.80395500	-6.24818100
C	2.14037300	-5.64411500	-8.08148900
H	2.34891000	-6.30912100	-10.12606500
H	1.61100300	-5.04172300	-6.06568200
H	3.17661500	-5.30724800	-8.00089700
C	-8.44077900	-3.71427400	-7.91722800
H	-9.10445400	-2.93691600	-8.32618600

H	-8.89367800	-4.69560500	-8.13070700
H	-8.41415100	-3.58734700	-6.82227000
H	3.17261800	-5.30157900	-7.99905900

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***anti*-TS_H-II**

C	-1.55947800	-3.68161400	1.36940500
C	-0.76990000	-2.55254100	0.68520300
C	-2.08066600	-3.01490600	-1.41083100
C	-1.66894200	-1.96223200	-0.37666200
C	-2.51691500	-2.12009100	-2.52769500
O	-1.15366900	-0.89689200	-1.11800000
C	-1.93044500	-0.84346000	-2.31713100
O	-1.91725700	0.18002000	-2.96894500
H	-2.40395400	-3.21271800	1.90551000
H	-0.46591300	-1.79524200	1.42597100
H	0.14953700	-2.94891600	0.21967700
H	-1.17011100	-3.59882800	-1.69588800
H	-2.61159700	-1.63933400	0.11666800
C	-0.97884300	-2.71355000	-4.30693500
I	0.55745200	-3.43497800	-6.10545600
H	-0.23209200	-2.64427800	-3.52145700
H	-1.61830500	-3.58944100	-4.33391100
H	-1.32085700	-1.78830100	-4.76243000
H	-3.37438300	-2.28267300	-3.17004300
C	-2.17406900	-4.66088800	0.35189500
H	-1.35339800	-5.24844800	-0.10695000
H	-2.83358500	-5.36313700	0.87079700
N	-2.91919800	-4.00085400	-0.71488800
C	-4.12884400	-4.42043100	-1.14763600
O	-4.73043600	-4.03557000	-2.12652800
O	-4.64618400	-5.37998700	-0.32093000
C	-5.93841000	-5.86526400	-0.63994200
H	-5.94668700	-6.92053300	-0.33199600
H	-6.08881000	-5.80422300	-1.72727800
C	-7.02657400	-5.10549900	0.08279900
C	-7.72034100	-5.68980500	1.14570600
C	-7.34590800	-3.79410200	-0.29530400
C	-8.71769100	-4.98608500	1.82147800
H	-7.47531500	-6.71129500	1.45097900
C	-8.33652200	-3.08824300	0.38283100
H	-6.79956400	-3.33759000	-1.12435800
C	-9.02638200	-3.68165900	1.44143400
H	-9.25141500	-5.45770500	2.65026700
H	-8.57281400	-2.06540900	0.08040200
H	-9.80416500	-3.12536800	1.97026500
C	-0.71215000	-4.44521700	2.38235000
H	-0.29890500	-3.76385100	3.14168100
H	-1.30022000	-5.21762100	2.90337200
H	0.13647100	-4.94509200	1.88672000

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