

Computational design of faster rotating second-generation light-driven molecular motors by control of steric effects

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Electronic Supplementary Information

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Supplementary computational methods

Detailed modeling of the full $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerization paths of the light-absorbing *anti*-(*M*)-stable-*E* and *anti*-(*M*)-stable-*Z* isomers of the motors of this work would require quantum chemical calculations with multi-reference methods. This holds true in particular for the description of the non-radiative decay from the excited state to the ground state that precedes the formation of the (*P*)-unstable-*Z* and (*P*)-unstable-*E* photoproducts, and is expected to occur through conical intersections at highly twisted molecular geometries where the two states are degenerate.¹⁻³ Although such calculations are beyond the scope of this work, we believe that a model of the photoisomerizations that – despite providing no information about the non-radiative decay – is of qualitative value can be obtained from TD-DFT calculations with a range-separated hybrid functional like ω B97X-D. This notion is supported by benchmark data on the performance of TD-DFT for the description of photoisomerizations around carbon-carbon double bonds in conjugated molecules.^{4,5}

Starting from the ground-state structures of *anti*-(*M*)-stable-*E* and *anti*-(*M*)-stable-*Z*, the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerization paths for motors **1** and **7** shown in Figs. S1 and S2 were computed at the ω B97X-D/SVP level of theory in three separate steps. First, TD-DFT singlepoint calculations were performed to locate the vertically excited FC point on the respective path. Second, TD-DFT geometry optimizations were performed to model the subsequent relaxation from the FC points to the *anti*-(*M*)-stable-*E** and *anti*-(*M*)-stable-*Z** minima. Third, starting from *anti*-(*M*)-stable-*E** and *anti*-(*M*)-stable-*Z**, additional points along the photoisomerization paths were located by carrying out a series

of constrained TD-DFT optimizations. For each constrained optimization, all geometric degrees of freedom except the α dihedral angle were allowed to relax. As a compromise between computational cost and structural detail, α was varied over the full range of possible values (180° to -180°) in steps of 10° . All TD-DFT optimizations were carried out in the gas phase within the TDA, and were followed by SMD/TD-DFT singlepoint calculations on the resulting geometries. In this regard, it has been noted that the TDA may actually improve the TD-DFT description of photoisomerization paths of organic molecules, especially with respect to the treatment of near-degeneracy effects.^{6,7}

Finally, structures of the (*P*)-unstable-*Z* and (*P*)-unstable-*E* photoproducts were obtained by starting ground-state SMD/ ω B97X-D/SVP geometry optimizations at different points along the photoisomerization paths. Notably, these optimizations were found to produce (irrespective of starting point) *syn*-folded isomers of the photoproducts. This is an indication that the stator-rotator folding changes from *anti* to *syn* during the photochemical steps of these motors, as a consequence of a ring flip of the stator relative to the olefinic plane.

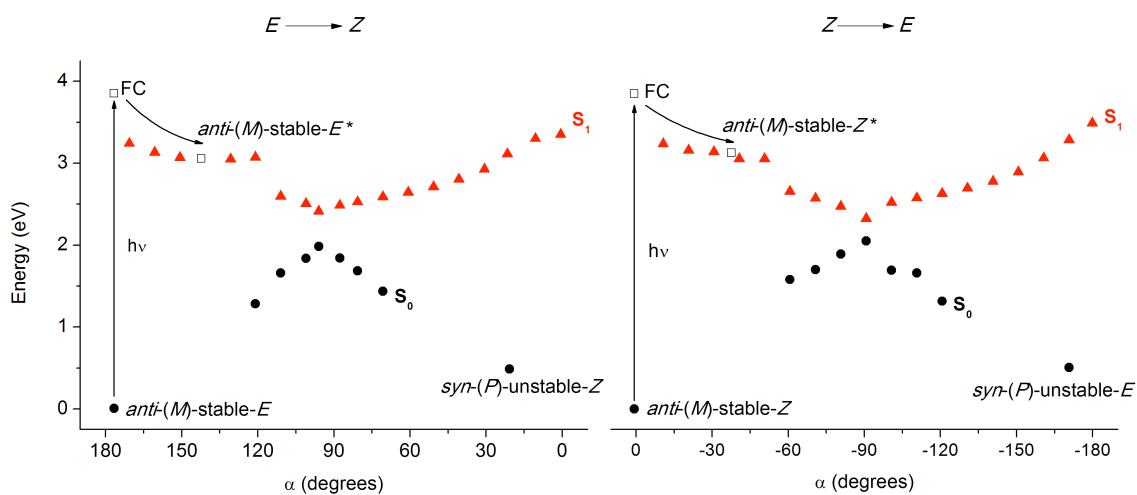


Fig. S1 Photoisomerization paths for the *anti*-(*M*)-stable-*E* and *anti*-(*M*)-stable-*Z* isomers of motor 1 obtained as described in the Supplementary computational methods section (the direction of photoisomerization is indicated by curved arrows). For a few points along the paths, shown also are the corresponding ground-state energies.

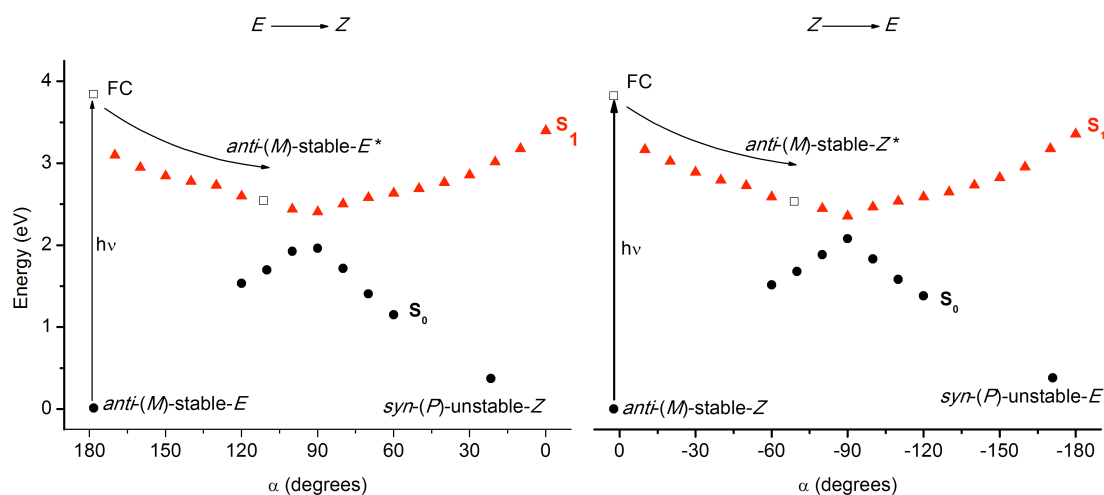


Fig. S2 Photoisomerization paths for the *anti-(M)*-stable-*E* and *anti-(M)*-stable-*Z* isomers of motor 7 obtained as described in the Supplementary computational methods section (the direction of photoisomerization is indicated by curved arrows). For a few points along the paths, shown also are the corresponding ground-state energies.

Table S1 Relative free energies (in kJ mol⁻¹) of *syn*- and *anti*-folded isomers of motor **1** calculated at different levels of theory^a

Functional	Basis set	<i>(M)</i> -stable- <i>E</i>		<i>(P)</i> -unstable- <i>Z</i>		<i>(M)</i> -stable- <i>Z</i>		<i>(P)</i> -unstable- <i>E</i>	
		<i>syn</i>	<i>anti</i>	<i>syn</i>	<i>anti</i>	<i>syn</i>	<i>anti</i>	<i>syn</i>	<i>anti</i>
B3LYP	SVP	27.1	0.0	41.0	35.9	27.8	2.9	41.1	35.0
PBE0	SVP	29.3	0.0	43.3	34.2	29.4	3.0	43.3	33.9
M06-2X	SVP	36.3	0.0	47.5	31.1	32.0	1.3	50.5	31.3
CAM-B3LYP	SVP	29.0	0.0	47.0	33.9	26.5	2.7	47.2	33.4
ωB97X-D	SVP	34.5	3.1	49.6	31.2	30.9	0.0	50.1	32.5
ωB97X-D	6-31++G(d,p)	31.9	0.0	47.2	29.7	30.3	0.9	48.8	30.6
ωB97X-D	cc-pVTZ	32.6	0.0	48.2	31.7	32.1	2.9	49.9	30.6

^a All energies given relative to the most stable isomer at the corresponding level of theory and obtained using an SMD description of the dichloromethane solvent.

Table S2 Geometric parameters (in Å and degrees) of all stationary points involved in the thermal steps of motor **1** calculated at the SMD/ωB97X-D/SVP level of theory

Stationary point	C9–C1'	α	β	γ	δ	δ'
<i>syn</i> -(<i>P</i>)-unstable- <i>Z</i>	1.363	20.8	55.1	6.3	−52.4	56.0
TS1	1.384	35.2	31.2	25.6	10.9	9.1
intermediate- <i>Z</i>	1.367	20.7	10.1	72.7	47.6	−45.8
TS2	1.361	13.9	−18.1	92.4	73.5	−66.1
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.355	−2.5	−51.9	115.8	76.4	−68.8
TS2'	1.360	1.3	13.9	59.1	64.4	−75.3
<i>anti</i> -(<i>P</i>)-unstable- <i>Z</i>	1.355	−5.3	40.9	4.7	57.7	−65.8
TS3	1.380	−20.0	−49.1	118.8	−3.2	−15.4
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.354	0.7	−37.4	101.5	−52.2	55.8
<i>syn</i> -(<i>P</i>)-unstable- <i>E</i>	1.362	−170.7	55.4	5.3	57.5	−55.7
TS4	1.384	−145.9	32.5	24.2	11.8	7.8
intermediate- <i>E</i>	1.367	−159.4	10.4	72.7	−45.9	47.7
TS5	1.360	−156.5	−19.8	93.1	−67.2	75.7
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.355	−165.9	−54.8	117.0	−67.7	74.0
TS5'	1.362	−168.2	14.5	60.2	−72.2	62.5
<i>anti</i> -(<i>P</i>)-unstable- <i>E</i>	1.354	178.8	41.5	3.0	−64.6	57.3
TS6	1.380	162.6	−49.5	119.0	−15.9	−3.0
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.355	176.7	−36.4	99.1	56.0	−52.4

Table S3 Geometric parameters (in Å and degrees) of all stationary points involved in the thermal steps of motor **1** calculated at the SMD/B3LYP/SVP level of theory

Stationary point	C9–Cl'	α	β	γ	δ	δ'
<i>syn</i> -(<i>P</i>)-unstable- <i>Z</i>	1.383	27.5	49.2	12.2	–36.1	44.8
TS1	1.402	39.2	29.5	27.7	12.0	5.8
intermediate- <i>Z</i>	1.382	25.2	10.2	71.9	46.0	–43.5
TS2	1.373	17.3	–15.2	90.3	69.1	–63.0
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.368	–5.5	–57.2	117.6	65.1	–62.1
TS2'	1.373	7.1	14.5	58.4	62.2	–71.8
<i>anti</i> -(<i>P</i>)-unstable- <i>Z</i>	1.364	–2.9	41.7	5.3	57.6	–64.0
TS3	1.395	–22.6	–49.3	118.4	–3.3	–14.3
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.365	–1.0	–36.6	99.4	–52.8	55.2
<i>syn</i> -(<i>P</i>)-unstable- <i>E</i>	1.384	–154.9	48.5	13.1	43.5	–33.7
TS4	1.402	–143.1	30.5	26.3	9.3	8.5
intermediate- <i>E</i>	1.383	–156.1	10.6	71.3	–43.0	45.5
TS5	1.373	–155.0	–18.3	92.3	–63.9	71.5
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.368	–170.1	–56.4	117.0	–62.9	66.5
TS5'	1.374	–166.1	15.2	58.3	–70.1	61.1
<i>anti</i> -(<i>P</i>)-unstable- <i>E</i>	1.364	179.0	41.5	4.3	–63.3	57.3
TS6	1.396	160.4	–48.9	118.1	–14.6	–3.0
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.366	177.4	–36.7	99.3	54.8	–52.0

Table S4 Geometric parameters (in Å and degrees) of all stationary points involved in the thermal steps of motor **1** calculated at the SMD/PBE0/SVP level of theory

Stationary point	C9–C1'	α	β	γ	δ	δ'
<i>syn</i> -(<i>P</i>)-unstable- <i>Z</i>	1.378	26.5	49.7	11.7	–36.9	45.4
TS1	1.396	37.9	29.6	27.7	12.1	6.1
intermediate- <i>Z</i>	1.377	24.1	10.5	72.3	45.7	–43.0
TS2	1.369	16.4	–15.5	91.1	69.7	–63.2
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.364	–5.1	–57.2	118.6	64.7	–61.7
TS2'	1.368	5.1	14.2	59.2	63.1	–73.0
<i>anti</i> -(<i>P</i>)-unstable- <i>Z</i>	1.361	–2.9	41.2	5.3	57.2	–63.9
TS3	1.390	–21.6	–49.2	118.7	–2.5	–15.0
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.361	–0.7	–36.1	99.9	–52.5	55.0
<i>syn</i> -(<i>P</i>)-unstable- <i>E</i>	1.377	–159.3	51.1	10.8	46.9	–39.1
TS4	1.396	–144.5	31.1	25.5	10.3	7.7
intermediate- <i>E</i>	1.378	–157.1	10.9	71.6	–42.7	45.4
TS5	1.368	–155.8	–19.0	93.2	–64.4	72.5
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.364	–170.3	–56.3	117.7	–62.1	65.3
TS5'	1.369	–167.0	15.0	59.0	–70.8	61.5
<i>anti</i> -(<i>P</i>)-unstable- <i>E</i>	1.361	178.9	40.8	4.3	–63.1	56.8
TS6	1.390	161.5	–49.3	118.7	–15.7	–1.9
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.362	177.6	–36.3	100.0	54.8	–51.8

Table S5 Geometric parameters (in Å and degrees) of all stationary points involved in the thermal steps of motor **1** calculated at the SMD/M06-2X/SVP level of theory

Stationary point	C9–C1'	α	β	γ	δ	δ'
<i>syn</i> -(<i>P</i>)-unstable- <i>Z</i>	1.365	22.7	54.3	8.5	−48.5	52.7
TS1	1.384	34.5	31.4	25.6	11.7	8.2
intermediate- <i>Z</i>	1.369	22.3	14.6	69.2	44.3	−41.0
TS2	1.362	14.4	−19.5	93.6	74.0	−65.0
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.356	−3.3	−52.9	116.9	74.3	−67.0
TS2'	1.361	1.6	13.8	60.8	63.6	−74.7
<i>anti</i> -(<i>P</i>)-unstable- <i>Z</i>	1.356	−4.2	40.3	5.6	56.5	−64.8
TS3	1.381	−19.5	−48.6	119.0	−3.1	−15.3
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.355	−0.4	−36.4	100.8	−51.6	55.3
<i>syn</i> -(<i>P</i>)-unstable- <i>E</i>	1.366	−165.1	54.6	8.8	52.3	−47.1
TS4	1.384	−146.7	32.8	23.7	12.6	7.0
intermediate- <i>E</i>	1.369	−159.3	13.8	69.7	−42.3	44.9
TS5	1.362	−156.6	−20.5	94.1	−65.6	75.4
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.356	−166.3	−55.0	117.8	−66.9	73.3
TS5'	1.368	−160.8	20.5	51.5	−57.2	51.5
<i>anti</i> -(<i>P</i>)-unstable- <i>E</i>	1.355	179.8	41.1	3.7	−63.3	55.8
TS6	1.381	162.3	−49.4	119.6	−16.8	−1.9
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.356	176.6	−35.2	98.9	55.6	−51.9

Table S6 Geometric parameters (in Å and degrees) of all stationary points involved in the thermal steps of motor **1** calculated at the SMD/CAM-B3LYP/SVP level of theory

Stationary point	C9–C1'	α	β	γ	δ	δ'
<i>syn</i> -(<i>P</i>)-unstable- <i>Z</i>	1.364	21.6	54.7	6.8	−49.4	53.9
TS1	1.384	36.8	30.9	27.3	12.1	6.8
intermediate- <i>Z</i>	1.367	21.3	7.0	75.5	50.3	−48.3
TS2	1.362	15.9	−14.6	90.2	69.9	−63.6
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.356	−4.0	−56.1	117.1	68.3	−63.9
TS2'	1.361	5.2	14.2	59.3	63.6	−73.2
<i>anti</i> -(<i>P</i>)-unstable- <i>Z</i>	1.354	−3.7	41.9	4.9	58.0	−64.6
TS3	1.380	−20.5	−50.2	118.6	−3.0	−14.7
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.354	0.1	−37.0	100.4	−53.5	55.9
<i>syn</i> -(<i>P</i>)-unstable- <i>E</i>	1.362	−169.8	55.5	5.1	56.8	−54.1
TS4	1.384	−145.4	32.2	25.4	10.1	8.7
intermediate- <i>E</i>	1.368	−158.0	10.2	72.6	−45.2	47.6
TS5	1.361	−156.0	−17.3	91.9	−64.5	72.2
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.355	−167.2	−55.4	116.9	−66.2	71.6
TS5'	1.362	−167.3	14.4	59.3	−71.8	62.7
<i>anti</i> -(<i>P</i>)-unstable- <i>E</i>	1.354	179.0	41.6	3.9	−63.8	57.5
TS6	1.380	162.2	−50.2	118.6	−15.4	−2.2
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.354	178.0	−37.4	100.8	55.6	−52.7

Table S7 Free-energy barriers (in kJ mol⁻¹) of different steps in the thermal isomerizations of motor **1** calculated at different levels of theory^a

Functional	Basis set	TS1	TS2	TS2'	TS3	TS4	TS5	TS5'	TS6
B3LYP	SVP	16.5	13.1	26.4	34.7	15.5	10.0	26.9	38.3
PBE0	SVP	14.4	14.3	27.2	32.8	14.3	11.3	27.8	34.6
M06-2X	SVP	17.4	20.2	28.3	38.8	18.0	18.4	30.0	36.1
CAM-B3LYP	SVP	20.8	10.1	21.7	44.0	20.7	8.5	26.1	41.6
ωB97X-D	SVP	24.1	14.3	25.8	42.8	21.7	10.9	22.4	40.2
ωB97X-D	6-31++G(d,p)	24.8	12.2	25.2	46.3	24.7	8.6	21.4	42.7
ωB97X-D	cc-pVTZ	26.4	10.6	24.0	44.4	24.0	8.9	19.8	44.0

^a All calculations performed using an SMD description of the dichloromethane solvent.

Table S8 Free-energy barriers (in kJ mol⁻¹) of different steps in the thermal isomerizations of motors **1–9**^a

Motor	TS1	TS2	TS3	TS4	TS5	TS6
1	24.1	14.3	42.8	21.7	10.9	40.2
2	20.6	25.5	43.0	17.0	13.5	37.3
3	22.4	15.2	44.3	20.8	13.6	43.6
4	22.5	12.9	45.0	20.8	13.0	44.8
5	21.8	12.9	43.7	21.7	14.0	43.3
6	7.2	9.1	71.3	9.4	5.3	75.3
7	17.6	18.7	26.4	18.3	20.2	27.7
8	20.7	21.3	23.7	22.7	21.8	26.7
9	24.4	21.6	25.9	19.3	24.0	24.8

^a All calculations performed at the ωB97X-D/SVP level of theory using an SMD description of the dichloromethane solvent.

Table S9 Net free-energy changes (in kJ mol⁻¹) during the thermal isomerizations of motors **1–9**^a

Motor	<i>syn</i> -(<i>P</i>)-unstable- <i>Z</i> → <i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	<i>syn</i> -(<i>P</i>)-unstable- <i>E</i> → <i>anti</i> -(<i>M</i>)-stable- <i>E</i>
1	-49.6	-47.0
2	-47.8	-46.5
3	-46.9	-48.0
4	-47.2	-48.4
5	-48.2	-48.1
6	-93.3	-89.0
7	-34.6	-32.0
8	-40.4	-37.7
9	-28.2	-32.3

^a All calculations performed at the ωB97X-D/SVP level of theory using an SMD description of the dichloromethane solvent.

Table S10 Geometric changes (in Å and degrees) during the FC relaxation of motors **1–9**^a

Motor	Isomer	C9–C1'	α
1	<i>anti-(M)</i> -stable- <i>E</i>	1.353 → 1.432	176.8 → 146.5
	<i>anti-(M)</i> -stable- <i>Z</i>	1.353 → 1.433	0.9 → -27.4
2	<i>anti-(M)</i> -stable- <i>E</i>	1.353 → 1.433	177.3 → 145.6
	<i>anti-(M)</i> -stable- <i>Z</i>	1.353 → 1.434	-1.2 → -38.7
3	<i>anti-(M)</i> -stable- <i>E</i>	1.354 → 1.433	176.6 → 144.7
	<i>anti-(M)</i> -stable- <i>Z</i>	1.354 → 1.433	1.7 → -28.4
4	<i>anti-(M)</i> -stable- <i>E</i>	1.353 → 1.431	176.7 → 145.4
	<i>anti-(M)</i> -stable- <i>Z</i>	1.353 → 1.428	-1.4 → -23.7
5	<i>anti-(M)</i> -stable- <i>E</i>	1.354 → 1.432	176.8 → 146.2
	<i>anti-(M)</i> -stable- <i>Z</i>	1.353 → 1.433	0.5 → -34.5
6	<i>anti-(M)</i> -stable- <i>E</i>	1.354 → 1.427	179.9 → 163.6
	<i>anti-(M)</i> -stable- <i>Z</i>	1.352 → 1.422	5.2 → -11.1
7	<i>anti-(M)</i> -stable- <i>E</i>	1.352 → 1.439	178.4 → 110.9
	<i>anti-(M)</i> -stable- <i>Z</i>	1.352 → 1.439	2.2 → -68.8
8	<i>anti-(M)</i> -stable- <i>E</i>	1.353 → 1.432	177.2 → 143.6
	<i>anti-(M)</i> -stable- <i>Z</i>	1.353 → 1.432	1.3 → -29.6
9	<i>anti-(M)</i> -stable- <i>E</i>	1.352 → 1.434	179.0 → 107.7
	<i>anti-(M)</i> -stable- <i>Z</i>	1.352 → 1.436	2.2 → -68.2

^a All calculations performed using ω B97X-D/SVP in the gas phase and employing the TDA to TD-DFT.

Table S11 Rotator–stator interatomic distances (r_{XY} , in Å) in intermediate-*Z*, TS2, intermediate-*E* and TS5 of motors **1** and **6–9** between every atom of the rotator substituent within the nominal van der Waals distance of any atom of the stator^a

Motor	r_{XY}				s_{XY}^b			
	Intermediate- <i>Z</i>	TS2	Intermediate- <i>E</i>	TS5	Intermediate- <i>Z</i>	TS2	Intermediate- <i>E</i>	TS5
1	H _{10'} –H ₈ = 1.92	H _{10'} –H ₈ = 2.09	H _{10'} –H ₁ = 1.94	H _{10'} –H ₁ = 2.08	0.28	0.11	0.26	0.12
	H _{10'} –C ₈ = 2.78	–	H _{10'} –C ₁ = 2.78	–	0.19	0.00	0.19	0.00
	H _{10'} –C ₉ = 2.89	–	H _{10'} –C ₉ = 2.89	–	0.01	0.00	0.01	0.00
	C _{10'} –H ₈ = 2.46	–	C _{10'} –H ₁ = 2.47	–	0.24	0.00	0.23	0.00
	C _{10'} –C ₈ = 3.33	–	C _{10'} –C ₁ = 3.33	–	0.14	0.00	0.14	0.00
	C _{10'} –C ₉ = 3.17	C _{10'} –C ₉ = 3.33	C _{10'} –C ₉ = 3.17	C _{10'} –C ₉ = 3.33	0.23	0.07	0.23	0.07
6^c	H _{11'a} –H ₈ = 1.88	H _{11'a} –H ₈ = 1.87	H _{11'a} –H ₁ = 1.90	H _{11'a} –H ₁ = 1.85	0.32	0.33	0.30	0.35
	H _{11'a} –C ₈ = 2.73	H _{11'a} –C ₈ = 2.68	H _{11'a} –C ₁ = 2.67	H _{11'a} –C ₁ = 2.61	0.24	0.29	0.30	0.36
	H _{11'b} –C ₉ = 2.54	–	H _{11'b} –C ₉ = 2.55	–	0.36	0.00	0.35	0.00
	H _{11'b} –C ₁ = 2.90	–	H _{11'b} –C ₉ = 2.87	–	0.07	0.00	0.10	0.00
	C _{11'} –H ₈ = 2.52	–	C _{11'} –H ₁ = 2.56	C _{11'} –H ₁ = 2.67	0.18	0.00	0.14	0.03
	C _{10'} –C ₈ = 3.36	–	C _{10'} –C ₁ = 3.36	–	0.04	0.00	0.04	0.00
	C _{11'} –C ₈ = 3.29	–	C _{11'} –C ₁ = 3.28	–	0.18	0.00	0.19	0.00
	C _{11'} –C ₉ = 3.23	C _{11'} –C ₉ = 3.23	C _{11'} –C ₉ = 3.21	C _{11'} –C ₉ = 3.22	0.17	0.17	0.19	0.18
	O _{10'} –H ₈ = 2.11	O _{10'} –H ₁ = 2.51	O _{10'} –H ₈ = 2.09	O _{10'} –H ₁ = 2.50	0.41	0.01	0.43	0.02
	O _{10'} –C ₈ = 2.99	O _{10'} –C ₁ = 3.11	O _{10'} –C ₁ = 2.96	O _{10'} –C ₁ = 3.14	0.30	0.18	0.33	0.15
7	O _{10'} –C ₉ = 2.98	O _{10'} –C ₉ = 3.12	O _{10'} –C ₉ = 2.98	O _{10'} –C ₉ = 3.13	0.24	0.10	0.24	0.09
8	N _{10'} –H ₈ = 2.11	N _{10'} –H ₈ = 2.49	N _{10'} –H ₁ = 2.10	N _{10'} –H ₁ = 2.52	0.44	0.06	0.45	0.03
	N _{10'} –C ₈ = 3.03	N _{10'} –C ₈ = 3.22	N _{10'} –C ₁ = 3.01	N _{10'} –C ₁ = 3.22	0.29	0.10	0.31	0.10
	N _{10'} –C ₉ = 3.05	N _{10'} –C ₉ = 3.20	N _{10'} –C ₉ = 3.04	N _{10'} –C ₉ = 3.21	0.20	0.05	0.21	0.04
9	O _{10'} –H ₈ = 2.10	O _{10'} –H ₈ = 2.48	O _{10'} –H ₁ = 2.08	–	0.42	0.04	0.44	0.00
	O _{10'} –C ₈ = 2.99	O _{10'} –C ₈ = 3.16	O _{10'} –C ₁ = 2.96	O _{10'} –C ₁ = 3.17	0.30	0.13	0.33	0.12
	O _{10'} –C ₉ = 2.97	O _{10'} –C ₉ = 3.13	O _{10'} –C ₉ = 2.96	O _{10'} –C ₉ = 3.15	0.25	0.09	0.26	0.07

^a The nominal van der Waals distances, taken from ref 8, are: H_{aliphatic}–H_{aromatic} = 2.20 Å, C_{aliphatic}–H_{aromatic} = 2.70 Å, C_{aromatic}–H_{aliphatic} = 2.97 Å, C_{aliphatic}–H_{aliphatic} = 2.90 Å, C_{aliphatic}–C_{aliphatic} = 3.40 Å, C_{aliphatic}–C_{aromatic} = 3.47 Å, O–H = 2.52 Å, N–H = 2.55 Å, O–C_{aliphatic} = 3.22 Å, O–C_{aromatic} = 3.29 Å, N–C_{aliphatic} = 3.25 Å and N–C_{aromatic} = 3.32 Å. ^b The magnitude (in Å) by which the distance is shorter than the corresponding van der Waals distance. ^c For motor **6**, C_{11'}, H_{11'a}, H_{11'b}, C_{12'} and H_{12'} denote the atoms of the methyl groups of the *tert*-butyl substituent.

Table S12 Free-energy barriers ($\Delta G^\ddagger$, in kJ mol⁻¹) and ΔS_{XY} values (in Å) for TS2 and TS5 during the thermal isomerizations of motors **1** and **6–9**

Motor	$\Delta G^\ddagger$		$S_{XY} = \Sigma S_{XY}$				ΔS_{XY}^a	
	TS2	TS5	Intermediate-Z	TS2	Intermediate-E	TS5	TS2	TS5
1	14.3	10.9	1.09	0.18	1.06	0.19	-0.91	-0.87
6	9.1	5.3	1.56	0.79	1.61	0.92	-0.77	-0.69
7	18.7	20.2	0.95	0.29	1.00	0.26	-0.66	-0.74
8	21.3	21.8	0.93	0.21	0.97	0.17	-0.72	-0.80
9	21.6	24.0	0.97	0.26	1.03	0.19	-0.71	-0.84

^a Difference between S_{XY} values for TS2/TS5 and intermediate-Z/intermediate-E.

Table S13 Rotator-stator interatomic distances (r_{XY} , in Å) in *syn-(M)-Stable-Z*, TS3, *syn-(M)-Stable-E* and TS6 of motors **1** and **6–9** between every atom of the rotator substituent within the nominal van der Waals distance of any atom of the stator^a

Motor	r_{XY}				s_{XY}^b			
	<i>syn-(M)-stable-Z</i>	TS3	<i>syn-(M)-stable-E</i>	TS6	<i>syn-(M)-stable-Z</i>	TS3	<i>syn-(M)-stable-E</i>	TS6
1	–	H _{10'} –H ₈ = 1.79	–	H _{10'} –H ₁ = 1.79	0.00	0.41	0.00	0.41
	–	H _{10'} –C ₈ = 2.86	–	H _{10'} –C ₁ = 2.85	0.00	0.11	0.00	0.12
	–	C _{10'} –H ₈ = 2.41	–	C _{10'} –H ₁ = 2.42	0.00	0.29	0.00	0.28
	–	C _{10'} –C ₈ = 3.38	–	C _{10'} –C ₁ = 3.38	0.00	0.09	0.00	0.09
6^c	–	H _{11'} –H ₈ = 1.84	–	H _{11'} –H ₁ = 1.80	0.00	0.36	0.00	0.40
	–	H _{12'} –H ₈ = 1.97	–	H _{12'} –H ₁ = 2.02	0.00	0.23	0.00	0.18
	H _{11'a} –C ₈ = 2.81	H _{11'a} –C ₈ = 2.76	H _{11'a} –C ₈ = 2.77	H _{11'a} –C ₁ = 2.75	0.16	0.21	0.20	0.22
	–	C _{11'} –H ₈ = 2.50	–	C _{11'} –H ₁ = 2.49	0.00	0.20	0.00	0.21
	–	C _{12'} –H ₈ = 2.60	–	C _{12'} –H ₁ = 2.65	0.00	0.10	0.00	0.05
	–	C _{10'} –H ₈ = 2.51	–	C _{10'} –H ₈ = 2.53	0.00	0.19	0.00	0.17
	7	O _{10'} –H ₈ = 2.04	–	O _{10'} –H ₁ = 2.03	0.00	0.48	0.00	0.49
	–	O _{10'} –C ₈ = 3.02	–	O _{10'} –C ₁ = 3.00	0.00	0.27	0.00	0.29
8	–	N _{10'} –H ₈ = 2.09	–	N _{10'} –H ₁ = 2.08	0.00	0.46	0.00	0.47
	–	N _{10'} –C ₈ = 3.08	–	N _{10'} –C ₁ = 3.07	0.00	0.24	0.00	0.25
9	–	O _{10'} –H ₈ = 2.05	–	O _{10'} –H ₁ = 2.05	0.00	0.47	0.00	0.47
	–	O _{10'} –C ₈ = 3.04	–	O _{10'} –C ₁ = 3.03	0.00	0.25	0.00	0.26

^a The nominal van der Waals distances, taken from ref 8, are: H_{aliphatic}–H_{aromatic} = 2.20 Å, C_{aliphatic}–H_{aromatic} = 2.70 Å, C_{aromatic}–H_{aliphatic} = 2.97 Å, C_{aliphatic}–H_{aliphatic} = 2.90 Å, C_{aliphatic}–C_{aliphatic} = 3.40 Å, C_{aliphatic}–C_{aromatic} = 3.47 Å, O–H = 2.52 Å, N–H = 2.55 Å, O–C_{aliphatic} = 3.22 Å, O–C_{aromatic} = 3.29 Å, N–C_{aliphatic} = 3.25 Å and N–C_{aromatic} = 3.32 Å. ^b The magnitude (in Å) by which the distance is shorter than the corresponding van der Waals distance. ^c For motor **6**, C_{11'}, H_{11'a}, H_{11'b}, C_{12'} and H_{12'} denote the atoms of the methyl groups of the *tert*-butyl substituent.

Table S14 Free-energy barriers ($\Delta G^\ddagger$, in kJ mol⁻¹) and ΔS_{XY} values (in Å) for TS3 and TS6 during the thermal isomerizations of motors **1** and **6–9**

Motor	$\Delta G^\ddagger$		$S_{XY} = \Sigma s_{XY}$				ΔS_{XY}^a	
	TS3	TS6	<i>syn-(M)</i> -stable- <i>Z</i>	TS3	<i>syn-(M)</i> -stable- <i>E</i>	TS6	TS3	TS6
1	42.8	40.2	0.00	0.90	0.00	0.90	0.90	0.90
6	71.3	75.3	0.16	1.29	0.20	1.23	1.13	1.03
7	26.4	27.7	0.00	0.75	0.00	0.78	0.75	0.78
8	23.7	26.7	0.00	0.70	0.00	0.72	0.70	0.72
9	25.9	24.8	0.00	0.72	0.00	0.73	0.72	0.73

^a Difference between S_{XY} values for TS3/TS6 and *syn-(M)*-stable-*Z*/*syn-(M)*-stable-*E*.

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Cartesian coordinates of all stationary points of motors 1–9

All geometries optimized at the ω B97X-D/SVP level of theory. Ground-state optimizations performed using an SMD description of the dichloromethane solvent. Excited-state optimizations performed in the gas phase within the TDA to TD-DFT.

motor 1

anti-(M)-stable-E

C	1.541465	2.531651	2.166868
C	0.947025	1.331829	1.785455
C	0.085298	1.278980	0.684165
C	-0.218947	2.473403	0.009164
C	0.375953	3.679288	0.387225
C	1.266403	3.702735	1.459066
C	-0.526495	0.007720	0.214790
S	-1.322823	2.419000	-1.382608
C	-2.470164	1.209564	-0.757785
C	-2.001212	0.127597	0.015720
C	-2.935328	-0.731574	0.592475
H	-2.618223	-1.530394	1.264022
C	-4.754760	0.442687	-0.490828
C	-3.832411	1.350781	-1.010565
H	2.227116	2.552347	3.016715
H	1.169459	0.410501	2.328198
H	0.136570	4.599568	-0.150926
H	1.733341	4.645599	1.752424
H	-5.814368	0.578275	-0.707619
H	-4.190985	2.190320	-1.610971
C	0.176478	-1.116932	-0.060630
C	1.643497	-1.353529	0.025984
C	-0.415316	-2.484281	-0.389826
C	1.842249	-2.683462	0.362746
H	-1.437648	-2.591494	-0.017880
C	0.540460	-3.438768	0.361252
H	0.633842	-4.422382	-0.124273
C	2.768498	-0.512252	-0.251613
C	4.070829	-1.029348	0.032750
C	4.219655	-2.367846	0.498697
C	3.131872	-3.197184	0.621602
C	5.211081	-0.213532	-0.211976
C	5.079494	1.037370	-0.764433
C	3.796819	1.516961	-1.122655
C	2.674616	0.762978	-0.874152
H	0.184569	-3.613548	1.391014
H	5.226272	-2.738872	0.708301
H	3.256940	-4.242463	0.914427
H	6.200025	-0.612357	0.029159
H	5.963347	1.650517	-0.954937
H	3.696867	2.490347	-1.608551
H	1.699585	1.132497	-1.186297
C	-0.426592	-2.732613	-1.900366
H	-1.071898	-2.000294	-2.409010
H	0.583985	-2.649879	-2.331444
H	-0.812616	-3.739269	-2.122959
C	-4.306189	-0.594365	0.335280
O	-5.111171	-1.497296	0.928038
C	-6.499448	-1.424934	0.705432
H	-6.746708	-1.551846	-0.362166
H	-6.951131	-2.248630	1.272130
H	-6.922778	-0.471707	1.065010

*anti-(M)-stable-E**

C	2.227278	1.909886	2.238040
C	1.390814	0.887595	1.827479
C	0.281492	1.119064	0.967237
C	0.049423	2.473700	0.599778
C	0.895061	3.501561	1.015959
C	1.997058	3.223792	1.820057
C	-0.521335	0.021293	0.457926
S	-1.199708	2.877973	-0.556518
C	-2.340093	1.565931	-0.322836
C	-1.920537	0.278378	0.120345
C	-2.924930	-0.703267	0.211081
H	-2.712908	-1.689589	0.609389
C	-4.630390	0.806303	-0.610689
C	-3.664727	1.807155	-0.679781
H	3.073517	1.681607	2.889241
H	1.577617	-0.129210	2.173780
H	0.689404	4.526294	0.697739
H	2.661670	4.031053	2.133617
H	-5.657053	1.030221	-0.898220
H	-3.950648	2.804468	-1.022382
C	0.109846	-1.258280	0.334395
C	1.477424	-1.440601	-0.014605
C	-0.458257	-2.649374	0.617292
C	1.929497	-2.698749	0.466300
H	-1.225637	-2.622408	1.403985
C	0.783412	-3.427622	1.102844
H	0.752368	-4.496810	0.841360
C	2.414063	-0.556256	-0.685052
C	3.801302	-0.922816	-0.661524
C	4.200788	-2.155572	-0.098864
C	3.271580	-3.049944	0.433511
C	4.750333	-0.041195	-1.257059
C	4.348466	1.107487	-1.896053
C	2.975450	1.420672	-1.988777
C	2.033398	0.595288	-1.403171
H	0.869882	-3.365036	2.202498
H	5.262595	-2.415312	-0.110488
H	3.602137	-4.005850	0.847102
H	5.810179	-0.304288	-1.208676
H	5.089650	1.771558	-2.346610
H	2.652176	2.317102	-2.521896
H	0.973939	0.836830	-1.502436
C	-1.031077	-3.305513	-0.651681
H	-1.826664	-2.700379	-1.107038
H	-0.232009	-3.427200	-1.399309
H	-1.443499	-4.299507	-0.418405
C	-4.250421	-0.459115	-0.147557
O	-5.096448	-1.501758	-0.004443
C	-6.451125	-1.328415	-0.317001
H	-6.597550	-1.069081	-1.380124
H	-6.944893	-2.287207	-0.117600
H	-6.920133	-0.549073	0.308745

syn-(*P*)-unstable-*Z*

C	-3.970942	-1.255247	2.333180
C	-2.662451	-1.125360	1.873369
C	-2.371641	-0.368000	0.731144
C	-3.422686	0.311000	0.097057
C	-4.737850	0.181757	0.548176
C	-5.011331	-0.612565	1.660481
C	-0.973371	-0.269595	0.233625
S	-3.050197	1.291174	-1.326080
C	-1.463145	1.917151	-0.821811
C	-0.546286	1.132563	-0.074822
C	0.671861	1.721993	0.255288

H	1.409317	1.196679	0.851416
C	1.012091	3.018194	-0.155832
C	0.110264	3.767892	-0.912802
C	-1.127142	3.206558	-1.225865
H	-4.179928	-1.859113	3.218959
H	-1.844664	-1.632210	2.391457
H	-5.545876	0.709261	0.035546
H	-6.040105	-0.711725	2.014145
H	0.339885	4.780373	-1.244805
H	-1.848436	3.797020	-1.796194
C	-0.274951	-1.402755	-0.058922
C	1.175088	-1.546803	-0.337625
C	-0.875886	-2.729365	-0.558314
C	1.335803	-2.388154	-1.425446
H	-0.614273	-3.526763	0.160080
C	0.004246	-2.954683	-1.823170
H	-0.432782	-2.401337	-2.673468
C	2.311822	-1.154382	0.433080
C	3.606190	-1.431930	-0.106529
C	3.723020	-2.150007	-1.330207
C	2.611904	-2.666474	-1.956673
C	4.759972	-1.046227	0.633931
C	4.642549	-0.480961	1.879884
C	3.360761	-0.291745	2.453818
C	2.227077	-0.617555	1.749150
H	0.063782	-4.014936	-2.111721
H	4.722169	-2.340393	-1.730589
H	2.714120	-3.290948	-2.847471
H	5.745664	-1.231653	0.198950
H	5.535857	-0.200469	2.442660
H	3.274538	0.113689	3.464582
H	1.242376	-0.478339	2.201053
C	-2.354149	-2.828330	-0.905079
H	-3.005934	-2.859633	-0.023512
H	-2.671193	-1.987467	-1.541101
H	-2.521254	-3.758491	-1.470793
O	2.226662	3.452274	0.235512
C	2.633058	4.751173	-0.120814
H	3.631537	4.897060	0.310002
H	2.697681	4.875435	-1.215309
H	1.954117	5.518112	0.289660

TS1

C	1.360478	2.464478	-1.107226
C	0.745613	1.224979	-0.943869
C	-0.516505	1.059031	-0.348473
C	-1.212742	2.250200	-0.047033
C	-0.602147	3.498167	-0.209644
C	0.687280	3.624788	-0.708113
C	-1.098971	-0.307876	-0.189659
S	-2.901432	2.320103	0.436389
C	-3.403394	0.640181	0.402100
C	-2.532428	-0.449598	0.183775
C	-3.068605	-1.719883	0.497765
H	-2.411133	-2.585484	0.495107
C	-4.396205	-1.920483	0.842067
C	-5.263738	-0.829913	0.927272
C	-4.754237	0.443916	0.734273
H	1.300090	0.365415	-1.311265
H	-1.159391	4.403744	0.045605
H	1.129896	4.615036	-0.814178
H	-6.316756	-0.967116	1.181666
H	-5.401880	1.315283	0.864288
C	-0.315260	-1.425531	-0.417464
C	1.122714	-1.580480	-0.120127

C	-0.715698	-2.700522	-1.184534
C	1.669190	-2.565259	-0.927313
H	-0.978999	-3.510219	-0.480353
C	0.625169	-3.118710	-1.844592
H	0.709002	-2.651968	-2.842258
C	1.914419	-0.992529	0.925346
C	3.293771	-1.358767	0.999041
C	3.829143	-2.317405	0.089236
C	3.028371	-2.932961	-0.841191
C	4.115031	-0.777893	2.004523
C	3.595103	0.106812	2.918494
C	2.219585	0.433737	2.875914
C	1.402946	-0.099689	1.905468
H	0.707230	-4.206468	-1.987171
H	4.888694	-2.574353	0.166946
H	3.433285	-3.694077	-1.512442
H	5.171577	-1.056375	2.042291
H	4.236012	0.545403	3.686810
H	1.801338	1.112850	3.622610
H	0.342919	0.153032	1.897662
C	-1.811024	-2.558380	-2.236887
H	-2.811700	-2.411586	-1.812691
H	-1.597834	-1.708729	-2.904298
H	-1.847042	-3.470672	-2.852693
H	-4.749777	-2.930556	1.059045
O	2.586280	2.448777	-1.670050
C	3.244313	3.672221	-1.892930
H	3.442437	4.207147	-0.948424
H	4.203297	3.432311	-2.368928
H	2.668387	4.329721	-2.566466

intermediate-Z

C	-4.918403	1.114668	0.568416
C	-3.543343	1.154844	0.789912
C	-2.650516	0.341749	0.071437
C	-3.224179	-0.573188	-0.843873
C	-4.602781	-0.612024	-1.069881
C	-5.453446	0.242936	-0.376021
C	-1.153131	0.366887	0.167251
S	-2.216795	-1.702493	-1.777308
C	-0.993674	-2.042954	-0.543444
C	-0.560741	-0.989757	0.281100
C	0.397632	-1.251805	1.258144
H	0.729774	-0.457686	1.929793
C	0.982404	-2.519170	1.375571
C	0.572247	-3.550915	0.522560
C	-0.425167	-3.307180	-0.423259
H	-5.572203	1.769631	1.148450
H	-3.171788	1.831550	1.553748
H	-5.010007	-1.330894	-1.785087
H	-6.530007	0.206477	-0.556076
H	1.004921	-4.548942	0.592370
H	-0.759438	-4.121070	-1.071015
C	-0.400515	1.508299	0.161818
C	1.042424	1.723345	-0.145462
C	-0.931160	2.848548	0.680432
C	1.352411	3.061750	0.078649
H	-1.920287	3.089388	0.266359
C	0.122310	3.889006	0.295960
H	0.248009	4.668505	1.062244
C	2.070706	0.878143	-0.706133
C	3.418760	1.360986	-0.687776
C	3.698456	2.694273	-0.271277
C	2.675871	3.552262	0.037937
C	4.471617	0.530673	-1.162349

C	4.210399	-0.694936	-1.724833
C	2.869715	-1.116836	-1.868694
C	1.836617	-0.354084	-1.374391
H	-0.125305	4.402752	-0.648540
H	4.736792	3.035640	-0.264651
H	2.872406	4.601906	0.268905
H	5.496514	0.905804	-1.098908
H	5.025625	-1.320112	-2.096050
H	2.645954	-2.052245	-2.387115
H	0.816974	-0.683338	-1.545253
C	-1.006175	2.781324	2.218039
H	-1.556283	1.903339	2.581943
H	0.008407	2.716563	2.643354
H	-1.485487	3.686044	2.622862
O	1.923088	-2.651208	2.330122
C	2.548841	-3.899639	2.503630
H	3.273323	-3.777862	3.318545
H	1.825048	-4.683235	2.784786
H	3.087999	-4.215884	1.594507

TS2

C	4.509933	-1.691501	1.049363
C	3.169845	-1.368100	1.255600
C	2.407646	-0.776707	0.241788
C	3.056465	-0.439378	-0.964452
C	4.396031	-0.771095	-1.177494
C	5.118735	-1.413632	-0.173850
C	0.945433	-0.438296	0.318307
S	2.154204	0.447674	-2.224329
C	1.295266	1.551005	-1.124042
C	0.798051	1.022435	0.080105
C	0.326038	1.891833	1.061008
H	-0.022338	1.504468	2.020443
C	0.220013	3.266229	0.807155
C	0.625280	3.772932	-0.434792
C	1.185542	2.914504	-1.382268
H	5.080089	-2.164080	1.852228
H	2.705453	-1.588984	2.216753
H	4.878698	-0.507410	-2.121523
H	6.167857	-1.668077	-0.339867
H	0.547603	4.836031	-0.662994
H	1.563172	3.327249	-2.320725
C	-0.005017	-1.407155	0.414238
C	-1.476868	-1.508382	0.084566
C	0.404027	-2.820387	0.845814
C	-1.776096	-2.863941	-0.047476
H	1.439074	-3.041104	0.559959
C	-0.579573	-3.743481	0.134718
H	-0.806876	-4.657810	0.703379
C	-2.543990	-0.561245	-0.159926
C	-3.860837	-1.069723	-0.426157
C	-4.097998	-2.469111	-0.503898
C	-3.067317	-3.352100	-0.339680
C	-4.943610	-0.171871	-0.638699
C	-4.759917	1.188382	-0.621404
C	-3.463655	1.698922	-0.397545
C	-2.402664	0.850531	-0.178660
H	-0.197974	-4.057734	-0.851815
H	-5.112164	-2.820884	-0.709246
H	-3.229453	-4.429475	-0.420661
H	-5.933552	-0.596021	-0.825955
H	-5.599739	1.866295	-0.789387
H	-3.291751	2.778120	-0.400047
H	-1.425704	1.281816	-0.024210
O	-0.292078	4.013885	1.802625

C	-0.431981	5.402193	1.616214
H	-0.866888	5.799724	2.541716
H	0.541221	5.891963	1.442759
H	-1.109879	5.635861	0.777768
C	0.263930	-2.966234	2.368115
H	-0.789579	-2.867571	2.675623
H	0.620465	-3.956012	2.693212
H	0.835340	-2.199977	2.910963

syn-(*M*)-stable-*Z*

C	1.138922	3.040217	-0.199786
C	0.574443	1.871308	-0.729827
C	-0.414010	1.171829	-0.047929
C	-0.936042	1.733462	1.138851
C	-0.383576	2.898162	1.663755
C	0.673443	3.542802	1.019246
C	-1.044679	-0.107757	-0.493664
S	-2.347234	0.985038	1.926629
C	-3.242249	0.521088	0.460158
C	-2.521698	0.026923	-0.641496
C	-3.220278	-0.335580	-1.797058
H	-2.662499	-0.705352	-2.660595
C	-4.611034	-0.246682	-1.841892
C	-5.317744	0.216895	-0.731427
C	-4.635319	0.610160	0.419235
H	0.932721	1.532269	-1.697835
H	-0.790654	3.329009	2.581588
H	1.091005	4.448513	1.459153
H	-6.407143	0.290360	-0.764405
H	-5.183976	0.995635	1.281904
C	-0.485937	-1.339865	-0.423259
C	0.871102	-1.726977	0.049867
C	-1.312167	-2.619410	-0.316693
C	0.706521	-2.755089	0.964463
H	-2.376745	-2.389184	-0.183443
C	-0.722233	-3.231895	0.978238
H	-0.797967	-4.329741	1.011105
C	2.181361	-1.270650	-0.282969
C	3.271119	-1.726994	0.523095
C	3.036590	-2.682519	1.552482
C	1.787325	-3.225086	1.741163
C	4.585279	-1.262721	0.233447
C	4.824162	-0.445764	-0.844962
C	3.759498	-0.081994	-1.705584
C	2.475881	-0.488124	-1.431483
H	-1.252581	-2.834043	1.860097
H	3.882699	-3.016055	2.159027
H	1.626985	-4.006743	2.487865
H	5.408332	-1.590365	0.874086
H	5.838835	-0.103645	-1.061429
H	3.963490	0.512290	-2.599362
H	1.666130	-0.249711	-2.120616
C	-1.156121	-3.541672	-1.525112
H	-1.550237	-3.065513	-2.435661
H	-0.099080	-3.794981	-1.705741
H	-1.708099	-4.480934	-1.367140
H	-5.145427	-0.540071	-2.748187
O	2.112523	3.606181	-0.939278
C	2.711788	4.796423	-0.486290
H	3.219128	4.655636	0.483164
H	3.459078	5.076741	-1.238937
H	1.975467	5.612886	-0.393894

TS2'

C	0.939597	-2.708272	1.139009
C	0.380961	-1.423161	1.208149
C	-0.501751	-0.984872	0.229350
C	-0.893221	-1.866873	-0.798218
C	-0.349093	-3.144187	-0.862378
C	0.576919	-3.567424	0.094615
C	-1.110145	0.372261	0.234508
S	-2.043776	-1.277399	-2.024924
C	-3.151770	-0.464813	-0.890407
C	-2.604370	0.220533	0.213986
C	-3.476127	0.559607	1.256112
H	-3.067004	0.937566	2.191689
C	-4.854701	0.398955	1.123560
C	-5.388196	-0.145997	-0.043828
C	-4.532104	-0.614195	-1.038212
H	0.685962	-0.757029	2.017344
H	-0.646333	-3.829307	-1.659735
H	0.993820	-4.571777	0.019361
H	-6.468047	-0.264358	-0.157307
H	-4.932973	-1.134450	-1.911281
C	-0.441711	1.550010	0.104080
C	1.023734	1.795423	-0.099046
C	-1.115508	2.938905	0.213492
C	1.276308	3.149322	0.070783
H	-1.852180	3.032927	-0.600770
C	0.025466	3.960863	0.037102
H	0.008852	4.740576	0.812759
C	2.140905	0.954674	-0.470444
C	3.463162	1.471858	-0.277744
C	3.654493	2.829705	0.109539
C	2.581968	3.674987	0.201388
C	4.591190	0.658771	-0.575528
C	4.440608	-0.584913	-1.139628
C	3.144250	-1.041070	-1.464122
C	2.034733	-0.293976	-1.139398
H	-0.030843	4.482839	-0.932700
H	4.673467	3.197667	0.254058
H	2.719875	4.741814	0.392754
H	5.587822	1.064243	-0.381873
H	5.314882	-1.194875	-1.378471
H	3.015378	-1.990280	-1.989575
H	1.057737	-0.648680	-1.449757
C	-1.824879	3.247324	1.538904
H	-2.796620	2.758014	1.628347
H	-1.201744	2.959068	2.401071
H	-2.010927	4.329835	1.606831
H	-5.513628	0.692448	1.943773
O	1.815586	-3.023634	2.111352
C	2.435654	-4.287037	2.090148
H	3.013547	-4.441101	1.163277
H	3.124599	-4.312510	2.943655
H	1.701860	-5.103623	2.199893

anti-(P)-unstable-Z

C	1.313008	-2.326742	1.292010
C	0.586255	-1.129163	1.248215
C	-0.412155	-0.938591	0.299655
C	-0.748805	-1.995821	-0.566682
C	-0.038381	-3.190740	-0.517213
C	1.004765	-3.357579	0.395893
C	-1.167619	0.340285	0.164991
S	-2.054733	-1.751199	-1.753049
C	-3.167035	-0.855204	-0.689522
C	-2.636893	0.076330	0.223838
C	-3.492728	0.597534	1.200589

H	-3.079776	1.237968	1.980289
C	-4.856940	0.317146	1.181528
C	-5.385177	-0.521520	0.199404
C	-4.536025	-1.131375	-0.721403
H	0.850663	-0.331159	1.944289
H	-0.295776	-4.009445	-1.193415
H	1.550357	-4.301049	0.409588
H	-6.455503	-0.738375	0.176084
H	-4.929944	-1.848545	-1.445455
C	-0.565277	1.530657	-0.070418
C	0.912203	1.773222	-0.119085
C	-1.135075	2.950745	-0.164733
C	1.158855	3.007928	0.457273
H	-0.921569	3.251657	-1.207287
C	-0.133305	3.730225	0.717105
H	-0.430681	3.657319	1.778740
C	1.991626	1.019847	-0.677564
C	3.322405	1.469096	-0.411993
C	3.533614	2.682764	0.303998
C	2.473608	3.465400	0.693305
C	4.421380	0.716130	-0.914593
C	4.218121	-0.394895	-1.696042
C	2.899845	-0.784557	-2.037354
C	1.819156	-0.094708	-1.544072
H	-0.077622	4.799101	0.461022
H	4.560822	3.004142	0.494875
H	2.639466	4.428225	1.182744
H	5.435516	1.052004	-0.682061
H	5.069722	-0.960934	-2.080578
H	2.740655	-1.634749	-2.704834
H	0.811837	-0.385543	-1.837959
C	-2.586020	3.306643	0.106922
H	-3.282437	2.731769	-0.517639
H	-2.862763	3.168846	1.160407
H	-2.729871	4.372520	-0.130473
H	-5.510387	0.751043	1.941640
O	2.287062	-2.393163	2.219945
C	3.114852	-3.530446	2.261347
H	3.641692	-3.684019	1.304250
H	3.857175	-3.348987	3.048785
H	2.548122	-4.442963	2.513825

TS3

C	-1.226782	2.690884	-0.694484
C	-0.685329	1.408732	-0.612966
C	0.637268	1.137393	-0.226508
C	1.456295	2.282027	-0.067181
C	0.916699	3.571243	-0.130715
C	-0.423386	3.798494	-0.412244
C	1.155530	-0.269846	-0.118413
S	3.209323	2.263072	0.053225
C	3.580569	0.558021	0.176460
C	2.613764	-0.469807	0.159235
C	3.096948	-1.743938	0.526857
H	2.385889	-2.544792	0.684286
C	4.438031	-2.024323	0.740010
C	5.383839	-1.004829	0.630421
C	4.943572	0.284402	0.378891
H	-1.362775	0.609634	-0.886899
H	1.574972	4.430245	0.025738
H	-0.806060	4.818484	-0.443558
H	6.446807	-1.201869	0.784330
H	5.660178	1.110171	0.358904
C	0.342920	-1.365117	-0.328853
C	-1.137907	-1.457595	-0.283070

C	0.737526	-2.683932	-1.021686
C	-1.568704	-2.238978	-1.341465
H	1.733243	-2.609572	-1.479353
C	-0.375498	-2.744433	-2.105663
H	-0.520189	-3.754961	-2.515747
C	-2.062465	-1.002119	0.706465
C	-3.447245	-1.282089	0.499121
C	-3.857102	-2.024369	-0.646793
C	-2.937292	-2.510659	-1.546555
C	-4.394349	-0.816134	1.453368
C	-3.990470	-0.114784	2.563878
C	-2.614503	0.143084	2.778045
C	-1.674681	-0.288008	1.871766
H	-0.131476	-2.069603	-2.943803
H	-4.923117	-2.222234	-0.785996
H	-3.257746	-3.109325	-2.402655
H	-5.453858	-1.027534	1.286524
H	-4.727339	0.239241	3.288508
H	-2.299460	0.687498	3.671346
H	-0.615521	-0.087897	2.043579
C	0.639860	-3.960606	-0.173314
H	1.305181	-3.968544	0.700636
H	-0.384785	-4.104380	0.202705
H	0.896702	-4.835212	-0.790125
H	4.739247	-3.038506	1.010715
O	-2.524948	2.757335	-1.055280
C	-3.127607	4.020884	-1.193167
H	-2.623657	4.633313	-1.960391
H	-4.163293	3.841338	-1.507613
H	-3.139521	4.575068	-0.239149

anti-(M)-stable-Z

C	1.202237	-2.535352	-1.186723
C	0.538753	-1.302064	-1.214083
C	-0.497593	-1.028560	-0.326730
C	-0.931702	-2.037237	0.552655
C	-0.283664	-3.268966	0.573094
C	0.792937	-3.520172	-0.279058
C	-1.171055	0.295857	-0.286472
S	-2.268062	-1.695660	1.673910
C	-3.272254	-0.700474	0.593662
C	-2.659429	0.181042	-0.318038
C	-3.480420	0.855416	-1.232476
H	-3.023902	1.476729	-2.004840
C	-4.867301	0.738096	-1.176756
C	-5.461598	-0.081346	-0.216695
C	-4.663595	-0.818418	0.654574
H	0.878150	-0.539713	-1.917605
H	-0.616447	-4.051348	1.259319
H	1.287587	-4.490536	-0.236108
H	-6.548586	-0.176303	-0.166661
H	-5.119808	-1.505210	1.371556
C	-0.508337	1.471235	-0.170764
C	0.957444	1.709996	-0.076365
C	-1.116262	2.865432	-0.286155
C	1.233018	2.911733	-0.708763
H	-2.074349	2.857010	-0.813617
C	-0.039395	3.611037	-1.108561
H	-0.005590	4.690510	-0.894667
C	2.005006	0.988491	0.578933
C	3.347226	1.434881	0.373853
C	3.595865	2.611971	-0.390480
C	2.559144	3.363238	-0.888448
C	4.416194	0.724684	0.989337
C	4.170360	-0.347239	1.812748

C	2.836363	-0.738911	2.080275
C	1.784266	-0.087871	1.481637
H	-0.228052	3.495076	-2.189540
H	4.631029	2.932801	-0.533231
H	2.752257	4.299276	-1.418221
H	5.440616	1.061183	0.809009
H	4.999346	-0.879935	2.284490
H	2.640320	-1.558162	2.776074
H	0.762783	-0.379308	1.721633
C	-1.331817	3.495117	1.092868
H	-2.025614	2.889155	1.695156
H	-0.384502	3.579558	1.648945
H	-1.759292	4.504582	0.992259
H	-5.485750	1.284249	-1.892425
O	2.216205	-2.680854	-2.061146
C	2.983853	-3.859787	-2.029350
H	2.380492	-4.750147	-2.275993
H	3.767117	-3.745599	-2.789283
H	3.462084	-4.007444	-1.045961

*anti-(M)-stable-Z**

C	1.777134	-1.743772	-1.361970
C	0.809873	-0.746353	-1.336094
C	-0.419305	-0.904695	-0.654016
C	-0.694154	-2.205118	-0.133922
C	0.259183	-3.212355	-0.197468
C	1.515423	-2.984698	-0.763950
C	-1.274275	0.233171	-0.377754
S	-2.131433	-2.510676	0.813566
C	-3.206918	-1.239945	0.266724
C	-2.716093	-0.005441	-0.237596
C	-3.704274	0.941861	-0.598791
H	-3.403462	1.877448	-1.058810
C	-5.060372	0.706196	-0.430124
C	-5.507956	-0.502478	0.105667
C	-4.575468	-1.475085	0.439199
H	1.052535	0.203454	-1.810719
H	0.038930	-4.189241	0.239345
H	2.255991	-3.783699	-0.762162
H	-6.573815	-0.692842	0.243728
H	-4.902539	-2.438419	0.837766
C	-0.651800	1.516160	-0.239316
C	0.687639	1.732831	0.197202
C	-1.234167	2.892955	-0.560627
C	1.143764	2.996772	-0.267970
H	-1.907117	2.855130	-1.428034
C	0.009766	3.735312	-0.913042
H	-0.070041	4.777512	-0.565580
C	1.622719	0.861466	0.894847
C	3.018167	1.192103	0.811239
C	3.419727	2.418598	0.248147
C	2.486673	3.337047	-0.244510
C	3.968262	0.269463	1.345882
C	3.561027	-0.868037	1.999258
C	2.183502	-1.123209	2.184726
C	1.241126	-0.254082	1.662879
H	0.159376	3.772498	-2.005977
H	4.485900	2.658188	0.220122
H	2.820462	4.292952	-0.655194
H	5.032307	0.495136	1.238059
H	4.301241	-1.565146	2.399487
H	1.858635	-2.001900	2.745303
H	0.180502	-0.451169	1.823806
C	-1.976318	3.489280	0.646266
H	-2.791844	2.837794	0.990132

H	-1.274193	3.620616	1.484135
H	-2.401427	4.472951	0.392537
H	-5.777739	1.471474	-0.733603
O	2.944560	-1.421607	-1.956971
C	4.048466	-2.264495	-1.776034
H	3.905750	-3.245782	-2.262432
H	4.906339	-1.764754	-2.242466
H	4.262560	-2.419235	-0.703844

syn-(P)-unstable-E

C	3.758228	-1.265258	-1.006885
C	2.378080	-1.054164	-0.880561
C	1.881036	0.011249	-0.133178
C	2.784899	0.918202	0.443790
C	4.155710	0.719044	0.314962
C	4.650521	-0.375713	-0.396589
C	0.413850	0.204133	0.016662
S	2.137268	2.272058	1.381869
C	0.710764	2.636575	0.383687
C	-0.026848	1.611347	-0.257254
C	-1.113689	2.012872	-1.043493
H	-1.681769	1.271985	-1.595288
C	-1.494483	3.349459	-1.147865
C	-0.782287	4.337077	-0.473838
C	0.331167	3.977382	0.280263
H	1.692998	-1.758797	-1.356523
H	4.857258	1.423379	0.768315
H	5.728918	-0.509007	-0.482046
H	-1.072239	5.387204	-0.551661
H	0.923061	4.744476	0.785430
C	-0.356582	-0.787258	0.544595
C	-1.838075	-0.869137	0.603182
C	0.105816	-1.846442	1.562574
C	-2.206722	-1.283777	1.871775
H	-0.061703	-2.847705	1.126694
C	-0.980518	-1.642485	2.659209
H	-0.671307	-0.817507	3.325720
C	-2.817969	-0.791943	-0.432819
C	-4.193183	-0.899509	-0.055711
C	-4.535772	-1.158051	1.301516
C	-3.562149	-1.396192	2.244385
C	-5.194348	-0.816144	-1.065208
C	-4.853214	-0.718718	-2.391872
C	-3.488179	-0.719531	-2.773271
C	-2.499237	-0.752770	-1.820069
H	-1.123309	-2.537753	3.282618
H	-5.593606	-1.228985	1.567897
H	-3.831454	-1.678690	3.265080
H	-6.244715	-0.863094	-0.765661
H	-5.630247	-0.671486	-3.158126
H	-3.222805	-0.699701	-3.832901
H	-1.448886	-0.768127	-2.119669
C	1.498681	-1.791935	2.171706
H	2.287708	-2.104976	1.477479
H	1.736188	-0.781011	2.536502
H	1.529777	-2.474827	3.035563
H	-2.354709	3.613020	-1.767354
O	4.130073	-2.342922	-1.725044
C	5.500505	-2.630261	-1.868904
H	5.987578	-2.797121	-0.893063
H	5.567255	-3.553091	-2.458565
H	6.033113	-1.826056	-2.404728

TS4

C	2.205030	2.820650	-1.388518
C	1.532593	1.625949	-1.189454
C	0.229975	1.549705	-0.644113
C	-0.411777	2.792100	-0.451819
C	0.267611	4.007903	-0.640788
C	1.580250	4.030601	-1.080842
C	-0.436982	0.229488	-0.436511
S	-2.118910	2.990459	-0.096318
C	-2.694644	1.338602	0.066934
C	-1.873994	0.193767	-0.045862
C	-2.452663	-1.015045	0.376834
H	-1.854101	-1.919959	0.441972
C	-3.792723	-1.139404	0.740733
C	-4.611585	-0.004998	0.743895
C	-4.038820	1.221810	0.433772
H	3.215224	2.805733	-1.802631
H	2.037834	0.710566	-1.486003
H	-0.261220	4.947129	-0.456844
H	2.095846	4.983015	-1.220477
H	-5.665530	-0.053442	1.017158
H	-4.655529	2.122628	0.495064
C	0.257754	-0.953000	-0.619498
C	1.681290	-1.217963	-0.325775
C	-0.251682	-2.227868	-1.321822
C	2.136487	-2.268809	-1.106382
H	-0.536678	-2.989871	-0.574067
C	1.040274	-2.754217	-2.000585
H	1.138760	-2.305944	-3.005512
C	2.523971	-0.676745	0.704353
C	3.862451	-1.169753	0.795765
C	4.307533	-2.199008	-0.084904
C	3.455149	-2.759006	-1.004979
C	4.732282	-0.641499	1.789557
C	4.296100	0.315259	2.674358
C	2.958477	0.771025	2.613556
C	2.096839	0.288977	1.655125
H	1.035533	-3.846646	-2.129624
H	5.336904	-2.555111	0.006727
H	3.788464	-3.572899	-1.653273
H	5.756228	-1.020729	1.842997
H	4.973482	0.712344	3.433925
H	2.604263	1.508175	3.337893
H	1.065903	0.641652	1.634832
C	-1.371800	-2.071468	-2.344761
H	-2.355194	-1.893016	-1.893199
H	-1.156079	-1.239948	-3.033960
H	-1.449439	-2.993798	-2.941351
O	-4.202505	-2.379862	1.077964
C	-5.542930	-2.572169	1.459907
H	-6.242348	-2.301446	0.650675
H	-5.657245	-3.641175	1.679153
H	-5.799275	-1.994993	2.364885

intermediate-E

C	1.521041	-2.394011	2.328155
C	0.928359	-1.230638	1.845369
C	0.097063	-1.260939	0.717760
C	-0.177845	-2.504941	0.127337
C	0.411769	-3.675989	0.607082
C	1.273676	-3.615816	1.700763
C	-0.518702	-0.009583	0.207372
S	-1.231139	-2.542698	-1.294152
C	-2.396356	-1.297758	-0.788042
C	-1.987475	-0.152264	-0.059707
C	-2.986581	0.744828	0.325544

H	-2.765975	1.615732	0.935328
C	-4.328781	0.568817	-0.038658
C	-4.705347	-0.543399	-0.794378
C	-3.730036	-1.475114	-1.146103
H	2.181065	-2.347482	3.197066
H	1.120811	-0.271936	2.332709
H	0.192654	-4.632977	0.127619
H	1.736507	-4.531124	2.076340
H	-5.740389	-0.712465	-1.090701
H	-4.023226	-2.366841	-1.705465
C	0.184572	1.146683	0.013607
C	1.645059	1.381315	-0.169239
C	-0.458501	2.532111	0.130296
C	1.873239	2.752759	-0.240178
H	-1.395907	2.602270	-0.438579
C	0.594617	3.522748	-0.369541
H	0.591205	4.466678	0.195528
C	2.765506	0.498762	-0.394013
C	4.081768	1.060506	-0.342917
C	4.256921	2.469588	-0.228104
C	3.171963	3.306571	-0.248888
C	5.215241	0.213688	-0.488590
C	5.070518	-1.123560	-0.767547
C	3.774643	-1.655196	-0.951492
C	2.660970	-0.867643	-0.770117
H	0.448452	3.782983	-1.431674
H	5.272470	2.871619	-0.188529
H	3.299975	4.391600	-0.254753
H	6.209979	0.659262	-0.404626
H	5.948358	-1.762283	-0.888380
H	3.650508	-2.698645	-1.250606
H	1.682813	-1.293046	-0.967834
C	-0.726531	2.821838	1.619724
H	-1.289862	2.021916	2.118836
H	0.228985	2.923169	2.159294
H	-1.282076	3.765266	1.735785
O	-5.178379	1.523369	0.390552
C	-6.543996	1.417729	0.066581
H	-6.994696	0.502726	0.486968
H	-7.039225	2.290787	0.509580
H	-6.707796	1.432457	-1.024349

TS5

C	0.644318	3.435877	-1.768163
C	0.335398	2.081912	-1.659690
C	-0.106393	1.547724	-0.442377
C	-0.361579	2.426596	0.622991
C	-0.030967	3.780050	0.527615
C	0.494823	4.277133	-0.663730
C	-0.478658	0.115171	-0.279356
S	-1.216580	1.776872	2.042002
C	-2.387996	0.781343	1.133140
C	-1.952583	0.052798	0.004387
C	-2.899053	-0.627397	-0.755796
H	-2.609559	-1.167742	-1.657025
C	-4.248219	-0.661712	-0.373747
C	-4.659843	0.013235	0.780568
C	-3.725667	0.745830	1.514952
H	1.011504	3.835253	-2.715990
H	0.473718	1.414165	-2.513199
H	-0.219740	4.449994	1.369619
H	0.746235	5.337145	-0.742681
H	-5.700513	0.002129	1.104614
H	-4.057422	1.309003	2.390419
C	0.305443	-0.992272	-0.181535

C	1.776316	-1.253839	0.044963
C	-0.351269	-2.377415	-0.155160
C	1.890691	-2.547158	0.552762
H	-1.364599	-2.329406	0.259228
C	0.566659	-3.222659	0.721807
H	0.591467	-4.283774	0.430781
C	2.990497	-0.480182	-0.093434
C	4.242294	-1.107430	0.226985
C	4.282741	-2.443106	0.711671
C	3.123264	-3.145598	0.888625
C	5.460274	-0.388769	0.074280
C	5.473231	0.913739	-0.359494
C	4.247399	1.547852	-0.654067
C	3.057359	0.870020	-0.523898
H	0.263320	-3.179705	1.781913
H	5.252100	-2.890430	0.945302
H	3.136532	-4.166607	1.277285
H	6.394705	-0.900984	0.318279
H	6.416438	1.453441	-0.469920
H	4.235048	2.588330	-0.988232
H	2.140774	1.392339	-0.751360
C	-0.421871	-2.955164	-1.575173
H	-0.970249	-2.293093	-2.259982
H	0.587765	-3.098264	-1.993084
H	-0.927363	-3.933071	-1.565699
O	-5.067533	-1.368507	-1.176283
C	-6.432023	-1.468921	-0.845468
H	-6.925856	-0.482499	-0.838518
H	-6.896849	-2.091093	-1.620449
H	-6.579429	-1.952978	0.134998

syn-(*M*)-stable-*E*

C	4.146362	-0.705492	0.856595
C	2.755264	-0.639806	1.022817
C	1.971705	0.124623	0.164010
C	2.591301	0.871666	-0.854719
C	3.972299	0.812307	-1.018509
C	4.754227	0.019253	-0.176114
C	0.485103	0.173079	0.249339
S	1.575689	1.842697	-1.945315
C	0.387675	2.423182	-0.753775
C	-0.034109	1.574726	0.292941
C	-0.854874	2.122587	1.283055
H	-1.113981	1.527393	2.154928
C	-1.341568	3.424712	1.179664
C	-0.986502	4.220092	0.091933
C	-0.098981	3.727851	-0.862404
H	2.293035	-1.214020	1.828131
H	4.456731	1.390548	-1.809024
H	5.833426	-0.010078	-0.327371
H	-1.370636	5.238602	0.001320
H	0.234692	4.366018	-1.684139
C	-0.234354	-0.933928	-0.055887
C	-1.691806	-1.064280	-0.320579
C	0.382717	-2.172944	-0.701914
C	-1.831339	-1.761159	-1.510008
H	1.431650	-1.994446	-0.969546
C	-0.497089	-2.286414	-1.973571
H	-0.564491	-3.313594	-2.363820
C	-2.846012	-0.693578	0.430592
C	-4.124837	-0.854053	-0.190016
C	-4.213652	-1.442302	-1.483654
C	-3.094334	-1.931798	-2.115438
C	-5.293840	-0.486253	0.534791
C	-5.211007	-0.053479	1.835989

C	-3.952411	0.004328	2.483804
C	-2.803479	-0.307449	1.797714
H	-0.084043	-1.649613	-2.774303
H	-5.199839	-1.551236	-1.942400
H	-3.178064	-2.448170	-3.074859
H	-6.265373	-0.582658	0.042930
H	-6.117170	0.212637	2.385200
H	-3.897865	0.283320	3.538796
H	-1.841164	-0.308677	2.309909
C	0.302394	-3.420953	0.176356
H	0.869871	-3.282566	1.108884
H	-0.739735	-3.657421	0.445600
H	0.722009	-4.291641	-0.350414
H	-1.999570	3.817095	1.958106
O	4.810697	-1.486211	1.730254
C	6.208613	-1.605952	1.616174
H	6.530700	-2.285220	2.415243
H	6.504449	-2.036577	0.644429
H	6.713991	-0.634574	1.750291

TSS'

C	0.939597	-2.708272	1.139009
C	0.380961	-1.423161	1.208149
C	-0.501751	-0.984872	0.229350
C	-0.893221	-1.866873	-0.798218
C	-0.349093	-3.144187	-0.862378
C	0.576919	-3.567424	0.094615
C	-1.110145	0.372261	0.234508
S	-2.043776	-1.277399	-2.024924
C	-3.151770	-0.464813	-0.890407
C	-2.604370	0.220533	0.213986
C	-3.476127	0.559607	1.256112
H	-3.067004	0.937566	2.191689
C	-4.854701	0.398955	1.123560
C	-5.388196	-0.145997	-0.043828
C	-4.532104	-0.614195	-1.038212
H	0.685962	-0.757029	2.017344
H	-0.646333	-3.829307	-1.659735
H	0.993820	-4.571777	0.019361
H	-6.468047	-0.264358	-0.157307
H	-4.932973	-1.134450	-1.911281
C	-0.441711	1.550010	0.104080
C	1.023734	1.795423	-0.099046
C	-1.115508	2.938905	0.213492
C	1.276308	3.149322	0.070783
H	-1.852180	3.032927	-0.600770
C	0.025466	3.960863	0.037102
H	0.008852	4.740576	0.812759
C	2.140905	0.954674	-0.470444
C	3.463162	1.471858	-0.277744
C	3.654493	2.829705	0.109539
C	2.581968	3.674987	0.201388
C	4.591190	0.658771	-0.575528
C	4.440608	-0.584913	-1.139628
C	3.144250	-1.041070	-1.464122
C	2.034733	-0.293976	-1.139398
H	-0.030843	4.482839	-0.932700
H	4.673467	3.197667	0.254058
H	2.719875	4.741814	0.392754
H	5.587822	1.064243	-0.381873
H	5.314882	-1.194875	-1.378471
H	3.015378	-1.990280	-1.989575
H	1.057737	-0.648680	-1.449757
C	-1.824879	3.247324	1.538904
H	-2.796620	2.758014	1.628347

H	-1.201744	2.959068	2.401071
H	-2.010927	4.329835	1.606831
H	-5.513628	0.692448	1.943773
O	1.815586	-3.023634	2.111352
C	2.435654	-4.287037	2.090148
H	3.013547	-4.441101	1.163277
H	3.124599	-4.312510	2.943655
H	1.701860	-5.103623	2.199893

anti-(P)-unstable-E

C	-4.288573	0.405960	0.373862
C	-2.920383	0.647558	0.556233
C	-1.961259	-0.121594	-0.094448
C	-2.384759	-1.247148	-0.830906
C	-3.742751	-1.495219	-1.009481
C	-4.701288	-0.656761	-0.437916
C	-0.490393	0.091332	0.046127
S	-1.166060	-2.398727	-1.432926
C	-0.093456	-2.362863	-0.010822
C	0.151314	-1.128648	0.615698
C	0.964421	-1.101994	1.752784
H	1.135883	-0.150715	2.261276
C	1.577910	-2.264453	2.212915
C	1.368718	-3.475069	1.550608
C	0.519747	-3.530663	0.446121
H	-2.621363	1.463866	1.212945
H	-4.068318	-2.367101	-1.581837
H	-5.758106	-0.871150	-0.597558
H	1.850330	-4.387678	1.908799
H	0.326855	-4.482103	-0.055091
C	0.209457	1.182941	-0.345283
C	1.682430	1.383992	-0.170426
C	-0.248070	2.551994	-0.861400
C	1.893193	2.712614	0.158056
H	0.181466	2.605935	-1.878950
C	0.616809	3.493587	0.008478
H	0.126715	3.659182	0.984798
C	2.795413	0.503018	-0.336192
C	4.081795	0.977011	0.069262
C	4.233526	2.317918	0.526550
C	3.169668	3.187830	0.529682
C	5.205607	0.109786	-0.042541
C	5.077706	-1.144896	-0.586279
C	3.819880	-1.579137	-1.071955
C	2.711425	-0.776554	-0.951887
H	0.775060	4.478670	-0.455889
H	5.227514	2.657033	0.829975
H	3.304452	4.233862	0.815539
H	6.180348	0.471388	0.295813
H	5.948226	-1.799540	-0.671051
H	3.731264	-2.556267	-1.552494
H	1.756170	-1.108627	-1.355812
C	-1.698510	2.986724	-0.979102
H	-2.297381	2.289626	-1.580204
H	-2.185860	3.113377	-0.003899
H	-1.723336	3.964573	-1.485487
H	2.226585	-2.225326	3.090782
O	-5.125131	1.242276	1.019139
C	-6.514202	1.060192	0.883836
H	-6.992829	1.845748	1.481850
H	-6.840548	1.165120	-0.164869
H	-6.837371	0.076814	1.265607

TS6

C	3.902515	-1.200538	0.536562
C	2.536141	-1.010865	0.330478
C	1.967591	0.210578	-0.059269
C	2.856289	1.308520	-0.088990
C	4.227646	1.129714	0.116520
C	4.773388	-0.115811	0.399424
C	0.494565	0.297727	-0.318632
S	2.355909	2.979349	-0.268659
C	0.606955	2.865139	-0.326190
C	-0.127542	1.661301	-0.434875
C	-1.483223	1.837034	-0.795033
H	-2.083834	0.970601	-1.043505
C	-2.103764	3.073744	-0.881312
C	-1.375750	4.236781	-0.633578
C	-0.018553	4.122405	-0.385934
H	1.905437	-1.868907	0.522390
H	4.890984	1.997955	0.072502
H	5.848114	-0.213546	0.551430
H	-1.848676	5.220151	-0.673065
H	0.589605	5.022172	-0.258836
C	-0.233720	-0.860618	-0.497361
C	-1.701482	-1.063706	-0.417078
C	0.244438	-2.157732	-1.181435
C	-2.095641	-1.890464	-1.454924
H	1.223001	-2.018314	-1.660554
C	-0.884348	-2.313794	-2.240411
H	-0.962100	-3.337033	-2.636629
C	-2.632923	-0.669152	0.591734
C	-3.995793	-1.063075	0.425835
C	-4.375465	-1.848372	-0.701902
C	-3.443450	-2.271933	-1.620780
C	-4.950541	-0.663734	1.402436
C	-4.573478	0.078724	2.495703
C	-3.217453	0.448813	2.669046
C	-2.271296	0.085452	1.739997
H	-0.709282	-1.632559	-3.090467
H	-5.425683	-2.131625	-0.810344
H	-3.737646	-2.905528	-2.461013
H	-5.994116	-0.960268	1.267623
H	-5.316289	0.380817	3.237437
H	-2.923253	1.025885	3.548873
H	-1.227310	0.371642	1.880182
C	0.259124	-3.428366	-0.318528
H	0.988337	-3.403561	0.502053
H	-0.730140	-3.612335	0.128345
H	0.510219	-4.296015	-0.947483
H	-3.160792	3.123797	-1.150660
O	4.282199	-2.449222	0.878206
C	5.646897	-2.703053	1.109820
H	5.730664	-3.768179	1.359422
H	6.257828	-2.501065	0.213380
H	6.036013	-2.108206	1.953872

motor 2

anti-(M)-stable-E

C	2.469137	2.355134	2.252382
C	1.746897	1.253638	1.801072
C	0.941067	1.344317	0.660314
C	0.821466	2.589793	0.019719
C	1.545310	3.697060	0.467953
C	2.380498	3.573183	1.576679
C	0.199400	0.176058	0.115758
S	-0.217042	2.727015	-1.415849
C	-1.530392	1.646759	-0.894091

C	-1.236515	0.486606	-0.150539
C	-2.298551	-0.270976	0.339247
H	-2.115016	-1.128391	0.987584
C	-3.903774	1.150633	-0.770124
C	-2.852234	1.959637	-1.200224
H	3.106723	2.262113	3.134146
H	1.823227	0.296342	2.321267
H	1.446445	4.657281	-0.043776
H	2.947266	4.439202	1.925784
H	-4.918206	1.432199	-1.041991
H	-3.078932	2.859988	-1.776386
C	0.769146	-1.020776	-0.163561
C	2.185812	-1.449863	-0.005281
C	0.029206	-2.290966	-0.573514
C	2.188844	-2.801809	0.301965
H	-1.023012	-2.270862	-0.277749
C	0.800839	-3.376641	0.209876
H	0.789691	-4.357007	-0.290564
C	3.424492	-0.758326	-0.195824
C	4.630175	-1.449390	0.141300
C	4.576054	-2.807161	0.570733
C	3.383623	-3.487262	0.611998
C	5.878403	-0.783545	-0.012796
C	5.941941	0.488601	-0.527405
C	4.755079	1.141622	-0.938693
C	3.532502	0.534122	-0.779239
H	0.363998	-3.514928	1.213832
H	5.512215	-3.313952	0.819246
H	3.353696	-4.546630	0.878602
H	6.791899	-1.313837	0.269230
H	6.906590	0.987293	-0.646500
H	4.811767	2.131993	-1.396369
H	2.632126	1.033905	-1.132403
C	0.096750	-2.505799	-2.088035
H	-0.395201	-1.677486	-2.620357
H	1.138549	-2.565706	-2.441403
H	-0.412541	-3.440955	-2.367619
C	-3.634696	0.030322	0.028238
O	-4.527709	-0.827156	0.554536
C	-5.966871	-0.746266	0.472188
C	-6.444113	-0.913183	-0.971293
H	-7.537204	-1.036227	-0.983875
H	-6.201824	-0.053500	-1.609629
H	-5.993883	-1.812486	-1.417823
C	-6.485566	0.537570	1.120578
H	-6.063848	0.650564	2.130697
H	-6.244948	1.440685	0.544878
H	-7.580564	0.484175	1.210629
C	-6.411039	-1.951849	1.298673
H	-7.508046	-2.021480	1.321443
H	-6.010331	-2.880615	0.866189
H	-6.043649	-1.864125	2.331899

*anti-(M)-stable-E**

C	2.897845	1.585333	2.440757
C	1.974228	0.723205	1.876034
C	0.999897	1.167259	0.939271
C	0.998306	2.561280	0.657728
C	1.930579	3.427021	1.229126
C	2.894774	2.942561	2.108698
C	0.095507	0.234554	0.287675
S	-0.073085	3.229907	-0.554092
C	-1.394972	2.078704	-0.545761
C	-1.200157	0.719745	-0.177416
C	-2.330378	-0.119881	-0.294926

H	-2.273519	-1.161192	-0.004374
C	-3.708180	1.670740	-1.146122
C	-2.626059	2.533087	-1.026417
H	3.633233	1.195815	3.147768
H	1.984068	-0.329775	2.158299
H	1.898538	4.489731	0.977287
H	3.627453	3.624588	2.544326
H	-4.666207	2.017021	-1.535450
H	-2.731489	3.581719	-1.314157
C	0.524905	-1.127824	0.170953
C	1.873967	-1.515280	-0.064075
C	-0.265303	-2.419543	0.393347
C	2.087670	-2.825369	0.441557
H	-1.097389	-2.270344	1.097388
C	0.800658	-3.356322	1.000309
H	0.629840	-4.418268	0.765766
C	2.984187	-0.786712	-0.649400
C	4.286513	-1.381854	-0.557639
C	4.445012	-2.665742	0.012153
C	3.354064	-3.391416	0.488058
C	5.401435	-0.671733	-1.090233
C	5.236411	0.537290	-1.722974
C	3.945189	1.087990	-1.868212
C	2.845944	0.429751	-1.349210
H	0.809502	-3.261792	2.101346
H	5.447674	-3.098791	0.056144
H	3.498255	-4.386431	0.916121
H	6.395659	-1.116294	-0.997443
H	6.102563	1.065966	-2.127267
H	3.809898	2.037747	-2.389653
H	1.852085	0.857628	-1.489517
C	-0.787387	-3.022243	-0.924602
H	-1.429432	-2.327683	-1.482390
H	0.063027	-3.282333	-1.573685
H	-1.361574	-3.940368	-0.723932
C	-3.558650	0.334243	-0.759590
O	-4.593022	-0.538819	-0.899927
C	-5.490772	-0.788220	0.202137
C	-6.171243	0.507585	0.644087
H	-6.909927	0.296833	1.431329
H	-5.443085	1.227442	1.046426
H	-6.693428	0.977166	-0.202719
C	-4.745656	-1.430586	1.374037
H	-4.225590	-2.343347	1.046097
H	-4.006873	-0.741961	1.809528
H	-5.457920	-1.705590	2.165851
C	-6.508325	-1.761100	-0.382295
H	-7.262655	-2.034052	0.369640
H	-7.015503	-1.304998	-1.244424
H	-6.003743	-2.675531	-0.725735

syn-(*P*)-unstable-*Z*

C	-4.756703	-0.584123	2.101255
C	-3.437169	-0.743877	1.685540
C	-2.894977	0.063932	0.676680
C	-3.695076	1.082904	0.140547
C	-5.020121	1.249296	0.549594
C	-5.553178	0.404397	1.521383
C	-1.495269	-0.152367	0.224089
S	-3.009844	2.120757	-1.113431
C	-1.330455	2.200691	-0.536044
C	-0.694359	1.106641	0.099295
C	0.637301	1.286220	0.487976
H	1.170379	0.504489	1.016368
C	1.334630	2.469274	0.231156

C	0.690950	3.529955	-0.406438
C	-0.641443	3.391504	-0.777546
H	-5.164696	-1.234108	2.878293
H	-2.810614	-1.519794	2.131825
H	-5.631252	2.042994	0.113170
H	-6.589797	0.535064	1.840029
H	1.226827	4.463524	-0.584237
H	-1.158695	4.227093	-1.255435
C	-1.107603	-1.395857	-0.180648
C	0.260956	-1.925833	-0.401838
C	-2.014901	-2.430846	-0.872079
C	0.264928	-2.662979	-1.574486
H	-2.046099	-3.347534	-0.255985
C	-1.132274	-2.754060	-2.113836
H	-1.313122	-1.993477	-2.894608
C	1.389203	-1.975940	0.473818
C	2.577191	-2.609680	-0.008522
C	2.586084	-3.208940	-1.299419
C	1.439691	-3.274088	-2.057795
C	3.717466	-2.682122	0.841201
C	3.670098	-2.207286	2.128874
C	2.468159	-1.651768	2.633459
C	1.359822	-1.539538	1.828491
H	-1.357727	-3.738856	-2.549230
H	3.509917	-3.673192	-1.653921
H	1.431294	-3.807521	-3.011240
H	4.629762	-3.142087	0.452485
H	4.548656	-2.275651	2.774346
H	2.420450	-1.316718	3.672103
H	0.433506	-1.124448	2.231346
C	-3.428903	-2.061402	-1.295483
H	-4.136355	-2.020708	-0.458333
H	-3.450404	-1.090243	-1.813648
H	-3.796171	-2.824341	-2.000018
O	2.613279	2.608990	0.673990
C	3.721765	2.200352	-0.168082
C	4.946198	2.512508	0.682443
H	4.914006	1.943178	1.623564
H	5.868357	2.247098	0.145116
H	4.980465	3.584750	0.926786
C	3.736852	3.013144	-1.460957
H	2.851773	2.802519	-2.079926
H	3.768144	4.092305	-1.247218
H	4.627184	2.754387	-2.053633
C	3.640977	0.706025	-0.467616
H	3.572960	0.130072	0.466217
H	2.770633	0.460111	-1.094001
H	4.542851	0.380253	-1.007321

TS1

C	-1.451755	-2.106292	-0.906277
C	-0.613743	-1.005143	-0.776514
C	0.699584	-1.085632	-0.260060
C	1.157480	-2.386085	0.035385
C	0.307331	-3.498759	-0.064882
C	-0.993378	-3.370075	-0.515902
C	1.577695	0.123248	-0.223203
S	2.820718	-2.804226	0.417729
C	3.655521	-1.264436	0.352612
C	3.019558	-0.028671	0.112793
C	3.806645	1.116381	0.374617
H	3.335247	2.096063	0.347465
C	5.154419	1.053357	0.692456
C	5.782900	-0.188029	0.806665
C	5.023152	-1.338014	0.663830

H	-0.999530	-0.057403	-1.144228
H	0.694276	-4.491010	0.182876
H	-1.638875	-4.242841	-0.622432
H	6.845890	-0.260780	1.045909
H	5.483988	-2.317910	0.815881
C	1.071127	1.373697	-0.527837
C	-0.259510	1.912907	-0.190724
C	1.727826	2.444776	-1.419292
C	-0.594147	2.930280	-1.071279
H	2.191199	3.233976	-0.799975
C	0.489353	3.098069	-2.090746
H	0.238453	2.550688	-3.016928
C	-1.071746	1.672765	0.968447
C	-2.271039	2.438158	1.109354
C	-2.614148	3.415412	0.131287
C	-1.783722	3.674419	-0.932878
C	-3.106427	2.219586	2.239276
C	-2.766599	1.301925	3.203742
C	-1.559925	0.573225	3.085983
C	-0.736349	0.753145	1.998377
H	0.663709	4.148149	-2.367731
H	-3.543597	3.976254	0.259060
H	-2.032850	4.451651	-1.659194
H	-4.028452	2.800127	2.327608
H	-3.417292	1.141521	4.066359
H	-1.276312	-0.135389	3.867524
H	0.195283	0.192312	1.931931
C	2.727537	1.958686	-2.461947
H	3.684345	1.637399	-2.032007
H	2.311316	1.113606	-3.032586
H	2.944197	2.772089	-3.171934
H	5.709935	1.976502	0.870022
O	-2.658494	-1.979844	-1.522231
C	-3.860979	-1.728143	-0.754229
C	-4.966826	-1.757237	-1.800694
H	-5.944997	-1.573136	-1.332862
H	-4.794340	-0.984105	-2.564532
H	-4.998145	-2.736795	-2.300828
C	-3.773285	-0.359681	-0.087719
H	-4.719043	-0.122912	0.422069
H	-2.972943	-0.338535	0.664855
H	-3.574650	0.426161	-0.831873
C	-4.076185	-2.820913	0.290947
H	-4.109007	-3.814977	-0.179910
H	-3.280748	-2.815890	1.051197
H	-5.032783	-2.656008	0.808913

intermediate-Z

C	5.384177	-0.064935	-1.064588
C	4.040373	0.294206	-1.146735
C	3.079134	-0.219789	-0.260083
C	3.530846	-1.178814	0.677516
C	4.878818	-1.536795	0.764110
C	5.813314	-0.968433	-0.096183
C	1.632125	0.168203	-0.193120
S	2.409747	-1.961263	1.815498
C	0.994674	-2.072193	0.758674
C	0.724717	-1.004523	-0.109980
C	-0.379319	-1.097434	-0.964865
H	-0.572157	-0.302299	-1.686778
C	-1.241536	-2.194861	-0.907863
C	-0.979570	-3.230407	-0.003673
C	0.142942	-3.175972	0.817802
H	6.097066	0.365167	-1.771566
H	3.745833	0.984082	-1.932311

H	5.192534	-2.278585	1.502445
H	6.865728	-1.250915	-0.023059
H	-1.646460	-4.093861	0.023768
H	0.363133	-4.001338	1.498856
C	1.182047	1.459084	-0.215587
C	-0.107082	2.045261	0.244783
C	1.928555	2.584333	-0.939198
C	-0.131326	3.397258	-0.086795
H	2.996162	2.611143	-0.679453
C	1.210022	3.878307	-0.549632
H	1.157043	4.600145	-1.378225
C	-1.198543	1.524337	1.031342
C	-2.386245	2.317531	1.137891
C	-2.414799	3.640923	0.613051
C	-1.283647	4.196514	0.073822
C	-3.517299	1.800740	1.828146
C	-3.462605	0.588615	2.471898
C	-2.247293	-0.132520	2.486662
C	-1.152485	0.323474	1.789426
H	1.706126	4.391147	0.291971
H	-3.335845	4.222089	0.705190
H	-1.268278	5.240657	-0.247573
H	-4.428693	2.403786	1.857157
H	-4.336064	0.202182	3.001723
H	-2.168981	-1.057623	3.062497
H	-0.219603	-0.226060	1.859641
C	1.760250	2.375576	-2.456647
H	2.031512	1.362042	-2.781444
H	0.706699	2.528934	-2.740994
H	2.371496	3.097935	-3.019393
O	-2.277344	-2.305834	-1.781779
C	-3.565585	-1.714851	-1.473421
C	-3.444913	-0.196558	-1.373527
H	-4.437749	0.251106	-1.217472
H	-2.809703	0.097423	-0.527130
H	-3.017314	0.224957	-2.295864
C	-4.433561	-2.112088	-2.659982
H	-5.450332	-1.709011	-2.544623
H	-4.006803	-1.718324	-3.594681
H	-4.497866	-3.207291	-2.742681
C	-4.118658	-2.294555	-0.173718
H	-4.203916	-3.390082	-0.236209
H	-3.477128	-2.037891	0.682365
H	-5.118811	-1.880437	0.022950

TS2

C	-3.355278	-3.818707	1.215237
C	-2.636303	-2.634900	1.374414
C	-2.007723	-2.022878	0.284151
C	-2.056115	-2.678179	-0.964292
C	-2.784772	-3.857792	-1.128453
C	-3.446868	-4.420992	-0.038997
C	-1.248519	-0.726186	0.311681
S	-1.146841	-1.999977	-2.344018
C	0.312329	-1.556410	-1.427432
C	0.138889	-0.997221	-0.151431
C	1.246002	-0.853870	0.682408
H	1.126065	-0.463306	1.694737
C	2.543698	-1.135974	0.226956
C	2.710217	-1.601403	-1.086068
C	1.595196	-1.831080	-1.892939
H	-3.844626	-4.272996	2.079627
H	-2.570995	-2.172934	2.360178
H	-2.813290	-4.348495	-2.104158
H	-4.009042	-5.348629	-0.167301

H	3.694363	-1.835124	-1.485086
H	1.737837	-2.260269	-2.887469
C	-1.875396	0.457900	0.548139
C	-1.599436	1.904480	0.208949
C	-3.264400	0.456598	1.196315
C	-2.819184	2.577870	0.263796
H	-3.813582	-0.462032	0.960165
C	-3.964144	1.683507	0.621043
H	-4.665129	2.154133	1.326997
C	-0.436077	2.660397	-0.203701
C	-0.591314	4.062329	-0.475153
C	-1.863886	4.686699	-0.368136
C	-2.962843	3.953046	-0.017712
C	0.530623	4.841854	-0.871592
C	1.774372	4.280668	-1.022550
C	1.935340	2.900878	-0.775728
C	0.867932	2.128576	-0.378958
H	-4.535258	1.433411	-0.289351
H	-1.946598	5.755763	-0.579517
H	-3.949991	4.415842	0.053465
H	0.375278	5.906665	-1.063545
H	2.625859	4.890130	-1.333587
H	2.914147	2.431886	-0.900419
H	1.033767	1.077263	-0.199424
O	3.512424	-0.940208	1.140146
C	4.924898	-0.775029	0.881014
C	-3.129481	0.578287	2.720651
H	-2.674251	1.542794	2.997759
H	-4.118573	0.518860	3.200557
H	-2.495645	-0.215980	3.140208
C	5.456459	-0.303351	2.233052
H	5.265472	-1.062073	3.006670
H	6.540084	-0.124741	2.179995
H	4.960589	0.631141	2.534147
C	5.168269	0.305222	-0.171796
H	4.793707	0.028181	-1.166074
H	4.686511	1.246580	0.132163
H	6.248813	0.488463	-0.264427
C	5.574908	-2.111025	0.516180
H	5.275947	-2.885061	1.238576
H	5.314629	-2.458498	-0.492180
H	6.669620	-2.009568	0.556131

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C	1.426633	-2.444995	0.286031
C	0.636108	-1.339823	0.613231
C	-0.655144	-1.177905	0.106714
C	-1.163406	-2.207512	-0.718774
C	-0.386213	-3.325218	-1.027809
C	0.909597	-3.447397	-0.536170
C	-1.542754	0.004077	0.327502
S	-2.790040	-2.118866	-1.429757
C	-3.639170	-1.308652	-0.104755
C	-2.952979	-0.347473	0.653052
C	-3.631053	0.273799	1.710367
H	-3.094167	0.996945	2.328381
C	-4.969260	-0.011859	1.969648
C	-5.648159	-0.942430	1.181508
C	-4.981457	-1.601823	0.151082
H	1.066820	-0.602949	1.283473
H	-0.804704	-4.118563	-1.651803
H	1.506311	-4.331701	-0.763262
H	-6.697598	-1.171418	1.379943
H	-5.500750	-2.351423	-0.450882
C	-1.249747	1.297170	0.029692

C	0.038785	1.916887	-0.367942
C	-2.306395	2.289147	-0.461864
C	-0.192248	2.651022	-1.520689
H	-3.270950	1.787631	-0.614604
C	-1.668424	2.681348	-1.824834
H	-2.000623	3.665400	-2.189275
C	1.292027	2.014274	0.304959
C	2.356945	2.689864	-0.369879
C	2.122066	3.285085	-1.641418
C	0.860575	3.307223	-2.191473
C	3.616429	2.817633	0.282238
C	3.795780	2.364019	1.566191
C	2.714050	1.773755	2.266589
C	1.497138	1.602532	1.651700
H	-1.932632	1.931842	-2.590229
H	2.953551	3.785200	-2.144791
H	0.670786	3.840039	-3.126460
H	4.434616	3.309190	-0.250740
H	4.763043	2.479194	2.060428
H	2.847874	1.461729	3.304912
H	0.659294	1.174075	2.205355
C	-2.513320	3.501847	0.443745
H	-2.919479	3.199561	1.420269
H	-1.568705	4.040717	0.619874
H	-3.224606	4.206274	-0.014470
H	-5.482622	0.490092	2.792716
O	2.664948	-2.547424	0.837998
C	3.833249	-2.154445	0.070412
C	4.169370	-3.231123	-0.960278
H	4.270220	-4.214003	-0.475549
H	3.395816	-3.298932	-1.739281
H	5.121283	-2.992957	-1.458610
C	3.605514	-0.805862	-0.605867
H	4.532996	-0.472815	-1.094768
H	2.820005	-0.858900	-1.374540
H	3.316195	-0.046372	0.133172
C	4.931562	-2.049244	1.120725
H	5.889395	-1.777885	0.653396
H	4.675015	-1.281941	1.866127
H	5.058080	-3.010320	1.641546

TS2'

C	-2.118987	-1.427779	0.157911
C	-0.990866	-0.790056	-0.365773
C	0.207292	-0.775492	0.346930
C	0.289750	-1.464407	1.569819
C	-0.837346	-2.085861	2.105428
C	-2.042583	-2.054624	1.406269
C	1.435727	-0.098655	-0.146137
S	1.845829	-1.461904	2.437722
C	2.877732	-1.744169	1.012434
C	2.540997	-1.112699	-0.202491
C	3.145382	-1.597892	-1.368831
H	2.788740	-1.251890	-2.337751
C	4.179647	-2.530416	-1.309165
C	4.601613	-3.031954	-0.078242
C	3.922987	-2.667606	1.082708
H	-1.066592	-0.265487	-1.319371
H	-0.776991	-2.600903	3.066911
H	-2.934747	-2.526120	1.821391
H	5.416752	-3.757125	-0.026279
H	4.174506	-3.134137	2.038068
C	1.584845	1.237288	-0.355493
C	0.600399	2.348500	-0.143828
C	2.859311	1.877639	-0.956463

C	1.103772	3.504935	-0.722740
H	3.700505	1.684575	-0.271581
C	2.557271	3.387553	-1.034872
H	2.811051	3.813305	-2.016995
C	-0.667310	2.450763	0.545825
C	-1.487586	3.593479	0.273549
C	-0.985661	4.667032	-0.517778
C	0.317331	4.659657	-0.936847
C	-2.769090	3.704222	0.879466
C	-3.197672	2.784935	1.805915
C	-2.330705	1.738413	2.189399
C	-1.107910	1.579637	1.577837
H	3.127938	3.964424	-0.287990
H	-1.634223	5.524603	-0.714477
H	0.749709	5.521292	-1.451009
H	-3.393258	4.563499	0.619985
H	-4.177687	2.887851	2.277274
H	-2.624687	1.051818	2.986722
H	-0.443244	0.798834	1.931195
C	3.264106	1.403800	-2.358908
H	3.745596	0.424034	-2.357008
H	2.395246	1.371556	-3.036308
H	3.992872	2.111373	-2.782642
H	4.648334	-2.876539	-2.233038
O	-3.303514	-1.362026	-0.504963
C	-3.663042	-2.392106	-1.459726
C	-3.806733	-3.742582	-0.760137
H	-4.163255	-4.497276	-1.477087
H	-2.846249	-4.095645	-0.355537
H	-4.534270	-3.680611	0.063241
C	-2.628555	-2.474839	-2.580650
H	-2.503335	-1.497846	-3.071304
H	-1.649040	-2.808117	-2.205986
H	-2.960798	-3.200162	-3.338154
C	-5.006251	-1.919943	-2.001242
H	-5.394033	-2.630844	-2.745530
H	-5.740297	-1.833657	-1.186192
H	-4.900859	-0.934776	-2.479402

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C	-1.265573	-2.147351	-0.858675
C	-0.402143	-1.054363	-0.967392
C	0.691301	-0.925142	-0.109021
C	0.962800	-1.946979	0.813963
C	0.106107	-3.042782	0.926717
C	-1.012980	-3.132170	0.103492
C	1.624809	0.235251	-0.176851
S	2.408952	-1.802358	1.843399
C	3.515886	-1.166717	0.599189
C	3.028192	-0.245515	-0.347618
C	3.840636	0.059884	-1.445079
H	3.440652	0.684543	-2.243639
C	5.146210	-0.418526	-1.525478
C	5.651944	-1.243750	-0.520613
C	4.827601	-1.642135	0.529703
H	-0.584577	-0.294673	-1.728221
H	0.318838	-3.834727	1.648507
H	-1.687735	-3.987438	0.172395
H	6.676333	-1.618650	-0.577643
H	5.191128	-2.349980	1.278331
C	1.212876	1.516106	-0.023872
C	-0.203241	1.960979	0.178607
C	1.950623	2.849367	-0.186833
C	-0.382122	3.142093	-0.522157
H	1.904874	3.304352	0.819879

C	0.935988	3.637018	-1.049693
H	1.072785	3.385408	-2.116711
C	-1.252648	1.460759	1.011534
C	-2.528486	2.102071	0.929243
C	-2.705216	3.229830	0.077963
C	-1.643624	3.769405	-0.607157
C	-3.597719	1.628534	1.740304
C	-3.405072	0.607002	2.637331
C	-2.122779	0.021102	2.772943
C	-1.078050	0.435532	1.982132
H	1.046422	4.727157	-0.948170
H	-3.693474	3.693591	0.022621
H	-1.765986	4.679623	-1.199234
H	-4.574602	2.110430	1.648651
H	-4.231254	0.257130	3.260462
H	-1.960734	-0.761359	3.517951
H	-0.090218	-0.000644	2.120931
C	3.387409	2.980721	-0.659906
H	4.083680	2.389610	-0.050481
H	3.515475	2.697803	-1.713015
H	3.683623	4.037631	-0.569407
H	5.768883	-0.151301	-2.382235
O	-2.300156	-2.314739	-1.724747
C	-3.559045	-1.626994	-1.507892
C	-4.498252	-2.266876	-2.522051
H	-5.495770	-1.807433	-2.464720
H	-4.109752	-2.132841	-3.542787
H	-4.598356	-3.345279	-2.328446
C	-3.401494	-0.133582	-1.786825
H	-2.724228	0.339678	-1.063541
H	-3.008473	0.033181	-2.801121
H	-4.376159	0.370785	-1.704039
C	-4.054098	-1.862296	-0.083800
H	-4.164689	-2.938048	0.121444
H	-3.363450	-1.433023	0.656460
H	-5.034274	-1.382730	0.056135

TS3

C	1.458386	-2.104939	-0.782937
C	0.601918	-1.022570	-0.616649
C	-0.743946	-1.132539	-0.206998
C	-1.202873	-2.458798	-0.043492
C	-0.337644	-3.556246	-0.176336
C	0.989132	-3.398160	-0.534867
C	-1.647632	0.068067	-0.138303
S	-2.877441	-2.935879	0.184770
C	-3.731694	-1.409018	0.205348
C	-3.104986	-0.148051	0.124010
C	-3.939459	0.951017	0.418696
H	-3.490881	1.930318	0.528778
C	-5.306515	0.841268	0.624545
C	-5.913853	-0.413949	0.584822
C	-5.116684	-1.532748	0.403491
H	1.026735	-0.059890	-0.875072
H	-0.736000	-4.564897	-0.035660
H	1.634268	-4.265656	-0.675705
H	-6.989289	-0.525938	0.737348
H	-5.562736	-2.530521	0.435808
C	-1.184474	1.339808	-0.401807
C	0.201879	1.856504	-0.325619
C	-1.909159	2.444123	-1.195714
C	0.442875	2.659735	-1.426348
H	-2.823362	2.057226	-1.666750
C	-0.810040	2.744745	-2.256985
H	-0.941902	3.723270	-2.742034

C	1.147392	1.779061	0.741837
C	2.386165	2.472111	0.579782
C	2.639614	3.199544	-0.619927
C	1.681568	3.311050	-1.601667
C	3.334097	2.442963	1.640590
C	3.063269	1.774135	2.810446
C	1.831181	1.095161	2.971325
C	0.900155	1.089437	1.958958
H	-0.816139	1.970441	-3.042757
H	3.602465	3.705229	-0.729114
H	1.868907	3.909956	-2.496129
H	4.282892	2.969943	1.510287
H	3.798046	1.763677	3.618673
H	1.621460	0.571026	3.906616
H	-0.049174	0.566872	2.089951
C	-2.214499	3.747901	-0.445588
H	-2.932848	3.631235	0.377008
H	-1.297341	4.180674	-0.017015
H	-2.636582	4.485370	-1.145220
H	-5.891843	1.737709	0.839716
O	2.699914	-1.871063	-1.284808
C	3.873476	-1.917119	-0.434959
C	4.914480	-1.127528	-1.220260
H	4.579428	-0.088773	-1.360624
H	5.876930	-1.116730	-0.687967
H	5.069934	-1.578510	-2.211999
C	4.326362	-3.363956	-0.242391
H	3.609663	-3.935087	0.365552
H	4.443557	-3.865508	-1.214964
H	5.294935	-3.389954	0.279542
C	3.591205	-1.249225	0.905255
H	2.850999	-1.811582	1.493656
H	4.517472	-1.188707	1.495491
H	3.211966	-0.229339	0.755160

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C	1.353798	-2.253187	-0.734333
C	0.479044	-1.180409	-0.924627
C	-0.665634	-1.043621	-0.134163
C	-0.962092	-2.037451	0.812759
C	-0.091689	-3.111199	1.007818
C	1.067993	-3.210724	0.245640
C	-1.611220	0.091889	-0.298288
S	-2.447076	-1.896845	1.780316
C	-3.524797	-1.272042	0.508851
C	-3.023364	-0.370348	-0.448668
C	-3.862425	-0.004812	-1.510127
H	-3.469868	0.623495	-2.311568
C	-5.185905	-0.436007	-1.560587
C	-5.689874	-1.267468	-0.559838
C	-4.853087	-1.704332	0.464095
H	0.694776	-0.442729	-1.698595
H	-0.327898	-3.881559	1.745348
H	1.749798	-4.052636	0.378121
H	-6.727618	-1.606525	-0.594227
H	-5.223864	-2.401620	1.219175
C	-1.258089	1.398727	-0.255375
C	0.079673	2.014862	-0.035219
C	-2.172287	2.578985	-0.573888
C	0.120549	3.209322	-0.738999
H	-3.021390	2.287866	-1.198320
C	-1.220918	3.519127	-1.346631
H	-1.488536	4.581902	-1.244510
C	1.182180	1.640352	0.796941
C	2.371809	2.431393	0.723810

C	2.407084	3.587853	-0.106452
C	1.292041	3.994232	-0.798201
C	3.500300	2.063961	1.509290
C	3.444172	0.995697	2.370513
C	2.238452	0.266221	2.508024
C	1.139698	0.581049	1.744870
H	-1.228980	3.279717	-2.423947
H	3.330233	4.171723	-0.149363
H	1.305059	4.915537	-1.385736
H	4.414112	2.657519	1.421829
H	4.316844	0.722568	2.968222
H	2.178001	-0.548970	3.232816
H	0.211287	0.031707	1.886452
C	-2.714399	3.220054	0.706443
H	-3.326433	2.501797	1.272868
H	-1.898458	3.561496	1.363273
H	-3.344732	4.089966	0.465520
H	-5.824488	-0.127299	-2.391219
O	2.431711	-2.427218	-1.544481
C	3.692031	-1.775580	-1.243206
C	4.648041	-2.344986	-2.282838
H	4.286381	-2.124664	-3.298324
H	5.649293	-1.905194	-2.165994
H	4.730575	-3.436696	-2.173453
C	4.152773	-2.127457	0.169274
H	3.449149	-1.749353	0.925330
H	4.252613	-3.216508	0.293150
H	5.132590	-1.667211	0.365997
C	3.551855	-0.264205	-1.401849
H	3.179162	-0.010587	-2.405976
H	2.860296	0.149497	-0.655817
H	4.527334	0.224653	-1.260476

*anti-(M)-stable-Z**

C	1.411927	-1.993705	-1.239713
C	0.524963	-0.925931	-1.207507
C	-0.729241	-1.010542	-0.552213
C	-1.065532	-2.266036	0.023172
C	-0.180297	-3.341890	-0.022130
C	1.059523	-3.209032	-0.635563
C	-1.599907	0.146487	-0.460978
S	-2.529213	-2.453756	0.962871
C	-3.570690	-1.234370	0.254316
C	-3.041800	-0.069125	-0.365346
C	-3.996185	0.848204	-0.869359
H	-3.656073	1.717064	-1.423915
C	-5.360947	0.653129	-0.723041
C	-5.848022	-0.479679	-0.067466
C	-4.947822	-1.425428	0.406209
H	0.784591	-0.003882	-1.724089
H	-0.464073	-4.292111	0.435968
H	1.764800	-4.040299	-0.674957
H	-6.921250	-0.635539	0.056044
H	-5.308566	-2.331829	0.898088
C	-0.984735	1.441244	-0.479518
C	0.241605	1.758413	0.172184
C	-1.420077	2.705098	-1.223461
C	0.818849	2.908094	-0.433191
H	-1.969536	2.464707	-2.145621
C	-0.068919	3.375869	-1.547248
H	-0.135074	4.472073	-1.622181
C	0.929333	1.121406	1.281952
C	2.220303	1.636247	1.646003
C	2.758126	2.757481	0.974273
C	2.057334	3.399261	-0.045018

C	2.924683	1.021668	2.721462
C	2.371881	-0.016204	3.433719
C	1.078704	-0.479124	3.113612
C	0.374908	0.089905	2.067590
H	0.321205	3.002725	-2.511760
H	3.736413	3.133538	1.284386
H	2.485930	4.271168	-0.544701
H	3.916522	1.402115	2.978698
H	2.926828	-0.474140	4.255547
H	0.625847	-1.287171	3.691608
H	-0.637908	-0.256417	1.859965
C	-2.256939	3.644613	-0.334539
H	-3.152253	3.153372	0.069014
H	-1.650051	3.981461	0.520057
H	-2.572966	4.532014	-0.905030
H	-6.054918	1.388995	-1.134832
O	2.601649	-1.921834	-1.889335
C	3.701556	-1.171559	-1.323101
C	4.920758	-1.715667	-2.059383
H	4.804990	-1.568102	-3.142901
H	5.834895	-1.200801	-1.729593
H	5.032695	-2.792679	-1.869010
C	3.806733	-1.428253	0.178121
H	2.912176	-1.073083	0.710161
H	3.931679	-2.502185	0.382877
H	4.674590	-0.892763	0.589736
C	3.528010	0.320268	-1.609423
H	3.352623	0.482838	-2.683265
H	2.689887	0.745911	-1.043378
H	4.432721	0.872746	-1.314671

syn-(P)-unstable-E

C	3.396537	0.091816	-0.853606
C	2.014791	-0.052713	-0.717129
C	1.237211	0.955778	-0.136197
C	1.858022	2.157084	0.228023
C	3.235632	2.321650	0.072309
C	4.004494	1.286239	-0.451500
C	-0.220721	0.736957	0.045696
S	0.870234	3.441250	0.930839
C	-0.637438	3.182599	0.025620
C	-1.074075	1.894102	-0.370915
C	-2.299694	1.827798	-1.048480
H	-2.670743	0.871406	-1.399472
C	-3.070062	2.961295	-1.299232
C	-2.630629	4.214643	-0.883603
C	-1.406988	4.321383	-0.230039
H	1.535765	-0.971690	-1.057526
H	3.711184	3.263564	0.355714
H	5.081586	1.405638	-0.581735
H	-3.224068	5.110327	-1.079372
H	-1.036474	5.300665	0.082698
C	-0.638709	-0.389393	0.692429
C	-1.990771	-0.994182	0.742562
C	0.125745	-1.100965	1.825249
C	-2.242255	-1.419546	2.036489
H	0.368667	-2.129865	1.502491
C	-1.016910	-1.215572	2.877163
H	-1.076217	-0.272426	3.449349
C	-2.866740	-1.382848	-0.317596
C	-4.109766	-1.993050	0.039077
C	-4.401405	-2.258359	1.407013
C	-3.467287	-2.021199	2.389325
C	-5.005446	-2.391305	-0.993824
C	-4.662936	-2.256396	-2.316846

C	-3.394397	-1.732135	-2.669201
C	-2.521627	-1.306059	-1.697022
H	-0.850996	-2.031178	3.596514
H	-5.361546	-2.717869	1.655686
H	-3.663240	-2.305118	3.426056
H	-5.965388	-2.831992	-0.712116
H	-5.354488	-2.576469	-3.099450
H	-3.107776	-1.670903	-3.721622
H	-1.541359	-0.912581	-1.975556
C	1.359803	-0.459473	2.444159
H	2.254014	-0.534625	1.813445
H	1.184802	0.604658	2.665912
H	1.583379	-0.968676	3.394824
H	-4.020408	2.853845	-1.826621
O	4.143417	-0.882207	-1.438908
C	4.620091	-2.004830	-0.654720
C	5.518185	-2.760053	-1.626243
H	5.943547	-3.653697	-1.147014
H	4.945215	-3.077436	-2.510518
H	6.344402	-2.116496	-1.963490
C	5.416441	-1.513163	0.551983
H	4.779932	-0.955962	1.256190
H	5.843768	-2.371067	1.091977
H	6.242677	-0.858041	0.237008
C	3.453397	-2.884692	-0.205885
H	2.805837	-2.364253	0.514711
H	2.843632	-3.194790	-1.067813
H	3.838264	-3.789790	0.287208

TS4

C	3.606753	2.400310	-0.791188
C	2.596585	1.461829	-0.925792
C	1.262620	1.697876	-0.521072
C	0.983828	3.018793	-0.113682
C	2.003316	3.974298	0.033220
C	3.317873	3.664670	-0.273988
C	0.228093	0.629967	-0.659873
S	-0.630018	3.657895	0.143049
C	-1.669959	2.281688	-0.185625
C	-1.206703	0.980978	-0.474450
C	-2.184142	-0.034553	-0.420357
H	-1.895200	-1.076382	-0.513604
C	-3.538487	0.213428	-0.237929
C	-3.979562	1.531544	-0.079493
C	-3.039002	2.546357	-0.027233
H	4.621090	2.148494	-1.107525
H	2.850364	0.505585	-1.376923
H	1.745433	4.980555	0.374467
H	4.101197	4.415703	-0.152092
H	-5.043474	1.743929	0.034634
H	-3.365965	3.572814	0.159735
C	0.600580	-0.668251	-0.960718
C	1.824944	-1.371651	-0.525122
C	-0.093558	-1.631131	-1.944018
C	2.113194	-2.406067	-1.401198
H	-0.725161	-2.352100	-1.393338
C	1.103006	-2.444971	-2.503235
H	1.501802	-1.947445	-3.405307
C	2.588074	-1.227927	0.684275
C	3.719080	-2.083983	0.861614
C	4.022084	-3.080536	-0.112093
C	3.219437	-3.260564	-1.211730
C	4.514831	-1.952515	2.033161
C	4.194663	-1.037244	3.006685
C	3.045806	-0.226067	2.856880

C	2.265817	-0.318016	1.727113
H	0.820303	-3.467587	-2.794089
H	4.892963	-3.720814	0.050536
H	3.432011	-4.050831	-1.935705
H	5.384412	-2.604687	2.149491
H	4.811849	-0.946739	3.903486
H	2.771559	0.476462	3.647242
H	1.376095	0.304458	1.639243
C	-0.895909	-1.007163	-3.081577
H	-1.840131	-0.553481	-2.757015
H	-0.304057	-0.230948	-3.591708
H	-1.143330	-1.783301	-3.822292
O	-4.427388	-0.816284	-0.277108
C	-4.787077	-1.513239	0.943016
C	-5.807989	-2.542192	0.475610
H	-6.160505	-3.149069	1.322348
H	-6.675330	-2.043754	0.017503
H	-5.360427	-3.213938	-0.272083
C	-3.563808	-2.202042	1.546351
H	-3.098235	-2.882334	0.816952
H	-2.809975	-1.472799	1.878273
H	-3.862951	-2.794129	2.424265
C	-5.411623	-0.548044	1.948779
H	-4.685833	0.203094	2.294811
H	-6.274225	-0.026660	1.507110
H	-5.761501	-1.103620	2.831666

intermediate-*E*

C	2.597299	-2.221050	2.341442
C	1.835100	-1.163198	1.853315
C	1.009280	-1.325525	0.732546
C	0.914227	-2.604061	0.159382
C	1.673803	-3.670402	0.644698
C	2.527531	-3.472709	1.728232
C	0.217088	-0.180428	0.213415
S	-0.130667	-2.817343	-1.250841
C	-1.456547	-1.737895	-0.763035
C	-1.214619	-0.533043	-0.058465
C	-2.332253	0.226449	0.295529
H	-2.237556	1.136707	0.878975
C	-3.643228	-0.129735	-0.062752
C	-3.850507	-1.307527	-0.787113
C	-2.752937	-2.101211	-1.115926
H	3.249233	-2.067645	3.204038
H	1.889804	-0.182106	2.330858
H	1.591277	-4.654642	0.177606
H	3.124331	-4.305939	2.105940
H	-4.841751	-1.639536	-1.085419
H	-2.921918	-3.037046	-1.654091
C	0.751849	1.063032	0.017269
C	2.167093	1.491771	-0.157902
C	-0.074462	2.348645	0.126449
C	2.213421	2.881692	-0.212463
H	-1.001105	2.295057	-0.461745
C	0.844843	3.475861	-0.350199
H	0.708065	4.405560	0.221887
C	3.391293	0.766757	-0.400061
C	4.623522	1.493546	-0.343808
C	4.614103	2.911427	-0.202372
C	3.429126	3.599892	-0.210141
C	5.855453	0.804356	-0.517063
C	5.881786	-0.534338	-0.825501
C	4.663841	-1.225841	-1.011922
C	3.459486	-0.593729	-0.804496
H	0.679319	3.724669	-1.412231

H	5.569236	3.440735	-0.155718
H	3.413189	4.692355	-0.199376
H	6.785762	1.372130	-0.431241
H	6.833739	-1.050730	-0.968139
H	4.673856	-2.269641	-1.334852
H	2.540795	-1.135719	-1.004710
C	-0.406084	2.592766	1.611109
H	-0.861463	1.720249	2.098154
H	0.516769	2.822461	2.167954
H	-1.090074	3.448715	1.719151
O	-4.579406	0.737080	0.367674
C	-5.987045	0.719679	0.047676
C	-6.491413	2.005804	0.699185
H	-5.985379	2.880405	0.264263
H	-7.574205	2.116732	0.544345
H	-6.292082	1.991599	1.780976
C	-6.678657	-0.483247	0.690616
H	-6.375504	-1.441138	0.248764
H	-6.460268	-0.515758	1.768514
H	-7.767468	-0.390366	0.563846
C	-6.213731	0.793495	-1.462967
H	-5.637355	1.626520	-1.892804
H	-5.935401	-0.128224	-1.989980
H	-7.279884	0.978038	-1.660977

TS5

C	1.779202	3.282835	-1.968719
C	1.261480	2.005575	-1.766877
C	0.816344	1.610898	-0.498447
C	0.775919	2.567040	0.528575
C	1.317380	3.840251	0.339237
C	1.840030	4.186696	-0.905986
C	0.241642	0.262550	-0.242177
S	-0.067018	2.124128	2.030069
C	-1.432928	1.273542	1.256004
C	-1.199380	0.433582	0.145403
C	-2.294984	-0.138794	-0.493875
H	-2.161210	-0.761095	-1.378315
C	-3.607496	0.039657	-0.022811
C	-3.815082	0.834264	1.111974
C	-2.728228	1.454991	1.729074
H	2.146546	3.571110	-2.955963
H	1.238522	1.282357	-2.585361
H	1.298696	4.570396	1.151691
H	2.260175	5.183741	-1.056245
H	-4.807589	1.008634	1.519414
H	-2.908228	2.105341	2.588419
C	0.864395	-0.945285	-0.161271
C	2.293736	-1.402814	0.015683
C	0.020819	-2.223901	-0.107203
C	2.249939	-2.707227	0.506059
H	-0.948231	-2.041703	0.371210
C	0.855959	-3.214754	0.696840
H	0.735058	-4.255660	0.360242
C	3.595725	-0.783949	-0.121664
C	4.760833	-1.560032	0.200623
C	4.636966	-2.897424	0.666630
C	3.400913	-3.457478	0.829267
C	6.057867	-0.991445	0.068196
C	6.232451	0.303548	-0.352890
C	5.095000	1.080687	-0.657768
C	3.830472	0.550816	-0.542515
H	0.598299	-3.187701	1.769386
H	5.544656	-3.459384	0.900709
H	3.288474	-4.477420	1.204717

H	6.920748	-1.614091	0.319166
H	7.234012	0.729099	-0.447202
H	5.211544	2.116351	-0.986457
H	2.988058	1.181803	-0.779392
C	-0.220772	-2.751345	-1.528508
H	-0.687862	-1.993753	-2.173946
H	0.727101	-3.050057	-2.004439
H	-0.879340	-3.633503	-1.502690
O	-4.544303	-0.590318	-0.755634
C	-5.946922	-0.726445	-0.440245
C	-6.449959	-1.645221	-1.552411
H	-5.918940	-2.608137	-1.525263
H	-7.526693	-1.835343	-1.436546
H	-6.281080	-1.184021	-2.536835
C	-6.661720	0.622843	-0.532146
H	-6.375172	1.319264	0.266246
H	-6.447890	1.101079	-1.499729
H	-7.748335	0.467143	-0.460068
C	-6.144884	-1.407496	0.914243
H	-5.574980	-2.348065	0.955533
H	-5.837965	-0.780827	1.761508
H	-7.209956	-1.646044	1.050410

syn-(*M*)-stable-*E*

C	3.568094	-0.075352	0.234758
C	2.202125	-0.225278	0.531091
C	1.228528	0.503327	-0.143641
C	1.621465	1.439340	-1.116380
C	2.971215	1.597881	-1.414740
C	3.943967	0.842501	-0.756493
C	-0.231285	0.329148	0.097647
S	0.367800	2.368137	-1.970718
C	-0.732207	2.641596	-0.598157
C	-0.914570	1.631137	0.370968
C	-1.665610	1.947882	1.506774
H	-1.741625	1.226994	2.316585
C	-2.312020	3.177034	1.626582
C	-2.192401	4.131868	0.618539
C	-1.381311	3.872975	-0.484120
H	1.915687	-0.945678	1.299632
H	3.285220	2.323907	-2.168430
H	4.986236	1.001889	-1.021615
H	-2.699429	5.095376	0.705367
H	-1.231099	4.638459	-1.249314
C	-0.832347	-0.830200	-0.263668
C	-2.281312	-1.137275	-0.394850
C	-0.136240	-1.894648	-1.109814
C	-2.465929	-1.725344	-1.636032
H	0.837180	-1.534904	-1.466590
C	-1.138015	-2.014600	-2.286826
H	-1.116482	-3.001784	-2.773331
C	-3.381055	-1.005587	0.503959
C	-4.692217	-1.263596	-0.006027
C	-4.852251	-1.721393	-1.344868
C	-3.758658	-1.996664	-2.132448
C	-5.809274	-1.127437	0.866365
C	-5.634897	-0.829184	2.195880
C	-4.328146	-0.679900	2.722656
C	-3.233268	-0.765453	1.896726
H	-0.908001	-1.257922	-3.056129
H	-5.863079	-1.908166	-1.716606
H	-3.884765	-2.421858	-3.131229
H	-6.811422	-1.292464	0.461721
H	-6.499540	-0.740550	2.857707
H	-4.191196	-0.508783	3.792935

H	-2.226635	-0.695835	2.309840
C	0.066677	-3.220032	-0.376814
H	0.752565	-3.095387	0.474668
H	-0.884798	-3.620194	0.009007
H	0.500572	-3.971982	-1.053901
H	-2.905379	3.388937	2.518757
O	4.379427	-0.859040	0.967082
C	5.818621	-0.942329	0.888456
C	6.144201	-1.989287	1.952033
H	5.643496	-2.940607	1.718941
H	7.228067	-2.166986	2.000422
H	5.800095	-1.650598	2.940591
C	6.470454	0.388913	1.265970
H	6.342402	1.167054	0.502259
H	6.052232	0.761549	2.213182
H	7.551270	0.239197	1.405678
C	6.266430	-1.449686	-0.482572
H	5.739299	-2.382307	-0.733917
H	6.090770	-0.725575	-1.288578
H	7.345573	-1.661783	-0.458558

TS5'

C	-3.632291	0.094707	-0.123477
C	-2.314592	0.353582	0.288003
C	-1.215977	-0.229598	-0.336729
C	-1.464138	-1.249309	-1.281147
C	-2.764944	-1.516301	-1.697600
C	-3.848424	-0.820705	-1.160697
C	0.223087	0.020120	0.009020
S	-0.120791	-2.298189	-1.799849
C	0.679239	-2.414023	-0.212531
C	0.809580	-1.236849	0.547368
C	1.432858	-1.306058	1.795953
H	1.519765	-0.397915	2.396829
C	1.966530	-2.509536	2.253962
C	1.870384	-3.660702	1.471745
C	1.216369	-3.619137	0.239595
H	-2.178255	1.016898	1.138276
H	-2.949312	-2.298981	-2.437327
H	-4.846532	-1.045861	-1.528948
H	2.290304	-4.603691	1.828930
H	1.117262	-4.524562	-0.363620
C	0.907126	1.166794	-0.258505
C	2.381459	1.418879	-0.183627
C	0.244155	2.514013	-0.636201
C	2.612541	2.781729	-0.299635
H	-0.301008	2.388087	-1.585319
C	1.412245	3.507247	-0.807327
H	1.235085	4.454666	-0.277308
C	3.537317	0.555169	-0.099196
C	4.796133	1.148440	0.239152
C	4.921570	2.565601	0.322065
C	3.868297	3.369406	-0.024012
C	5.945513	0.324636	0.390301
C	5.895901	-1.020591	0.114623
C	4.692716	-1.581589	-0.367618
C	3.553836	-0.816076	-0.469091
H	1.582420	3.768388	-1.865289
H	5.891274	2.994713	0.586626
H	3.981491	4.455073	-0.072906
H	6.885057	0.794803	0.692630
H	6.789177	-1.640622	0.219144
H	4.663921	-2.629513	-0.675572
H	2.660093	-1.260138	-0.893297
C	-0.723738	3.099219	0.403777

H	-1.712220	2.637170	0.375755
H	-0.316206	3.004994	1.423358
H	-0.873995	4.170046	0.200487
H	2.466104	-2.547593	3.224338
O	-4.566729	0.802894	0.539469
C	-5.983539	0.524107	0.591090
C	-6.468895	1.467502	1.689649
H	-6.246716	2.512183	1.425512
H	-7.554328	1.366712	1.832693
H	-5.967754	1.238257	2.641693
C	-6.660165	0.890663	-0.730980
H	-6.389194	1.916041	-1.024199
H	-6.394389	0.213987	-1.553564
H	-7.752566	0.847610	-0.608083
C	-6.248306	-0.923512	1.002914
H	-5.951048	-1.650299	0.235862
H	-5.708860	-1.161015	1.932264
H	-7.324154	-1.058538	1.187808

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C	-3.606503	0.049013	-0.140819
C	-2.274493	0.385445	0.140521
C	-1.209273	-0.332635	-0.395079
C	-1.487900	-1.513525	-1.109754
C	-2.806964	-1.861232	-1.390859
C	-3.865333	-1.069512	-0.945255
C	0.223275	-0.007711	-0.133739
S	-0.145619	-2.599089	-1.549481
C	0.791615	-2.427633	-0.044168
C	0.894487	-1.155031	0.543932
C	1.593064	-1.026159	1.748307
H	1.653174	-0.046574	2.227383
C	2.235776	-2.123301	2.316390
C	2.172174	-3.370511	1.693423
C	1.437748	-3.529711	0.519254
H	-2.088852	1.242220	0.787472
H	-3.023552	-2.773558	-1.951687
H	-4.881094	-1.363182	-1.201923
H	2.676367	-4.232566	2.135903
H	1.355666	-4.511784	0.047701
C	0.876368	1.119327	-0.503768
C	2.306061	1.437494	-0.197548
C	0.373257	2.430991	-1.116437
C	2.386534	2.788417	0.095704
H	0.894177	2.481263	-2.090652
C	1.078785	3.465663	-0.209502
H	0.484850	3.630403	0.707547
C	3.491054	0.639349	-0.223201
C	4.694130	1.222265	0.282940
C	4.701623	2.583885	0.702743
C	3.582055	3.369868	0.571076
C	5.885714	0.443280	0.303301
C	5.904928	-0.831915	-0.206467
C	4.733454	-1.377275	-0.786771
C	3.560977	-0.661330	-0.795032
H	1.212395	4.442293	-0.698872
H	5.633441	3.006843	1.087118
H	3.611967	4.431456	0.828553
H	6.794127	0.889778	0.716491
H	6.827808	-1.416463	-0.191423
H	4.764312	-2.371223	-1.239089
H	2.674469	-1.079368	-1.269939
C	-1.086886	2.747859	-1.389430
H	-1.572676	1.982998	-2.009739
H	-1.673693	2.874696	-0.470743

H	-1.134550	3.700601	-1.940167
H	2.790437	-2.003544	3.249521
O	-4.521872	0.889953	0.380757
C	-5.895108	0.567158	0.697920
C	-6.307197	1.715913	1.616232
H	-6.173974	2.680951	1.104998
H	-7.363592	1.618189	1.905434
H	-5.693093	1.720332	2.529266
C	-5.994846	-0.759101	1.450054
H	-5.777435	-1.628358	0.815276
H	-5.298571	-0.769988	2.302307
H	-7.015835	-0.880685	1.840826
C	-6.757025	0.587455	-0.565223
H	-6.619446	1.537778	-1.102324
H	-6.522194	-0.234790	-1.253585
H	-7.819051	0.497291	-0.292467

TS6

C	3.577262	0.038518	-0.369954
C	2.195214	-0.108672	-0.366647
C	1.292585	0.967485	-0.459156
C	1.881550	2.247252	-0.412751
C	3.274565	2.411027	-0.437712
C	4.128588	1.320457	-0.446698
C	-0.181093	0.702414	-0.509382
S	0.980025	3.737828	-0.231155
C	-0.674768	3.180949	-0.054083
C	-1.116627	1.856190	-0.279368
C	-2.518316	1.722689	-0.399276
H	-2.937653	0.775556	-0.714801
C	-3.414106	2.754922	-0.164442
C	-2.943014	4.019154	0.186061
C	-1.574454	4.227414	0.210679
H	1.820696	-1.117911	-0.266571
H	3.693095	3.421050	-0.433085
H	5.210669	1.454509	-0.479505
H	-3.630045	4.840658	0.399217
H	-1.178389	5.226357	0.412769
C	-0.630938	-0.566015	-0.812913
C	-1.973349	-1.164403	-0.605395
C	0.033271	-1.571978	-1.773674
C	-2.314532	-1.896304	-1.729836
H	0.863050	-1.109018	-2.324331
C	-1.173077	-1.865692	-2.709854
H	-1.060299	-2.807659	-3.266713
C	-2.799049	-1.199051	0.560017
C	-4.037260	-1.905447	0.474943
C	-4.390061	-2.576880	-0.732030
C	-3.539991	-2.589549	-1.813432
C	-4.892764	-1.934311	1.611846
C	-4.535992	-1.303273	2.779284
C	-3.296769	-0.623348	2.868281
C	-2.450290	-0.571271	1.785950
H	-1.300055	-1.050381	-3.442185
H	-5.344914	-3.107120	-0.773470
H	-3.800373	-3.139599	-2.720951
H	-5.842435	-2.470923	1.539138
H	-5.203019	-1.330389	3.644080
H	-3.013004	-0.137943	3.804915
H	-1.495064	-0.048738	1.862618
C	0.489118	-2.904823	-1.161742
H	1.267815	-2.803353	-0.393804
H	-0.356968	-3.431509	-0.693676
H	0.892941	-3.555042	-1.952495
H	-4.484658	2.566063	-0.266305

O	4.373742	-1.064880	-0.359423
C	4.839390	-1.616047	0.897973
C	3.658162	-2.053164	1.763008
H	4.026436	-2.555042	2.670015
H	3.046742	-1.195678	2.081714
H	3.013825	-2.758806	1.216829
C	5.668485	-2.820769	0.471892
H	6.496077	-2.504999	-0.180891
H	6.090552	-3.330449	1.350192
H	5.045350	-3.537442	-0.083669
C	5.705116	-0.600188	1.640969
H	6.539262	-0.261336	1.008052
H	5.122373	0.279145	1.954096
H	6.126518	-1.059918	2.547352

motor 3

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C	1.169507	2.590111	2.115150
C	0.648881	1.346216	1.768956
C	-0.236354	1.215888	0.692914
C	-0.641277	2.375848	0.011484
C	-0.119886	3.625931	0.352990
C	0.797570	3.727713	1.396906
C	-0.767977	-0.100866	0.252010
S	-1.785089	2.229097	-1.340379
C	-2.818416	0.941104	-0.678049
C	-2.252200	-0.090339	0.090244
C	-3.116978	-1.009027	0.701376
H	-2.700778	-1.762339	1.373988
C	-5.022396	0.013985	-0.345694
C	-4.196785	0.982581	-0.904994
H	1.875766	2.671400	2.944175
H	0.949682	0.451943	2.319176
H	-0.437390	4.518404	-0.191464
H	1.208649	4.704501	1.661376
H	-6.099517	0.056113	-0.528304
H	-4.626385	1.789112	-1.504185
C	0.009248	-1.172606	-0.036032
C	1.491056	-1.298112	0.017075
C	-0.485836	-2.583616	-0.340315
C	1.798315	-2.605379	0.360166
H	-1.488102	-2.762597	0.058375
C	0.557554	-3.457045	0.393156
H	0.713097	-4.434757	-0.088539
C	2.540807	-0.373555	-0.285557
C	3.883499	-0.778540	-0.008914
C	4.144614	-2.097522	0.463348
C	3.128826	-3.011505	0.604086
C	4.948581	0.130991	-0.261853
C	4.708413	1.362795	-0.820632
C	3.388234	1.727429	-1.179216
C	2.335870	0.882475	-0.919646
H	0.241653	-3.650061	1.432762
H	5.180188	-2.383300	0.665828
H	3.341266	-4.040978	0.902689
H	5.969250	-0.178702	-0.021942
H	5.534430	2.050557	-1.015882
H	3.204983	2.684517	-1.673165
H	1.330572	1.162299	-1.229439
C	-0.515409	-2.846597	-1.848163
H	-1.222762	-2.166774	-2.347066
H	0.476798	-2.697310	-2.303495
H	-0.832378	-3.880684	-2.053487
C	-4.497142	-0.984503	0.486694

C	-5.401266	-2.007179	1.121768
H	-6.292814	-1.534880	1.561037
H	-5.755294	-2.735484	0.374049
H	-4.883809	-2.566597	1.914015

*anti-(M)-stable-E**

C	1.736848	2.040648	2.316705
C	1.024721	0.944101	1.863769
C	-0.086942	1.075508	0.986035
C	-0.450485	2.404875	0.636075
C	0.269713	3.507460	1.094303
C	1.374850	3.331671	1.922862
C	-0.770482	-0.089337	0.451930
S	-1.716001	2.704292	-0.536438
C	-2.712040	1.271406	-0.367407
C	-2.175525	0.033561	0.072431
C	-3.081404	-1.054416	0.113138
H	-2.740875	-2.004622	0.513282
C	-4.884054	0.274951	-0.752362
C	-4.044860	1.379430	-0.775462
H	2.587868	1.889345	2.983931
H	1.312704	-0.055216	2.191674
H	-0.037536	4.511262	0.791319
H	1.939133	4.198841	2.271077
H	-5.922669	0.376651	-1.076830
H	-4.422078	2.347075	-1.115040
C	-0.015297	-1.302045	0.341705
C	1.365642	-1.345031	-0.000477
C	-0.429906	-2.740762	0.656936
C	1.946225	-2.536367	0.510790
H	-1.210906	-2.778676	1.430204
C	0.884508	-3.356160	1.182247
H	0.973058	-4.433627	0.973948
C	2.204050	-0.384911	-0.694932
C	3.619500	-0.621397	-0.694066
C	4.144956	-1.797141	-0.111879
C	3.315323	-2.758111	0.464579
C	4.471456	0.326780	-1.331609
C	3.953610	1.421117	-1.982467
C	2.556626	1.610868	-2.042703
C	1.705617	0.717378	-1.419166
H	0.956313	-3.228628	2.277498
H	5.225805	-1.957375	-0.142162
H	3.742116	-3.666373	0.896974
H	5.551214	0.158937	-1.305738
H	4.621683	2.136852	-2.466916
H	2.142023	2.466041	-2.580353
H	0.627215	0.864659	-1.497200
C	-0.892865	-3.500007	-0.599849
H	-1.741880	-3.008731	-1.094652
H	-0.067882	-3.548825	-1.327149
H	-1.187561	-4.529310	-0.341436
C	-4.408213	-0.961010	-0.290140
C	-5.320672	-2.158186	-0.236735
H	-6.235517	-1.937068	0.334104
H	-5.633374	-2.456958	-1.249878
H	-4.828229	-3.022172	0.230845

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C	-3.645847	-1.676496	2.296244
C	-2.382642	-1.348013	1.811136
C	-2.229914	-0.491408	0.711757
C	-3.381946	0.079083	0.151761
C	-4.653169	-0.243877	0.632619

C	-4.783423	-1.133432	1.697119
C	-0.870594	-0.184514	0.194622
S	-3.204092	1.179520	-1.217763
C	-1.668914	1.956932	-0.773720
C	-0.634869	1.265093	-0.097298
C	0.536028	1.983796	0.164868
H	1.344868	1.505712	0.705518
C	0.729268	3.309168	-0.240081
C	-0.305384	3.953480	-0.920123
C	-1.498440	3.282909	-1.174526
H	-3.742864	-2.359129	3.143207
H	-1.489342	-1.774391	2.273971
H	-5.539212	0.206218	0.178597
H	-5.777966	-1.385422	2.072091
H	-0.189770	4.991557	-1.242358
H	-2.313841	3.799066	-1.687452
C	-0.023985	-1.210366	-0.109984
C	1.436398	-1.166366	-0.364107
C	-0.445661	-2.592868	-0.641891
C	1.720847	-1.963981	-1.459936
H	-0.096754	-3.367575	0.064393
C	0.475502	-2.678689	-1.895192
H	-0.012571	-2.161802	-2.740770
C	2.501791	-0.654208	0.438565
C	3.832264	-0.771417	-0.072084
C	4.061812	-1.457631	-1.298021
C	3.032873	-2.087583	-1.960332
C	4.914448	-0.254316	0.696313
C	4.702537	0.286274	1.940679
C	3.394728	0.315825	2.486076
C	2.324402	-0.139790	1.754671
H	0.667919	-3.716242	-2.206352
H	5.085975	-1.528876	-1.673355
H	3.228554	-2.683441	-2.855067
H	5.925059	-0.319275	0.284474
H	5.542487	0.669378	2.524566
H	3.238628	0.700969	3.496427
H	1.320355	-0.120000	2.184343
C	-1.894429	-2.867571	-1.017353
H	-2.548155	-3.010809	-0.148475
H	-2.307989	-2.051675	-1.630351
H	-1.935237	-3.791929	-1.615350
C	2.039080	3.993890	0.047297
H	2.357827	3.825193	1.087119
H	2.836950	3.598706	-0.602298
H	1.973970	5.077903	-0.123153

TS1

C	1.080819	2.636193	-1.510595
C	0.635560	1.358714	-1.196751
C	-0.586368	1.081874	-0.542020
C	-1.439077	2.187200	-0.365178
C	-1.010765	3.489691	-0.670886
C	0.244451	3.720130	-1.204130
C	-0.959558	-0.322128	-0.195918
S	-3.121056	2.079261	0.125735
C	-3.361688	0.359686	0.377263
C	-2.342811	-0.611639	0.271978
C	-2.665825	-1.882265	0.801713
H	-1.884326	-2.633016	0.890284
C	-3.935016	-2.218003	1.246917
C	-4.955938	-1.266368	1.217328
C	-4.654922	0.023261	0.809870
H	1.275442	0.527424	-1.483412
H	-1.689585	4.329021	-0.496506

H	0.561857	4.742784	-1.424008
H	-5.966034	-1.514132	1.550300
H	-5.423016	0.800416	0.847473
C	-0.033742	-1.342906	-0.320988
C	1.423456	-1.264373	-0.089365
C	-0.278885	-2.754805	-0.888345
C	2.070033	-2.265102	-0.797047
H	-0.385632	-3.488995	-0.069117
C	1.076588	-3.068557	-1.574876
H	1.046819	-2.728097	-2.625449
C	2.167309	-0.445205	0.827457
C	3.586540	-0.609455	0.865889
C	4.213700	-1.602653	0.057655
C	3.469163	-2.436201	-0.740752
C	4.358646	0.207351	1.737824
C	3.757672	1.130017	2.559707
C	2.349014	1.258560	2.558971
C	1.576545	0.492729	1.716544
H	1.303820	-4.144897	-1.588558
H	5.300467	-1.708001	0.109024
H	3.949585	-3.221899	-1.328856
H	5.444254	0.078794	1.748352
H	4.361490	1.752205	3.224303
H	1.869404	1.968405	3.236974
H	0.492222	0.598077	1.740902
C	-1.429653	-2.918490	-1.875940
H	-2.420466	-2.868978	-1.408604
H	-1.383813	-2.142092	-2.655748
H	-1.348832	-3.898751	-2.370954
H	-4.122205	-3.221719	1.634068
C	2.418138	2.854413	-2.165558
H	2.940799	1.902821	-2.336950
H	2.309921	3.366676	-3.134587
H	3.064408	3.485768	-1.535282

intermediate-Z

C	-4.687699	1.634575	0.235680
C	-3.328524	1.542528	0.527822
C	-2.522096	0.513627	0.010648
C	-3.178901	-0.466641	-0.771701
C	-4.541713	-0.374469	-1.068016
C	-5.298403	0.685406	-0.579258
C	-1.038182	0.375010	0.179862
S	-2.307032	-1.856406	-1.453535
C	-1.150004	-2.122790	-0.143281
C	-0.612818	-1.007263	0.517323
C	0.305874	-1.226516	1.549212
H	0.702924	-0.361112	2.086941
C	0.755090	-2.508161	1.882173
C	0.226569	-3.596617	1.179495
C	-0.731008	-3.411551	0.183375
H	-5.269598	2.457140	0.657064
H	-2.902724	2.292050	1.187738
H	-5.012617	-1.150464	-1.676326
H	-6.362939	0.752080	-0.813734
H	0.554818	-4.610356	1.423478
H	-1.153930	-4.274230	-0.336978
C	-0.148223	1.407014	0.056031
C	1.317137	1.393381	-0.212342
C	-0.510805	2.860895	0.375716
C	1.801324	2.695843	-0.137187
H	-1.438407	3.175712	-0.122519
C	0.690595	3.698902	-0.069253
H	0.898494	4.534905	0.615087
C	2.232667	0.357358	-0.628849

C	3.633401	0.652989	-0.610940
C	4.083440	1.978408	-0.344096
C	3.180343	2.996272	-0.182467
C	4.571686	-0.362450	-0.944991
C	4.155172	-1.600027	-1.372446
C	2.772796	-1.852215	-1.518837
C	1.844491	-0.903402	-1.156887
H	0.546196	4.134047	-1.072782
H	5.158330	2.176435	-0.335430
H	3.513713	4.030526	-0.068920
H	5.637391	-0.125861	-0.885458
H	4.884387	-2.368496	-1.638447
H	2.432691	-2.804410	-1.932849
H	0.792471	-1.109544	-1.325994
C	-0.658013	3.002248	1.903322
H	-1.341217	2.260963	2.339579
H	0.320145	2.857876	2.390021
H	-1.020970	4.008128	2.165646
C	1.794849	-2.691514	2.955173
H	1.978908	-3.755213	3.161449
H	2.750985	-2.235539	2.651925
H	1.489193	-2.207181	3.895379

TS2

C	4.489283	-1.676284	0.870158
C	3.161419	-1.352250	1.144469
C	2.384159	-0.650562	0.215844
C	3.005795	-0.213065	-0.972590
C	4.333088	-0.543363	-1.253417
C	5.071001	-1.289316	-0.336441
C	0.934481	-0.287936	0.364076
S	2.091781	0.799142	-2.125302
C	1.275760	1.813158	-0.913503
C	0.813428	1.190216	0.255516
C	0.390803	1.987969	1.322733
H	0.086581	1.502182	2.253975
C	0.290281	3.378565	1.200700
C	0.647101	3.962690	-0.021184
C	1.162663	3.194525	-1.064659
H	5.071919	-2.234648	1.606206
H	2.718365	-1.659581	2.092163
H	4.795450	-0.196357	-2.180419
H	6.111108	-1.541340	-0.554678
H	0.559839	5.044875	-0.148078
H	1.504750	3.676796	-1.983271
C	-0.039205	-1.237750	0.400820
C	-1.513935	-1.273644	0.070167
C	0.334827	-2.688935	0.720330
C	-1.848058	-2.605635	-0.171566
H	1.359713	-2.917025	0.405281
C	-0.680301	-3.532043	-0.044030
H	-0.937291	-4.470942	0.469298
C	-2.551460	-0.280200	-0.111452
C	-3.871449	-0.725325	-0.462680
C	-4.143572	-2.106222	-0.662779
C	-3.144357	-3.030029	-0.533761
C	-4.922613	0.218370	-0.630480
C	-4.707234	1.565593	-0.479007
C	-3.410020	2.016540	-0.155414
C	-2.378746	1.122401	0.018464
H	-0.309837	-3.799184	-1.048405
H	-5.159092	-2.409855	-0.929591
H	-3.333817	-4.092771	-0.702410
H	-5.915290	-0.158423	-0.890604
H	-5.523065	2.279456	-0.612961

H	-3.214404	3.085695	-0.042264
H	-1.400688	1.510755	0.256635
C	0.210070	-2.938730	2.230043
H	-0.830858	-2.802035	2.564922
H	0.510582	-3.969729	2.473161
H	0.835847	-2.250596	2.816345
C	-0.197804	4.207075	2.358369
H	0.536396	4.202588	3.179783
H	-0.367078	5.252309	2.064198
H	-1.140049	3.806673	2.763176

syn-(M)-stable-Z

C	-0.655157	3.391205	0.216714
C	-0.350559	2.100697	0.667619
C	0.621124	1.304913	0.060532
C	1.386999	1.881591	-0.976442
C	1.104323	3.167717	-1.434974
C	0.072753	3.906199	-0.858186
C	0.945345	-0.111361	0.410911
S	2.735186	0.988725	-1.718245
C	3.327155	0.136932	-0.277390
C	2.396401	-0.327873	0.665936
C	2.867417	-0.996371	1.801890
H	2.148069	-1.340988	2.548331
C	4.229199	-1.235641	1.973322
C	5.140741	-0.794937	1.012666
C	4.694073	-0.099106	-0.109428
H	-0.895685	1.710935	1.523092
H	1.703103	3.602067	-2.239236
H	-0.143173	4.909893	-1.233497
H	6.209439	-0.978331	1.144470
H	5.408021	0.266782	-0.851112
C	0.138533	-1.185840	0.225081
C	-1.275916	-1.238879	-0.227353
C	0.680251	-2.586523	-0.058870
C	-1.343223	-2.156198	-1.263712
H	1.769417	-2.564020	-0.191985
C	-0.029507	-2.880409	-1.407940
H	-0.165038	-3.956097	-1.598576
C	-2.468129	-0.641412	0.277472
C	-3.673243	-0.824868	-0.470828
C	-3.665998	-1.655376	-1.627378
C	-2.535899	-2.350595	-1.991727
C	-4.877786	-0.233116	0.005788
C	-4.909301	0.437807	1.203994
C	-3.738999	0.521088	1.999164
C	-2.552650	-0.002936	1.545466
H	0.559767	-2.462392	-2.241846
H	-4.597588	-1.782166	-2.184913
H	-2.559009	-3.050713	-2.830447
H	-5.788690	-0.348279	-0.587679
H	-5.842456	0.876041	1.565293
H	-3.785032	0.995822	2.982027
H	-1.663613	0.024638	2.177356
C	0.332873	-3.616247	1.014880
H	0.803131	-3.357555	1.975413
H	-0.755187	-3.681835	1.176259
H	0.692058	-4.614459	0.720442
H	4.581075	-1.766374	2.860715
C	-1.748082	4.180660	0.886158
H	-1.862648	5.174853	0.431753
H	-2.714449	3.657995	0.806870
H	-1.540919	4.317879	1.959007

TS2'

C	0.654968	-2.786331	1.588462
C	0.251943	-1.451796	1.463220
C	-0.567619	-1.035538	0.414271
C	-1.051455	-1.990896	-0.496194
C	-0.668463	-3.325665	-0.383798
C	0.188292	-3.711780	0.647277
C	-0.998578	0.376544	0.234877
S	-2.105292	-1.436751	-1.821043
C	-3.110166	-0.336670	-0.843326
C	-2.498547	0.417058	0.180175
C	-3.340441	1.004080	1.133027
H	-2.906260	1.445594	2.028073
C	-4.724771	1.007103	0.970012
C	-5.301913	0.382150	-0.134665
C	-4.494990	-0.325246	-1.022885
H	0.612449	-0.706323	2.177243
H	-1.041387	-4.066969	-1.094441
H	0.485534	-4.760634	0.729066
H	-6.385225	0.391306	-0.273854
H	-4.943252	-0.904997	-1.833231
C	-0.173918	1.434504	0.003615
C	1.313794	1.450462	-0.176171
C	-0.643271	2.908820	-0.042452
C	1.756110	2.764585	-0.134391
H	-1.352768	3.025000	-0.877413
C	0.634926	3.735437	-0.292128
H	0.719160	4.589688	0.395957
C	2.304255	0.426410	-0.424301
C	3.682338	0.763194	-0.227819
C	4.060578	2.112418	0.032212
C	3.121602	3.107796	-0.006224
C	4.683252	-0.232752	-0.396522
C	4.364066	-1.489838	-0.850234
C	3.024753	-1.778864	-1.193569
C	2.031143	-0.849786	-0.985155
H	0.668640	4.152420	-1.312500
H	5.118390	2.342334	0.183354
H	3.408269	4.158088	0.085816
H	5.723582	0.036943	-0.196185
H	5.142667	-2.243036	-0.991107
H	2.773128	-2.742616	-1.642430
H	1.021082	-1.080782	-1.306141
C	-1.309599	3.443481	1.233320
H	-2.347966	3.123548	1.340100
H	-0.751251	3.138786	2.133300
H	-1.322713	4.543383	1.202974
H	-5.354978	1.491232	1.719391
C	1.611570	-3.194622	2.675519
H	1.575803	-4.277673	2.860723
H	2.646141	-2.939425	2.391079
H	1.396468	-2.673409	3.619999

anti-(P)-unstable-Z

C	1.076973	-2.438196	1.695083
C	0.500859	-1.185003	1.472996
C	-0.450284	-0.983776	0.469576
C	-0.895648	-2.087625	-0.273116
C	-0.339693	-3.349946	-0.061370
C	0.651234	-3.513741	0.903432
C	-1.027711	0.354695	0.157414
S	-2.145754	-1.841380	-1.517263
C	-3.147527	-0.674431	-0.619849
C	-2.519152	0.294028	0.185641
C	-3.319978	1.050244	1.049073

H	-2.842228	1.730930	1.754124
C	-4.708570	0.949386	1.011561
C	-5.320945	0.060219	0.127640
C	-4.540144	-0.773115	-0.670250
H	0.823871	-0.328416	2.070278
H	-0.684574	-4.206741	-0.645139
H	1.088888	-4.503620	1.057990
H	-6.409703	-0.019437	0.089574
H	-5.010952	-1.523556	-1.309663
C	-0.265386	1.423852	-0.176538
C	1.231951	1.466444	-0.166534
C	-0.632285	2.885344	-0.456225
C	1.617956	2.714407	0.292637
H	-0.330095	3.033583	-1.509491
C	0.425849	3.624908	0.394455
H	0.072831	3.718936	1.437294
C	2.221768	0.522813	-0.584059
C	3.588629	0.820439	-0.289784
C	3.931085	2.066256	0.311245
C	2.971514	3.018872	0.555474
C	4.596158	-0.116127	-0.657021
C	4.277377	-1.266436	-1.336667
C	2.933433	-1.516763	-1.707697
C	1.935830	-0.645357	-1.343618
H	0.637918	4.639318	0.024179
H	4.983273	2.270856	0.525426
H	3.246510	3.999765	0.950925
H	5.636186	0.108318	-0.405537
H	5.059731	-1.974785	-1.618611
H	2.688914	-2.406144	-2.293319
H	0.910956	-0.833346	-1.659884
C	-2.031935	3.459230	-0.322602
H	-2.771416	2.902067	-0.912982
H	-2.375732	3.501609	0.719230
H	-2.016527	4.492898	-0.703049
H	-5.315235	1.564797	1.679562
C	2.165362	-2.614984	2.719287
H	2.113852	-3.604087	3.197449
H	3.156296	-2.528272	2.243441
H	2.108967	-1.846405	3.503311

TS3

C	-0.911888	2.972364	-0.920663
C	-0.548006	1.636388	-0.767065
C	0.719908	1.191697	-0.342509
C	1.695620	2.210334	-0.245088
C	1.354894	3.562769	-0.386401
C	0.058598	3.950214	-0.688294
C	1.021043	-0.265643	-0.131039
S	3.425476	1.939642	-0.120008
C	3.538667	0.214699	0.155219
C	2.428763	-0.655077	0.204118
C	2.710944	-1.948526	0.692873
H	1.887069	-2.618236	0.904890
C	3.993262	-2.404822	0.960110
C	5.082152	-1.550859	0.785087
C	4.842963	-0.238206	0.412198
H	-1.307346	0.904073	-1.013330
H	2.134530	4.321825	-0.277806
H	-0.184894	5.011347	-0.782957
H	6.102056	-1.888904	0.980009
H	5.673802	0.468888	0.339280
C	0.060504	-1.244235	-0.283679
C	-1.419887	-1.120061	-0.286004
C	0.272498	-2.662115	-0.848198

C	-1.932452	-1.918791	-1.293844
H	1.280212	-2.778107	-1.269366
C	-0.806897	-2.657241	-1.966605
H	-1.089738	-3.669586	-2.291472
C	-2.295346	-0.463555	0.632662
C	-3.700643	-0.566275	0.400499
C	-4.184325	-1.334051	-0.698778
C	-3.320652	-2.013973	-1.525571
C	-4.595101	0.098499	1.285552
C	-4.122732	0.824171	2.352642
C	-2.729018	0.908709	2.591522
C	-1.838321	0.280804	1.753046
H	-0.442556	-2.105905	-2.849945
H	-5.264116	-1.394923	-0.857524
H	-3.701289	-2.631984	-2.342322
H	-5.669673	0.017780	1.101614
H	-4.819389	1.331267	3.024104
H	-2.361207	1.474591	3.450577
H	-0.765480	0.348381	1.942466
C	-0.040064	-3.827142	0.102643
H	0.573849	-3.838639	1.013593
H	-1.091743	-3.796135	0.427117
H	0.121218	-4.783538	-0.417430
H	4.136738	-3.423385	1.326729
C	-2.322211	3.320274	-1.316708
H	-2.624357	2.780122	-2.227440
H	-3.032750	3.037330	-0.523300
H	-2.436199	4.397374	-1.503705

anti-(M)-stable-Z

C	-0.867613	-2.738392	1.555509
C	-0.396170	-1.427772	1.432905
C	0.570954	-1.079583	0.487065
C	1.132939	-2.091344	-0.308355
C	0.682053	-3.406579	-0.196612
C	-0.321669	-3.718849	0.718258
C	1.032593	0.320547	0.296793
S	2.382950	-1.671288	-1.499334
C	3.242739	-0.429020	-0.560153
C	2.521091	0.433418	0.286782
C	3.248181	1.305296	1.109407
H	2.717072	1.920720	1.837832
C	4.634831	1.393583	1.015692
C	5.327643	0.588155	0.111043
C	4.634047	-0.340135	-0.661005
H	-0.814786	-0.644215	2.069933
H	1.119137	-4.190568	-0.819675
H	-0.672850	-4.751267	0.794874
H	6.414596	0.657366	0.029188
H	5.175672	-1.013997	-1.329073
C	0.203033	1.371240	0.089261
C	-1.284679	1.400905	0.031280
C	0.617554	2.837974	0.024013
C	-1.704871	2.624599	0.529283
H	1.578030	3.019040	0.514509
C	-0.531281	3.530027	0.791322
H	-0.716207	4.560404	0.450657
C	-2.245063	0.470406	-0.480028
C	-3.628805	0.756650	-0.262986
C	-4.012748	1.976994	0.365058
C	-3.073867	2.915187	0.717786
C	-4.609418	-0.164361	-0.727832
C	-4.246461	-1.290617	-1.425905
C	-2.881352	-1.530623	-1.714448
C	-1.909857	-0.673373	-1.255787

H	-0.305903	3.576495	1.870649
H	-5.077010	2.172721	0.519617
H	-3.376782	3.875275	1.142711
H	-5.663524	0.052037	-0.534896
H	-5.008304	-1.987883	-1.781974
H	-2.597579	-2.400067	-2.312156
H	-0.867140	-0.855345	-1.509775
C	0.722004	3.318753	-1.426262
H	1.499307	2.758446	-1.967818
H	-0.230096	3.185541	-1.964261
H	0.985408	4.387215	-1.459895
H	5.178079	2.089510	1.658681
C	-1.967681	-3.061574	2.530110
H	-2.939353	-2.714772	2.141125
H	-2.046247	-4.143365	2.708791
H	-1.807492	-2.561751	3.497131

anti-(M)-stable- Z^*

C	-1.568478	-2.036379	1.673282
C	-0.780896	-0.908957	1.488837
C	0.431783	-0.921727	0.746411
C	0.879075	-2.197174	0.300827
C	0.115531	-3.341603	0.511071
C	-1.115510	-3.259276	1.157864
C	1.100462	0.309390	0.373166
S	2.290033	-2.348357	-0.719618
C	3.194622	-0.905407	-0.304002
C	2.553634	0.271689	0.167057
C	3.410564	1.367308	0.432026
H	2.999719	2.273571	0.864415
C	4.777487	1.317532	0.202987
C	5.369599	0.158278	-0.299806
C	4.572868	-0.953585	-0.538082
H	-1.118367	0.042268	1.903228
H	0.475405	-4.303260	0.137601
H	-1.718546	-4.161720	1.284256
H	6.444594	0.112657	-0.483440
H	5.016880	-1.881191	-0.906912
C	0.295888	1.485706	0.222287
C	-1.077226	1.491599	-0.158453
C	0.687012	2.943115	0.470634
C	-1.689055	2.698442	0.280459
H	1.397296	3.035196	1.303646
C	-0.648898	3.611520	0.855316
H	-0.735350	4.642517	0.477560
C	-1.904160	0.473946	-0.792699
C	-3.329803	0.627310	-0.692388
C	-3.878526	1.808991	-0.157339
C	-3.064962	2.857096	0.285413
C	-4.163944	-0.422256	-1.185604
C	-3.625321	-1.519747	-1.812174
C	-2.229685	-1.607670	-2.010519
C	-1.396117	-0.613773	-1.527675
H	-0.758160	3.661969	1.952700
H	-4.966139	1.910827	-0.116612
H	-3.512639	3.775661	0.672254
H	-5.246545	-0.325117	-1.070457
H	-4.278150	-2.314662	-2.180106
H	-1.804186	-2.457886	-2.547052
H	-0.321466	-0.685305	-1.699785
C	1.278938	3.593024	-0.790912
H	2.170328	3.060088	-1.149812
H	0.531163	3.581019	-1.598767
H	1.556336	4.640029	-0.591809
H	5.389457	2.192339	0.432937

C	-2.917205	-1.921974	2.329297
H	-3.677135	-1.670014	1.570073
H	-3.219168	-2.863237	2.810496
H	-2.931923	-1.124546	3.085777

syn-(P)-unstable-E

C	-3.746898	-1.596031	1.547709
C	-2.413627	-1.264167	1.287239
C	-2.066190	-0.265245	0.370850
C	-3.090831	0.456251	-0.254919
C	-4.428308	0.143127	-0.011479
C	-4.747887	-0.883344	0.874488
C	-0.638940	0.046900	0.095750
S	-2.649238	1.733239	-1.396597
C	-1.206761	2.362128	-0.567931
C	-0.331669	1.512990	0.151458
C	0.754596	2.121343	0.792760
H	1.425072	1.521713	1.398912
C	1.005970	3.487332	0.678651
C	0.159784	4.296682	-0.074052
C	-0.957353	3.732216	-0.682982
H	-1.611754	-1.806764	1.795857
H	-5.222710	0.706358	-0.506999
H	-5.799003	-1.118497	1.061962
H	0.350927	5.367528	-0.171638
H	-1.651123	4.360461	-1.246983
C	0.202889	-0.922060	-0.359309
C	1.677561	-0.851499	-0.521793
C	-0.194820	-2.144324	-1.207157
C	2.008806	-1.372784	-1.760892
H	0.125078	-3.059386	-0.677047
C	0.782875	-1.952485	-2.403908
H	0.335339	-1.247782	-3.127514
C	2.705788	-0.548674	0.421239
C	4.057471	-0.557306	-0.045357
C	4.339739	-0.935030	-1.388569
C	3.341056	-1.383239	-2.222587
C	5.105717	-0.257225	0.871050
C	4.840762	-0.037589	2.200348
C	3.510258	-0.126732	2.681122
C	2.472529	-0.372149	1.814693
H	0.986570	-2.893017	-2.937303
H	5.379173	-0.924323	-1.726949
H	3.574887	-1.754450	-3.223350
H	6.133312	-0.231925	0.498769
H	5.654935	0.178454	2.895847
H	3.311235	-0.003943	3.748185
H	1.451220	-0.455537	2.192810
C	-1.622073	-2.326064	-1.700537
H	-2.316527	-2.637109	-0.910792
H	-2.009180	-1.403044	-2.158320
H	-1.627992	-3.110406	-2.473806
H	1.872946	3.915895	1.186297
C	-4.091532	-2.712269	2.497442
H	-4.164856	-3.673268	1.961773
H	-3.323835	-2.828936	3.276059
H	-5.059373	-2.538362	2.989818

TS4

C	1.533262	2.801782	-1.679672
C	1.022259	1.552687	-1.366879
C	-0.217582	1.364826	-0.713873
C	-0.989280	2.533340	-0.544366
C	-0.473170	3.805017	-0.845516

C	0.794935	3.949232	-1.383709
C	-0.693303	-0.007193	-0.363064
S	-2.679077	2.544774	-0.070519
C	-3.038283	0.847898	0.198924
C	-2.093809	-0.192710	0.104508
C	-2.505135	-1.434993	0.640794
H	-1.769719	-2.230977	0.732326
C	-3.792163	-1.703400	1.090977
C	-4.734217	-0.664979	1.048992
C	-4.348662	0.598358	0.637345
H	2.506237	2.878331	-2.169165
H	1.607852	0.681757	-1.650646
H	-1.093672	4.688088	-0.669789
H	1.186307	4.943826	-1.607367
H	-5.760857	-0.837141	1.382636
H	-5.067302	1.421836	0.672543
C	0.155512	-1.093790	-0.480402
C	1.613532	-1.122521	-0.243209
C	-0.190506	-2.488479	-1.038970
C	2.187013	-2.170906	-0.945180
H	-0.345472	-3.208590	-0.214679
C	1.138897	-2.899711	-1.725081
H	1.134896	-2.557158	-2.775425
C	2.409625	-0.361740	0.680063
C	3.811318	-0.636865	0.732910
C	4.367089	-1.675510	-0.070183
C	3.568235	-2.449302	-0.876390
C	4.635399	0.118418	1.612548
C	4.099279	1.083675	2.430485
C	2.704916	1.320803	2.416638
C	1.884239	0.618535	1.564569
H	1.288189	-3.989447	-1.739508
H	5.442038	-1.863946	-0.008459
H	3.992226	-3.269858	-1.460240
H	5.708140	-0.091328	1.632666
H	4.742493	1.657610	3.101437
H	2.275563	2.064389	3.092165
H	0.811200	0.807143	1.578131
C	-1.352673	-2.579667	-2.022222
H	-2.336530	-2.466955	-1.550759
H	-1.261722	-1.808597	-2.803578
H	-1.336624	-3.563558	-2.516402
C	-4.168624	-3.063565	1.614851
H	-4.601511	-2.996410	2.625121
H	-4.926315	-3.536571	0.969662
H	-3.298801	-3.734278	1.658312

intermediate-*E*

C	1.111860	-2.381419	2.346636
C	0.599240	-1.187461	1.847592
C	-0.242926	-1.176526	0.727196
C	-0.615162	-2.407787	0.165361
C	-0.107002	-3.610228	0.661590
C	0.769651	-3.593215	1.744758
C	-0.769512	0.108283	0.200428
S	-1.683710	-2.402343	-1.244348
C	-2.739145	-1.049554	-0.777875
C	-2.243961	0.071252	-0.070106
C	-3.179414	1.050887	0.292751
H	-2.865707	1.900238	0.893942
C	-4.530334	0.986750	-0.069476
C	-4.968301	-0.109626	-0.814424
C	-4.081062	-1.127956	-1.150744
H	1.783209	-2.366725	3.207971
H	0.864560	-0.236979	2.316262

H	-0.401397	-4.557380	0.203435
H	1.170431	-4.532730	2.131812
H	-6.017386	-0.188358	-1.110873
H	-4.439729	-2.004483	-1.695872
C	0.022179	1.206233	0.003436
C	1.496221	1.315324	-0.178017
C	-0.500957	2.641429	0.123380
C	1.846148	2.660922	-0.234062
H	-1.421898	2.798475	-0.455488
C	0.640354	3.541982	-0.356832
H	0.717237	4.474592	0.221698
C	2.531717	0.337995	-0.413977
C	3.893424	0.775975	-0.355157
C	4.195100	2.162362	-0.223561
C	3.190169	3.094316	-0.236386
C	4.943781	-0.170484	-0.511774
C	4.676206	-1.485104	-0.807612
C	3.336836	-1.892286	-0.999946
C	2.300979	-1.007180	-0.809180
H	0.523645	3.829821	-1.415456
H	5.243025	2.469865	-0.177645
H	3.414323	4.163711	-0.229737
H	5.975507	0.179756	-0.421513
H	5.490431	-2.202128	-0.934942
H	3.118163	-2.915751	-1.313692
H	1.286913	-1.335538	-1.012960
C	-0.760040	2.943901	1.612085
H	-1.392017	2.189808	2.099964
H	0.194209	2.963859	2.162650
H	-1.239074	3.928435	1.729368
C	-5.470027	2.088663	0.342812
H	-5.396301	2.289850	1.422607
H	-5.230245	3.029166	-0.178906
H	-6.514669	1.835304	0.113562

TS5

C	-0.190049	3.410907	1.777461
C	0.027929	2.038417	1.683921
C	0.452515	1.465490	0.478027
C	0.785746	2.315609	-0.588613
C	0.546290	3.689303	-0.508882
C	0.034731	4.230433	0.669249
C	0.726394	0.010178	0.331672
S	1.619823	1.601187	-1.988233
C	2.695513	0.519641	-1.060263
C	2.194896	-0.159759	0.066249
C	3.087900	-0.909081	0.839199
H	2.723477	-1.399760	1.742953
C	4.429213	-1.066151	0.476714
C	4.881539	-0.432458	-0.687784
C	4.029986	0.369420	-1.441981
H	-0.546152	3.841997	2.715504
H	-0.171921	1.388529	2.539071
H	0.793635	4.338014	-1.352376
H	-0.147306	5.305371	0.735564
H	5.924393	-0.546046	-0.995577
H	4.408482	0.892583	-2.323421
C	-0.134880	-1.039128	0.235930
C	-1.616399	-1.194435	-0.017822
C	0.419049	-2.468865	0.248880
C	-1.819083	-2.487659	-0.497773
H	1.436824	-2.505013	-0.156390
C	-0.548855	-3.269163	-0.616440
H	-0.662086	-4.314020	-0.289990
C	-2.767753	-0.321833	0.060326

C	-4.053794	-0.851567	-0.297497
C	-4.187056	-2.192072	-0.751120
C	-3.084858	-2.993107	-0.863232
C	-5.212326	-0.030205	-0.216897
C	-5.134344	1.279625	0.186930
C	-3.873453	1.816181	0.523685
C	-2.739833	1.038916	0.460694
H	-0.225808	-3.289162	-1.671386
H	-5.180832	-2.562206	-1.015260
H	-3.169196	-4.019839	-1.227232
H	-6.174834	-0.470267	-0.490440
H	-6.032331	1.899162	0.241720
H	-3.787517	2.859581	0.837032
H	-1.794282	1.489601	0.719382
C	0.435496	-3.016240	1.682878
H	1.014992	-2.373766	2.360614
H	-0.586109	-3.087558	2.089574
H	0.878985	-4.023823	1.702766
C	5.368497	-1.880888	1.325904
H	6.029224	-2.503996	0.704661
H	6.013971	-1.227371	1.935441
H	4.819167	-2.540065	2.013024

syn-(*M*)-stable-*E*

C	4.124874	-1.288239	1.264964
C	2.750525	-1.026356	1.253048
C	2.178608	-0.142289	0.333529
C	3.015350	0.534124	-0.566381
C	4.389798	0.292065	-0.567460
C	4.932445	-0.619856	0.335830
C	0.709682	0.091907	0.265122
S	2.292113	1.667082	-1.725697
C	1.019636	2.349108	-0.686419
C	0.349646	1.543063	0.260912
C	-0.568915	2.171552	1.107469
H	-1.046156	1.601042	1.898780
C	-0.885913	3.521207	0.964018
C	-0.265289	4.284919	-0.021769
C	0.704547	3.702073	-0.833709
H	2.096406	-1.531747	1.968949
H	5.039875	0.822775	-1.267241
H	6.010659	-0.800518	0.328782
H	-0.509388	5.342665	-0.142292
H	1.235617	4.303909	-1.575105
C	-0.105129	-0.937454	-0.076014
C	-1.557169	-0.931714	-0.386655
C	0.415065	-2.224735	-0.715468
C	-1.725454	-1.600870	-1.588389
H	1.485125	-2.141137	-0.943816
C	-0.426642	-2.232528	-2.020336
H	-0.569805	-3.241562	-2.436473
C	-2.694159	-0.501593	0.358515
C	-3.970139	-0.556274	-0.285140
C	-4.077154	-1.104568	-1.594796
C	-2.985627	-1.663393	-2.219151
C	-5.123744	-0.132837	0.434430
C	-5.034127	0.250279	1.750535
C	-3.785233	0.202232	2.418360
C	-2.647970	-0.161951	1.738930
H	0.070616	-1.618742	-2.790876
H	-5.060425	-1.132115	-2.071315
H	-3.091545	-2.156356	-3.188631
H	-6.091414	-0.146988	-0.073962
H	-5.929327	0.558709	2.295504
H	-3.729987	0.442614	3.482739

H	-1.695498	-0.241059	2.265492
C	0.185438	-3.475805	0.130541
H	0.739814	-3.416092	1.079130
H	-0.881196	-3.613597	0.369342
H	0.529684	-4.372931	-0.406671
H	-1.619977	3.974385	1.633872
C	4.706091	-2.283429	2.233783
H	4.603222	-3.310371	1.845919
H	5.776512	-2.100915	2.405462
H	4.189123	-2.247110	3.203771

TS5'

C	-4.542463	0.735608	0.472149
C	-3.172767	0.809272	0.749158
C	-2.218659	0.135809	-0.020565
C	-2.689980	-0.784336	-0.977765
C	-4.050122	-0.869609	-1.276982
C	-4.964276	-0.082554	-0.582168
C	-0.731645	0.180380	0.183376
S	-1.550856	-1.962043	-1.679279
C	-0.624615	-2.270522	-0.189304
C	-0.270401	-1.168396	0.610172
C	0.443145	-1.393333	1.790054
H	0.703427	-0.543628	2.425319
C	0.848074	-2.681878	2.135113
C	0.530013	-3.761237	1.310333
C	-0.216754	-3.560549	0.148847
H	-2.842500	1.390332	1.609175
H	-4.399265	-1.583976	-2.026262
H	-6.028594	-0.157325	-0.820291
H	0.847936	-4.771197	1.578926
H	-0.490643	-4.406654	-0.485828
C	0.068762	1.238565	-0.121191
C	1.563781	1.304690	-0.178592
C	-0.450424	2.667472	-0.411851
C	1.952436	2.632370	-0.283195
H	-1.090306	2.634426	-1.308418
C	0.813210	3.512442	-0.675078
H	0.802362	4.464179	-0.123556
C	2.605321	0.303861	-0.213986
C	3.951185	0.726323	0.033259
C	4.258521	2.114061	0.137461
C	3.289723	3.052370	-0.100219
C	4.996134	-0.237525	0.072949
C	4.756108	-1.556275	-0.228864
C	3.458257	-1.948227	-0.625629
C	2.420047	-1.045456	-0.616909
H	0.923960	3.770975	-1.741501
H	5.292591	2.410736	0.330970
H	3.531138	4.117549	-0.132043
H	6.008069	0.102559	0.308711
H	5.568176	-2.286631	-0.210932
H	3.276100	-2.973499	-0.956199
H	1.447164	-1.360465	-0.978272
C	-1.241016	3.340185	0.719652
H	-2.268604	2.979080	0.795450
H	-0.744321	3.199305	1.693175
H	-1.302343	4.421948	0.527689
H	1.418033	-2.844089	3.052514
C	-5.527995	1.534815	1.282341
H	-5.162592	1.700565	2.306276
H	-6.504503	1.032588	1.340022
H	-5.693191	2.525958	0.828144

anti-(P)-unstable-E

C	-4.516526	0.675416	0.508964
C	-3.136794	0.833944	0.665810
C	-2.217220	0.022745	-0.005592
C	-2.708758	-1.070889	-0.739819
C	-4.082959	-1.247189	-0.911397
C	-4.975230	-0.360475	-0.315084
C	-0.735672	0.164324	0.110232
S	-1.566372	-2.288354	-1.361518
C	-0.457980	-2.305556	0.032068
C	-0.138796	-1.088138	0.656544
C	0.705400	-1.106294	1.771191
H	0.935113	-0.166814	2.278620
C	1.275421	-2.298678	2.209795
C	0.990874	-3.494468	1.548463
C	0.111013	-3.504005	0.467317
H	-2.761137	1.615673	1.327607
H	-4.457405	-2.097193	-1.486722
H	-6.049572	-0.506734	-0.455372
H	1.438951	-4.430620	1.888926
H	-0.139073	-4.442532	-0.032972
C	0.008977	1.224443	-0.286139
C	1.495225	1.342472	-0.156159
C	-0.387330	2.625128	-0.767203
C	1.791424	2.652252	0.181342
H	0.014048	2.674307	-1.796314
C	0.554557	3.502903	0.090692
H	0.106273	3.673673	1.086141
C	2.550027	0.404403	-0.377802
C	3.876189	0.800502	-0.019664
C	4.119727	2.124292	0.447667
C	3.106271	3.050737	0.506699
C	4.944096	-0.126209	-0.188373
C	4.724796	-1.363815	-0.741888
C	3.426454	-1.719348	-1.183168
C	2.370773	-0.858224	-1.007915
H	0.748888	4.487556	-0.360569
H	5.142723	2.404073	0.712989
H	3.309868	4.083496	0.800105
H	5.950673	0.175224	0.113786
H	5.552449	-2.065338	-0.869864
H	3.265185	-2.681817	-1.674347
H	1.383791	-1.127871	-1.381008
C	-1.814539	3.140608	-0.833071
H	-2.465931	2.491036	-1.432860
H	-2.267239	3.270724	0.158433
H	-1.799166	4.129829	-1.317049
H	1.949957	-2.294751	3.068815
C	-5.478885	1.614921	1.184733
H	-5.733856	2.455047	0.517280
H	-6.418989	1.108906	1.448389
H	-5.046810	2.042977	2.100825

TS6

C	3.845288	-1.928463	0.782777
C	2.542077	-1.521127	0.518648
C	2.181631	-0.235095	0.061917
C	3.233331	0.699970	0.028685
C	4.559777	0.314795	0.280415
C	4.872256	-0.988512	0.622821
C	0.750892	0.076745	-0.256371
S	3.019180	2.420917	-0.209441
C	1.279159	2.589920	-0.351098
C	0.363162	1.517140	-0.448821
C	-0.931726	1.893955	-0.872606

H	-1.657082	1.126658	-1.114373
C	-1.337670	3.210294	-1.032201
C	-0.437145	4.249344	-0.802314
C	0.872820	3.927934	-0.490979
H	1.755231	-2.239242	0.711758
H	5.351818	1.066555	0.224818
H	5.912281	-1.266452	0.812662
H	-0.738510	5.294002	-0.903919
H	1.616651	4.721224	-0.377015
C	-0.152629	-0.953093	-0.418215
C	-1.636730	-0.915551	-0.397693
C	0.132884	-2.346105	-1.012522
C	-2.118969	-1.726878	-1.410716
H	1.138872	-2.394616	-1.450650
C	-0.962917	-2.384950	-2.114637
H	-1.190003	-3.406158	-2.454840
C	-2.531348	-0.335079	0.552981
C	-3.932014	-0.527892	0.350785
C	-4.389613	-1.301239	-0.755657
C	-3.502768	-1.905992	-1.615834
C	-4.847276	0.047963	1.275849
C	-4.399071	0.771671	2.354577
C	-3.009084	0.946140	2.562849
C	-2.098643	0.408623	1.683600
H	-0.645891	-1.797018	-2.992748
H	-5.466432	-1.430560	-0.891984
H	-3.861311	-2.531527	-2.436869
H	-5.918072	-0.101417	1.114107
H	-5.111929	1.206630	3.058954
H	-2.659263	1.510250	3.430589
H	-1.028755	0.545591	1.850966
C	-0.095494	-3.546941	-0.082099
H	0.532554	-3.542260	0.819150
H	-1.141659	-3.585683	0.258450
H	0.113785	-4.480928	-0.625445
H	-2.362008	3.418454	-1.347765
C	4.144112	-3.329197	1.246396
H	3.221600	-3.908327	1.393390
H	4.765719	-3.865290	0.511506
H	4.699769	-3.324829	2.197092

motor 4

anti-(M)-stable-E

C	1.017256	2.640630	2.080413
C	0.548078	1.373296	1.745061
C	-0.312572	1.194272	0.656289
C	-0.747228	2.328118	-0.051729
C	-0.276304	3.600980	0.278819
C	0.617669	3.752482	1.337235
C	-0.785121	-0.149682	0.227063
S	-1.854937	2.108719	-1.423097
C	-2.857157	0.803881	-0.742448
C	-2.267564	-0.199540	0.048142
C	-3.094575	-1.136966	0.672927
H	-2.660412	-1.870395	1.355668
C	-5.040546	-0.179608	-0.390429
C	-4.236912	0.799623	-0.959626
H	1.705166	2.760381	2.920182
H	0.872111	0.499218	2.314379
H	-0.615128	4.472609	-0.286242
H	0.988383	4.747607	1.593144
H	-6.118406	-0.172130	-0.570812
H	-4.694097	1.582780	-1.569636
C	0.039936	-1.191740	-0.034938

C	1.524894	-1.253762	0.042428
C	-0.389641	-2.627304	-0.323178
C	1.881360	-2.540519	0.414077
H	-1.391358	-2.840703	0.059543
C	0.676446	-3.442618	0.444020
H	0.879892	-4.422120	-0.015750
C	2.539124	-0.290117	-0.258229
C	3.892801	-0.631484	0.048889
C	4.201935	-1.930353	0.547169
C	3.223698	-2.884782	0.686745
C	4.921237	0.320920	-0.198076
C	4.637506	1.532543	-0.780120
C	3.309711	1.832615	-1.169520
C	2.291059	0.945466	-0.916638
H	0.351666	-3.628580	1.482245
H	5.245105	-2.167891	0.771854
H	3.474898	-3.899004	1.006811
H	5.949840	0.060817	0.065676
H	5.435803	2.253819	-0.969743
H	3.094046	2.773131	-1.681890
H	1.280316	1.175074	-1.249337
C	-0.378654	-2.917875	-1.826187
H	-1.102569	-2.276439	-2.351283
H	0.615752	-2.736899	-2.264994
H	-0.649476	-3.967538	-2.018237
C	-4.483344	-1.156362	0.456639
N	-5.272518	-2.131751	1.028810
H	-4.891842	-2.602079	1.842108
H	-6.259857	-1.919926	1.116592

*anti-(M)-stable-E**

C	1.477612	2.150841	2.453648
C	0.842956	1.028286	1.952895
C	-0.207468	1.117390	0.998933
C	-0.596668	2.431863	0.623043
C	0.046313	3.562479	1.128963
C	1.094436	3.428522	2.034025
C	-0.804650	-0.074031	0.418548
S	-1.783538	2.677149	-0.637141
C	-2.736060	1.212533	-0.528562
C	-2.190177	-0.008774	-0.044655
C	-3.051540	-1.124813	-0.049496
H	-2.711000	-2.060620	0.383550
C	-4.845049	0.138828	-1.058964
C	-4.040589	1.266203	-1.028448
H	2.284995	2.031850	3.179148
H	1.147862	0.039670	2.297864
H	-0.278312	4.553592	0.803207
H	1.598293	4.316060	2.421383
H	-5.858695	0.199431	-1.461642
H	-4.428860	2.215776	-1.404739
C	0.006999	-1.250523	0.346121
C	1.410304	-1.237613	0.101264
C	-0.375911	-2.709965	0.596827
C	1.996370	-2.421205	0.621629
H	-1.201246	-2.794657	1.318934
C	0.921132	-3.297419	1.193118
H	1.061965	-4.363939	0.958409
C	2.259923	-0.236091	-0.516922
C	3.679720	-0.423718	-0.422423
C	4.205818	-1.593774	0.170924
C	3.372442	-2.596203	0.665227
C	4.538664	0.567293	-0.980873
C	4.027875	1.656125	-1.646299
C	2.632536	1.797524	-1.802413

C	1.773629	0.862468	-1.255347
H	0.912709	-3.204155	2.294140
H	5.291188	-1.716503	0.212428
H	3.799771	-3.501296	1.103923
H	5.619433	0.436644	-0.882527
H	4.701808	2.404985	-2.068788
H	2.225453	2.647638	-2.353693
H	0.698625	0.972316	-1.406403
C	-0.735860	-3.447105	-0.705479
H	-1.573616	-2.972517	-1.234841
H	0.131377	-3.443265	-1.383528
H	-1.003911	-4.494613	-0.494601
C	-4.356192	-1.078596	-0.548880
N	-5.140967	-2.215315	-0.575177
H	-4.862765	-2.977862	0.027668
H	-6.141668	-2.080080	-0.623192

syn-(*P*)-unstable-*Z*

C	-3.496416	-1.994695	2.157980
C	-2.259169	-1.554956	1.694296
C	-2.164942	-0.663171	0.616431
C	-3.353807	-0.172030	0.056448
C	-4.599121	-0.608309	0.515748
C	-4.668061	-1.529968	1.558514
C	-0.827419	-0.243484	0.120353
S	-3.244159	0.964868	-1.288914
C	-1.781696	1.851198	-0.799344
C	-0.697337	1.226442	-0.136765
C	0.416536	2.015709	0.157927
H	1.259392	1.586768	0.687432
C	0.509088	3.369804	-0.207914
C	-0.578900	3.959222	-0.871057
C	-1.708479	3.201343	-1.149667
H	-3.546340	-2.702793	2.988013
H	-1.339222	-1.920602	2.156968
H	-5.513938	-0.219996	0.061676
H	-5.642723	-1.869565	1.916347
H	-0.540436	5.013518	-1.156035
H	-2.558350	3.672048	-1.650725
C	0.094525	-1.198486	-0.196413
C	1.551749	-1.047098	-0.425188
C	-0.221065	-2.594156	-0.766474
C	1.908946	-1.798291	-1.532381
H	0.169622	-3.359770	-0.072141
C	0.723169	-2.586512	-2.005451
H	0.213800	-2.084114	-2.847187
C	2.565751	-0.482618	0.408243
C	3.910109	-0.498957	-0.078654
C	4.207121	-1.139081	-1.315075
C	3.234864	-1.820979	-2.010598
C	4.941223	0.070611	0.721936
C	4.671425	0.566848	1.973677
C	3.354645	0.497519	2.493513
C	2.330388	-0.010759	1.731156
H	0.991838	-3.600565	-2.336968
H	5.240125	-1.132226	-1.672420
H	3.485997	-2.381028	-2.914593
H	5.961171	0.082390	0.328567
H	5.473556	0.990121	2.582543
H	3.155003	0.847207	3.509144
H	1.319626	-0.067531	2.141346
C	-1.641626	-2.958137	-1.172589
H	-2.296800	-3.166979	-0.318149
H	-2.100853	-2.156876	-1.772309
H	-1.610204	-3.867981	-1.793041

N	1.663376	4.080181	0.046130
H	1.580189	5.089742	0.068173
H	2.274869	3.710687	0.765221

TS1

C	-3.833427	-2.382762	1.191941
C	-2.582700	-1.986818	0.745358
C	-2.313652	-0.692732	0.241350
C	-3.368797	0.236317	0.375888
C	-4.644902	-0.162751	0.809648
C	-4.891504	-1.471297	1.190614
C	-0.946257	-0.341958	-0.230410
S	-3.196838	1.966951	0.166132
C	-1.527043	2.147706	-0.354192
C	-0.629763	1.080724	-0.561085
C	0.571553	1.403849	-1.221374
H	1.247223	0.606379	-1.521748
C	0.963539	2.709151	-1.528384
C	0.083214	3.758498	-1.207773
C	-1.152593	3.464245	-0.661036
H	-3.977807	-3.401281	1.558240
H	-1.771203	-2.707428	0.811620
H	-5.442770	0.582398	0.869028
H	-5.888504	-1.766222	1.524838
H	0.355298	4.793587	-1.428002
H	-1.859122	4.277278	-0.471834
C	0.016715	-1.324819	-0.379561
C	1.470671	-1.198249	-0.148622
C	-0.178627	-2.733818	-0.973032
C	2.151204	-2.165154	-0.871843
H	-0.258092	-3.487293	-0.168375
C	1.185968	-2.986550	-1.666329
H	1.143522	-2.625455	-2.709577
C	2.186223	-0.372052	0.784485
C	3.609655	-0.495363	0.828245
C	4.270310	-1.454140	0.005366
C	3.554623	-2.294086	-0.812649
C	4.352945	0.326777	1.720449
C	3.720854	1.215828	2.555784
C	2.308988	1.304575	2.547750
C	1.563804	0.532963	1.686331
H	1.450218	-4.053904	-1.702178
H	5.359418	-1.528656	0.061376
H	4.061072	-3.053984	-1.412726
H	5.441711	0.228828	1.735964
H	4.302607	1.841879	3.236277
H	1.805047	1.988005	3.235185
H	0.476882	0.608038	1.704583
N	2.156011	2.949858	-2.185392
H	2.519222	3.893369	-2.110360
H	2.876442	2.246308	-2.064365
C	-1.325098	-2.917905	-1.961938
H	-1.214061	-3.886503	-2.473820
H	-2.315897	-2.907701	-1.491973
H	-1.305498	-2.127032	-2.728134

intermediate-Z

C	-4.604016	1.814190	0.198509
C	-3.258030	1.652047	0.520906
C	-2.482217	0.612212	-0.019629
C	-3.157115	-0.307775	-0.858789
C	-4.505746	-0.143273	-1.186692
C	-5.230556	0.927145	-0.672516
C	-1.008999	0.404775	0.178807

S	-2.315267	-1.702076	-1.567933
C	-1.231574	-2.069071	-0.216714
C	-0.657942	-1.004251	0.493559
C	0.201069	-1.283328	1.559231
H	0.624820	-0.453577	2.130845
C	0.558329	-2.601444	1.889419
C	-0.007805	-3.651012	1.140817
C	-0.901788	-3.384806	0.109952
H	-5.162653	2.642386	0.639944
H	-2.818574	2.354763	1.222489
H	-4.991408	-0.871906	-1.840342
H	-6.284503	1.049471	-0.931399
H	0.245790	-4.685495	1.385766
H	-1.349956	-4.214494	-0.442493
C	-0.075435	1.400478	0.092377
C	1.392655	1.336123	-0.155138
C	-0.388436	2.861258	0.432492
C	1.921493	2.619969	-0.058107
H	-1.298661	3.217955	-0.069426
C	0.847205	3.661767	0.014245
H	1.077919	4.478547	0.714395
C	2.275772	0.273758	-0.576326
C	3.685662	0.523119	-0.550536
C	4.178951	1.828528	-0.263493
C	3.310026	2.873790	-0.090468
C	4.591996	-0.517050	-0.896633
C	4.137558	-1.735175	-1.340274
C	2.748083	-1.942460	-1.488734
C	1.849258	-0.969257	-1.117038
H	0.729873	4.117989	-0.983454
H	5.259857	1.990171	-0.248585
H	3.677592	3.894468	0.039506
H	5.664493	-0.314831	-0.832190
H	4.842597	-2.522816	-1.615268
H	2.378374	-2.879376	-1.912207
H	0.791734	-1.143046	-1.287607
C	-0.548038	2.982355	1.960476
H	-1.261980	2.258336	2.376126
H	0.418719	2.795530	2.455537
H	-0.878448	3.995894	2.236175
N	1.469980	-2.855700	2.891502
H	1.606784	-2.121841	3.576869
H	1.451380	-3.784260	3.297176

TS2

C	4.520719	-1.701912	0.989454
C	3.185078	-1.373608	1.218259
C	2.406004	-0.782754	0.216999
C	3.032750	-0.456544	-1.004778
C	4.367193	-0.793763	-1.239570
C	5.107886	-1.430694	-0.245647
C	0.947505	-0.434090	0.317149
S	2.107478	0.418422	-2.255560
C	1.272314	1.535932	-1.150924
C	0.801942	1.025331	0.067055
C	0.353275	1.903603	1.055979
H	0.029763	1.502723	2.019915
C	0.241324	3.282061	0.804688
C	0.632472	3.762269	-0.461303
C	1.167073	2.903180	-1.414120
H	5.104690	-2.172806	1.783373
H	2.738093	-1.591281	2.188587
H	4.832683	-0.535658	-2.193670
H	6.153741	-1.687014	-0.428869
H	0.546758	4.829582	-0.680293

H	1.526375	3.307021	-2.363764
C	-0.008517	-1.394948	0.435799
C	-1.481927	-1.488059	0.109967
C	0.389039	-2.802412	0.894349
C	-1.796882	-2.842764	0.009747
H	1.418048	-3.043331	0.602944
C	-0.611960	-3.732256	0.217200
H	-0.848725	-4.623936	0.817061
C	-2.535102	-0.534767	-0.170614
C	-3.853465	-1.033336	-0.448620
C	-4.106929	-2.431406	-0.494786
C	-3.090564	-3.321783	-0.287522
C	-4.920666	-0.127605	-0.702563
C	-4.721897	1.230709	-0.707603
C	-3.425164	1.731180	-0.464879
C	-2.378447	0.875229	-0.210092
H	-0.239982	-4.084212	-0.760144
H	-5.121608	-2.776050	-0.710057
H	-3.264708	-4.399052	-0.341991
H	-5.912036	-0.543439	-0.900992
H	-5.550276	1.914867	-0.904973
H	-3.241752	2.808313	-0.477859
H	-1.400659	1.299396	-0.039788
C	0.264123	-2.908522	2.420995
H	-0.780356	-2.759437	2.739130
H	0.581972	-3.905975	2.762249
H	0.874687	-2.156300	2.940544
N	-0.297823	4.129866	1.748155
H	-0.287572	3.804022	2.707920
H	-0.069349	5.113207	1.657274

syn-(*M*)-stable-*Z*

C	0.467150	3.438665	-0.317841
C	0.265643	2.101634	-0.705743
C	-0.666773	1.279959	-0.075385
C	-1.493856	1.845102	0.919423
C	-1.315480	3.175738	1.301622
C	-0.333833	3.962149	0.711568
C	-0.904029	-0.165336	-0.377842
S	-2.785846	0.892466	1.689215
C	-3.310220	-0.039135	0.273029
C	-2.337591	-0.475639	-0.641918
C	-2.748480	-1.210640	-1.759999
H	-1.997991	-1.534208	-2.484898
C	-4.089805	-1.541980	-1.941232
C	-5.041706	-1.128400	-1.008133
C	-4.656479	-0.368332	0.095093
H	0.860061	1.710479	-1.526590
H	-1.962919	3.609662	2.067813
H	-0.202862	5.000234	1.027017
H	-6.094824	-1.383063	-1.147385
H	-5.402699	-0.023573	0.814854
C	-0.040983	-1.186953	-0.150587
C	1.373735	-1.149561	0.301985
C	-0.508183	-2.602832	0.187278
C	1.488806	-2.022603	1.371858
H	-1.597337	-2.633623	0.318889
C	0.212606	-2.804657	1.547610
H	0.400740	-3.863413	1.783086
C	2.534321	-0.516942	-0.232545
C	3.750563	-0.615929	0.513589
C	3.787072	-1.399785	1.701646
C	2.692013	-2.131569	2.100036
C	4.924319	0.010661	0.005571
C	4.918070	0.636933	-1.216786

C	3.740027	0.638872	-2.004719
C	2.581984	0.077675	-1.523679
H	-0.398533	-2.381269	2.362900
H	4.725943	-1.461458	2.257998
H	2.751543	-2.796468	2.965231
H	5.843055	-0.040821	0.595905
H	5.828219	1.102918	-1.601322
H	3.758650	1.078621	-3.004721
H	1.688202	0.041549	-2.148662
C	-0.103304	-3.655094	-0.843533
H	-0.586199	-3.462983	-1.813373
H	0.986855	-3.667084	-1.003591
H	-0.406986	-4.658754	-0.507815
H	-4.393300	-2.123799	-2.814404
N	1.453950	4.197196	-0.909402
H	1.796988	3.878455	-1.808073
H	1.354590	5.203684	-0.847353

TS2'

C	0.464039	-2.851638	1.600691
C	0.138876	-1.488097	1.477320
C	-0.617939	-1.027458	0.403881
C	-1.125707	-1.939421	-0.538094
C	-0.821024	-3.294861	-0.420367
C	-0.025916	-3.745820	0.628850
C	-0.977430	0.406098	0.232884
S	-2.108707	-1.307016	-1.884022
C	-3.094480	-0.189029	-0.907468
C	-2.473366	0.514289	0.146501
C	-3.308223	1.118322	1.094691
H	-2.873711	1.523453	2.006958
C	-4.687354	1.187424	0.902768
C	-5.266807	0.614248	-0.228493
C	-4.472782	-0.108360	-1.116451
H	0.517427	-0.773047	2.212143
H	-1.209091	-4.010263	-1.149664
H	0.210226	-4.809744	0.712071
H	-6.345253	0.676385	-0.390479
H	-4.928479	-0.647016	-1.950695
C	-0.104477	1.429230	0.026070
C	1.386347	1.387202	-0.130030
C	-0.515759	2.920914	-0.022824
C	1.878088	2.683448	-0.076554
H	-1.197113	3.067168	-0.876332
C	0.798302	3.699670	-0.235641
H	0.904419	4.536572	0.470764
C	2.340641	0.326584	-0.369798
C	3.729625	0.613972	-0.168663
C	4.156067	1.947189	0.097856
C	3.254071	2.975930	0.062369
C	4.696373	-0.415340	-0.336512
C	4.335354	-1.660801	-0.789970
C	2.986584	-1.905369	-1.129527
C	2.024727	-0.942820	-0.924064
H	0.865882	4.135040	-1.246567
H	5.221065	2.137682	0.253437
H	3.578006	4.014674	0.161997
H	5.744880	-0.180909	-0.134337
H	5.087957	-2.440228	-0.929535
H	2.701017	-2.862487	-1.572217
H	1.006954	-1.144178	-1.240745
C	-1.196246	3.476035	1.236303
H	-2.248524	3.195074	1.313627
H	-0.674334	3.147184	2.149555
H	-1.166772	4.575814	1.210541

H	-5.311893	1.683320	1.649242
N	1.284957	-3.289442	2.615196
H	1.373195	-2.686719	3.424828
H	1.244786	-4.275298	2.845703

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C	0.867440	-2.562701	1.711787
C	0.389298	-1.259648	1.489571
C	-0.499639	-0.984656	0.452590
C	-0.989029	-2.036527	-0.339074
C	-0.528130	-3.335837	-0.125467
C	0.402227	-3.595709	0.875066
C	-0.993760	0.392517	0.161912
S	-2.168671	-1.673180	-1.624630
C	-3.141530	-0.491631	-0.714982
C	-2.487639	0.410021	0.147019
C	-3.272847	1.175602	1.016226
H	-2.781554	1.802644	1.760678
C	-4.663242	1.153524	0.933953
C	-5.294565	0.335296	-0.003437
C	-4.535080	-0.508705	-0.811042
H	0.747776	-0.441158	2.118856
H	-0.900910	-4.157810	-0.741763
H	0.763058	-4.615736	1.029135
H	-6.384319	0.318510	-0.077433
H	-5.025243	-1.206130	-1.494497
C	-0.170394	1.428747	-0.126175
C	1.327151	1.394747	-0.093519
C	-0.458758	2.914198	-0.373200
C	1.769278	2.611912	0.397320
H	-0.134986	3.074208	-1.418335
C	0.622665	3.577315	0.510125
H	0.260253	3.660827	1.550706
C	2.274747	0.415894	-0.528542
C	3.653559	0.646746	-0.228849
C	4.050450	1.859765	0.404530
C	3.133835	2.847449	0.672748
C	4.620422	-0.320712	-0.623995
C	4.253064	-1.437786	-1.333365
C	2.898818	-1.623436	-1.704097
C	1.938850	-0.721279	-1.314229
H	0.889247	4.589623	0.170454
H	5.110400	2.011947	0.624124
H	3.451496	3.804787	1.093241
H	5.669223	-0.146737	-0.368922
H	5.004718	-2.170238	-1.636425
H	2.615810	-2.487137	-2.310486
H	0.906612	-0.860260	-1.631114
C	-1.828658	3.555948	-0.240253
H	-2.588065	3.056134	-0.856023
H	-2.183829	3.585247	0.798322
H	-1.754150	4.598295	-0.588848
H	-5.256432	1.775627	1.607890
N	1.805888	-2.810505	2.690450
H	1.880212	-2.123032	3.431148
H	1.877236	-3.765953	3.020512

TS3

C	-0.804758	3.036720	-0.882025
C	-0.492363	1.680691	-0.748578
C	0.756550	1.189408	-0.322018
C	1.769925	2.164180	-0.185924
C	1.477819	3.529715	-0.323012
C	0.207621	3.978521	-0.632814

C	1.003518	-0.284059	-0.148751
S	3.488143	1.831299	-0.022918
C	3.536637	0.094946	0.169170
C	2.395295	-0.735955	0.173764
C	2.628189	-2.059779	0.605519
H	1.778758	-2.706317	0.785270
C	3.890617	-2.575231	0.856844
C	5.011387	-1.754688	0.723779
C	4.822452	-0.419323	0.409485
H	-1.280093	0.985253	-1.011081
H	2.282281	4.259679	-0.195035
H	0.004007	5.048441	-0.718438
H	6.017230	-2.138909	0.906071
H	5.679357	0.258799	0.370096
C	0.007421	-1.221355	-0.333116
C	-1.466936	-1.041504	-0.324114
C	0.163490	-2.623924	-0.953037
C	-2.013140	-1.781416	-1.359084
H	1.164889	-2.760991	-1.382857
C	-0.917757	-2.533326	-2.065791
H	-1.239250	-3.520162	-2.430915
C	-2.313320	-0.388288	0.623597
C	-3.722687	-0.431609	0.396670
C	-4.239160	-1.137550	-0.728795
C	-3.404631	-1.816202	-1.586512
C	-4.588355	0.228253	1.313801
C	-4.084589	0.891360	2.406584
C	-2.687580	0.917090	2.639238
C	-1.824018	0.294212	1.769518
H	-0.534868	-1.960233	-2.927249
H	-5.321251	-1.153218	-0.883023
H	-3.811720	-2.387443	-2.424346
H	-5.666105	0.193812	1.133751
H	-4.759128	1.395070	3.102749
H	-2.295250	1.434114	3.517997
H	-0.748456	0.316905	1.953848
C	-0.190648	-3.813588	-0.048418
H	0.423289	-3.883447	0.859962
H	-1.240179	-3.757035	0.279601
H	-0.064913	-4.754133	-0.605901
H	3.994586	-3.613773	1.177957
N	-2.087085	3.433435	-1.207092
H	-2.179318	4.338878	-1.653236
H	-2.684962	2.724641	-1.617121

anti-(M)-stable-Z

C	-0.664018	-2.837534	1.558196
C	-0.287913	-1.488588	1.440537
C	0.623356	-1.072404	0.470390
C	1.229271	-2.025829	-0.363827
C	0.873110	-3.370664	-0.250199
C	-0.071214	-3.772336	0.687190
C	1.002582	0.355898	0.302949
S	2.408221	-1.495168	-1.585723
C	3.230562	-0.243358	-0.626923
C	2.483433	0.549071	0.266016
C	3.180259	1.433744	1.100808
H	2.633613	1.994641	1.861329
C	4.557166	1.604406	0.977705
C	5.270942	0.870363	0.029616
C	4.611385	-0.070281	-0.757509
H	-0.742001	-0.745355	2.100545
H	1.341056	-4.116629	-0.897487
H	-0.344494	-4.827739	0.765149
H	6.349782	1.004851	-0.075522

H	5.172764	-0.689630	-1.461102
C	0.118213	1.367168	0.130816
C	-1.369778	1.327166	0.089472
C	0.462480	2.853139	0.086657
C	-1.842129	2.523375	0.607743
H	1.418008	3.070783	0.571926
C	-0.709712	3.478271	0.875268
H	-0.945500	4.504390	0.553650
C	-2.290406	0.362242	-0.431373
C	-3.685063	0.586745	-0.210439
C	-4.120055	1.778996	0.437607
C	-3.221667	2.750663	0.805003
C	-4.626766	-0.365946	-0.691541
C	-4.217516	-1.464449	-1.407557
C	-2.843286	-1.644703	-1.695784
C	-1.907860	-0.755932	-1.222448
H	-0.476486	3.517641	1.953259
H	-5.191529	1.926644	0.595988
H	-3.564911	3.689934	1.245616
H	-5.688881	-0.196221	-0.495734
H	-4.949839	-2.186682	-1.775685
H	-2.523313	-2.493373	-2.304952
H	-0.858026	-0.893331	-1.475082
C	0.530956	3.362262	-1.356031
H	1.327814	2.847247	-1.913917
H	-0.419151	3.194332	-1.887841
H	0.744802	4.442151	-1.373933
H	5.076472	2.309090	1.630923
N	-1.624241	-3.227086	2.466109
H	-1.631308	-4.205490	2.729739
H	-1.799933	-2.599286	3.241813

*anti-(M)-stable-Z**

C	-1.144962	-2.441073	1.450824
C	-0.454353	-1.227607	1.450988
C	0.651527	-0.993115	0.615885
C	1.196894	-2.128830	-0.059212
C	0.566299	-3.372449	0.009112
C	-0.620312	-3.524183	0.712478
C	1.118232	0.358750	0.343480
S	2.531495	-1.963039	-1.158299
C	3.285267	-0.477717	-0.617857
C	2.552041	0.534313	0.056670
C	3.302490	1.676617	0.423613
H	2.830620	2.459394	1.008013
C	4.642391	1.827651	0.098783
C	5.319479	0.832931	-0.608629
C	4.636127	-0.324361	-0.951959
H	-0.862478	-0.394423	2.023845
H	0.988113	-4.220492	-0.535070
H	-1.137570	-4.486321	0.713110
H	6.373282	0.947137	-0.868557
H	5.148641	-1.131981	-1.480120
C	0.163230	1.420479	0.349766
C	-1.246560	1.301330	0.128839
C	0.433051	2.903806	0.611040
C	-1.915682	2.422115	0.688271
H	1.199890	3.044442	1.383107
C	-0.912446	3.438257	1.143708
H	-1.142512	4.449929	0.773385
C	-2.050040	0.237992	-0.455170
C	-3.452129	0.214013	-0.131314
C	-4.041611	1.306807	0.532877
C	-3.286908	2.430347	0.888955
C	-4.219410	-0.924461	-0.531383

C	-3.659351	-1.932063	-1.280639
C	-2.314909	-1.838953	-1.700680
C	-1.544906	-0.751070	-1.314516
H	-0.902303	3.496392	2.245646
H	-5.114440	1.281348	0.740923
H	-3.768088	3.287589	1.366223
H	-5.275503	-0.965165	-0.251043
H	-4.263933	-2.792571	-1.577960
H	-1.883853	-2.609007	-2.343015
H	-0.510762	-0.680912	-1.653097
C	0.858047	3.635365	-0.670688
H	1.771151	3.203801	-1.104900
H	0.057173	3.563013	-1.422749
H	1.043964	4.700984	-0.464041
H	5.168698	2.730955	0.414784
N	-2.324293	-2.567269	2.147484
H	-2.924343	-3.335303	1.876507
H	-2.835198	-1.706199	2.303993

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C	-3.600523	-1.964102	1.465118
C	-2.286469	-1.528858	1.218960
C	-2.016962	-0.509732	0.303723
C	-3.082624	0.130377	-0.343433
C	-4.392937	-0.284140	-0.104852
C	-4.651528	-1.325997	0.779421
C	-0.617116	-0.071202	0.055196
S	-2.718421	1.426504	-1.494317
C	-1.370466	2.188841	-0.620600
C	-0.447377	1.417721	0.126814
C	0.552385	2.116718	0.813948
H	1.250516	1.574377	1.442541
C	0.683221	3.500847	0.715204
C	-0.202835	4.235251	-0.067864
C	-1.240628	3.576387	-0.721356
H	-1.453765	-2.011046	1.738024
H	-5.224646	0.212703	-0.610661
H	-5.682259	-1.642241	0.958639
H	-0.105952	5.319736	-0.154037
H	-1.967368	4.143621	-1.308051
C	0.318317	-0.950035	-0.398614
C	1.778978	-0.726903	-0.556307
C	0.050362	-2.197728	-1.260094
C	2.161551	-1.194039	-1.802139
H	0.464183	-3.079937	-0.739188
C	1.002716	-1.891089	-2.453056
H	0.483843	-1.227494	-3.167832
C	2.770584	-0.320656	0.386858
C	4.112319	-0.169909	-0.084365
C	4.430217	-0.501273	-1.431744
C	3.485145	-1.051842	-2.266878
C	5.122776	0.243188	0.830578
C	4.840672	0.417034	2.163090
C	3.532770	0.165613	2.648478
C	2.526331	-0.190425	1.783524
H	1.302679	-2.798361	-2.998545
H	5.460194	-0.369438	-1.773441
H	3.755028	-1.385085	-3.271895
H	6.138361	0.392650	0.454553
H	5.627270	0.721457	2.857264
H	3.326678	0.251388	3.717824
H	1.523840	-0.397632	2.164437
C	-1.349443	-2.523562	-1.756827
H	-2.007069	-2.910834	-0.969334
H	-1.830496	-1.642150	-2.207150

H	-1.272980	-3.297510	-2.536862
H	1.487197	4.002590	1.258342
N	-3.846164	-3.022767	2.315163
H	-3.126970	-3.227880	2.999452
H	-4.783964	-3.088106	2.694404

TS4

C	-2.256594	2.721758	1.490694
C	-1.552376	1.547746	1.281451
C	-0.258389	1.510415	0.711378
C	0.348685	2.769661	0.517871
C	-0.365256	3.965279	0.713073
C	-1.672534	3.948926	1.168847
C	0.428977	0.206205	0.470523
S	2.045037	3.005858	0.146115
C	2.653196	1.365839	-0.030896
C	1.865089	0.201658	0.076604
C	2.465429	-0.994012	-0.367223
H	1.862391	-1.896205	-0.439629
C	3.805016	-1.095824	-0.751265
C	4.586799	0.073522	-0.743285
C	3.998863	1.282179	-0.416985
H	-3.259708	2.679236	1.919819
H	-2.024006	0.615999	1.583684
H	0.132144	4.919744	0.519929
H	-2.215914	4.885546	1.310351
H	5.639105	0.033911	-1.034588
H	4.595549	2.196747	-0.477412
C	-0.260456	-0.985376	0.613562
C	-1.682028	-1.242280	0.303754
C	0.246960	-2.281547	1.277332
C	-2.140888	-2.320652	1.043594
H	0.543655	-3.019591	0.509526
C	-1.048663	-2.836091	1.926447
H	-1.154754	-2.426550	2.947077
C	-2.519643	-0.664701	-0.710916
C	-3.859469	-1.150125	-0.823119
C	-4.308505	-2.210898	0.016936
C	-3.459278	-2.806230	0.917858
C	-4.725752	-0.581100	-1.797424
C	-4.284632	0.404141	-2.647620
C	-2.944323	0.849712	-2.571040
C	-2.087063	0.330343	-1.628657
H	-1.041719	-3.932539	2.014998
H	-5.337821	-2.562381	-0.091650
H	-3.796090	-3.644729	1.532283
H	-5.752234	-0.951387	-1.863832
H	-4.959698	0.833901	-3.391207
H	-2.585606	1.609298	-3.269598
H	-1.055025	0.678107	-1.593718
C	1.356166	-2.152496	2.315640
H	2.338820	-1.934280	1.880161
H	1.120851	-1.355808	3.038915
H	1.445396	-3.097870	2.873322
N	4.355092	-2.318449	-1.090919
H	5.167043	-2.285212	-1.697540
H	3.696200	-3.039227	-1.364509

intermediate-*E*

C	0.998754	-2.407055	2.320461
C	0.521800	-1.196629	1.825297
C	-0.302475	-1.154721	0.692347
C	-0.695166	-2.371838	0.112053
C	-0.221975	-3.590158	0.604374

C	0.637671	-3.604528	1.701230
C	-0.786213	0.149628	0.169916
S	-1.734733	-2.320041	-1.317251
C	-2.766630	-0.949765	-0.844392
C	-2.257233	0.155810	-0.124341
C	-3.163222	1.160332	0.238749
H	-2.836107	2.000423	0.844997
C	-4.518182	1.130207	-0.135448
C	-4.980906	0.038889	-0.888258
C	-4.111303	-0.991451	-1.218232
H	1.656868	-2.416341	3.192066
H	0.802841	-0.257339	2.307299
H	-0.530709	-4.525544	0.131652
H	1.010468	-4.556946	2.084861
H	-6.030696	-0.012281	-1.187151
H	-4.489979	-1.855780	-1.769730
C	0.040452	1.225750	-0.003207
C	1.519579	1.290765	-0.161703
C	-0.439168	2.675516	0.126742
C	1.913506	2.624865	-0.192128
H	-1.344320	2.868588	-0.465663
C	0.738513	3.545778	-0.320971
H	0.835269	4.467002	0.272691
C	2.526157	0.284228	-0.398674
C	3.900344	0.675876	-0.312719
C	4.244857	2.049482	-0.154439
C	3.270881	3.013884	-0.167722
C	4.920962	-0.302526	-0.469607
C	4.614179	-1.602551	-0.791193
C	3.265099	-1.961671	-1.010512
C	2.256479	-1.045576	-0.820263
H	0.648657	3.852676	-1.376858
H	5.301460	2.321547	-0.087946
H	3.529503	4.075175	-0.141136
H	5.962417	0.011049	-0.358481
H	5.406133	-2.344149	-0.918415
H	3.017576	-2.971849	-1.345271
H	1.234954	-1.334987	-1.045284
C	-0.714749	2.966650	1.614817
H	-1.377904	2.226042	2.081556
H	0.229803	2.949711	2.182005
H	-1.164998	3.964125	1.737486
N	-5.358182	2.173871	0.196560
H	-6.350757	1.968114	0.194452
H	-5.074837	2.748213	0.982356

TS5

C	-0.085885	3.384961	1.772303
C	0.099870	2.007656	1.675765
C	0.504931	1.427345	0.466997
C	0.851927	2.270414	-0.601898
C	0.643033	3.648756	-0.518611
C	0.151298	4.200162	0.663585
C	0.740093	-0.035006	0.316852
S	1.654584	1.528747	-2.005772
C	2.715665	0.431679	-1.076626
C	2.204501	-0.241932	0.050610
C	3.072532	-0.998903	0.836875
H	2.698238	-1.486067	1.738376
C	4.423901	-1.169488	0.485850
C	4.898351	-0.532576	-0.675488
C	4.055670	0.272624	-1.433046
H	-0.427226	3.822961	2.712663
H	-0.112139	1.361354	2.530767
H	0.898967	4.292803	-1.363179

H	-0.006016	5.278917	0.732133
H	5.945749	-0.650593	-0.964431
H	4.453464	0.795125	-2.306600
C	-0.149619	-1.059526	0.217709
C	-1.636179	-1.173987	-0.028852
C	0.365751	-2.503746	0.222795
C	-1.877273	-2.461495	-0.506599
H	1.380710	-2.564484	-0.186454
C	-0.628296	-3.274450	-0.639784
H	-0.765217	-4.318194	-0.318964
C	-2.763415	-0.271276	0.059021
C	-4.067664	-0.770696	-0.276033
C	-4.240759	-2.108387	-0.724428
C	-3.160081	-2.935715	-0.853941
C	-5.204204	0.079353	-0.180694
C	-5.087046	1.389439	0.212646
C	-3.807330	1.897831	0.521121
C	-2.694426	1.092282	0.445298
H	-0.313848	-3.295673	-1.697336
H	-5.247442	-2.454477	-0.971821
H	-3.274862	-3.960107	-1.216253
H	-6.181726	-0.338543	-0.435173
H	-5.968320	2.031487	0.278478
H	-3.690084	2.941962	0.821533
H	-1.733076	1.522350	0.680045
C	0.373483	-3.057567	1.654427
H	0.969886	-2.431972	2.333226
H	-0.648240	-3.106331	2.064230
H	0.792995	-4.075501	1.668730
N	5.247239	-1.981852	1.237293
H	6.244361	-1.828598	1.138143
H	4.964006	-2.148635	2.196192

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C	4.169430	-1.435527	1.137979
C	2.787613	-1.185690	1.223217
C	2.159100	-0.303905	0.344734
C	2.919233	0.382572	-0.615737
C	4.292647	0.149737	-0.705104
C	4.909980	-0.754701	0.152174
C	0.689651	-0.053822	0.358009
S	2.098892	1.509738	-1.722962
C	0.951627	2.219425	-0.562299
C	0.370862	1.405715	0.434286
C	-0.393679	2.033120	1.422293
H	-0.768429	1.451436	2.260587
C	-0.677261	3.396259	1.359820
C	-0.171721	4.168934	0.316016
C	0.665462	3.584941	-0.632139
H	2.191488	-1.704688	1.978322
H	4.891018	0.682975	-1.448087
H	5.985557	-0.931398	0.071475
H	-0.393599	5.236937	0.259441
H	1.120450	4.194759	-1.416234
C	-0.158982	-1.036982	-0.027914
C	-1.597090	-0.944630	-0.398236
C	0.318253	-2.339752	-0.667635
C	-1.748654	-1.592911	-1.614070
H	1.397553	-2.306708	-0.861766
C	-0.479821	-2.310723	-1.995334
H	-0.674790	-3.314151	-2.404067
C	-2.734374	-0.396949	0.265829
C	-3.965282	-0.334466	-0.460135
C	-4.041396	-0.886043	-1.770429
C	-2.968273	-1.545503	-2.322428

C	-5.111748	0.224112	0.172872
C	-5.066171	0.631186	1.484121
C	-3.875843	0.467632	2.234868
C	-2.743659	-0.034574	1.640130
H	0.075498	-1.740135	-2.759204
H	-4.990174	-0.823317	-2.309654
H	-3.053479	-2.026237	-3.300192
H	-6.041089	0.298334	-0.398048
H	-5.955354	1.049462	1.961462
H	-3.864082	0.730104	3.295397
H	-1.842872	-0.206251	2.229319
C	0.006106	-3.579619	0.169631
H	0.525021	-3.542787	1.139324
H	-1.074191	-3.674611	0.364603
H	0.335658	-4.489299	-0.355871
H	-1.293517	3.854693	2.136368
N	4.771485	-2.358049	1.967270
H	5.775834	-2.279226	2.078119
H	4.290214	-2.569698	2.833748

TSS'

C	-4.313691	0.468088	0.352313
C	-2.947887	0.631337	0.647560
C	-1.953317	-0.002132	-0.097299
C	-2.346417	-0.962265	-1.052470
C	-3.697123	-1.138133	-1.354741
C	-4.672300	-0.399780	-0.694474
C	-0.474727	0.127793	0.135131
S	-1.122376	-2.076714	-1.715148
C	-0.223830	-2.320634	-0.196651
C	0.048331	-1.188447	0.594277
C	0.743407	-1.355144	1.794450
H	0.940318	-0.482791	2.421875
C	1.210585	-2.613828	2.170697
C	0.974160	-3.721353	1.356082
C	0.247466	-3.579912	0.173047
H	-2.669979	1.250358	1.499041
H	-3.994927	-1.881482	-2.098352
H	-5.726974	-0.543277	-0.942649
H	1.340775	-4.707840	1.648976
H	0.038194	-4.449186	-0.454905
C	0.275465	1.221416	-0.171340
C	1.766271	1.364917	-0.198830
C	-0.310216	2.616439	-0.499890
C	2.087864	2.709177	-0.317650
H	-0.924864	2.534230	-1.410837
C	0.913631	3.522266	-0.748830
H	0.840793	4.480331	-0.213102
C	2.859336	0.419972	-0.195784
C	4.175635	0.916225	0.072669
C	4.408101	2.319512	0.160142
C	3.397020	3.201680	-0.113631
C	5.268245	0.009181	0.150382
C	5.104034	-1.324823	-0.134681
C	3.837345	-1.790337	-0.552360
C	2.753624	-0.943196	-0.580465
H	1.035043	3.770298	-1.816601
H	5.420897	2.672806	0.370383
H	3.583117	4.277462	-0.158381
H	6.255684	0.405465	0.401783
H	5.952556	-2.011097	-0.087509
H	3.716124	-2.828647	-0.869973
H	1.806532	-1.313754	-0.957280
C	-1.162965	3.267349	0.598749
H	-2.170979	2.852066	0.656138

H	-0.683817	3.171015	1.586470
H	-1.275720	4.340731	0.383981
H	1.765289	-2.729942	3.104345
N	-5.272138	1.103480	1.113882
H	-4.977204	1.933747	1.614723
H	-6.192765	1.192436	0.699846

anti-(P)-unstable-E

C	-4.506723	0.840178	0.479016
C	-3.115505	0.949829	0.643537
C	-2.231815	0.118739	-0.043253
C	-2.750295	-0.943964	-0.805953
C	-4.130697	-1.072521	-0.969591
C	-5.000464	-0.173171	-0.363580
C	-0.746827	0.201143	0.090630
S	-1.639623	-2.183409	-1.444653
C	-0.559799	-2.276777	-0.031961
C	-0.206349	-1.083744	0.622312
C	0.618716	-1.153664	1.748956
H	0.874580	-0.233028	2.278046
C	1.138291	-2.374291	2.173205
C	0.821509	-3.545889	1.484007
C	-0.040230	-3.502490	0.388888
H	-2.718987	1.710847	1.316857
H	-4.535496	-1.898298	-1.559866
H	-6.079057	-0.280526	-0.504502
H	1.230087	-4.504087	1.812832
H	-0.314937	-4.421592	-0.134093
C	0.042714	1.237301	-0.280285
C	1.530283	1.299443	-0.126642
C	-0.294226	2.658028	-0.747817
C	1.867905	2.592741	0.235187
H	0.128188	2.706044	-1.768586
C	0.663656	3.488711	0.138556
H	0.205444	3.660139	1.129417
C	2.554119	0.327477	-0.346622
C	3.888130	0.670388	0.036571
C	4.171797	1.977631	0.527169
C	3.191082	2.938790	0.585803
C	4.924619	-0.291604	-0.130907
C	4.669390	-1.512428	-0.705835
C	3.365763	-1.814708	-1.170741
C	2.339089	-0.918755	-0.997938
H	0.900242	4.472591	-0.293861
H	5.200102	2.216712	0.811139
H	3.427045	3.959191	0.897742
H	5.936814	-0.031093	0.189959
H	5.473260	-2.241347	-0.832390
H	3.177520	-2.763683	-1.678324
H	1.348628	-1.147170	-1.389013
C	-1.700203	3.226113	-0.835010
H	-2.362063	2.607317	-1.455439
H	-2.170079	3.359443	0.147890
H	-1.638633	4.219978	-1.305773
H	1.798615	-2.411132	3.042474
N	-5.359546	1.733776	1.093886
H	-6.318315	1.429335	1.218963
H	-4.991007	2.224666	1.900678

TS6

C	3.824884	-2.027008	0.722458
C	2.521483	-1.588211	0.468492
C	2.195222	-0.295228	0.018813
C	3.264760	0.620947	-0.028571

C	4.578619	0.203373	0.227248
C	4.873584	-1.104336	0.566513
C	0.767729	0.049339	-0.284905
S	3.086147	2.347105	-0.280015
C	1.349534	2.552411	-0.381500
C	0.408868	1.498882	-0.465975
C	-0.885323	1.904556	-0.866173
H	-1.630176	1.153384	-1.098557
C	-1.267470	3.229045	-1.014394
C	-0.341698	4.248663	-0.795746
C	0.966092	3.899361	-0.508228
H	1.723126	-2.292720	0.664817
H	5.389034	0.935577	0.172653
H	5.907057	-1.404593	0.755120
H	-0.623268	5.299778	-0.887660
H	1.727694	4.676917	-0.403187
C	-0.159984	-0.960319	-0.440411
C	-1.642602	-0.890526	-0.399886
C	0.086523	-2.354290	-1.052044
C	-2.156284	-1.681312	-1.413565
H	1.085766	-2.421425	-1.502455
C	-1.023936	-2.355461	-2.140249
H	-1.277513	-3.366906	-2.490794
C	-2.511592	-0.299406	0.567860
C	-3.918753	-0.460727	0.383824
C	-4.408137	-1.214795	-0.722322
C	-3.546275	-1.829838	-1.600461
C	-4.808585	0.127526	1.325776
C	-4.330093	0.833649	2.403156
C	-2.933919	0.977163	2.593087
C	-2.047467	0.426667	1.697505
H	-0.704875	-1.763010	-3.014569
H	-5.489257	-1.320341	-0.844369
H	-3.929316	-2.439822	-2.422147
H	-5.884468	0.002282	1.177850
H	-5.023708	1.278841	3.120236
H	-2.560101	1.527810	3.459470
H	-0.972639	0.540354	1.850095
C	-0.158747	-3.560322	-0.132887
H	0.492178	-3.590615	0.751580
H	-1.196784	-3.569949	0.233834
H	0.005914	-4.492626	-0.694148
H	-2.292533	3.459106	-1.311957
N	4.075459	-3.338087	1.082809
H	4.933537	-3.500374	1.598073
H	3.288894	-3.852023	1.464355

motor 5

anti-(M)-stable-E

C	1.573703	2.507323	2.145260
C	0.962413	1.313300	1.772299
C	0.092756	1.267204	0.676954
C	-0.203763	2.463889	0.002730
C	0.408972	3.663743	0.371232
C	1.309573	3.679301	1.434700
C	-0.530717	0.000786	0.207937
S	-1.323849	2.418252	-1.375996
C	-2.474517	1.218698	-0.739471
C	-2.006893	0.129705	0.021831
C	-2.942379	-0.726968	0.607593
H	-2.623521	-1.531998	1.270987
C	-4.758981	0.478840	-0.443055
C	-3.840782	1.380288	-0.972832
H	2.266486	2.521901	2.989382

H	1.179127	0.391367	2.316463
H	0.175539	4.585066	-0.167683
H	1.791951	4.616728	1.720452
H	-5.828539	0.607892	-0.630306
H	-4.197958	2.228386	-1.561825
C	0.166675	-1.124777	-0.079071
C	1.633061	-1.364239	0.003080
C	-0.427843	-2.490744	-0.409203
C	1.831440	-2.693847	0.340324
H	-1.450069	-2.595961	-0.036195
C	0.528506	-3.447600	0.338620
H	0.618540	-4.430695	-0.148764
C	2.756590	-0.519579	-0.265236
C	4.057610	-1.027479	0.038998
C	4.206515	-2.366879	0.502533
C	3.121208	-3.202091	0.610381
C	5.193829	-0.198009	-0.176509
C	5.060745	1.054107	-0.725947
C	3.781156	1.520532	-1.112736
C	2.662268	0.754321	-0.889562
H	0.175668	-3.623311	1.369342
H	5.212292	-2.732335	0.725984
H	3.247753	-4.247154	0.903589
H	6.182045	-0.585735	0.084845
H	5.940621	1.680018	-0.891767
H	3.682851	2.493801	-1.599234
H	1.688708	1.111913	-1.220224
C	-0.440409	-2.738439	-1.919920
H	-1.077909	-2.000256	-2.429815
H	0.571872	-2.666310	-2.349090
H	-0.833794	-3.742178	-2.142777
C	-4.310576	-0.568924	0.368388
O	-5.149599	-1.449078	0.950385
H	-6.064165	-1.229807	0.728126

*anti-(M)-stable-E**

C	1.912947	1.903479	2.508888
C	1.167023	0.885655	1.941486
C	0.157336	1.139225	0.972316
C	-0.073447	2.506352	0.656185
C	0.681066	3.529662	1.229487
C	1.687385	3.233943	2.144817
C	-0.552379	0.052540	0.319225
S	-1.194888	2.945977	-0.612936
C	-2.313006	1.595073	-0.584024
C	-1.908176	0.295221	-0.167425
C	-2.883523	-0.720307	-0.253450
H	-2.681612	-1.721549	0.111293
C	-4.522954	0.796073	-1.182873
C	-3.595682	1.826477	-1.081795
H	2.683347	1.659073	3.243060
H	1.347291	-0.145937	2.245492
H	0.478295	4.565860	0.948533
H	2.279223	4.039206	2.584094
H	-5.524381	0.991938	-1.575302
H	-3.872462	2.834314	-1.399797
C	0.121016	-1.207206	0.218820
C	1.523548	-1.342763	0.017949
C	-0.432568	-2.621139	0.400953
C	1.955046	-2.603077	0.511030
H	-1.288640	-2.636584	1.090633
C	0.769179	-3.371680	1.013190
H	0.798581	-4.438254	0.741844
C	2.501059	-0.418262	-0.527626
C	3.886705	-0.765536	-0.390062

C	4.256976	-2.008230	0.171600
C	3.300789	-2.930540	0.595398
C	4.871242	0.144600	-0.873818
C	4.509885	1.308334	-1.509550
C	3.145687	1.609286	-1.709416
C	2.167658	0.754460	-1.235834
H	0.733436	-3.317120	2.116220
H	5.319918	-2.251892	0.247006
H	3.609628	-3.892067	1.012607
H	5.926211	-0.108911	-0.741705
H	5.277971	1.993975	-1.874598
H	2.856951	2.520447	-2.237333
H	1.118118	0.989443	-1.420275
C	-0.824192	-3.267272	-0.940227
H	-1.585058	-2.684217	-1.476589
H	0.062178	-3.338744	-1.589282
H	-1.217511	-4.282748	-0.776935
C	-4.160644	-0.484889	-0.751554
O	-5.014144	-1.532372	-0.786585
H	-5.866221	-1.246349	-1.127933

syn-(*P*)-unstable-*Z*

C	-3.919448	-1.364463	2.315783
C	-2.625271	-1.198838	1.829003
C	-2.367989	-0.372400	0.726286
C	-3.439790	0.335522	0.163559
C	-4.740873	0.176372	0.646323
C	-4.980339	-0.684940	1.715227
C	-0.981355	-0.243524	0.205570
S	-3.120270	1.389101	-1.216548
C	-1.505735	1.978948	-0.760209
C	-0.562007	1.164626	-0.084370
C	0.687012	1.727214	0.189091
H	1.449315	1.173295	0.724799
C	1.018404	3.025305	-0.210496
C	0.084132	3.807298	-0.890417
C	-1.175674	3.277408	-1.149736
H	-4.100731	-2.026271	3.165452
H	-1.792257	-1.732657	2.292794
H	-5.563841	0.731839	0.190312
H	-5.998193	-0.808823	2.091908
H	0.331364	4.826273	-1.199928
H	-1.919419	3.891676	-1.663133
C	-0.276715	-1.369906	-0.104254
C	1.176314	-1.518755	-0.356975
C	-0.877228	-2.684856	-0.634759
C	1.354565	-2.350477	-1.449824
H	-0.635414	-3.497241	0.073999
C	0.026382	-2.895272	-1.886042
H	-0.387750	-2.320545	-2.733718
C	2.297207	-1.150260	0.448421
C	3.601698	-1.450013	-0.054549
C	3.741459	-2.163610	-1.278437
C	2.639934	-2.650069	-1.944843
C	4.740387	-1.086573	0.719704
C	4.597931	-0.520215	1.962436
C	3.303728	-0.307708	2.499046
C	2.184735	-0.612300	1.762046
H	0.080202	-3.949981	-2.194299
H	4.748217	-2.374064	-1.648618
H	2.757453	-3.269382	-2.837347
H	5.734663	-1.290975	0.313769
H	5.479257	-0.255765	2.551092
H	3.196678	0.099048	3.507283
H	1.190822	-0.452987	2.186139

C	-2.349328	-2.763938	-1.011610
H	-3.016940	-2.815973	-0.142988
H	-2.648775	-1.900944	-1.626545
H	-2.513401	-3.675715	-1.607748
O	2.255741	3.465632	0.098220
H	2.373949	4.368213	-0.225921

TS1

C	1.368428	2.463240	-1.152582
C	0.758120	1.227167	-0.977034
C	-0.515916	1.073383	-0.396197
C	-1.218066	2.267885	-0.131281
C	-0.606030	3.517078	-0.304977
C	0.688811	3.629191	-0.783748
C	-1.100913	-0.289568	-0.215806
S	-2.916772	2.351158	0.314185
C	-3.409413	0.669026	0.348821
C	-2.533908	-0.423002	0.163833
C	-3.060717	-1.684844	0.524804
H	-2.399035	-2.547179	0.548816
C	-4.385511	-1.880125	0.882523
C	-5.258552	-0.791840	0.934200
C	-4.757825	0.477350	0.694288
H	1.318346	0.361207	-1.319734
H	-1.168785	4.425185	-0.072707
H	1.152442	4.611316	-0.908912
H	-6.309064	-0.925347	1.201054
H	-5.409163	1.349340	0.797962
C	-0.322064	-1.414679	-0.422169
C	1.114101	-1.577739	-0.118228
C	-0.731754	-2.704792	-1.158194
C	1.651590	-2.587247	-0.901221
H	-0.993847	-3.497643	-0.434335
C	0.604546	-3.144044	-1.812609
H	0.691006	-2.691916	-2.816800
C	1.907403	-0.983302	0.922272
C	3.278520	-1.374929	1.019176
C	3.804164	-2.364281	0.137474
C	3.001645	-2.980606	-0.791185
C	4.101434	-0.789166	2.020690
C	3.590996	0.125655	2.909712
C	2.222753	0.478263	2.845619
C	1.405021	-0.060633	1.879163
H	0.674311	-4.234613	-1.939501
H	4.856076	-2.644795	0.235457
H	3.398683	-3.765549	-1.439345
H	5.150975	-1.090167	2.075513
H	4.233308	0.569269	3.673936
H	1.809492	1.180785	3.573166
H	0.351001	0.214881	1.856445
C	-1.831358	-2.585127	-2.208186
H	-2.829598	-2.428731	-1.781840
H	-1.621185	-1.750041	-2.894693
H	-1.869521	-3.510292	-2.804050
H	-4.732388	-2.883336	1.138690
O	2.604839	2.478463	-1.694046
H	2.910640	3.390322	-1.785459

intermediate-Z

C	-4.946991	1.070565	0.488666
C	-3.577354	1.130217	0.738215
C	-2.661338	0.300453	0.068983
C	-3.209417	-0.649840	-0.826221
C	-4.582416	-0.708762	-1.079942

C	-5.455251	0.162256	-0.435829
C	-1.166389	0.349603	0.184768
S	-2.177978	-1.797983	-1.706456
C	-0.961296	-2.078346	-0.452402
C	-0.548597	-0.992799	0.336718
C	0.415939	-1.204735	1.324980
H	0.731164	-0.380876	1.968265
C	1.016411	-2.456480	1.481611
C	0.621813	-3.521945	0.664399
C	-0.375154	-3.332571	-0.289510
H	-5.617742	1.741349	1.029894
H	-3.230303	1.837601	1.485283
H	-4.967576	-1.454586	-1.779501
H	-6.527397	0.111394	-0.637381
H	1.081641	-4.506394	0.787967
H	-0.697402	-4.174155	-0.907227
C	-0.430400	1.502497	0.167682
C	1.007815	1.726251	-0.145870
C	-0.971909	2.841310	0.678606
C	1.314497	3.065294	0.076965
H	-1.955666	3.080994	0.251189
C	0.083614	3.887094	0.309627
H	0.210489	4.651628	1.090539
C	2.030552	0.886919	-0.723938
C	3.376727	1.374045	-0.724486
C	3.657435	2.707184	-0.307098
C	2.635687	3.560086	0.019154
C	4.423241	0.551114	-1.225071
C	4.154877	-0.671760	-1.790817
C	2.813709	-1.099584	-1.909859
C	1.787520	-0.343760	-1.391314
H	-0.166160	4.420071	-0.623555
H	4.694292	3.052887	-0.315189
H	2.832461	4.609378	0.251464
H	5.448341	0.928322	-1.179091
H	4.965171	-1.289822	-2.183907
H	2.582809	-2.033241	-2.428387
H	0.765369	-0.676001	-1.542274
C	-1.067241	2.772953	2.215282
H	-1.622952	1.895434	2.572733
H	-0.057414	2.709032	2.651803
H	-1.550947	3.678513	2.613164
O	1.961403	-2.582782	2.434853
H	2.300841	-3.487506	2.442414

TS2

C	4.525256	-1.747291	0.968360
C	3.192156	-1.420118	1.212912
C	2.408793	-0.805938	0.229228
C	3.028519	-0.457361	-0.989614
C	4.360771	-0.791456	-1.239924
C	5.105796	-1.450766	-0.264061
C	0.952692	-0.453834	0.344307
S	2.099108	0.442214	-2.220496
C	1.274519	1.543115	-1.092517
C	0.812442	1.009888	0.120679
C	0.374765	1.873414	1.127289
H	0.056559	1.476996	2.093430
C	0.273043	3.246215	0.883229
C	0.636956	3.757648	-0.369068
C	1.162096	2.910713	-1.341962
H	5.112864	-2.236896	1.748096
H	2.750369	-1.657070	2.181109
H	4.820881	-0.514377	-2.191266
H	6.149934	-1.705463	-0.458846

H	0.547251	4.829261	-0.567507
H	1.508790	3.327362	-2.290396
C	-0.007813	-1.411511	0.451557
C	-1.480131	-1.494574	0.120610
C	0.384509	-2.825010	0.894399
C	-1.799367	-2.846712	0.001637
H	1.411845	-3.067385	0.598422
C	-0.621208	-3.744498	0.210316
H	-0.866943	-4.636367	0.806283
C	-2.526901	-0.533583	-0.157836
C	-3.842143	-1.023428	-0.464471
C	-4.100135	-2.419884	-0.531636
C	-3.091041	-3.316827	-0.318148
C	-4.902057	-0.110850	-0.723694
C	-4.699320	1.246754	-0.705721
C	-3.406270	1.739275	-0.430046
C	-2.366854	0.876436	-0.168929
H	-0.248769	-4.096531	-0.766790
H	-5.112630	-2.757771	-0.766961
H	-3.268759	-4.392684	-0.386795
H	-5.891081	-0.520600	-0.945048
H	-5.521963	1.936303	-0.908111
H	-3.220580	2.816118	-0.422155
H	-1.392737	1.295475	0.030129
C	0.263111	-2.943312	2.420466
H	-0.779984	-2.792752	2.742389
H	0.577928	-3.944848	2.752335
H	0.877925	-2.197546	2.944420
O	-0.192957	4.026197	1.878397
H	-0.211031	4.949219	1.592621

syn-(*M*)-stable-*Z*

C	1.104128	3.079718	-0.055304
C	0.600468	1.887686	-0.586363
C	-0.465519	1.222129	0.015363
C	-1.096516	1.833554	1.121903
C	-0.597744	3.024564	1.648306
C	0.515344	3.639077	1.081338
C	-1.049798	-0.081678	-0.425382
S	-2.557731	1.114879	1.842256
C	-3.330530	0.540186	0.349470
C	-2.518281	0.003970	-0.663521
C	-3.121469	-0.448610	-1.842033
H	-2.491256	-0.848780	-2.639624
C	-4.506441	-0.407452	-1.992166
C	-5.304496	0.100131	-0.965875
C	-4.719070	0.583212	0.203531
H	1.064978	1.498966	-1.487503
H	-1.091233	3.490561	2.504432
H	0.903276	4.571194	1.501073
H	-6.390073	0.136446	-1.081412
H	-5.340562	1.002080	0.998389
C	-0.467179	-1.300365	-0.312293
C	0.905203	-1.654549	0.133787
C	-1.271970	-2.586407	-0.128879
C	0.783927	-2.644331	1.095815
H	-2.337281	-2.363233	0.011620
C	-0.645012	-3.113196	1.189214
H	-0.720234	-4.206150	1.296812
C	2.195424	-1.248737	-0.317089
C	3.333232	-1.711182	0.415881
C	3.153321	-2.615674	1.500837
C	1.908043	-3.113776	1.807565
C	4.633350	-1.312393	-0.006545
C	4.806696	-0.559525	-1.142422

C	3.685413	-0.195566	-1.928568
C	2.416183	-0.532204	-1.524828
H	-1.151078	-2.654069	2.055547
H	4.035931	-2.957178	2.047854
H	1.786917	-3.868215	2.588757
H	5.497873	-1.641697	0.576047
H	5.810139	-0.269683	-1.462500
H	3.833789	0.346012	-2.865614
H	1.557747	-0.290976	-2.153229
C	-1.121739	-3.578664	-1.280895
H	-1.521988	-3.158891	-2.215939
H	-0.066024	-3.843890	-1.452070
H	-1.672806	-4.506556	-1.063124
H	-4.965163	-0.770987	-2.914306
O	2.151896	3.645141	-0.688488
H	2.406981	4.460572	-0.237014

TS2'

C	0.956705	-2.656526	1.234157
C	0.385683	-1.379496	1.263104
C	-0.499118	-0.986124	0.262688
C	-0.869247	-1.901297	-0.740359
C	-0.305360	-3.174472	-0.765898
C	0.615231	-3.549245	0.211722
C	-1.130926	0.360172	0.235511
S	-2.018927	-1.362469	-1.990684
C	-3.148208	-0.535454	-0.887300
C	-2.622463	0.185968	0.205218
C	-3.511812	0.540149	1.227151
H	-3.119840	0.943340	2.159046
C	-4.886498	0.359430	1.082787
C	-5.399147	-0.221283	-0.076447
C	-4.524912	-0.705104	-1.047338
H	0.669048	-0.683438	2.055008
H	-0.584233	-3.885679	-1.546834
H	1.058004	-4.548905	0.192227
H	-6.476232	-0.354155	-0.200062
H	-4.908755	-1.252795	-1.911291
C	-0.475009	1.544918	0.100679
C	0.986784	1.798263	-0.110161
C	-1.155081	2.930314	0.218679
C	1.235032	3.152983	0.056000
H	-1.901927	3.024267	-0.585931
C	-0.020181	3.958140	0.032964
H	-0.033063	4.736622	0.810269
C	2.103862	0.962096	-0.490336
C	3.425582	1.482086	-0.306295
C	3.614891	2.840600	0.080214
C	2.540070	3.682503	0.177621
C	4.552824	0.670732	-0.611182
C	4.400707	-0.570740	-1.179653
C	3.103179	-1.026579	-1.501062
C	1.994962	-0.282695	-1.165799
H	-0.087213	4.482773	-0.934711
H	4.633807	3.210742	0.219681
H	2.674443	4.749578	0.370147
H	5.550519	1.074808	-0.420199
H	5.274242	-1.179570	-1.423928
H	2.974051	-1.970823	-2.035339
H	1.015728	-0.633418	-1.473465
C	-1.847630	3.227099	1.556499
H	-2.825403	2.749923	1.647897
H	-1.221184	2.915583	2.407909
H	-2.019120	4.310488	1.644577
H	-5.558117	0.664635	1.888322

O	1.828402	-2.973260	2.211583
H	2.160238	-3.871048	2.078675

anti-(P)-unstable-Z

C	1.295902	-2.314418	1.362487
C	0.575305	-1.118581	1.291934
C	-0.416857	-0.948998	0.328174
C	-0.744006	-2.019609	-0.522382
C	-0.030165	-3.214397	-0.449232
C	0.999589	-3.358253	0.477981
C	-1.178044	0.323799	0.171428
S	-2.049895	-1.803361	-1.714734
C	-3.169301	-0.895486	-0.668948
C	-2.646286	0.054986	0.228445
C	-3.507608	0.594715	1.190189
H	-3.099384	1.253243	1.957216
C	-4.870988	0.309901	1.171310
C	-5.391882	-0.550913	0.204633
C	-4.537215	-1.176578	-0.700488
H	0.825828	-0.306158	1.976565
H	-0.277145	-4.044952	-1.114716
H	1.562495	-4.294199	0.529622
H	-6.461141	-0.773096	0.180967
H	-4.927071	-1.908407	-1.411929
C	-0.581470	1.514934	-0.073692
C	0.895015	1.764432	-0.113992
C	-1.156916	2.930900	-0.189281
C	1.131240	3.006551	0.450748
H	-0.933249	3.220573	-1.232686
C	-0.166218	3.726191	0.691598
H	-0.473762	3.668392	1.751304
C	1.980379	1.014877	-0.666333
C	3.307510	1.479892	-0.408662
C	3.508716	2.699980	0.299183
C	2.442232	3.476430	0.682943
C	4.412261	0.740462	-0.918018
C	4.217923	-0.374744	-1.695725
C	2.902438	-0.784711	-2.023520
C	1.816167	-0.107274	-1.524849
H	-0.113960	4.791286	0.419627
H	4.533042	3.033643	0.484184
H	2.600948	4.445300	1.162775
H	5.423621	1.090542	-0.694695
H	5.073585	-0.930320	-2.086264
H	2.749866	-1.641242	-2.684549
H	0.811056	-0.412941	-1.810772
C	-2.611943	3.288045	0.058343
H	-3.300512	2.696138	-0.559089
H	-2.902065	3.177146	1.111483
H	-2.755167	4.346904	-0.209594
H	-5.529092	0.759260	1.918300
O	2.262948	-2.407447	2.297309
H	2.693957	-3.270316	2.238995

TS3

C	-1.214222	2.708623	-0.727198
C	-0.686898	1.425632	-0.628777
C	0.640314	1.153552	-0.245599
C	1.465978	2.293295	-0.102674
C	0.935963	3.588433	-0.183708
C	-0.401233	3.813497	-0.465278
C	1.154336	-0.254206	-0.129113
S	3.220069	2.269066	0.007761
C	3.584577	0.564600	0.153495

C	2.610932	-0.456728	0.154579
C	3.085377	-1.728048	0.542352
H	2.368663	-2.520224	0.718340
C	4.425437	-2.015075	0.754426
C	5.377915	-1.003813	0.626010
C	4.946278	0.284405	0.355670
H	-1.365210	0.622712	-0.889232
H	1.599924	4.445744	-0.042699
H	-0.796832	4.830776	-0.520965
H	6.440138	-1.206356	0.778122
H	5.667411	1.105659	0.321190
C	0.341798	-1.349877	-0.335901
C	-1.138904	-1.441748	-0.292580
C	0.736044	-2.673872	-1.018703
C	-1.567729	-2.227659	-1.348491
H	1.735237	-2.606653	-1.469972
C	-0.371947	-2.735927	-2.107774
H	-0.517540	-3.748645	-2.512305
C	-2.062559	-0.996195	0.701853
C	-3.445093	-1.293894	0.504055
C	-3.854351	-2.036256	-0.641786
C	-2.934748	-2.511333	-1.547921
C	-4.390155	-0.849355	1.470682
C	-3.985745	-0.153181	2.584158
C	-2.611800	0.124284	2.787367
C	-1.674147	-0.285176	1.868839
H	-0.121915	-2.066443	-2.948114
H	-4.918905	-2.246549	-0.773545
H	-3.254072	-3.112604	-2.402525
H	-5.447574	-1.077106	1.312340
H	-4.720888	0.182458	3.319223
H	-2.295744	0.664705	3.682703
H	-0.616449	-0.070194	2.031946
C	0.626997	-3.944862	-0.163603
H	1.267137	-3.939570	0.729095
H	-0.406535	-4.095224	0.184945
H	0.907603	-4.822084	-0.765967
H	4.721153	-3.026219	1.041803
O	-2.511055	2.819793	-1.085774
H	-2.756036	3.752028	-1.147945

anti-(M)-stable-Z

C	1.164250	-2.580694	-1.212719
C	0.529136	-1.336192	-1.237446
C	-0.499629	-1.047842	-0.341045
C	-0.940790	-2.045839	0.545185
C	-0.312410	-3.290579	0.565310
C	0.746554	-3.555557	-0.299249
C	-1.165630	0.280805	-0.302668
S	-2.266460	-1.683962	1.673791
C	-3.271511	-0.694849	0.589180
C	-2.654460	0.170101	-0.334644
C	-3.471169	0.833730	-1.260629
H	-3.010159	1.440457	-2.042294
C	-4.858571	0.726554	-1.201084
C	-5.457551	-0.071641	-0.225804
C	-4.663494	-0.801147	0.655479
H	0.871618	-0.579578	-1.945741
H	-0.651417	-4.065703	1.256628
H	1.238530	-4.531939	-0.281267
H	-6.545262	-0.154279	-0.170933
H	-5.124044	-1.472636	1.383982
C	-0.508911	1.459113	-0.181471
C	0.953293	1.720188	-0.082733
C	-1.140772	2.844699	-0.273340

C	1.208063	2.943889	-0.682551
H	-2.093339	2.829700	-0.810230
C	-0.074245	3.631663	-1.067576
H	-0.060806	4.704704	-0.822018
C	2.016601	0.999848	0.549772
C	3.349944	1.478458	0.357703
C	3.575917	2.680742	-0.373248
C	2.524973	3.424827	-0.850643
C	4.433846	0.770764	0.949228
C	4.211239	-0.328807	1.742013
C	2.885715	-0.754115	1.999278
C	1.820007	-0.106738	1.421059
H	-0.254732	3.545366	-2.152828
H	4.604628	3.025098	-0.507534
H	2.700258	4.377410	-1.356575
H	5.450979	1.131947	0.775521
H	5.050984	-0.860875	2.194963
H	2.707020	-1.598357	2.669472
H	0.805608	-0.426691	1.652527
C	-1.383992	3.435103	1.118590
H	-2.092436	2.814009	1.687616
H	-0.448824	3.500945	1.697242
H	-1.806623	4.448548	1.038533
H	-5.474966	1.263217	-1.925612
O	2.169223	-2.788366	-2.086520
H	2.531912	-3.675915	-1.966302

*anti-(M)-stable-Z**

C	1.502323	-2.080522	-1.602157
C	0.692792	-0.964958	-1.435648
C	-0.444079	-0.983870	-0.591945
C	-0.755318	-2.226032	0.032742
C	0.057229	-3.341777	-0.141079
C	1.197195	-3.276354	-0.938431
C	-1.208486	0.223476	-0.334056
S	-2.051633	-2.341603	1.202336
C	-3.119541	-1.052541	0.684449
C	-2.626240	0.094211	0.003602
C	-3.592238	1.080105	-0.315176
H	-3.296704	1.946252	-0.897998
C	-4.924561	0.961132	0.049824
C	-5.369057	-0.159812	0.753480
C	-4.463203	-1.168033	1.056276
H	0.958363	-0.057389	-1.976614
H	-0.196687	-4.276546	0.364056
H	1.834465	-4.156678	-1.058145
H	-6.416602	-0.256968	1.044713
H	-4.792263	-2.065153	1.585843
C	-0.522585	1.476645	-0.441570
C	0.842880	1.676073	-0.088116
C	-1.022953	2.806535	-1.008131
C	1.355543	2.802539	-0.785401
H	-1.772661	2.655717	-1.797955
C	0.260661	3.426879	-1.597478
H	0.266829	4.527148	-1.556989
C	1.726770	0.914359	0.776436
C	3.123691	1.241698	0.747661
C	3.583477	2.333471	-0.022318
C	2.705160	3.124839	-0.760873
C	4.022127	0.475385	1.545768
C	3.563703	-0.522656	2.372337
C	2.180372	-0.788938	2.455835
C	1.286406	-0.072862	1.681032
H	0.375857	3.139189	-2.657809
H	4.650706	2.569493	-0.010062

H	3.078805	3.975360	-1.336053
H	5.088942	0.709138	1.500230
H	4.266855	-1.097939	2.979004
H	1.810133	-1.560742	3.133889
H	0.218374	-0.271672	1.778396
C	-1.591453	3.721093	0.091904
H	-2.417070	3.246579	0.639665
H	-0.800858	3.957937	0.820368
H	-1.957275	4.665146	-0.341461
H	-5.626938	1.749622	-0.228644
O	2.574919	-1.959411	-2.414939
H	3.061922	-2.787978	-2.432428

syn-(P)-unstable-E

C	3.795609	-1.294030	-0.951112
C	2.414414	-1.100708	-0.848477
C	1.898879	-0.022328	-0.127695
C	2.784304	0.901717	0.447232
C	4.161416	0.713920	0.344916
C	4.669513	-0.386865	-0.341591
C	0.429227	0.171358	-0.006510
S	2.108984	2.268031	1.348803
C	0.708445	2.610651	0.307018
C	-0.004077	1.569340	-0.334771
C	-1.060005	1.946585	-1.172823
H	-1.599733	1.188563	-1.730232
C	-1.444861	3.278430	-1.316351
C	-0.765038	4.283011	-0.633525
C	0.324735	3.946437	0.164929
H	1.739832	-1.817554	-1.321055
H	4.849278	1.431147	0.798952
H	5.750339	-0.531302	-0.421402
H	-1.061654	5.328934	-0.737924
H	0.893440	4.727867	0.674792
C	-0.355326	-0.787116	0.557963
C	-1.839000	-0.823674	0.628651
C	0.081434	-1.808699	1.623597
C	-2.207168	-1.152063	1.922092
H	-0.130506	-2.824037	1.242958
C	-0.984237	-1.504653	2.717298
H	-0.641314	-0.649960	3.327516
C	-2.827375	-0.762927	-0.399719
C	-4.200652	-0.791148	-0.001900
C	-4.535932	-0.960628	1.371162
C	-3.560839	-1.188470	2.314973
C	-5.210892	-0.721954	-1.003616
C	-4.883304	-0.712179	-2.337053
C	-3.524532	-0.791518	-2.732926
C	-2.525253	-0.813523	-1.790088
H	-1.147419	-2.354414	3.396941
H	-5.591827	-0.970891	1.653879
H	-3.827618	-1.405002	3.352168
H	-6.257832	-0.705728	-0.689379
H	-5.667649	-0.672663	-3.096359
H	-3.272059	-0.841048	-3.794579
H	-1.480704	-0.890142	-2.100060
C	1.482880	-1.780731	2.213661
H	2.249581	-2.156299	1.525157
H	1.766075	-0.764934	2.528484
H	1.498129	-2.422675	3.108634
H	-2.283897	3.525381	-1.970643
O	4.228028	-2.366607	-1.644718
H	5.193924	-2.391196	-1.644737

TS4

S100

C	-2.247563	2.728282	1.469809
C	-1.547610	1.551381	1.260505
C	-0.245811	1.511059	0.709761
C	0.370049	2.768312	0.534509
C	-0.338416	3.966580	0.729663
C	-1.652228	3.954491	1.167166
C	0.441877	0.206371	0.472397
S	2.074039	3.001226	0.189170
C	2.675173	1.362356	-0.013474
C	1.878957	0.200870	0.082905
C	2.476469	-0.992509	-0.368939
H	1.890342	-1.904012	-0.452741
C	3.810990	-1.076615	-0.749574
C	4.607462	0.072920	-0.732682
C	4.021679	1.281698	-0.392362
H	-3.256953	2.687812	1.884168
H	-2.029519	0.620531	1.548628
H	0.167771	4.919273	0.551341
H	-2.191703	4.893235	1.309222
H	5.660218	0.028132	-1.023467
H	4.621515	2.194621	-0.438803
C	-0.244078	-0.987194	0.612168
C	-1.663423	-1.250220	0.299029
C	0.268757	-2.281178	1.274824
C	-2.118474	-2.330422	1.038323
H	0.569924	-3.015615	0.505724
C	-1.025189	-2.843080	1.921157
H	-1.134172	-2.437094	2.942830
C	-2.500899	-0.676794	-0.718004
C	-3.838315	-1.167814	-0.832422
C	-4.284360	-2.229944	0.007713
C	-3.434699	-2.821571	0.910465
C	-4.705007	-0.603526	-1.808918
C	-4.266175	0.382834	-2.659097
C	-2.927959	0.833959	-2.580123
C	-2.070365	0.319124	-1.635440
H	-1.013559	-3.939717	2.006080
H	-5.311943	-2.585893	-0.102734
H	-3.769004	-3.661506	1.524209
H	-5.729649	-0.978489	-1.877219
H	-4.941351	0.808924	-3.404676
H	-2.570886	1.594187	-3.278817
H	-1.039670	0.670735	-1.599035
C	1.375651	-2.147676	2.315009
H	2.358351	-1.924626	1.882134
H	1.135002	-1.353537	3.039302
H	1.468816	-3.093711	2.870756
O	4.277390	-2.283959	-1.134533
H	5.201126	-2.206297	-1.406946

intermediate-*E*

C	1.591289	-2.296647	2.349561
C	0.967599	-1.158825	1.845857
C	0.118413	-1.233365	0.732943
C	-0.145743	-2.498968	0.185663
C	0.473511	-3.645845	0.687282
C	1.354729	-3.540043	1.761530
C	-0.523565	-0.003039	0.201485
S	-1.218538	-2.600255	-1.216230
C	-2.388076	-1.343888	-0.749831
C	-1.989005	-0.169403	-0.066454
C	-2.996144	0.740593	0.278792
H	-2.780558	1.635875	0.853499
C	-4.331864	0.537306	-0.080392

C	-4.698388	-0.607855	-0.788847
C	-3.722181	-1.547174	-1.103430
H	2.266198	-2.213040	3.204131
H	1.150030	-0.184522	2.305001
H	0.261038	-4.619691	0.239876
H	1.842526	-4.435867	2.152313
H	-5.741323	-0.777807	-1.068564
H	-4.008957	-2.462584	-1.626532
C	0.168678	1.161071	0.005483
C	1.627238	1.391520	-0.177312
C	-0.471705	2.547178	0.135325
C	1.869322	2.761058	-0.211095
H	-1.395227	2.635920	-0.453774
C	0.597233	3.544758	-0.320726
H	0.597257	4.468053	0.277575
C	2.734335	0.502362	-0.433088
C	4.057716	1.043827	-0.370656
C	4.250235	2.447320	-0.215417
C	3.175510	3.298115	-0.208480
C	5.177162	0.184025	-0.546005
C	5.009943	-1.142468	-0.862900
C	3.705210	-1.649024	-1.058474
C	2.605023	-0.849619	-0.850136
H	0.461511	3.845213	-1.373546
H	5.271265	2.834542	-0.166432
H	3.315480	4.381437	-0.182782
H	6.179579	0.610343	-0.452982
H	5.876724	-1.792077	-1.004395
H	3.565193	-2.680876	-1.389340
H	1.617340	-1.249972	-1.056344
C	-0.772223	2.808150	1.624140
H	-1.347920	1.999943	2.094691
H	0.170865	2.896702	2.187026
H	-1.330036	3.749528	1.747021
O	-5.219266	1.482645	0.292349
H	-6.106126	1.238946	-0.003827

TS5

C	-0.655537	3.407923	1.808008
C	-0.332356	2.058237	1.687930
C	0.105146	1.538121	0.463146
C	0.342074	2.425884	-0.598886
C	-0.003142	3.774752	-0.491818
C	-0.524711	4.257453	0.707410
C	0.486039	0.109942	0.287634
S	1.187327	1.789880	-2.029557
C	2.374858	0.796383	-1.138646
C	1.957223	0.058420	-0.011065
C	2.916546	-0.619720	0.740528
H	2.636807	-1.161945	1.643411
C	4.257726	-0.635852	0.343320
C	4.651560	0.050341	-0.809693
C	3.711527	0.778227	-1.534818
H	-1.020545	3.796686	2.760998
H	-0.459175	1.382808	2.537211
H	0.169079	4.452372	-1.331280
H	-0.789555	5.313516	0.795033
H	5.699287	0.038970	-1.121757
H	4.031220	1.348374	-2.410217
C	-0.294678	-1.000484	0.194501
C	-1.765569	-1.264233	-0.027319
C	0.366489	-2.383708	0.179779
C	-1.882635	-2.566600	-0.510995
H	1.372598	-2.339207	-0.252958
C	-0.561325	-3.251243	-0.664548

H	-0.588976	-4.302083	-0.338849
C	-2.976876	-0.480802	0.085582
C	-4.228492	-1.105853	-0.238868
C	-4.272075	-2.450386	-0.698182
C	-3.115947	-3.164563	-0.846840
C	-5.443636	-0.376148	-0.119760
C	-5.454022	0.934855	0.287720
C	-4.228225	1.566285	0.587341
C	-3.040750	0.878255	0.487922
H	-0.264223	-3.246198	-1.727230
H	-5.242040	-2.893577	-0.937225
H	-3.132247	-4.192922	-1.215597
H	-6.377297	-0.888009	-0.367125
H	-6.394527	1.484007	0.372003
H	-4.212942	2.613296	0.899937
H	-2.125037	1.400470	0.717804
C	0.464657	-2.935545	1.608826
H	1.010719	-2.253522	2.275436
H	-0.536840	-3.088362	2.042158
H	0.985927	-3.905374	1.609577
O	5.124785	-1.329882	1.108149
H	6.015928	-1.259996	0.740730

syn-(*M*)-stable-*E*

C	4.160786	-0.718183	0.773766
C	2.775733	-0.689435	0.970659
C	1.965423	0.106934	0.162052
C	2.553078	0.915325	-0.826523
C	3.933971	0.890903	-1.018773
C	4.736434	0.070001	-0.229620
C	0.479226	0.135537	0.272401
S	1.504229	1.927792	-1.847301
C	0.346709	2.439326	-0.595658
C	-0.042723	1.530565	0.411134
C	-0.819260	2.021438	1.464948
H	-1.049316	1.375483	2.308408
C	-1.296525	3.330873	1.461194
C	-0.977562	4.189381	0.410757
C	-0.132750	3.751141	-0.606510
H	2.335293	-1.312073	1.751949
H	4.393425	1.518731	-1.785790
H	5.818796	0.051662	-0.383833
H	-1.351221	5.215668	0.401210
H	0.177648	4.435747	-1.399321
C	-0.237602	-0.954282	-0.093407
C	-1.693360	-1.069460	-0.378814
C	0.386004	-2.162054	-0.790242
C	-1.820425	-1.714747	-1.599043
H	1.435302	-1.968239	-1.045590
C	-0.485746	-2.232597	-2.068873
H	-0.556293	-3.248214	-2.487715
C	-2.857031	-0.705296	0.361394
C	-4.124851	-0.815282	-0.291803
C	-4.197254	-1.353130	-1.608114
C	-3.073942	-1.838342	-2.235449
C	-5.301373	-0.443262	0.418322
C	-5.238164	-0.051997	1.733650
C	-3.993909	-0.046764	2.411075
C	-2.837530	-0.366862	1.741563
H	-0.066999	-1.576248	-2.850684
H	-5.175598	-1.424158	-2.090490
H	-3.145705	-2.312922	-3.217278
H	-6.263979	-0.500651	-0.096667
H	-6.149231	0.221867	2.270690
H	-3.957500	0.200246	3.474717

H	-1.888174	-0.412195	2.274956
C	0.308932	-3.445618	0.036032
H	0.873890	-3.346112	0.975059
H	-0.732415	-3.700580	0.290121
H	0.735197	-4.289811	-0.527804
H	-1.916748	3.680745	2.289330
O	4.890702	-1.519059	1.575873
H	5.826693	-1.449769	1.345684

TSS'

C	-4.317669	0.437066	0.359110
C	-2.963556	0.615067	0.662155
C	-1.969009	-0.019926	-0.081644
C	-2.367412	-0.985278	-1.031269
C	-3.716032	-1.167215	-1.333999
C	-4.693300	-0.428808	-0.671700
C	-0.490671	0.114957	0.144768
S	-1.143216	-2.094524	-1.700992
C	-0.232551	-2.332087	-0.188480
C	0.039709	-1.199225	0.600644
C	0.741970	-1.364016	1.796987
H	0.938607	-0.491423	2.424084
C	1.215940	-2.621140	2.169525
C	0.979381	-3.729218	1.355635
C	0.245021	-3.590117	0.177194
H	-2.705475	1.243150	1.511754
H	-4.013064	-1.915718	-2.072234
H	-5.750337	-0.572462	-0.911299
H	1.351635	-4.714370	1.645740
H	0.035091	-4.459723	-0.450037
C	0.252434	1.213291	-0.162447
C	1.742186	1.363753	-0.194345
C	-0.341643	2.605991	-0.485153
C	2.056241	2.709926	-0.311801
H	-0.960604	2.522783	-1.393057
C	0.876915	3.517375	-0.738792
H	0.801659	4.475234	-0.203220
C	2.840137	0.424355	-0.195317
C	4.154290	0.927514	0.070604
C	4.379395	2.331958	0.159934
C	3.363147	3.209251	-0.109881
C	5.252262	0.026763	0.143910
C	5.095000	-1.307816	-0.142562
C	3.829793	-1.779993	-0.556992
C	2.741095	-0.939004	-0.580948
H	0.993522	3.765248	-1.807145
H	5.390778	2.690145	0.368653
H	3.543228	4.286096	-0.152857
H	6.238050	0.428402	0.393241
H	5.947626	-1.989174	-0.098683
H	3.713523	-2.818657	-0.875288
H	1.795007	-1.314971	-0.955037
C	-1.191805	3.250377	0.619771
H	-2.202629	2.841756	0.673583
H	-0.713397	3.143916	1.606731
H	-1.300212	4.325855	0.414023
H	1.776327	-2.735669	3.099949
O	-5.211465	1.122607	1.100790
H	-6.109921	0.912059	0.813846

anti-(P)-unstable-E

C	-4.293830	0.373679	0.365900
C	-2.933066	0.631446	0.554969
C	-1.964813	-0.132512	-0.095229

C	-2.374661	-1.259104	-0.834608
C	-3.731757	-1.518986	-1.023315
C	-4.692806	-0.688125	-0.452894
C	-0.496021	0.089732	0.054154
S	-1.145375	-2.407141	-1.423821
C	-0.083384	-2.362114	0.005142
C	0.150390	-1.125112	0.629794
C	0.960118	-1.089517	1.769022
H	1.123069	-0.135830	2.275715
C	1.580471	-2.246451	2.234114
C	1.381353	-3.460097	1.574212
C	0.536746	-3.524561	0.466957
H	-2.639668	1.446774	1.215522
H	-4.047592	-2.391545	-1.599806
H	-5.755843	-0.894233	-0.604437
H	1.869217	-4.368199	1.935423
H	0.353882	-4.478538	-0.033146
C	0.200448	1.183242	-0.337608
C	1.673225	1.387293	-0.166585
C	-0.259505	2.551634	-0.852202
C	1.883532	2.716458	0.160097
H	0.171891	2.608687	-1.868734
C	0.603425	3.493572	0.020189
H	0.115743	3.651044	0.999113
C	2.785942	0.508372	-0.342145
C	4.075908	0.984996	0.048648
C	4.229238	2.326924	0.502342
C	3.163106	3.194121	0.518058
C	5.199577	0.119043	-0.074235
C	5.068156	-1.136901	-0.614151
C	3.806117	-1.572722	-1.087541
C	2.698256	-0.771216	-0.957267
H	0.754896	4.481779	-0.439582
H	5.226214	2.668699	0.792878
H	3.298449	4.240666	0.801925
H	6.177823	0.481932	0.252361
H	5.938040	-1.791346	-0.706498
H	3.715011	-2.549835	-1.567734
H	1.740059	-1.102351	-1.355062
C	-1.711078	2.981806	-0.973070
H	-2.302464	2.285905	-1.583117
H	-2.205233	3.099249	-0.000126
H	-1.736362	3.962943	-1.472839
H	2.227443	-2.200037	3.112863
O	-5.173112	1.175851	1.000087
H	-6.076839	0.889176	0.813285

TS6

C	3.908307	-1.193182	0.519325
C	2.544604	-1.010280	0.312503
C	1.975501	0.215272	-0.077997
C	2.864139	1.310521	-0.116149
C	4.239155	1.134421	0.085964
C	4.777893	-0.109002	0.374162
C	0.500667	0.305841	-0.332750
S	2.369237	2.981690	-0.303722
C	0.620072	2.873554	-0.343213
C	-0.119095	1.671832	-0.443864
C	-1.478733	1.851791	-0.786708
H	-2.085886	0.987711	-1.026689
C	-2.096157	3.090812	-0.867990
C	-1.360160	4.251675	-0.635131
C	-0.000951	4.133168	-0.401765
H	1.914019	-1.869583	0.499511
H	4.901282	2.002808	0.033970

H	5.853878	-0.226358	0.527115
H	-1.828095	5.237565	-0.674165
H	0.612813	5.030773	-0.286546
C	-0.232365	-0.849900	-0.505409
C	-1.701009	-1.054354	-0.427664
C	0.245899	-2.155336	-1.170509
C	-2.090748	-1.892181	-1.458572
H	1.227613	-2.026430	-1.645459
C	-0.875846	-2.325889	-2.233546
H	-0.951385	-3.355921	-2.612298
C	-2.633367	-0.667923	0.583399
C	-3.991826	-1.079833	0.426242
C	-4.367879	-1.872195	-0.697376
C	-3.435032	-2.287652	-1.618891
C	-4.945150	-0.700412	1.412227
C	-4.571406	0.042419	2.506232
C	-3.220135	0.434159	2.668962
C	-2.275638	0.089751	1.730766
H	-0.693981	-1.659829	-3.093996
H	-5.414453	-2.171246	-0.797889
H	-3.724201	-2.930086	-2.454087
H	-5.983667	-1.017180	1.284934
H	-5.312418	0.325366	3.257436
H	-2.927119	1.012026	3.548596
H	-1.235622	0.393637	1.863001
C	0.248870	-3.410837	-0.285687
H	0.915136	-3.345528	0.585140
H	-0.760797	-3.621407	0.099302
H	0.568592	-4.280517	-0.879458
H	-3.156341	3.143050	-1.123900
O	4.326607	-2.427396	0.873308
H	5.283243	-2.422465	1.008568

motor 6

anti-(M)-stable-E

C	-1.825680	3.124833	-1.772042
C	-1.157834	1.909863	-1.643473
C	-0.261209	1.695661	-0.591066
C	0.003641	2.754743	0.294164
C	-0.666224	3.974179	0.171258
C	-1.593001	4.150888	-0.854620
C	0.431909	0.397247	-0.378055
S	1.170037	2.504411	1.613076
C	2.352979	1.510902	0.730273
C	1.904467	0.569114	-0.216333
C	2.850926	-0.113367	-0.977254
H	2.542054	-0.795239	-1.770538
C	4.657198	0.932700	0.249995
C	3.715872	1.676337	0.962342
H	-2.537573	3.269519	-2.587507
H	-1.348619	1.100697	-2.351820
H	-0.455326	4.785797	0.871656
H	-2.117619	5.104149	-0.950268
H	5.717554	1.081374	0.454786
H	4.059406	2.405709	1.699653
C	-0.201218	-0.795819	-0.270893
C	-1.652974	-1.077916	-0.424278
C	0.469749	-2.165771	-0.204591
C	-1.778658	-2.314834	-1.032011
H	1.483704	-2.124868	-0.612968
C	-0.441670	-2.995717	-1.142598
H	-0.503773	-4.061167	-0.877570
C	-2.817877	-0.359439	-0.011279
C	-4.088440	-0.856284	-0.437722

C	-4.165074	-2.076253	-1.170525
C	-3.037225	-2.816415	-1.430270
C	-5.267041	-0.147025	-0.073314
C	-5.201965	0.966459	0.728816
C	-3.950545	1.406410	1.224112
C	-2.791517	0.760900	0.864033
H	-0.060093	-2.946173	-2.176670
H	-5.148733	-2.435983	-1.483594
H	-3.108342	-3.782222	-1.936534
H	-6.231421	-0.520645	-0.427919
H	-6.114798	1.498374	1.006869
H	-3.906092	2.260495	1.904023
H	-1.838528	1.093406	1.273362
C	0.626716	-2.742798	1.241896
C	4.223123	0.046799	-0.743453
O	5.042777	-0.685412	-1.522534
C	6.435196	-0.574484	-1.347854
H	6.745345	-0.882042	-0.334688
H	6.896241	-1.250937	-2.078416
H	6.791690	0.451832	-1.539121
C	1.474570	-1.776006	2.080957
H	2.463250	-1.608767	1.624933
H	0.985327	-0.796170	2.192177
H	1.634022	-2.187688	3.090475
C	-0.715771	-2.965124	1.951098
H	-1.255362	-2.019896	2.114074
H	-1.377721	-3.638696	1.385147
H	-0.545715	-3.423520	2.938762
C	1.375690	-4.080229	1.147702
H	2.348324	-3.956129	0.644453
H	1.568075	-4.485386	2.153910
H	0.803247	-4.840447	0.594289

*anti-(M)-stable-E**

C	-2.481700	2.379039	-1.855782
C	-1.549238	1.375806	-1.665492
C	-0.461682	1.524564	-0.758904
C	-0.332794	2.795626	-0.127801
C	-1.280624	3.797822	-0.315249
C	-2.374118	3.583954	-1.154962
C	0.418081	0.420248	-0.427290
S	0.909557	3.046082	1.083614
C	2.162509	1.971210	0.480496
C	1.826726	0.771639	-0.204272
C	2.900988	0.002602	-0.679850
H	2.733920	-0.882543	-1.286173
C	4.535713	1.486045	0.314364
C	3.489932	2.303202	0.737785
H	-3.311291	2.218364	-2.547066
H	-1.639541	0.441409	-2.220425
H	-1.166865	4.749009	0.209732
H	-3.119794	4.370193	-1.287754
H	5.563447	1.771844	0.535432
H	3.714474	3.228074	1.273833
C	-0.122053	-0.900136	-0.377886
C	-1.512911	-1.200599	-0.263557
C	0.588572	-2.246911	-0.513430
C	-1.766995	-2.457973	-0.877915
H	1.505543	-2.176358	-1.107306
C	-0.463565	-3.074731	-1.284866
H	-0.423235	-4.155988	-1.090007
C	-2.623723	-0.452882	0.303673
C	-3.950597	-0.899009	-0.020042
C	-4.138323	-2.100039	-0.731278
C	-3.055588	-2.898323	-1.123608

C	-5.057759	-0.123350	0.440541
C	-4.867846	0.977211	1.240972
C	-3.565888	1.342630	1.647697
C	-2.471940	0.621565	1.199321
H	-0.310565	-2.941817	-2.370234
H	-5.159355	-2.426757	-0.945135
H	-3.227565	-3.844694	-1.641590
H	-6.067154	-0.434393	0.159049
H	-5.727005	1.558684	1.583309
H	-3.418375	2.189338	2.320840
H	-1.470628	0.900759	1.530990
C	0.996647	-2.914418	0.857877
C	4.230806	0.334259	-0.420168
O	5.152880	-0.518939	-0.916630
C	6.512220	-0.247687	-0.711588
H	6.769537	-0.231817	0.362024
H	7.070638	-1.057283	-1.197065
H	6.811518	0.713468	-1.164923
C	1.848451	-1.962238	1.707346
H	2.787107	-1.693544	1.204236
H	1.310235	-1.030037	1.936745
H	2.105022	-2.446060	2.662824
C	-0.224111	-3.326238	1.694040
H	-0.827760	-2.455972	1.991132
H	-0.885505	-4.027941	1.165059
H	0.115507	-3.824865	2.615477
C	1.840651	-4.158766	0.540595
H	2.738953	-3.889768	-0.037946
H	2.175867	-4.642936	1.470947
H	1.277857	-4.908905	-0.035390

syn-(*P*)-unstable-*Z*

C	3.663332	-1.256485	-2.503431
C	2.442255	-1.096974	-1.863357
C	2.167627	-0.000229	-1.018558
C	3.144151	1.011166	-0.975969
C	4.375730	0.865775	-1.628833
C	4.651147	-0.278769	-2.365114
C	0.847987	0.059507	-0.338974
S	2.889365	2.506930	-0.098593
C	1.135673	2.529021	0.119336
C	0.303987	1.380813	0.064814
C	-0.992587	1.542486	0.578665
H	-1.662754	0.694599	0.675512
C	-1.499402	2.769170	1.009268
C	-0.687938	3.907039	0.967064
C	0.626762	3.760310	0.539388
H	3.837511	-2.133584	-3.130340
H	1.659712	-1.840958	-2.020841
H	5.117881	1.665741	-1.562004
H	5.616571	-0.387190	-2.864067
H	-1.045964	4.886679	1.282735
H	1.285633	4.632792	0.551653
C	0.228543	-1.149514	-0.044567
C	-1.183141	-1.525669	-0.170428
C	0.973991	-2.331207	0.626054
C	-1.382891	-2.795834	0.360354
H	1.823361	-2.690371	0.031257
C	-0.091964	-3.440635	0.747173
H	-0.142522	-3.890756	1.747372
C	-2.248080	-0.934749	-0.946667
C	-3.540877	-1.541269	-0.885034
C	-3.726191	-2.757259	-0.165781
C	-2.655363	-3.402426	0.400783
C	-4.624188	-0.953000	-1.594004

C	-4.432698	0.149065	-2.392086
C	-3.135290	0.692224	-2.531654
C	-2.076410	0.167691	-1.825985
H	0.105212	-4.273670	0.051668
H	-4.726115	-3.196549	-0.124743
H	-2.777423	-4.379063	0.875392
H	-5.612355	-1.412834	-1.509552
H	-5.270814	0.588280	-2.937802
H	-2.968554	1.531766	-3.210524
H	-1.083738	0.594375	-1.960019
C	1.575991	-1.952184	2.034750
O	-2.774344	2.756373	1.449371
C	-3.338635	3.950723	1.933362
H	-4.368490	3.714086	2.228903
H	-2.794133	4.332933	2.813609
H	-3.365932	4.734936	1.157882
C	2.214860	-3.215104	2.640522
H	2.972275	-3.637967	1.960221
H	2.719622	-2.967944	3.587577
H	1.483075	-4.004924	2.862698
C	2.695123	-0.907997	1.926188
H	2.324158	0.086744	1.646942
H	3.188815	-0.797283	2.904845
H	3.461776	-1.208328	1.195120
C	0.491650	-1.412237	2.976669
H	0.038540	-0.490217	2.579378
H	-0.315902	-2.141851	3.145900
H	0.926531	-1.172021	3.960038

TS1

C	-4.411217	0.497643	-1.786220
C	-3.114320	0.671219	-1.330332
C	-2.365114	-0.351806	-0.706816
C	-2.972613	-1.627054	-0.717576
C	-4.293959	-1.807876	-1.160486
C	-5.028394	-0.749281	-1.669148
C	-0.978505	-0.105611	-0.224655
S	-2.139743	-3.129803	-0.354673
C	-0.620921	-2.585141	0.339050
C	-0.207889	-1.235561	0.372105
C	0.951083	-0.972464	1.122678
H	1.291135	0.049248	1.271978
C	1.740885	-1.968874	1.692185
C	1.350355	-3.307568	1.575286
C	0.158347	-3.589677	0.920688
H	-4.935067	1.336789	-2.248774
H	-2.654291	1.641053	-1.486531
H	-4.736022	-2.807037	-1.118790
H	-6.055471	-0.904339	-2.006026
H	1.931367	-4.121259	2.008875
H	-0.183977	-4.626872	0.870309
C	-0.402031	1.161807	-0.258698
C	1.001111	1.455195	-0.605960
C	-1.049442	2.492788	0.207993
C	1.280081	2.794259	-0.373760
H	-1.908190	2.800382	-0.399053
C	0.062299	3.552145	0.034270
H	0.243180	4.134898	0.947555
C	1.991387	0.655734	-1.293774
C	3.297290	1.212198	-1.466359
C	3.566375	2.554569	-1.066258
C	2.562491	3.348961	-0.577435
C	4.313695	0.441529	-2.093620
C	4.049063	-0.812165	-2.590306
C	2.738415	-1.330681	-2.501128

C	1.742873	-0.619411	-1.869205
H	-0.190012	4.287756	-0.746686
H	4.574719	2.952111	-1.206710
H	2.743738	4.400352	-0.341046
H	5.310673	0.878777	-2.193388
H	4.836483	-1.392266	-3.076904
H	2.507502	-2.301931	-2.944881
H	0.739440	-1.038293	-1.839273
C	-1.584771	2.464678	1.692250
O	2.846370	-1.548384	2.340723
C	3.695167	-2.503752	2.928167
H	4.528945	-1.949555	3.377086
H	3.183020	-3.074822	3.721554
H	4.099469	-3.207377	2.180458
C	-2.146588	3.860746	2.018177
H	-2.919737	4.156553	1.290433
H	-2.612711	3.856351	3.015833
H	-1.374209	4.643210	2.025253
C	-2.734082	1.468539	1.888683
H	-3.561274	1.653805	1.187025
H	-2.410109	0.426345	1.769581
H	-3.133276	1.568104	2.910836
C	-0.471076	2.110751	2.686216
H	-0.839662	2.215711	3.719176
H	-0.141607	1.069371	2.559730
H	0.410903	2.761815	2.585275

intermediate-Z

C	-4.938157	-0.049625	-0.390257
C	-3.636789	0.297618	-0.036464
C	-2.525680	-0.500659	-0.359985
C	-2.813206	-1.715574	-1.032831
C	-4.119197	-2.067803	-1.387390
C	-5.187354	-1.232848	-1.078592
C	-1.081933	-0.162278	-0.130960
S	-1.538740	-2.846002	-1.530800
C	-0.414566	-2.604449	-0.191058
C	-0.261840	-1.309230	0.335133
C	0.653177	-1.119129	1.371221
H	0.778248	-0.132512	1.820284
C	1.459261	-2.166582	1.834512
C	1.320722	-3.442620	1.276971
C	0.371579	-3.653224	0.275271
H	-5.760030	0.615022	-0.115127
H	-3.499169	1.221307	0.510943
H	-4.295382	-3.015407	-1.902266
H	-6.204422	-1.516266	-1.357684
H	1.927655	-4.280885	1.619255
H	0.251400	-4.653752	-0.147098
C	-0.527918	1.082786	-0.310020
C	0.856355	1.455180	-0.734021
C	-1.261482	2.399175	-0.036383
C	0.900962	2.835049	-0.907780
H	-2.297975	2.371394	-0.392735
C	-0.457824	3.451087	-0.803882
H	-0.447684	4.443335	-0.335606
C	2.032004	0.699831	-1.110372
C	3.257870	1.418088	-1.299673
C	3.268628	2.842514	-1.288796
C	2.095224	3.538439	-1.172737
C	4.457273	0.710034	-1.586850
C	4.452118	-0.650330	-1.777769
C	3.223784	-1.344599	-1.732083
C	2.056810	-0.688871	-1.411413
H	-0.861233	3.587640	-1.821785

H	4.218587	3.361866	-1.438368
H	2.075221	4.628038	-1.252546
H	5.384989	1.280015	-1.685512
H	5.378346	-1.182493	-2.006150
H	3.190343	-2.411757	-1.964672
H	1.128356	-1.246690	-1.438747
C	-1.299724	2.760653	1.516476
O	2.328649	-1.852733	2.813979
C	3.204387	-2.842987	3.296353
H	3.828404	-2.362771	4.060505
H	2.659691	-3.682463	3.761015
H	3.858534	-3.232969	2.498173
C	-2.178755	4.011106	1.681832
H	-2.302107	4.250796	2.749851
H	-1.749559	4.899414	1.194815
H	-3.183426	3.847362	1.259043
C	0.106603	3.055431	2.065110
H	0.618122	3.865674	1.525923
H	0.031153	3.365106	3.119314
H	0.753438	2.165736	2.027368
C	-1.900810	1.661837	2.409131
H	-1.726303	1.924240	3.464126
H	-2.987906	1.564475	2.291457
H	-1.445773	0.676322	2.241034

TS2

C	-4.892347	-0.056487	0.000353
C	-3.570774	0.190500	0.368544
C	-2.491156	-0.428960	-0.279482
C	-2.812742	-1.375291	-1.282769
C	-4.135911	-1.622312	-1.656167
C	-5.180360	-0.951844	-1.025720
C	-1.022933	-0.185701	-0.050810
S	-1.533304	-2.280173	-2.128838
C	-0.461798	-2.527705	-0.740631
C	-0.302248	-1.464444	0.164433
C	0.477810	-1.655296	1.303124
H	0.598080	-0.853351	2.032417
C	1.166064	-2.858474	1.509069
C	1.049392	-3.890861	0.569723
C	0.219971	-3.723929	-0.541568
H	-5.699505	0.456787	0.527634
H	-3.390213	0.888046	1.181815
H	-4.346451	-2.358800	-2.435349
H	-6.213494	-1.149886	-1.319246
H	1.574219	-4.837336	0.700557
H	0.104959	-4.545061	-1.252983
C	-0.440365	1.047913	-0.124585
C	0.927473	1.521594	-0.547972
C	-1.238319	2.317051	0.155821
C	0.808861	2.879985	-0.846198
H	-2.296393	2.171134	-0.085959
C	-0.608654	3.356456	-0.762279
H	-0.707542	4.394181	-0.417334
C	2.213752	0.898692	-0.784942
C	3.336348	1.754020	-1.055442
C	3.158625	3.154402	-1.227758
C	1.904649	3.699379	-1.185367
C	4.635330	1.198872	-1.222327
C	4.840024	-0.158147	-1.201686
C	3.728033	-1.012491	-1.044926
C	2.466057	-0.499523	-0.847127
H	-1.062637	3.306701	-1.766916
H	4.034384	3.773210	-1.438849
H	1.744088	4.762827	-1.377047

H	5.469362	1.884185	-1.395165
H	5.840675	-0.573742	-1.339893
H	3.861247	-2.095843	-1.094304
H	1.640481	-1.193116	-0.781144
O	1.916027	-2.925940	2.625198
C	2.622912	-4.110306	2.905846
H	3.149220	-3.943898	3.853988
H	1.943700	-4.971539	3.023951
H	3.365534	-4.339290	2.122889
C	-1.177845	2.761216	1.682684
C	-2.400378	3.658383	1.925929
H	-2.385875	4.075722	2.945335
H	-2.422216	4.503935	1.219817
H	-3.342410	3.099996	1.805453
C	-1.215245	1.573326	2.655581
H	-1.352558	1.946233	3.682973
H	-2.024353	0.859588	2.456396
H	-0.270931	1.011558	2.632495
C	0.088535	3.561292	2.039403
H	1.007651	2.979830	1.878053
H	0.175223	4.501404	1.476152
H	0.053841	3.828957	3.107562

syn-(*M*)-stable-*Z*

C	-2.612946	-2.430970	-0.593852
C	-1.516107	-1.642205	-0.968063
C	-0.412381	-1.505976	-0.135933
C	-0.348670	-2.288050	1.037531
C	-1.430101	-3.083367	1.405574
C	-2.578326	-3.137020	0.612929
C	0.770701	-0.632939	-0.399242
S	1.146021	-2.291955	2.007523
C	2.319505	-2.228745	0.669137
C	2.027632	-1.434168	-0.455791
C	2.915408	-1.446426	-1.534584
H	2.670650	-0.875121	-2.430712
C	4.106871	-2.167659	-1.465664
C	4.414445	-2.901990	-0.319962
C	3.513954	-2.948283	0.743591
H	-1.559239	-1.131339	-1.927007
H	-1.381306	-3.685143	2.316238
H	-3.414488	-3.760206	0.930551
H	5.350053	-3.462656	-0.260635
H	3.732944	-3.553945	1.626261
C	0.794074	0.703524	-0.176554
C	-0.320844	1.521002	0.378972
C	2.064744	1.486712	0.150047
C	0.188898	2.188094	1.478658
H	2.918344	0.798696	0.221921
C	1.684154	2.023252	1.556653
H	2.187906	2.962852	1.825389
C	-1.673083	1.722244	-0.020524
C	-2.526481	2.455724	0.862211
C	-1.991010	3.022054	2.053770
C	-0.648975	2.927951	2.339395
C	-3.889076	2.650197	0.498299
C	-4.368582	2.202089	-0.708686
C	-3.495466	1.567245	-1.626404
C	-2.182900	1.339110	-1.290633
H	1.953737	1.278125	2.323358
H	-2.660223	3.578161	2.715411
H	-0.231425	3.417620	3.222698
H	-4.544531	3.185216	1.190579
H	-5.415149	2.363574	-0.977354
H	-3.866671	1.267380	-2.609229

H	-1.500154	0.892049	-2.013123
C	2.484784	2.598203	-0.866208
H	4.798955	-2.155818	-2.310670
O	-3.645953	-2.446198	-1.458829
C	-4.800927	-3.179005	-1.128814
H	-5.259243	-2.817457	-0.192564
H	-5.513134	-3.029981	-1.950039
H	-4.589243	-4.257639	-1.034125
C	3.812869	3.207017	-0.391194
H	4.183388	3.940646	-1.124796
H	3.709462	3.730389	0.571637
H	4.586718	2.431328	-0.273050
C	2.714535	1.965535	-2.243312
H	3.514948	1.211585	-2.205542
H	1.802689	1.479566	-2.624669
H	3.014467	2.733819	-2.973675
C	1.447241	3.720214	-1.012176
H	0.494055	3.351537	-1.419859
H	1.235658	4.220898	-0.055174
H	1.828478	4.486539	-1.706587

TS2'

C	2.126262	-1.724413	1.713647
C	1.043702	-0.897179	1.382959
C	0.245886	-1.179570	0.280235
C	0.492033	-2.349672	-0.462052
C	1.551749	-3.183184	-0.127858
C	2.382535	-2.870273	0.951028
C	-0.914973	-0.313709	-0.086729
S	-0.538163	-2.654435	-1.880558
C	-2.080765	-2.267547	-1.077481
C	-2.136329	-1.197714	-0.153483
C	-3.239633	-1.181371	0.708881
H	-3.271494	-0.473092	1.530522
C	-4.312532	-2.056877	0.546938
C	-4.302016	-2.999218	-0.477615
C	-3.164155	-3.126276	-1.270005
H	0.861864	-0.003276	1.982775
H	1.744979	-4.087904	-0.709003
H	3.211503	-3.536138	1.191273
H	-5.146035	-3.677323	-0.621528
H	-3.092290	-3.928995	-2.007627
C	-0.776512	1.019397	-0.362863
C	0.541551	1.706141	-0.562396
C	-1.869039	2.138374	-0.437264
C	0.363122	3.076181	-0.513761
H	-2.502249	1.926216	-1.312398
C	-1.067018	3.433830	-0.708661
H	-1.366472	4.285215	-0.092881
C	1.868373	1.233429	-0.878046
C	2.966437	2.127393	-0.674924
C	2.721443	3.497512	-0.366334
C	1.440002	3.983074	-0.382084
C	4.293954	1.665129	-0.892670
C	4.532437	0.413672	-1.408312
C	3.438886	-0.402165	-1.778309
C	2.148839	0.001398	-1.523475
H	-1.191576	3.761753	-1.754434
H	3.573032	4.163793	-0.206338
H	1.240183	5.051578	-0.271420
H	5.122813	2.345589	-0.679933
H	5.555520	0.073801	-1.584982
H	3.615177	-1.353395	-2.286277
H	1.319766	-0.607535	-1.872325
C	-2.866764	2.309760	0.792470

H	-5.160782	-1.994799	1.232260
O	2.857783	-1.341335	2.777740
C	3.994115	-2.091370	3.131732
H	4.737622	-2.112646	2.316650
H	4.439581	-1.594404	4.002662
H	3.734007	-3.126929	3.409887
C	-3.219562	3.785582	1.085705
H	-4.057301	3.805565	1.801099
H	-2.394028	4.344210	1.550270
H	-3.547733	4.326160	0.184233
C	-4.223410	1.677449	0.417055
H	-4.132883	0.738706	-0.135406
H	-4.845178	1.492706	1.307947
H	-4.779106	2.370731	-0.234752
C	-2.254614	1.777626	2.097904
H	-1.351520	2.357089	2.350549
H	-2.967432	1.894432	2.929843
H	-1.945639	0.728088	2.060966

anti-(P)-unstable-Z

C	2.622101	-1.842463	1.145269
C	1.471389	-1.043564	1.186552
C	0.444099	-1.232670	0.270313
C	0.526831	-2.296939	-0.648237
C	1.662651	-3.098939	-0.684146
C	2.721407	-2.867570	0.196362
C	-0.783630	-0.381744	0.217797
S	-0.834592	-2.572046	-1.767885
C	-2.138770	-2.293631	-0.588021
C	-1.976594	-1.263222	0.356202
C	-2.857750	-1.212408	1.438841
H	-2.663480	-0.505206	2.245486
C	-3.973429	-2.045858	1.488001
C	-4.196193	-2.973616	0.469845
C	-3.260064	-3.123582	-0.553032
H	1.419951	-0.239063	1.922180
H	1.730472	-3.920626	-1.400985
H	3.603237	-3.506193	0.143337
H	-5.074446	-3.622537	0.498078
H	-3.383223	-3.907082	-1.304351
C	-0.740569	0.950234	-0.023220
C	0.539775	1.737203	-0.023929
C	-1.777078	2.094117	-0.123928
C	0.303996	2.914568	0.661751
H	-1.509784	2.525246	-1.105847
C	-1.170626	3.078257	0.910995
H	-1.443739	2.776780	1.936821
C	1.814778	1.499747	-0.619903
C	2.882734	2.384876	-0.275441
C	2.627134	3.514794	0.554053
C	1.352281	3.805228	0.978832
C	4.177481	2.149297	-0.819820
C	4.394302	1.124546	-1.708290
C	3.314475	0.302242	-2.116255
C	2.060384	0.486848	-1.587865
H	-1.496602	4.118237	0.769371
H	3.459006	4.178437	0.804265
H	1.147876	4.713375	1.551459
H	4.994609	2.815851	-0.531393
H	5.390476	0.958862	-2.125195
H	3.478953	-0.479147	-2.862017
H	1.230728	-0.133903	-1.924957
C	-3.329885	2.039185	-0.183393
H	-4.670240	-1.973326	2.325912
O	3.577573	-1.547880	2.047947

C	4.779232	-2.279817	2.034706
H	5.308057	-2.174444	1.072057
H	5.408851	-1.863296	2.830871
H	4.608911	-3.350414	2.239229
C	-3.780338	3.378563	-0.805510
H	-4.880048	3.428595	-0.841189
H	-3.431249	4.246625	-0.226140
H	-3.406403	3.487387	-1.836410
C	-3.817008	0.933889	-1.131895
H	-3.233189	0.929815	-2.067069
H	-3.750201	-0.064914	-0.689332
H	-4.872334	1.105304	-1.397893
C	-4.003462	1.935645	1.190578
H	-3.852255	2.856496	1.775141
H	-5.090201	1.797322	1.071318
H	-3.628760	1.098306	1.786578

TS3

C	-1.920719	2.837355	-0.575190
C	-1.125194	1.692379	-0.526348
C	0.241450	1.691542	-0.204098
C	0.812400	2.983127	-0.074887
C	0.018607	4.134539	-0.099785
C	-1.351404	4.085535	-0.318502
C	1.047373	0.419146	-0.117980
S	2.533484	3.334396	-0.056778
C	3.251258	1.751681	0.127137
C	2.520665	0.544026	0.144648
C	3.271600	-0.587304	0.520153
H	2.751498	-1.518314	0.683320
C	4.642646	-0.575617	0.727399
C	5.349128	0.619131	0.598530
C	4.641942	1.778192	0.324318
H	-1.641714	0.776206	-0.775779
H	0.495648	5.109149	0.035439
H	-1.934337	5.006494	-0.321852
H	6.429896	0.657153	0.749839
H	5.163763	2.738058	0.281401
C	0.483445	-0.823747	-0.321656
C	-0.957300	-1.195882	-0.353065
C	1.135549	-2.052437	-0.988924
C	-1.181786	-1.956201	-1.484192
H	2.127303	-1.798230	-1.383543
C	0.134914	-2.202378	-2.172090
H	0.187178	-3.167541	-2.689659
C	-1.986283	-1.010919	0.617308
C	-3.278101	-1.540114	0.321528
C	-3.496031	-2.230673	-0.907211
C	-2.467734	-2.448238	-1.794402
C	-4.322307	-1.372307	1.273348
C	-4.096398	-0.717240	2.460243
C	-2.810238	-0.201629	2.753912
C	-1.780947	-0.342499	1.853403
H	0.341950	-1.417233	-2.919145
H	-4.498004	-2.613156	-1.118722
H	-2.634985	-3.015588	-2.713087
H	-5.310804	-1.779776	1.045388
H	-4.905440	-0.597415	3.184517
H	-2.637368	0.309467	3.703874
H	-0.790225	0.056033	2.081408
C	1.269899	-3.384749	-0.109947
H	5.152223	-1.500505	1.006332
O	-3.219109	2.633605	-0.880503
C	-4.080823	3.742883	-0.950358
H	-3.758325	4.465328	-1.719669

H	-5.069832	3.354353	-1.223663
H	-4.159949	4.261814	0.020221
C	0.976378	-3.140548	1.382197
H	1.554244	-2.316949	1.823478
H	-0.087437	-2.914340	1.545153
H	1.211284	-4.048518	1.960382
C	0.322569	-4.518708	-0.547217
H	-0.736720	-4.234000	-0.482750
H	0.527043	-4.868036	-1.569591
H	0.468515	-5.381925	0.120916
C	2.697788	-3.932465	-0.285614
H	3.471933	-3.249898	0.093331
H	2.812675	-4.888630	0.249299
H	2.913045	-4.118480	-1.350306

anti-(M)-stable-Z

C	2.469112	-2.327873	-0.931751
C	1.408061	-1.437204	-1.142038
C	0.279862	-1.469731	-0.328926
C	0.179403	-2.459062	0.667569
C	1.226115	-3.353372	0.870056
C	2.379239	-3.284829	0.086471
C	-0.840828	-0.503443	-0.473058
S	-1.271421	-2.512294	1.695108
C	-2.482539	-2.119389	0.453942
C	-2.164257	-1.188246	-0.551281
C	-3.093740	-0.983574	-1.578974
H	-2.834334	-0.326246	-2.411042
C	-4.341428	-1.602031	-1.549929
C	-4.673059	-2.459471	-0.499845
C	-3.734885	-2.737362	0.491405
H	1.500751	-0.687371	-1.929563
H	1.150214	-4.120251	1.644698
H	3.187884	-3.992745	0.268350
H	-5.652082	-2.942625	-0.469543
H	-3.968127	-3.450383	1.285692
C	-0.696743	0.843470	-0.446449
C	0.559674	1.637666	-0.368373
C	-1.801055	1.864288	-0.717570
C	0.375585	2.788660	-1.114729
H	-2.614518	1.415826	-1.296122
C	-1.048825	2.904527	-1.582577
H	-1.430260	3.930124	-1.476219
C	1.773292	1.447845	0.364844
C	2.836963	2.376482	0.140523
C	2.641645	3.486170	-0.731897
C	1.421701	3.714383	-1.319906
C	4.068621	2.202021	0.831549
C	4.226468	1.193841	1.751276
C	3.142860	0.329800	2.040291
C	1.950744	0.454697	1.367285
H	-1.135371	2.641245	-2.650499
H	3.470145	4.182484	-0.885478
H	1.255748	4.601661	-1.935846
H	4.883551	2.902147	0.629350
H	5.175427	1.072806	2.278761
H	3.251251	-0.438917	2.809061
H	1.118813	-0.200152	1.621606
C	-2.477895	2.448042	0.567833
H	-5.057595	-1.416751	-2.353471
O	3.530328	-2.187071	-1.748526
C	4.655329	-3.010478	-1.556703
H	4.415870	-4.076419	-1.710672
H	5.397508	-2.704585	-2.304435
H	5.090221	-2.878912	-0.551152

C	-3.586712	3.418059	0.133091
H	-4.148784	3.774179	1.011021
H	-3.187981	4.306014	-0.380562
H	-4.301926	2.925950	-0.545751
C	-3.128488	1.305484	1.360144
H	-3.869206	0.763410	0.751456
H	-2.382975	0.576131	1.711301
H	-3.647566	1.705900	2.245641
C	-1.494746	3.185697	1.485829
H	-0.722464	2.510984	1.885730
H	-0.985004	4.014874	0.970846
H	-2.035927	3.614491	2.344715

*anti-(M)-stable-Z**

C	2.536611	-1.794939	-1.008346
C	1.365594	-1.074296	-1.213760
C	0.173339	-1.385994	-0.526550
C	0.164758	-2.574967	0.266312
C	1.333110	-3.301046	0.454749
C	2.534243	-2.895774	-0.137183
C	-0.956099	-0.480315	-0.499258
S	-1.253266	-3.004738	1.202717
C	-2.525546	-2.288530	0.224416
C	-2.277171	-1.121670	-0.537939
C	-3.334354	-0.673713	-1.360687
H	-3.154864	0.142120	-2.058143
C	-4.584698	-1.273876	-1.338873
C	-4.829935	-2.365460	-0.502181
C	-3.789828	-2.884838	0.258851
H	1.403424	-0.212679	-1.879413
H	1.322581	-4.185124	1.096226
H	3.440852	-3.469388	0.052950
H	-5.814646	-2.835570	-0.474451
H	-3.945621	-3.774633	0.873071
C	-0.742235	0.924451	-0.445136
C	0.503322	1.574989	-0.189901
C	-1.760526	2.041385	-0.664325
C	0.489332	2.853576	-0.812645
H	-2.567947	1.745562	-1.341415
C	-0.892080	3.135234	-1.326079
H	-1.219203	4.163128	-1.112517
C	1.702036	1.149062	0.514710
C	2.914028	1.872530	0.240130
C	2.866413	3.059746	-0.509850
C	1.652172	3.582241	-0.985347
C	4.133931	1.376854	0.797957
C	4.135168	0.308364	1.662069
C	2.919292	-0.307032	2.036398
C	1.724963	0.134500	1.484253
H	-0.918077	3.016247	-2.423059
H	3.797132	3.605214	-0.686318
H	1.635386	4.534565	-1.520258
H	5.068281	1.884917	0.545750
H	5.076633	-0.050113	2.085945
H	2.913835	-1.116477	2.768366
H	0.788144	-0.340792	1.778671
C	-2.468428	2.527726	0.658397
H	-5.373617	-0.896404	-1.992908
O	3.630593	-1.343293	-1.652114
C	4.884312	-1.871775	-1.317899
H	4.967761	-2.940583	-1.582858
H	5.626171	-1.307307	-1.895750
H	5.096129	-1.745482	-0.242084
C	-3.562246	3.532918	0.266160
H	-4.109420	3.872455	1.159330

H	-3.150140	4.427403	-0.224912
H	-4.293209	3.075896	-0.420010
C	-3.136693	1.350675	1.382402
H	-3.879933	0.847486	0.747595
H	-2.399410	0.597750	1.699098
H	-3.653534	1.713344	2.284696
C	-1.491005	3.196262	1.635449
H	-0.715553	2.496732	1.980121
H	-0.983593	4.067657	1.195491
H	-2.040733	3.548479	2.522481

syn-(P)-unstable-E

C	3.319108	-1.169484	-1.676568
C	2.046420	-0.903992	-1.167185
C	1.749623	0.256284	-0.435599
C	2.767358	1.226112	-0.348933
C	4.036230	0.978671	-0.873788
C	4.335320	-0.220468	-1.513703
C	0.363772	0.436057	0.072020
S	2.502750	2.786728	0.412601
C	0.742808	2.916018	0.408669
C	-0.138085	1.810258	0.324609
C	-1.478886	2.079164	0.680314
H	-2.183083	1.256855	0.760906
C	-1.946379	3.354750	0.961471
C	-1.074043	4.442467	0.926682
C	0.269635	4.210527	0.671832
H	1.264343	-1.636887	-1.367006
H	4.812028	1.744314	-0.791208
H	5.338278	-0.379680	-1.909793
H	-1.428135	5.455901	1.126600
H	0.981307	5.040022	0.696929
C	-0.370608	-0.711919	0.346349
C	-1.774854	-1.009197	0.046470
C	0.196133	-1.890586	1.176440
C	-2.128699	-2.231403	0.608241
H	1.086233	-2.343384	0.721729
C	-0.953087	-2.919799	1.219983
H	-1.175857	-3.279249	2.233445
C	-2.682389	-0.404909	-0.901712
C	-4.004940	-0.938779	-1.001510
C	-4.365721	-2.099066	-0.256506
C	-3.429395	-2.765186	0.493350
C	-4.935171	-0.343618	-1.897245
C	-4.564616	0.698007	-2.713920
C	-3.233038	1.169843	-2.680677
C	-2.321195	0.636771	-1.797628
H	-0.720837	-3.819633	0.626260
H	-5.385269	-2.482909	-0.344391
H	-3.676939	-3.704457	0.993830
H	-5.948812	-0.750552	-1.942085
H	-5.284461	1.140237	-3.406402
H	-2.919896	1.959574	-3.367467
H	-1.297225	1.006548	-1.805596
C	0.635624	-1.452455	2.626956
H	-2.999088	3.494681	1.215686
O	3.466647	-2.342876	-2.325102
C	4.703705	-2.637331	-2.928222
H	5.515596	-2.706223	-2.184330
H	4.589317	-3.613353	-3.416319
H	4.975115	-1.888063	-3.691248
C	1.075781	-2.708210	3.401168
H	0.255848	-3.419384	3.575744
H	1.876818	-3.242651	2.864348
H	1.470669	-2.423514	4.388971

C	1.844484	-0.507583	2.606137
H	2.674922	-0.921851	2.013301
H	1.600554	0.485633	2.207350
H	2.209183	-0.355211	3.634360
C	-0.515096	-0.757973	3.367012
H	-0.214804	-0.513805	4.398653
H	-0.796552	0.184544	2.871505
H	-1.415220	-1.389972	3.428392

TS4

C	-2.387245	2.174426	2.106217
C	-1.623831	1.188711	1.503253
C	-0.406534	1.451806	0.830882
C	0.060467	2.778792	0.934307
C	-0.708357	3.784686	1.543623
C	-1.941045	3.497826	2.105875
C	0.353424	0.339840	0.191880
S	1.643688	3.310795	0.401785
C	2.413812	1.820752	-0.126242
C	1.756672	0.574779	-0.245421
C	2.465937	-0.419206	-0.939577
H	1.993653	-1.364582	-1.184326
C	3.782073	-0.268781	-1.371320
C	4.445544	0.943192	-1.148996
C	3.737598	1.977046	-0.550710
H	-3.326601	1.905290	2.593385
H	-1.986063	0.164555	1.556291
H	-0.312511	4.803021	1.587106
H	-2.529183	4.290795	2.572502
H	5.477459	1.105659	-1.459820
H	4.226913	2.946566	-0.423169
C	-0.245828	-0.910723	0.058368
C	-1.635093	-1.154922	-0.366346
C	0.360267	-2.278694	0.470483
C	-1.952396	-2.497283	-0.217653
H	1.221723	-2.577867	-0.137634
C	-0.775292	-3.299804	0.223682
H	-1.016162	-3.892067	1.117475
C	-2.570774	-0.297889	-1.060380
C	-3.875662	-0.815021	-1.333008
C	-4.192549	-2.169538	-1.017473
C	-3.233450	-3.010556	-0.515933
C	-4.839448	0.011481	-1.972233
C	-4.522033	1.283841	-2.384046
C	-3.208978	1.767820	-2.194111
C	-2.264987	1.000674	-1.548669
H	-0.510488	-4.029639	-0.558242
H	-5.199733	-2.536131	-1.231249
H	-3.448772	-4.067549	-0.341181
H	-5.838444	-0.396077	-2.148822
H	-5.269085	1.907485	-2.880321
H	-2.934667	2.756916	-2.568230
H	-1.256851	1.393534	-1.437192
C	0.866804	-2.338766	1.962927
C	-0.251302	-1.975614	2.948701
H	0.084106	-2.149153	3.983704
H	-0.523124	-0.913252	2.865691
H	-1.163315	-2.572923	2.795032
C	2.056180	-1.406781	2.224727
H	2.891557	-1.607690	1.536928
H	1.786025	-0.346495	2.135890
H	2.422025	-1.561700	3.252347
C	1.360303	-3.771188	2.238342
H	2.129120	-4.071065	1.507696
H	1.813012	-3.829486	3.240621

H	0.554613	-4.518735	2.204525
O	4.324130	-1.333739	-1.997512
C	5.626033	-1.227596	-2.520925
H	6.374772	-1.056761	-1.728594
H	5.845067	-2.184704	-3.010688
H	5.701041	-0.420626	-3.269536

intermediate-*E*

C	1.783756	-2.057123	2.612373
C	1.100846	-1.076064	1.900060
C	0.250047	-1.406819	0.833490
C	0.057678	-2.769380	0.550986
C	0.731635	-3.761128	1.266974
C	1.605945	-3.402754	2.290684
C	-0.455813	-0.325297	0.097725
S	-0.974441	-3.211077	-0.809840
C	-2.204823	-1.940359	-0.649658
C	-1.892587	-0.626925	-0.207208
C	-2.958372	0.276967	-0.160456
H	-2.828407	1.291425	0.193827
C	-4.259338	-0.058883	-0.555911
C	-4.538805	-1.350203	-1.004346
C	-3.500406	-2.278473	-1.034249
H	2.455181	-1.768764	3.423812
H	1.239344	-0.023443	2.154412
H	0.568899	-4.813840	1.023974
H	2.135456	-4.179106	2.847464
H	-5.540213	-1.651333	-1.311670
H	-3.711556	-3.299321	-1.362010
C	0.185404	0.846956	-0.228025
C	1.621696	1.071394	-0.561497
C	-0.479518	2.227050	-0.240974
C	1.788553	2.406030	-0.917564
H	-1.469702	2.199076	-0.709456
C	0.472368	3.101999	-1.061072
H	0.498502	4.155455	-0.754569
C	2.757370	0.192174	-0.722824
C	4.049933	0.790240	-0.878465
C	4.174727	2.199301	-1.046946
C	3.055468	2.983731	-1.145116
C	5.205443	-0.035692	-0.952267
C	5.099114	-1.405258	-0.974588
C	3.816723	-1.997086	-0.968812
C	2.686209	-1.221465	-0.847548
H	0.191090	3.092214	-2.128127
H	5.172681	2.629565	-1.163110
H	3.133554	4.050410	-1.368232
H	6.183588	0.446480	-1.028603
H	5.993037	-2.029374	-1.043274
H	3.714412	-3.079441	-1.077376
H	1.716676	-1.703237	-0.905170
C	-0.659134	2.832910	1.223322
O	-5.168399	0.931910	-0.458083
C	-6.501855	0.674009	-0.827656
H	-6.952189	-0.118765	-0.206545
H	-7.055729	1.607520	-0.667585
H	-6.585178	0.391280	-1.890864
C	-1.499704	4.112849	1.092969
H	-1.675223	4.557401	2.085496
H	-1.009051	4.878622	0.473477
H	-2.482963	3.896429	0.644514
C	0.696947	3.178376	1.863217
H	1.290756	3.884414	1.265662
H	0.530857	3.647819	2.845519
H	1.310111	2.278853	2.025370

C	-1.385078	1.907733	2.214849
H	-2.451428	1.784238	1.988420
H	-0.930230	0.910216	2.278072
H	-1.330598	2.354296	3.219862

TS5

C	1.434068	-2.647757	2.511572
C	0.862583	-1.515719	1.936841
C	0.132392	-1.604384	0.743682
C	-0.066276	-2.874967	0.178562
C	0.510683	-4.013150	0.745295
C	1.271849	-3.894922	1.907338
C	-0.464575	-0.389997	0.133861
S	-1.015633	-2.985219	-1.309306
C	-2.249326	-1.767764	-0.909299
C	-1.919831	-0.586181	-0.195989
C	-2.973190	0.281362	0.098470
H	-2.822346	1.183514	0.681293
C	-4.285486	0.048194	-0.335195
C	-4.581198	-1.099543	-1.072069
C	-3.553802	-2.005126	-1.334427
H	2.013573	-2.554404	3.432394
H	1.007601	-0.537223	2.397284
H	0.356409	-4.990830	0.282779
H	1.722547	-4.785254	2.351419
H	-5.590870	-1.316283	-1.420893
H	-3.782268	-2.925124	-1.878045
C	0.230748	0.755147	-0.148257
C	1.673783	1.013293	-0.491639
C	-0.458922	2.114234	-0.232519
C	1.745315	2.298729	-1.028794
H	-1.484118	2.006728	-0.601817
C	0.389951	2.904216	-1.220852
H	0.366180	3.992539	-1.078715
C	2.892531	0.228884	-0.487953
C	4.130292	0.909616	-0.750427
C	4.138316	2.275348	-1.149757
C	2.959033	2.938021	-1.353904
C	5.361829	0.201040	-0.691525
C	5.396083	-1.152598	-0.464087
C	4.178618	-1.850834	-0.321464
C	2.975131	-1.182527	-0.334787
H	0.059346	2.710258	-2.255680
H	5.097888	2.762415	-1.340495
H	2.944544	3.962279	-1.733791
H	6.286953	0.757454	-0.863872
H	6.347816	-1.687580	-0.431812
H	4.182866	-2.937885	-0.210818
H	2.066650	-1.765662	-0.272055
C	-0.551193	2.856147	1.174196
O	-5.185301	0.989502	0.012986
C	-6.532125	0.817665	-0.357378
H	-6.963494	-0.096689	0.084250
H	-7.075822	1.688362	0.029781
H	-6.655171	0.781597	-1.453215
C	-1.670376	3.900413	1.042088
H	-1.748803	4.508490	1.957363
H	-1.482684	4.586586	0.200969
H	-2.649096	3.422976	0.872057
C	0.751533	3.578308	1.564845
H	1.596358	2.880090	1.657920
H	1.037702	4.367963	0.855903
H	0.614479	4.061435	2.545283
C	-0.872821	1.917361	2.347626
H	-1.737382	1.264931	2.178744

H	-0.017926	1.271934	2.591018
H	-1.092089	2.519834	3.243440

syn-(M)-stable-E

C	4.205017	-0.012756	0.775362
C	2.823186	-0.054627	1.011525
C	1.934639	0.579747	0.152092
C	2.439451	1.337017	-0.922993
C	3.810973	1.390632	-1.152633
C	4.698351	0.704248	-0.320654
C	0.452449	0.513375	0.292828
S	1.297694	2.206159	-1.975861
C	0.146094	2.734725	-0.724714
C	-0.154143	1.878955	0.356101
C	-0.943828	2.384945	1.392145
H	-1.113308	1.781889	2.281687
C	-1.515927	3.653436	1.306397
C	-1.280235	4.453602	0.189727
C	-0.427221	4.004715	-0.816313
H	2.455020	-0.607044	1.875604
H	4.204661	1.977677	-1.985810
H	5.767479	0.758603	-0.526098
H	-1.732282	5.445101	0.114587
H	-0.187241	4.650116	-1.664633
C	-0.228404	-0.613704	-0.028389
C	-1.680297	-0.705131	-0.337612
C	0.404001	-1.813832	-0.733532
C	-1.786080	-1.297764	-1.582714
H	1.456791	-1.598163	-0.961737
C	-0.443596	-1.810957	-2.037888
H	-0.521905	-2.795501	-2.520981
C	-2.848091	-0.375699	0.406597
C	-4.110655	-0.481321	-0.256155
C	-4.167141	-0.967854	-1.593220
C	-3.032376	-1.408568	-2.234435
C	-5.295146	-0.157186	0.464521
C	-5.241893	0.182566	1.794637
C	-3.999022	0.189959	2.475104
C	-2.834990	-0.081244	1.797475
H	0.009588	-1.122769	-2.770762
H	-5.141493	-1.037110	-2.083802
H	-3.093588	-1.848045	-3.233140
H	-6.255377	-0.210455	-0.055300
H	-6.159914	0.415927	2.339040
H	-3.969343	0.400372	3.546857
H	-1.883648	-0.112367	2.329823
C	0.391476	-3.178562	0.028650
H	-2.147493	4.016350	2.120260
O	4.972330	-0.693061	1.649244
C	6.368484	-0.709117	1.468778
H	6.781035	-1.324046	2.278340
H	6.650662	-1.159890	0.502167
H	6.801622	0.303357	1.536385
C	1.121108	-3.026616	1.368234
H	2.172790	-2.739065	1.220415
H	0.644093	-2.267352	2.007962
H	1.112169	-3.981312	1.917994
C	-1.020455	-3.718091	0.299513
H	-1.596887	-3.060228	0.966946
H	-1.601644	-3.850946	-0.625747
H	-0.950010	-4.703625	0.787544
C	1.159655	-4.204808	-0.818644
H	1.234490	-5.165644	-0.285046
H	0.665478	-4.402285	-1.782092
H	2.184224	-3.858121	-1.029386

TS5'

C	-4.187613	-0.580338	0.079046
C	-2.903646	-0.103569	0.379851
C	-1.762009	-0.622757	-0.221601
C	-1.931643	-1.782784	-1.018224
C	-3.202538	-2.253437	-1.331046
C	-4.344878	-1.634148	-0.822571
C	-0.339383	-0.182463	0.012036
S	-0.513844	-2.770974	-1.450547
C	0.324570	-2.596184	0.109163
C	0.381673	-1.310728	0.674437
C	1.052928	-1.143808	1.889592
H	1.084237	-0.152375	2.347513
C	1.699926	-2.219136	2.495476
C	1.663370	-3.482250	1.903916
C	0.966046	-3.677179	0.711751
H	-2.842643	0.698143	1.106987
H	-3.310600	-3.147290	-1.949882
H	-5.328566	-2.022270	-1.086346
H	2.166323	-4.327115	2.379762
H	0.918671	-4.667226	0.252586
C	0.278607	0.984723	-0.345538
C	1.763789	1.185235	-0.361740
C	-0.356654	2.366369	-0.721942
C	2.048830	2.532748	-0.483771
H	-0.890979	2.236123	-1.675333
C	0.861917	3.289884	-0.962283
H	0.783040	4.270824	-0.488291
C	2.886612	0.277782	-0.384650
C	4.182727	0.803590	-0.083806
C	4.370246	2.211877	0.034782
C	3.338590	3.065394	-0.256484
C	5.298384	-0.076690	-0.020394
C	5.173541	-1.403278	-0.357142
C	3.929562	-1.884320	-0.824981
C	2.824564	-1.064957	-0.839403
H	1.000653	3.487357	-2.038574
H	5.366599	2.594667	0.270162
H	3.494624	4.146149	-0.296432
H	6.271153	0.335505	0.260893
H	6.039243	-2.068556	-0.319661
H	3.845005	-2.908572	-1.196064
H	1.895966	-1.429915	-1.268135
C	-1.408654	3.023747	0.280893
H	2.233420	-2.070287	3.436797
O	-5.200580	0.049278	0.707309
C	-6.524701	-0.330108	0.416809
H	-7.174082	0.305618	1.031596
H	-6.768016	-0.166684	-0.646799
H	-6.715522	-1.386028	0.673070
C	-1.262923	4.558469	0.392780
H	-2.139338	4.951054	0.932927
H	-0.374029	4.871449	0.960001
H	-1.242376	5.050657	-0.591721
C	-2.827060	2.838223	-0.301841
H	-2.989042	1.861474	-0.765862
H	-3.604542	2.985002	0.464962
H	-2.994361	3.590245	-1.090045
C	-1.227303	2.501617	1.715330
H	-0.235698	2.798473	2.094588
H	-1.983475	2.942701	2.384239
H	-1.280785	1.413087	1.816664

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C	3.993573	-0.597968	-0.805951
C	2.652167	-0.211330	-0.931155
C	1.685713	-0.714458	-0.071366
C	2.029867	-1.752786	0.815524
C	3.359215	-2.141047	0.943475
C	4.352179	-1.541009	0.164265
C	0.257943	-0.308269	-0.141173
S	0.720362	-2.607179	1.669041
C	-0.440432	-2.642879	0.314244
C	-0.566381	-1.501804	-0.498125
C	-1.421305	-1.552596	-1.602717
H	-1.497577	-0.682770	-2.258590
C	-2.195476	-2.684129	-1.846933
C	-2.110326	-3.786968	-0.995900
C	-1.220096	-3.776526	0.076970
H	2.374876	0.502160	-1.706708
H	3.634680	-2.936035	1.640318
H	5.387918	-1.856504	0.290728
H	-2.719918	-4.673899	-1.182799
H	-1.121244	-4.654244	0.719981
C	-0.272155	0.906257	0.131077
C	-1.709290	1.248933	-0.137398
C	0.288924	2.302622	0.489231
C	-1.729026	2.497773	-0.732626
H	-0.323709	2.534923	1.379296
C	-0.364512	3.129715	-0.648593
H	0.198590	3.003803	-1.589564
C	-2.930137	0.572260	0.155820
C	-4.136562	1.122885	-0.378605
C	-4.097051	2.347665	-1.105078
C	-2.922401	3.048446	-1.246489
C	-5.370099	0.456335	-0.127792
C	-5.417614	-0.668501	0.658596
C	-4.231398	-1.168089	1.251676
C	-3.022634	-0.563755	1.007972
H	-0.423450	4.205983	-0.433784
H	-5.031324	2.748101	-1.507445
H	-2.909465	4.021129	-1.744210
H	-6.285234	0.870586	-0.559239
H	-6.370915	-1.167485	0.847655
H	-4.279804	-2.036131	1.913434
H	-2.120019	-0.941830	1.486868
C	1.711521	2.740279	0.950114
H	-2.875437	-2.702546	-2.701475
O	4.857631	-0.006105	-1.653266
C	6.226327	-0.325721	-1.570510
H	6.732799	0.266079	-2.343146
H	6.648195	-0.060884	-0.586305
H	6.408845	-1.395731	-1.766522
C	2.710096	3.018448	-0.179773
H	3.656808	3.387580	0.246772
H	2.950449	2.130387	-0.770779
H	2.337859	3.795743	-0.865310
C	2.294962	1.745666	1.964041
H	1.540969	1.457270	2.714391
H	2.666295	0.830081	1.490625
H	3.140994	2.205319	2.499861
C	1.509676	4.075877	1.699909
H	1.059276	4.848380	1.058369
H	0.862561	3.947183	2.582330
H	2.478542	4.465084	2.050342

TS6

C	3.934579	-0.704593	0.524083
C	2.560498	-0.543324	0.347559

C	1.953477	0.657510	-0.042492
C	2.825404	1.766857	-0.124890
C	4.205498	1.615871	0.039994
C	4.783490	0.387810	0.334444
C	0.468786	0.711079	-0.266664
S	2.297713	3.423702	-0.337362
C	0.550635	3.285015	-0.296944
C	-0.175493	2.071525	-0.366246
C	-1.547767	2.241736	-0.659404
H	-2.157585	1.376885	-0.881166
C	-2.182412	3.473760	-0.718167
C	-1.455222	4.643034	-0.506627
C	-0.086918	4.537066	-0.325458
H	1.952185	-1.407654	0.563918
H	4.850322	2.494684	-0.046580
H	5.863902	0.311488	0.454524
H	-1.936869	5.622804	-0.521975
H	0.521173	5.440703	-0.228855
C	-0.242867	-0.459416	-0.433551
C	-1.717394	-0.658040	-0.435929
C	0.245934	-1.763956	-1.096204
C	-2.050473	-1.398739	-1.553499
H	1.254679	-1.633098	-1.506569
C	-0.784587	-1.801220	-2.262641
H	-0.854586	-2.766980	-2.777176
C	-2.699127	-0.339991	0.547892
C	-4.050084	-0.715064	0.280244
C	-4.369896	-1.393761	-0.932992
C	-3.390453	-1.742217	-1.833674
C	-5.050230	-0.405428	1.243723
C	-4.726592	0.237457	2.414831
C	-3.382249	0.595429	2.682213
C	-2.392548	0.316223	1.769577
H	-0.500070	-1.046947	-3.015932
H	-5.413622	-1.657493	-1.122292
H	-3.639041	-2.299745	-2.739923
H	-6.085403	-0.689500	1.036532
H	-5.503860	0.469748	3.146404
H	-3.133626	1.096554	3.620597
H	-1.355926	0.590894	1.975816
C	0.234468	-3.097640	-0.210848
H	-3.251614	3.512013	-0.936667
O	4.343641	-1.940147	0.884556
C	5.721383	-2.180751	1.044483
H	5.825497	-3.237717	1.319183
H	6.277345	-2.001293	0.108528
H	6.152904	-1.559878	1.847760
C	0.030291	-2.812364	1.289220
H	0.739689	-2.087807	1.711294
H	-0.981992	-2.428338	1.484010
H	0.145612	-3.746401	1.861714
C	1.570465	-3.827404	-0.436744
H	1.576986	-4.791640	0.096631
H	1.717700	-4.039728	-1.508318
H	2.441576	-3.254841	-0.087893
C	-0.873555	-4.097239	-0.597453
H	-1.881313	-3.671229	-0.497305
H	-0.758483	-4.483798	-1.620410
H	-0.820348	-4.965091	0.078504

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C	1.719117	-2.778825	-1.980974
C	1.075416	-1.576809	-1.700979

C	0.182863	-1.477262	-0.627802
C	-0.102303	-2.630740	0.122185
C	0.543784	-3.838267	-0.153885
C	1.463380	-3.905906	-1.198380
C	-0.479831	-0.196806	-0.265218
S	-1.249376	-2.526020	1.474196
C	-2.409169	-1.387258	0.750816
C	-1.953459	-0.346227	-0.083808
C	-2.897225	0.448352	-0.732804
H	-2.587298	1.205853	-1.453560
C	-4.706435	-0.694891	0.397972
C	-3.772155	-1.543628	0.991221
H	2.428240	-2.835176	-2.809539
H	1.283225	-0.688771	-2.301943
H	0.318568	-4.727218	0.440189
H	1.969100	-4.850398	-1.411141
H	-5.766250	-0.842237	0.606345
H	-4.121420	-2.349292	1.641376
C	0.188167	0.961962	-0.061317
C	1.642169	1.253870	-0.163814
C	-0.450914	2.329024	0.144649
C	1.782776	2.549677	-0.636140
H	-1.504253	2.377766	-0.160629
C	0.443314	3.231240	-0.732013
H	0.470214	4.271960	-0.376894
C	2.798411	0.489087	0.186534
C	4.078712	1.032752	-0.144361
C	4.172065	2.327039	-0.732652
C	3.049317	3.091192	-0.941502
C	5.250472	0.285627	0.163454
C	5.167776	-0.921959	0.812722
C	3.904666	-1.423173	1.210388
C	2.753635	-0.735673	0.907864
H	0.067384	3.242991	-1.769055
H	5.162744	2.720145	-0.975267
H	3.131049	4.104773	-1.341534
H	6.222661	0.701715	-0.113693
H	6.074932	-1.484034	1.046520
H	3.843916	-2.360778	1.767845
H	1.792887	-1.118209	1.249014
C	-4.268683	0.295345	-0.488869
O	-5.083469	1.137083	-1.153335
C	-6.473233	1.049680	-0.944614
H	-6.738282	1.238741	0.109421
H	-6.932760	1.825540	-1.569531
H	-6.871791	0.066955	-1.248416
O	-0.345470	2.645017	1.514420
C	-1.152584	3.716267	1.913385
H	-0.989745	3.875557	2.988482
H	-0.905396	4.657297	1.386543
H	-2.226478	3.504197	1.747284

*anti-(M)-stable-E**

C	1.956826	3.225645	1.606025
C	1.427028	1.978197	1.330096
C	0.136116	1.815446	0.756868
C	-0.594816	3.004154	0.482938
C	-0.050298	4.262224	0.765770
C	1.217567	4.377942	1.321446
C	-0.366902	0.490001	0.476633
S	-2.204777	3.008196	-0.193195
C	-2.552747	1.316549	-0.475583
C	-1.657702	0.265887	-0.132468
C	-2.050470	-1.051204	-0.448429
H	-1.383951	-1.875478	-0.193215

C	-4.146418	-0.286140	-1.366830
C	-3.774769	1.024854	-1.077631
H	2.954073	3.305780	2.042846
H	2.006021	1.080185	1.549813
H	-0.634628	5.159268	0.545564
H	1.629418	5.367057	1.531444
H	-5.112067	-0.469549	-1.837562
H	-4.455597	1.839488	-1.336827
C	0.443857	-0.639721	0.847858
C	1.657265	-1.076675	0.273100
C	0.212926	-1.379986	2.154072
C	2.239601	-2.094952	1.067311
H	0.361848	-0.655214	2.990113
C	1.313291	-2.467063	2.187681
H	0.834642	-3.441439	1.983949
C	2.346996	-0.613946	-0.909941
C	3.642785	-1.164299	-1.184191
C	4.195771	-2.150346	-0.331168
C	3.495089	-2.617442	0.772589
C	4.346221	-0.708255	-2.335139
C	3.797183	0.223496	-3.182335
C	2.510117	0.745645	-2.921984
C	1.806108	0.332074	-1.810434
H	1.823547	-2.546829	3.159648
H	5.184647	-2.552891	-0.564220
H	3.928225	-3.392116	1.410812
H	5.336915	-1.123137	-2.538320
H	4.351015	0.558009	-4.062578
H	2.070602	1.477760	-3.602823
H	0.807510	0.731346	-1.626632
C	-3.270511	-1.335282	-1.052527
O	-3.527575	-2.638047	-1.297009
C	-4.737290	-2.990804	-1.906345
H	-4.843635	-2.535250	-2.906873
H	-4.728325	-4.082144	-2.015830
H	-5.607952	-2.702643	-1.290535
O	-1.092428	-1.884834	2.247300
C	-1.465606	-2.295418	3.528213
H	-2.516760	-2.609609	3.482744
H	-0.860474	-3.149659	3.888077
H	-1.371936	-1.474503	4.265618

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C	-3.990673	-0.639306	2.300389
C	-2.670893	-0.658998	1.856353
C	-2.278998	0.068457	0.725707
C	-3.234605	0.870953	0.086492
C	-4.560867	0.894882	0.524283
C	-4.940576	0.127608	1.624202
C	-0.870616	0.011845	0.246437
S	-2.744708	1.815508	-1.325337
C	-1.094252	2.240188	-0.820549
C	-0.281832	1.350834	-0.071176
C	0.998639	1.784873	0.263928
H	1.662193	1.170331	0.861703
C	1.498315	3.028357	-0.146606
C	0.697930	3.880743	-0.909111
C	-0.598245	3.476542	-1.226725
H	-4.278944	-1.224581	3.176537
H	-1.924545	-1.261048	2.380686
H	-5.293893	1.520726	0.009412
H	-5.977978	0.148468	1.965918
H	1.051974	4.855594	-1.244217
H	-1.238528	4.149643	-1.801999
C	-0.303285	-1.196886	-0.012877

C	1.096160	-1.568023	-0.321189
C	-1.096586	-2.437760	-0.455429
C	1.094192	-2.462878	-1.381211
H	-0.965762	-3.248749	0.287069
C	-0.317591	-2.817091	-1.745031
H	-0.706453	-2.186995	-2.562519
C	2.302357	-1.329216	0.406292
C	3.521176	-1.836187	-0.142624
C	3.489586	-2.623410	-1.328488
C	2.294980	-2.976128	-1.912662
C	4.741804	-1.602516	0.552727
C	4.749771	-0.969278	1.771272
C	3.529542	-0.559815	2.363551
C	2.339442	-0.735959	1.699824
H	-0.441571	-3.871723	-2.029978
H	4.433730	-2.996762	-1.733709
H	2.272368	-3.650534	-2.772006
H	5.673243	-1.963875	0.109095
H	5.691533	-0.805673	2.299957
H	3.535499	-0.106280	3.357258
H	1.401045	-0.435555	2.170537
O	2.755684	3.309163	0.249756
C	3.328175	4.543194	-0.109286
H	4.337064	4.557220	0.321761
H	3.408838	4.654980	-1.204027
H	2.756165	5.394155	0.298329
O	-2.442682	-2.215947	-0.713495
C	-3.318992	-3.209890	-0.262640
H	-4.341262	-2.877446	-0.490600
H	-3.147057	-4.178723	-0.767828
H	-3.240684	-3.367829	0.828798

TS1

C	1.704893	2.427246	-1.145126
C	0.978999	1.267333	-0.882000
C	-0.301483	1.267717	-0.303280
C	-0.889717	2.540268	-0.125167
C	-0.163775	3.708904	-0.380691
C	1.137348	3.674550	-0.862698
C	-1.014057	-0.016698	-0.026956
S	-2.576089	2.815671	0.281492
C	-3.212653	1.196610	0.490809
C	-2.443510	0.018623	0.395119
C	-3.078904	-1.154557	0.863647
H	-2.502795	-2.070723	0.960300
C	-4.408330	-1.194585	1.250148
C	-5.176996	-0.028196	1.220172
C	-4.566598	1.163310	0.868540
H	1.462022	0.335974	-1.162643
H	-0.640119	4.679012	-0.214610
H	1.669771	4.608292	-1.043165
H	-6.230333	-0.041143	1.508402
H	-5.131457	2.098836	0.904223
C	-0.372460	-1.226629	-0.192485
C	1.051415	-1.575654	-0.025999
C	-1.000691	-2.495804	-0.776973
C	1.365300	-2.659959	-0.832875
H	-1.226960	-3.232423	0.022610
C	0.162509	-3.081573	-1.618820
H	0.141992	-2.598088	-2.610386
C	2.013256	-1.082627	0.917552
C	3.316922	-1.667073	0.904604
C	3.612906	-2.733755	0.006559
C	2.650332	-3.240816	-0.832443
C	4.301879	-1.186809	1.811834

C	4.008610	-0.189746	2.710582
C	2.706172	0.361483	2.750513
C	1.735680	-0.072630	1.877416
H	0.093241	-4.168892	-1.763020
H	4.618682	-3.161369	0.017451
H	2.872983	-4.081405	-1.493910
H	5.298615	-1.634949	1.784922
H	4.772556	0.169687	3.403776
H	2.467547	1.134814	3.484293
H	0.735084	0.356434	1.929923
H	-4.841956	-2.136103	1.593783
O	2.930427	2.247934	-1.678791
C	3.700495	3.376930	-2.012339
H	3.950411	3.980003	-1.122638
H	4.631290	3.000489	-2.454963
H	3.189525	4.017217	-2.751494
O	-2.140589	-2.222829	-1.525994
C	-2.957924	-3.332285	-1.770796
H	-3.843460	-2.978871	-2.316515
H	-2.452006	-4.100042	-2.384899
H	-3.293610	-3.809769	-0.830115

intermediate-Z

C	-4.919502	0.119400	0.343944
C	-3.578890	0.416946	0.577248
C	-2.550050	-0.261639	-0.091672
C	-2.922860	-1.326694	-0.942880
C	-4.267593	-1.620478	-1.184272
C	-5.269092	-0.884932	-0.556213
C	-1.090236	0.049760	0.023140
S	-1.694380	-2.333653	-1.741997
C	-0.484699	-2.341723	-0.447049
C	-0.271973	-1.161100	0.286127
C	0.673641	-1.159254	1.308067
H	0.834840	-0.258663	1.903368
C	1.459190	-2.290245	1.563976
C	1.267921	-3.450006	0.802922
C	0.286165	-3.471102	-0.189354
H	-5.694145	0.674347	0.878040
H	-3.305911	1.177440	1.303503
H	-4.529038	-2.444680	-1.852428
H	-6.318446	-1.120265	-0.747080
H	1.858244	-4.348759	0.981814
H	0.124014	-4.388250	-0.760577
C	-0.556140	1.297267	-0.109033
C	0.845802	1.724220	-0.350727
C	-1.364150	2.568647	0.178533
C	0.937297	3.099954	-0.182061
H	-2.288674	2.624179	-0.426045
C	-0.413586	3.739971	-0.095698
H	-0.479060	4.509888	0.685391
C	2.015839	1.016257	-0.806324
C	3.274949	1.693160	-0.743142
C	3.329439	3.070673	-0.382519
C	2.174485	3.779368	-0.174034
C	4.461705	1.003826	-1.116944
C	4.409953	-0.272124	-1.623760
C	3.154678	-0.893306	-1.813294
C	1.996032	-0.267027	-1.415999
H	-0.638617	4.236263	-1.053958
H	4.303505	3.564237	-0.337213
H	2.201911	4.855486	0.012600
H	5.418155	1.524409	-1.020617
H	5.326886	-0.788398	-1.916922
H	3.098546	-1.874736	-2.289987

H	1.042806	-0.747841	-1.615367
O	2.364728	-2.170525	2.553139
C	3.196219	-3.264458	2.855960
H	3.847735	-2.945650	3.679088
H	2.615499	-4.143701	3.183267
H	3.826442	-3.548083	1.995742
O	-1.702466	2.525206	1.556333
C	-2.604699	3.516894	1.968108
H	-2.839379	3.327367	3.024729
H	-2.187034	4.536524	1.886077
H	-3.545341	3.486361	1.384440

TS2

C	4.605828	-0.570978	0.993622
C	3.222944	-0.546064	1.168464
C	2.386862	-0.098111	0.141192
C	2.968974	0.397613	-1.041055
C	4.352684	0.362355	-1.221841
C	5.168731	-0.134774	-0.206253
C	0.888743	-0.082008	0.200320
S	1.904668	1.086076	-2.298921
C	0.821932	1.961468	-1.187754
C	0.446625	1.328550	0.012233
C	-0.150161	2.085740	1.017257
H	-0.374763	1.638697	1.987620
C	-0.518263	3.418265	0.786593
C	-0.245761	4.006808	-0.454869
C	0.452906	3.283426	-1.421784
H	5.247383	-0.935552	1.799096
H	2.771920	-0.907989	2.093688
H	4.793286	0.745012	-2.145433
H	6.251765	-0.157176	-0.346600
H	-0.525763	5.039014	-0.664465
H	0.735262	3.773503	-2.356403
C	0.190162	-1.246943	0.205102
C	-1.230215	-1.667777	-0.058766
C	0.983744	-2.548604	0.375406
C	-1.218322	-3.026341	-0.363786
H	1.979537	-2.472556	-0.089078
C	0.148203	-3.628756	-0.305025
H	0.162619	-4.579204	0.248330
C	-2.501943	-0.982194	-0.099786
C	-3.672636	-1.728224	-0.464690
C	-3.581771	-3.112935	-0.775256
C	-2.374405	-3.752249	-0.721587
C	-4.939776	-1.084501	-0.513802
C	-5.077758	0.247854	-0.211280
C	-3.935200	0.986694	0.163370
C	-2.699018	0.385381	0.216019
H	0.521187	-3.837496	-1.321169
H	-4.491893	-3.652599	-1.049441
H	-2.289182	-4.816810	-0.952313
H	-5.810645	-1.680707	-0.798735
H	-6.057130	0.729425	-0.255160
H	-4.026421	2.045543	0.418165
H	-1.848585	0.980910	0.510702
O	-1.136130	4.044817	1.805560
C	-1.525685	5.389060	1.649228
H	-1.985106	5.694009	2.597649
H	-0.662360	6.044560	1.444581
H	-2.268314	5.506995	0.841830
O	1.132954	-2.776723	1.762631
C	2.091726	-3.748611	2.075447
H	2.153050	-3.816893	3.170618
H	1.829477	-4.748390	1.682263

H 3.090518 -3.479146 1.681164

syn-(*M*)-stable-*Z*

C	-1.429198	3.123584	0.090021
C	-0.894139	1.874824	0.434371
C	0.355099	1.454892	-0.014389
C	1.103645	2.360679	-0.806734
C	0.572719	3.602015	-1.148443
C	-0.695162	3.992392	-0.719944
C	0.962917	0.113117	0.235392
S	2.711445	1.954318	-1.442728
C	3.309207	0.960298	-0.108707
C	2.407744	0.147778	0.596391
C	2.902478	-0.647063	1.640828
H	2.205792	-1.276133	2.198513
C	4.261193	-0.665262	1.944825
C	5.148381	0.128226	1.215651
C	4.673667	0.948939	0.195348
H	-1.502243	1.241769	1.071296
H	1.162683	4.289947	-1.758965
H	-1.080671	4.970697	-1.006996
H	6.215225	0.120799	1.450187
H	5.361554	1.586631	-0.365059
C	0.396301	-1.096838	-0.018227
C	-0.986297	-1.484254	-0.379639
C	1.246389	-2.286885	-0.449519
C	-0.915380	-2.347640	-1.462709
H	2.290371	-1.997969	-0.650715
C	0.519155	-2.700760	-1.755514
H	0.650730	-3.767209	-1.990442
C	-2.235245	-1.262943	0.274158
C	-3.417794	-1.739619	-0.373350
C	-3.310567	-2.480776	-1.583743
C	-2.080359	-2.825490	-2.095499
C	-4.679957	-1.524818	0.250556
C	-4.764281	-0.942923	1.491573
C	-3.583030	-0.571990	2.181020
C	-2.353690	-0.728726	1.588087
H	0.920430	-2.118789	-2.601899
H	-4.227001	-2.831701	-2.065174
H	-2.004109	-3.468492	-2.975702
H	-5.582975	-1.859577	-0.266751
H	-5.737335	-0.795597	1.965692
H	-3.651730	-0.166318	3.192987
H	-1.444453	-0.470254	2.135101
H	4.627952	-1.300478	2.754010
O	-2.649813	3.394345	0.591460
C	-3.250066	4.632407	0.296193
H	-3.418890	4.758798	-0.786781
H	-4.220240	4.639722	0.808263
H	-2.646944	5.478336	0.667974
O	1.211674	-3.295383	0.530888
C	2.200881	-4.273246	0.368237
H	2.078149	-5.013392	1.171234
H	2.120645	-4.800560	-0.600542
H	3.217382	-3.840533	0.441220

TS2'

C	1.693364	-2.079745	1.634430
C	0.785507	-1.035830	1.413282
C	-0.160248	-1.113727	0.394332
C	-0.242331	-2.291302	-0.370145
C	0.645969	-3.337352	-0.144164
C	1.624711	-3.234661	0.845638

C	-1.096185	0.014994	0.135559
S	-1.415581	-2.361418	-1.697243
C	-2.758892	-1.519600	-0.892413
C	-2.517408	-0.452903	0.003541
C	-3.620910	0.042676	0.713405
H	-3.445174	0.803658	1.466452
C	-4.914091	-0.409995	0.461517
C	-5.140606	-1.396187	-0.496304
C	-4.056239	-1.968742	-1.154118
H	0.855488	-0.138250	2.030680
H	0.585070	-4.247716	-0.745291
H	2.313855	-4.065378	0.997054
H	-6.152902	-1.750002	-0.704116
H	-4.210401	-2.788111	-1.860327
C	-0.648697	1.293423	-0.027002
C	0.743442	1.756462	-0.270808
C	-1.504977	2.560119	0.102795
C	0.839890	3.109075	0.015144
H	-2.133687	2.679415	-0.801900
C	-0.501286	3.727873	0.243826
H	-0.593659	4.155460	1.254827
C	1.892849	1.091532	-0.827628
C	3.154464	1.759433	-0.753866
C	3.224215	3.100514	-0.275382
C	2.079419	3.787143	0.036625
C	4.321231	1.107919	-1.240515
C	4.242074	-0.118793	-1.854719
C	2.977707	-0.722571	-2.043271
C	1.839275	-0.132104	-1.545697
H	-0.678375	4.542966	-0.474489
H	4.199947	3.590425	-0.225608
H	2.116705	4.842899	0.315391
H	5.282625	1.618656	-1.141239
H	5.143130	-0.605819	-2.234388
H	2.899076	-1.660283	-2.598521
H	0.873401	-0.587033	-1.747607
H	-5.749387	0.011638	1.025377
O	2.590644	-1.886287	2.620249
C	3.572362	-2.867609	2.851880
H	4.196946	-3.037224	1.958451
H	4.208885	-2.490024	3.661731
H	3.126570	-3.825947	3.168458
O	-2.324713	2.505325	1.244693
C	-3.365182	3.444369	1.235604
H	-3.921853	3.334197	2.176675
H	-2.991420	4.483156	1.175279
H	-4.059544	3.277223	0.390188

anti-(P)-unstable-Z

C	1.799302	-2.191794	1.320384
C	0.884740	-1.133277	1.245828
C	-0.134868	-1.137381	0.299969
C	-0.291650	-2.258661	-0.535457
C	0.610336	-3.315537	-0.459031
C	1.667913	-3.282250	0.451641
C	-1.083428	0.002794	0.146734
S	-1.625612	-2.274438	-1.711786
C	-2.864172	-1.517005	-0.680350
C	-2.502172	-0.468627	0.186500
C	-3.459954	-0.013159	1.102174
H	-3.178040	0.752503	1.822378
C	-4.761474	-0.505345	1.080779
C	-5.128534	-1.482450	0.153680
C	-4.174396	-2.004561	-0.714675
H	1.011306	-0.284898	1.920686

H	0.494438	-4.183386	-1.112579
H	2.365891	-4.119035	0.485437
H	-6.150644	-1.867410	0.130645
H	-4.436865	-2.812295	-1.401888
C	-0.651304	1.269106	-0.060889
C	0.760999	1.747846	-0.114290
C	-1.434241	2.577248	-0.089022
C	0.816239	2.993703	0.490426
H	-1.354541	2.969803	-1.125186
C	-0.565533	3.483006	0.817405
H	-0.834863	3.290709	1.870395
C	1.935796	1.187933	-0.707469
C	3.179341	1.850107	-0.466980
C	3.205148	3.073560	0.263185
C	2.042662	3.661522	0.698068
C	4.374280	1.299541	-1.010328
C	4.338650	0.177563	-1.801826
C	3.096408	-0.429293	-2.108567
C	1.928517	0.064359	-1.578982
H	-0.693771	4.556628	0.619002
H	4.169074	3.560676	0.431825
H	2.061173	4.629881	1.203580
H	5.322906	1.800728	-0.800721
H	5.261464	-0.233365	-2.217772
H	3.064961	-1.290681	-2.780009
H	0.977731	-0.393620	-1.847332
H	-5.494698	-0.125744	1.796105
O	2.766938	-2.071847	2.249747
C	3.734077	-3.087307	2.363884
H	4.302553	-3.215901	1.427201
H	4.425548	-2.775562	3.156559
H	3.281088	-4.052728	2.646945
O	-2.768989	2.491976	0.272924
C	-3.536165	3.616913	-0.056640
H	-4.580537	3.391095	0.199807
H	-3.225660	4.517798	0.503293
H	-3.481409	3.843464	-1.138060

TS3

C	-1.693126	2.619045	-0.845773
C	-0.961783	1.438677	-0.728795
C	0.369605	1.388066	-0.285453
C	0.996035	2.643789	-0.105231
C	0.264437	3.832062	-0.207562
C	-1.081955	3.840294	-0.545442
C	1.083611	0.081117	-0.131700
S	2.724184	2.885375	0.092289
C	3.344427	1.253865	0.222400
C	2.543368	0.092065	0.186488
C	3.191093	-1.101743	0.580405
H	2.594313	-1.999231	0.730419
C	4.553833	-1.175704	0.827597
C	5.341772	-0.027390	0.734159
C	4.726839	1.183773	0.462433
H	-1.486997	0.533733	-1.013561
H	0.771445	4.785704	-0.037403
H	-1.617705	4.787514	-0.607582
H	6.417684	-0.066651	0.917317
H	5.315019	2.105452	0.456405
C	0.438763	-1.123479	-0.323625
C	-0.994272	-1.476954	-0.220287
C	1.064312	-2.359182	-0.976812
C	-1.294525	-2.439207	-1.171218
H	1.999173	-2.115180	-1.508829
C	-0.057579	-2.793611	-1.946982

H	0.001184	-3.860690	-2.205308
C	-1.975849	-1.089413	0.746301
C	-3.289771	-1.634024	0.614463
C	-3.573360	-2.564039	-0.427523
C	-2.591068	-2.977711	-1.296265
C	-4.294164	-1.245726	1.544328
C	-4.010276	-0.373543	2.567456
C	-2.699397	0.140124	2.715819
C	-1.708624	-0.208317	1.827926
H	0.008145	-2.216786	-2.884617
H	-4.586838	-2.965630	-0.508060
H	-2.806516	-3.718706	-2.069746
H	-5.298910	-1.661669	1.432409
H	-4.789932	-0.082735	3.275167
H	-2.472861	0.815503	3.544121
H	-0.700302	0.187831	1.956070
H	4.996830	-2.130696	1.118038
O	-2.969293	2.482620	-1.259116
C	-3.784335	3.626364	-1.337973
H	-4.772785	3.284275	-1.669707
H	-3.891382	4.120207	-0.357095
H	-3.399422	4.356870	-2.070135
O	1.297000	-3.379890	-0.023774
C	2.150809	-4.397718	-0.473181
H	2.219012	-5.150242	0.324420
H	1.773074	-4.893895	-1.385292
H	3.166253	-4.011709	-0.686273

anti-(M)-stable-Z

C	1.726747	-2.502790	-1.081740
C	0.866902	-1.401140	-1.174677
C	-0.216049	-1.268402	-0.311527
C	-0.494134	-2.295735	0.608482
C	0.355906	-3.394612	0.699217
C	1.476220	-3.496085	-0.126894
C	-1.096047	-0.070727	-0.328857
S	-1.901705	-2.146485	1.684026
C	-3.025342	-1.367403	0.546487
C	-2.543005	-0.428977	-0.385943
C	-3.436109	0.067115	-1.345413
H	-3.064761	0.725211	-2.133195
C	-4.786013	-0.274622	-1.314030
C	-5.263946	-1.143957	-0.333004
C	-4.380517	-1.707356	0.584280
H	1.087720	-0.625227	-1.909760
H	0.148115	-4.189480	1.419555
H	2.129982	-4.362721	-0.028584
H	-6.322298	-1.412096	-0.301118
H	-4.738504	-2.431863	1.319550
C	-0.635772	1.197710	-0.232929
C	0.759849	1.701329	-0.141141
C	-1.476731	2.456785	-0.394915
C	0.818901	2.910854	-0.815762
H	-2.445252	2.282981	-0.882547
C	-0.554314	3.348001	-1.253516
H	-0.730622	4.420963	-1.087042
C	1.919042	1.193799	0.524728
C	3.160483	1.866707	0.301719
C	3.195357	3.048763	-0.492994
C	2.042115	3.586660	-1.011531
C	4.341787	1.363719	0.916115
C	4.293303	0.279284	1.757834
C	3.050442	-0.336210	2.043258
C	1.896509	0.110210	1.445200
H	-0.720741	3.145750	-2.325043

H	4.156528	3.545999	-0.647151
H	2.067143	4.524989	-1.570928
H	5.290031	1.871092	0.719823
H	5.205785	-0.095530	2.227245
H	3.006427	-1.166168	2.752433
H	0.944016	-0.353367	1.697004
H	-5.466214	0.132967	-2.065110
O	2.763788	-2.519279	-1.940522
C	3.726628	-3.540115	-1.829930
H	3.291967	-4.536113	-2.020596
H	4.488764	-3.335706	-2.592206
H	4.206945	-3.538879	-0.836799
O	-1.688711	2.992515	0.891216
C	-2.689576	3.969055	0.944922
H	-2.771073	4.308334	1.987034
H	-2.461847	4.849197	0.314343
H	-3.671275	3.566366	0.628505

*anti-(M)-stable-Z**

C	1.272053	0.178719	2.059152
C	1.872704	1.022703	1.097391
C	3.219805	1.464397	1.312587
C	3.910710	1.002726	2.468905
C	3.302516	0.169318	3.376224
C	1.965723	-0.242089	3.174252
C	3.834626	2.352440	0.396525
C	3.148413	2.825918	-0.713655
C	1.843711	2.404802	-0.952753
C	1.196353	1.483462	-0.093667
C	0.924924	2.796935	-2.072629
C	-0.260858	1.809077	-1.959808
C	-0.064359	1.123724	-0.618866
C	-0.943963	0.073228	-0.178117
C	-0.532679	-1.298106	-0.389797
C	-1.334571	-2.414127	-0.017021
S	-2.924966	-2.265963	0.698976
C	-3.156855	-0.543780	0.868318
C	-2.203523	0.415171	0.435704
C	-0.871281	-3.711052	-0.228463
C	0.372874	-3.956283	-0.805027
C	1.175901	-2.872821	-1.186801
C	0.722196	-1.573842	-0.976618
C	-2.509685	1.781015	0.673151
C	-3.687865	2.171367	1.280816
C	-4.618892	1.206743	1.682590
C	-4.350826	-0.140710	1.478093
O	2.391509	-2.992641	-1.759674
C	2.932557	-4.270209	-1.950471
O	-1.521590	2.417655	-2.060136
C	-1.899599	2.756618	-3.360996
H	-1.775525	2.518374	0.342697
H	1.375811	-0.753003	-1.271443
H	-1.498171	-4.557971	0.062083
H	0.695584	-4.987004	-0.949588
H	-5.553907	1.504818	2.161535
H	-5.069593	-0.897431	1.802146
H	-0.190026	1.030440	-2.756052
H	0.532511	3.816837	-1.912035
H	1.417087	2.782593	-3.056894
H	4.862464	2.672555	0.584467
H	3.632315	3.524411	-1.401392
H	4.940959	1.332071	2.627255
H	3.848063	-0.171135	4.259343
H	1.479141	-0.894096	3.902803
H	0.235280	-0.131822	1.920004

H	-3.888632	3.231845	1.444676
H	2.311235	-4.884617	-2.625837
H	3.918409	-4.128714	-2.409721
H	3.059006	-4.807505	-0.994158
H	-2.911928	3.179180	-3.313115
H	-1.225760	3.511667	-3.809573
H	-1.914859	1.871730	-4.026461

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C	-3.694617	-0.902025	1.227440
C	-2.311510	-0.741381	1.072033
C	-1.792268	0.226160	0.216469
C	-2.675897	1.099902	-0.437655
C	-4.049693	0.954514	-0.276352
C	-4.569010	-0.052449	0.541085
C	-0.321180	0.360931	0.041775
S	-2.010910	2.348726	-1.501003
C	-0.547802	2.753228	-0.576722
C	0.172137	1.770815	0.145507
C	1.304397	2.201764	0.847639
H	1.864529	1.494757	1.450260
C	1.743821	3.523127	0.798148
C	1.045726	4.465559	0.048466
C	-0.108294	4.079271	-0.627248
H	-1.642068	-1.410979	1.616098
H	-4.735493	1.633046	-0.789422
H	-5.649920	-0.146334	0.646603
H	1.382370	5.503600	0.002263
H	-0.684591	4.814893	-1.193571
C	0.407369	-0.714061	-0.359225
C	1.872404	-0.894734	-0.476398
C	-0.152503	-1.860522	-1.220329
C	2.147615	-1.483704	-1.701417
H	-0.045622	-2.820406	-0.679760
C	0.864541	-1.836902	-2.394073
H	0.540061	-1.049524	-3.094926
C	2.908153	-0.758433	0.497434
C	4.251728	-1.006920	0.077083
C	4.506077	-1.458547	-1.248920
C	3.471837	-1.743802	-2.110297
C	5.307027	-0.870773	1.023985
C	5.042381	-0.582740	2.340240
C	3.702057	-0.436378	2.776831
C	2.664880	-0.520632	1.879604
H	0.912445	-2.789591	-2.940918
H	5.541837	-1.636816	-1.549606
H	3.668481	-2.172466	-3.095839
H	6.334967	-1.029166	0.687335
H	5.859005	-0.495464	3.060521
H	3.493614	-0.263003	3.835047
H	1.633504	-0.425785	2.225778
H	2.638557	3.810272	1.354909
O	-4.085726	-1.900790	2.045367
C	-5.461237	-2.122536	2.242352
H	-5.974379	-2.375872	1.298939
H	-5.546283	-2.972868	2.930604
H	-5.955107	-1.247612	2.698262
O	-1.452072	-1.691609	-1.680972
C	-2.308198	-2.786177	-1.506976
H	-3.287154	-2.508011	-1.921612
H	-1.946336	-3.684047	-2.041549
H	-2.445094	-3.044370	-0.441378

TS4

C	2.408637	2.755975	-1.490724
C	1.683876	1.611413	-1.201092
C	0.381146	1.636396	-0.651300
C	-0.203498	2.917367	-0.552973
C	0.531289	4.083471	-0.829298
C	1.841371	4.012658	-1.271295
C	-0.343967	0.368704	-0.338880
S	-1.897552	3.220030	-0.217560
C	-2.543609	1.616575	0.091286
C	-1.778382	0.429785	0.065158
C	-2.411728	-0.712695	0.580374
H	-1.860230	-1.636818	0.725711
C	-3.752109	-0.744401	0.957177
C	-4.516950	0.424557	0.879911
C	-3.888972	1.594764	0.473982
H	3.415175	2.663952	-1.903788
H	2.146012	0.654523	-1.428151
H	0.046792	5.056558	-0.711515
H	2.399712	4.927745	-1.479640
H	-5.569629	0.447480	1.161949
H	-4.459971	2.527189	0.469710
C	0.287864	-0.853665	-0.439440
C	1.702619	-1.210370	-0.223357
C	-0.342882	-2.141345	-0.983227
C	2.022560	-2.335575	-0.969911
H	-0.600407	-2.837174	-0.158318
C	0.834325	-2.777849	-1.766311
H	0.844826	-2.337216	-2.777601
C	2.646166	-0.685689	0.721609
C	3.942726	-1.284191	0.769556
C	4.248048	-2.394913	-0.070320
C	3.300138	-2.929836	-0.909023
C	4.908479	-0.775374	1.681956
C	4.602326	0.262709	2.528705
C	3.305712	0.828307	2.509741
C	2.354013	0.367012	1.629969
H	0.752651	-3.869290	-1.866164
H	5.247544	-2.833462	-0.012767
H	3.528226	-3.804389	-1.522983
H	5.900190	-1.234806	1.703138
H	5.351476	0.643072	3.226911
H	3.055825	1.634106	3.203766
H	1.357146	0.807564	1.637609
O	-4.216668	-1.937462	1.389294
C	-5.565842	-2.042471	1.773359
H	-6.248503	-1.797944	0.941694
H	-5.728995	-3.087155	2.066332
H	-5.799301	-1.392191	2.633858
O	-1.455637	-1.893736	-1.781787
C	-2.353270	-2.964078	-1.885495
H	-3.169372	-2.648528	-2.550025
H	-1.883412	-3.867268	-2.316611
H	-2.786999	-3.230297	-0.903028

intermediate-*E*

C	1.730170	-2.309727	2.397091
C	1.071060	-1.207157	1.860695
C	0.263312	-1.338274	0.724418
C	0.080150	-2.618361	0.175846
C	0.740218	-3.727338	0.708478
C	1.575844	-3.567563	1.812532
C	-0.428806	-0.158707	0.144499
S	-0.946263	-2.784844	-1.258692
C	-2.204366	-1.609960	-0.811510
C	-1.879381	-0.422298	-0.113526

C	-2.927711	0.405984	0.282155
H	-2.717471	1.282163	0.888016
C	-4.256705	0.131790	-0.066573
C	-4.558552	-1.013696	-0.807977
C	-3.525340	-1.884645	-1.155058
H	2.368440	-2.186660	3.274545
H	1.192221	-0.219879	2.312115
H	0.594753	-4.714658	0.263909
H	2.090986	-4.435539	2.229950
H	-5.582005	-1.258180	-1.092908
H	-3.763258	-2.805416	-1.693248
C	0.198467	1.018380	-0.138896
C	1.644757	1.336754	-0.261132
C	-0.558127	2.350024	-0.225537
C	1.801925	2.714697	-0.339222
H	-1.373871	2.314890	-0.971727
C	0.496145	3.411878	-0.562087
H	0.374230	4.311688	0.056830
C	2.816225	0.510308	-0.412611
C	4.097377	1.137755	-0.299887
C	4.192933	2.555488	-0.194662
C	3.068834	3.335070	-0.284906
C	5.276261	0.345610	-0.375105
C	5.209554	-1.000240	-0.643486
C	3.952184	-1.597467	-0.887067
C	2.794042	-0.863267	-0.775179
H	0.434217	3.735476	-1.613997
H	5.182667	3.010598	-0.106124
H	3.141461	4.425067	-0.299843
H	6.243228	0.838967	-0.246266
H	6.122523	-1.596403	-0.709859
H	3.895080	-2.649269	-1.177209
H	1.846121	-1.335272	-1.014689
O	-5.169121	1.027739	0.360564
C	-6.525922	0.825251	0.046367
H	-6.909933	-0.115064	0.477173
H	-7.077171	1.665750	0.486190
H	-6.697035	0.819571	-1.043605
O	-1.104229	2.600923	1.059701
C	-2.014662	3.667433	1.098937
H	-2.413948	3.723701	2.121132
H	-1.545412	4.638328	0.858136
H	-2.858131	3.512001	0.398861

TS5

C	0.875062	3.554988	-1.770489
C	0.509510	2.216981	-1.644532
C	0.065779	1.710663	-0.416220
C	-0.154290	2.614312	0.637712
C	0.234037	3.951316	0.524761
C	0.775070	4.412762	-0.673420
C	-0.375486	0.300099	-0.220460
S	-1.063401	2.039470	2.057174
C	-2.270745	1.085793	1.150860
C	-1.850306	0.316567	0.046230
C	-2.799312	-0.353605	-0.717648
H	-2.489679	-0.935668	-1.586161
C	-4.153592	-0.335532	-0.354054
C	-4.559215	0.385713	0.774973
C	-3.614727	1.105580	1.510004
H	1.242416	3.929489	-2.728362
H	0.592039	1.541351	-2.498999
H	0.073629	4.639044	1.358245
H	1.071350	5.460052	-0.765127
H	-5.604826	0.417874	1.081232

H	-3.943251	1.698589	2.366807
C	0.334902	-0.848205	-0.070075
C	1.782656	-1.212038	0.113174
C	-0.445976	-2.154114	0.123516
C	1.829399	-2.466586	0.715394
H	-1.392319	-1.985159	0.660020
C	0.476604	-3.066862	0.925560
H	0.426520	-4.112212	0.586368
C	3.036839	-0.540271	-0.136909
C	4.252544	-1.176530	0.283112
C	4.221821	-2.450413	0.914306
C	3.030006	-3.089058	1.118046
C	5.503239	-0.537123	0.060090
C	5.581041	0.682497	-0.566260
C	4.392698	1.304056	-1.006278
C	3.171541	0.706642	-0.796738
H	0.213154	-3.058155	1.995981
H	5.164513	-2.909417	1.222714
H	2.991785	-4.071698	1.593973
H	6.410057	-1.044791	0.398881
H	6.548327	1.162980	-0.729447
H	4.436535	2.267416	-1.520235
H	2.283801	1.206565	-1.152567
O	-4.983499	-1.047968	-1.141100
C	-6.353927	-1.100460	-0.822575
H	-6.821664	-0.102141	-0.861703
H	-6.825845	-1.740976	-1.578032
H	-6.524026	-1.542150	0.173992
O	-0.726606	-2.663756	-1.165345
C	-1.701277	-3.669810	-1.180904
H	-1.866998	-3.955969	-2.228911
H	-1.392469	-4.571933	-0.620666
H	-2.661162	-3.314984	-0.758277

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C	4.013667	-0.547454	0.908846
C	2.615369	-0.485268	0.980985
C	1.895714	0.376256	0.156317
C	2.589206	1.217200	-0.731616
C	3.978968	1.164012	-0.798225
C	4.697067	0.281287	0.010288
C	0.406751	0.407924	0.168251
S	1.667563	2.284614	-1.808815
C	0.349145	2.724292	-0.701670
C	-0.150808	1.793236	0.235942
C	-1.110923	2.246999	1.145757
H	-1.454990	1.583509	1.932618
C	-1.635847	3.535336	1.069454
C	-1.187882	4.415420	0.086941
C	-0.177900	4.015663	-0.784231
H	2.090834	-1.151220	1.668524
H	4.520083	1.817404	-1.486847
H	5.784444	0.259321	-0.063980
H	-1.599834	5.424424	0.014985
H	0.219424	4.716088	-1.522832
C	-0.272992	-0.728634	-0.128113
C	-1.719834	-0.970666	-0.351978
C	0.419593	-1.907603	-0.800904
C	-1.845197	-1.686538	-1.532669
H	1.445480	-1.661496	-1.116107
C	-0.496099	-2.135596	-2.027786
H	-0.499360	-3.183676	-2.362851
C	-2.878253	-0.681910	0.430486
C	-4.158070	-0.914257	-0.164150
C	-4.240235	-1.505464	-1.456632

C	-3.108098	-1.934076	-2.109487
C	-5.331910	-0.617706	0.585413
C	-5.248444	-0.198173	1.890679
C	-3.982816	-0.084793	2.517028
C	-2.831569	-0.320958	1.805010
H	-0.146896	-1.515294	-2.870054
H	-5.227732	-1.668061	-1.896235
H	-3.181540	-2.458690	-3.065199
H	-6.305592	-0.761579	0.109712
H	-6.157181	0.012297	2.459334
H	-3.923203	0.175565	3.576438
H	-1.861742	-0.280426	2.302918
H	-2.396796	3.849274	1.787118
O	4.609977	-1.430846	1.732285
C	6.013210	-1.540719	1.718493
H	6.274301	-2.307046	2.458803
H	6.389577	-1.858801	0.731290
H	6.500361	-0.592573	2.002566
O	0.445071	-3.004476	0.079990
C	1.339595	-4.012813	-0.297975
H	1.295597	-4.802508	0.464876
H	1.085775	-4.462188	-1.276218
H	2.379151	-3.635564	-0.352735

TSS'

C	-4.283881	-0.038014	-0.024839
C	-2.981672	0.336056	0.330941
C	-1.866865	-0.403602	-0.060477
C	-2.103486	-1.617061	-0.752985
C	-3.397579	-1.990556	-1.106076
C	-4.496369	-1.200383	-0.769818
C	-0.432568	-0.051919	0.216472
S	-0.772588	-2.724348	-1.159415
C	0.204585	-2.487109	0.298475
C	0.314187	-1.189724	0.824838
C	1.111724	-1.000519	1.960695
H	1.184234	-0.001791	2.397134
C	1.824291	-2.058420	2.518414
C	1.731523	-3.334361	1.960712
C	0.911094	-3.554084	0.856272
H	-2.842744	1.238839	0.914934
H	-3.561166	-2.930421	-1.638740
H	-5.496205	-1.520977	-1.063227
H	2.285390	-4.168322	2.397523
H	0.816910	-4.554234	0.426683
C	0.193770	1.124714	-0.077842
C	1.657959	1.369075	-0.173821
C	-0.470125	2.491856	-0.285963
C	1.914801	2.724333	-0.044612
H	-0.863213	2.559029	-1.320372
C	0.655605	3.529107	-0.059555
H	0.476632	4.029108	0.906111
C	2.753837	0.486263	-0.472644
C	4.082148	0.990712	-0.314958
C	4.289610	2.367537	-0.009746
C	3.228644	3.233811	0.057904
C	5.188447	0.126371	-0.544139
C	5.000580	-1.159329	-0.991185
C	3.691921	-1.617529	-1.268997
C	2.602830	-0.815670	-1.018890
H	0.692355	4.310098	-0.833571
H	5.313826	2.731179	0.106513
H	3.387297	4.304558	0.206166
H	6.196850	0.517535	-0.385185
H	5.857763	-1.811744	-1.172630

H	3.543293	-2.609945	-1.701306
H	1.609942	-1.163581	-1.293653
H	2.452066	-1.886357	3.395342
O	-5.263496	0.786085	0.400228
C	-6.598230	0.480394	0.077726
H	-7.216689	1.274469	0.514696
H	-6.762467	0.462921	-1.013341
H	-6.911742	-0.487383	0.505026
O	-1.509907	2.716870	0.629732
C	-2.360132	3.773058	0.273873
H	-3.137510	3.850256	1.046614
H	-1.825900	4.739391	0.219402
H	-2.850177	3.593267	-0.701824

anti-(P)-unstable-E

C	-4.258017	0.025239	0.326908
C	-2.915653	0.352168	0.554290
C	-1.885504	-0.372757	-0.038840
C	-2.220276	-1.526724	-0.780021
C	-3.554453	-1.860238	-0.999379
C	-4.581090	-1.077466	-0.471560
C	-0.428890	-0.081722	0.146107
S	-0.935465	-2.603526	-1.379746
C	0.132013	-2.513539	0.038464
C	0.293431	-1.273524	0.678697
C	1.117625	-1.205607	1.807007
H	1.226397	-0.251932	2.328235
C	1.819408	-2.326481	2.243466
C	1.688919	-3.540287	1.567034
C	0.832768	-3.640567	0.471745
H	-2.691166	1.218572	1.171668
H	-3.804772	-2.755981	-1.572848
H	-5.617040	-1.357558	-0.662881
H	2.239436	-4.420966	1.905337
H	0.701964	-4.596021	-0.041574
C	0.223281	1.064881	-0.164889
C	1.687304	1.329780	-0.047178
C	-0.325734	2.441561	-0.530553
C	1.861033	2.647410	0.344227
H	-0.057828	2.621056	-1.593744
C	0.549088	3.376027	0.340837
H	0.100426	3.437806	1.347287
C	2.827037	0.518640	-0.347068
C	4.117216	1.042601	-0.025217
C	4.240384	2.364224	0.493537
C	3.139198	3.172972	0.633019
C	5.271558	0.251008	-0.283716
C	5.163278	-0.981209	-0.880963
C	3.891904	-1.464369	-1.274664
C	2.756877	-0.733642	-1.016802
H	0.636471	4.395563	-0.060985
H	5.238488	2.741142	0.731247
H	3.243847	4.208022	0.966903
H	6.251671	0.652717	-0.013347
H	6.057513	-1.576544	-1.079274
H	3.811990	-2.422159	-1.794075
H	1.789831	-1.101886	-1.355782
H	2.473844	-2.252126	3.114654
O	-5.166623	0.830005	0.916956
C	-6.535714	0.560782	0.739356
H	-7.081944	1.337148	1.289969
H	-6.828665	0.608948	-0.323530
H	-6.816057	-0.425967	1.145800
O	-1.690726	2.608142	-0.360653
C	-2.222218	3.762493	-0.949360

H	-3.310458	3.733578	-0.799852
H	-1.831541	4.688266	-0.489239
H	-2.014812	3.799646	-2.035350

TS6

C	3.837013	-0.846796	0.631508
C	2.468912	-0.721525	0.391383
C	1.869709	0.473864	-0.040394
C	2.710061	1.609077	-0.068926
C	4.080097	1.491532	0.183093
C	4.664773	0.272930	0.503566
C	0.404026	0.499068	-0.337665
S	2.141830	3.250666	-0.309002
C	0.401612	3.060945	-0.399813
C	-0.276684	1.823971	-0.487394
C	-1.636535	1.917691	-0.861681
H	-2.188612	1.011608	-1.084836
C	-2.312634	3.120110	-0.992032
C	-1.639933	4.322963	-0.775299
C	-0.282376	4.284293	-0.506593
H	1.859343	-1.603177	0.578888
H	4.709454	2.384770	0.142955
H	5.737708	0.223063	0.688334
H	-2.157279	5.281461	-0.852708
H	0.277868	5.216796	-0.397363
C	-0.263143	-0.696546	-0.507146
C	-1.697759	-1.034979	-0.382387
C	0.339364	-1.949231	-1.151085
C	-2.020761	-2.001116	-1.322432
H	1.274686	-1.727302	-1.690926
C	-0.796068	-2.378102	-2.107838
H	-0.751578	-3.449100	-2.353142
C	-2.657559	-0.640033	0.602652
C	-3.977583	-1.175888	0.497464
C	-4.287708	-2.104032	-0.538516
C	-3.324041	-2.528430	-1.423172
C	-4.958919	-0.782963	1.449929
C	-4.646104	0.082557	2.470349
C	-3.328569	0.586282	2.592449
C	-2.360056	0.234973	1.681556
H	-0.731875	-1.812443	-3.052367
H	-5.305458	-2.498228	-0.599537
H	-3.559281	-3.271140	-2.189147
H	-5.968787	-1.191477	1.358582
H	-5.408011	0.375865	3.196048
H	-3.079273	1.256105	3.418674
H	-1.346093	0.623356	1.788511
H	-3.368159	3.113653	-1.271392
O	4.264281	-2.075685	0.992322
C	5.623487	-2.256218	1.309091
H	5.747160	-3.314131	1.572207
H	6.279195	-2.027715	0.451499
H	5.927695	-1.637102	2.170418
O	0.558865	-2.963438	-0.188059
C	1.431497	-3.975822	-0.614033
H	1.464305	-4.738900	0.175661
H	1.092220	-4.457936	-1.548734
H	2.455613	-3.587147	-0.771491

motor 8

anti-(M)-stable-E

C	1.518509	2.515296	2.171414
C	0.931427	1.316428	1.776165
C	0.072868	1.271517	0.672302
C	-0.236422	2.470617	0.008539
C	0.352782	3.675216	0.399554
C	1.240544	3.691757	1.473693
C	-0.530335	0.002136	0.186101
S	-1.343995	2.425812	-1.380879
C	-2.483645	1.205489	-0.763103
C	-2.006155	0.115138	-0.006711
C	-2.932199	-0.753680	0.568549
H	-2.606191	-1.557805	1.229315
C	-4.763977	0.430833	-0.482096
C	-3.848503	1.346444	-1.001147
H	2.201417	2.530948	3.023545
H	1.156584	0.390922	2.310472
H	0.110414	4.599809	-0.129722
H	1.702514	4.633670	1.777728
H	-5.826012	0.568122	-0.685460
H	-4.214901	2.192726	-1.587103
C	0.184709	-1.109891	-0.103800
C	1.649597	-1.344924	0.001637
C	-0.393664	-2.478451	-0.453155
C	1.840618	-2.671645	0.352783
H	-1.435921	-2.588069	-0.126432
C	0.533397	-3.419167	0.343710
H	0.621399	-4.412394	-0.122442
C	2.775760	-0.503324	-0.258394
C	4.074547	-1.020490	0.042261
C	4.216479	-2.357618	0.512694
C	3.125554	-3.185210	0.628862
C	5.217127	-0.202977	-0.187381
C	5.090888	1.049223	-0.737711
C	3.811815	1.530564	-1.108113
C	2.687512	0.775132	-0.875891
H	0.145241	-3.563438	1.366186
H	5.220227	-2.729509	0.734277
H	3.246832	-4.228970	0.928750
H	6.203627	-0.601329	0.064396
H	5.976583	1.663251	-0.916554
H	3.717422	2.506266	-1.590496
H	1.715022	1.145493	-1.195967
C	-4.306034	-0.615320	0.327082
N	-0.223107	-2.710006	-1.885560
H	-0.606655	-3.624487	-2.124061
H	-0.781134	-2.031864	-2.403850
O	-5.103491	-1.525640	0.918200
C	-6.496287	-1.438284	0.731179
H	-6.771963	-1.548709	-0.331257
H	-6.941071	-2.265370	1.298342
H	-6.901303	-0.485951	1.113591

*anti-(M)-stable-E**

C	2.242618	1.986673	2.228619
C	1.422338	0.952733	1.811395
C	0.284495	1.174264	0.986684
C	0.002496	2.531372	0.669443
C	0.830839	3.571009	1.093217
C	1.963634	3.303791	1.857073
C	-0.503984	0.061727	0.480596
S	-1.319953	2.951505	-0.395367
C	-2.387289	1.570600	-0.225546
C	-1.899896	0.276921	0.120163
C	-2.840143	-0.771896	0.079347

H	-2.558770	-1.789391	0.329337
C	-4.629646	0.709463	-0.602228
C	-3.722023	1.766267	-0.570788
H	3.111307	1.763817	2.851597
H	1.644119	-0.065399	2.130408
H	0.582075	4.599119	0.819340
H	2.611981	4.121766	2.176997
H	-5.666709	0.901072	-0.875271
H	-4.062691	2.771416	-0.830641
C	0.141368	-1.214843	0.411117
C	1.495775	-1.405455	0.024943
C	-0.370555	-2.577090	0.880230
C	1.999209	-2.592647	0.616452
H	-1.120856	-2.453294	1.682473
C	0.911079	-3.247521	1.415420
H	0.882573	-4.339920	1.293797
C	2.371575	-0.571523	-0.770712
C	3.757866	-0.931450	-0.825900
C	4.213627	-2.101388	-0.174760
C	3.342912	-2.932852	0.525600
C	4.647744	-0.110875	-1.576423
C	4.188500	0.983419	-2.270396
C	2.812979	1.301166	-2.258201
C	1.927007	0.530779	-1.530436
H	1.050499	-3.024303	2.488970
H	5.274173	-2.357249	-0.244347
H	3.718480	-3.833844	1.016462
H	5.708369	-0.374261	-1.601015
H	4.883795	1.600962	-2.843297
H	2.444735	2.158573	-2.825295
H	0.862880	0.773666	-1.546642
C	-4.174481	-0.572443	-0.273658
N	-0.865005	-3.366727	-0.252755
H	-1.522958	-4.080572	0.052709
H	-1.332158	-2.787745	-0.944706
O	-4.953006	-1.676844	-0.264329
C	-6.308082	-1.556163	-0.598545
H	-6.445560	-1.184558	-1.629134
H	-6.742470	-2.560530	-0.523996
H	-6.844272	-0.885795	0.095813

syn-(P)-unstable-Z

C	-4.011213	-1.294585	2.265387
C	-2.693803	-1.139623	1.836907
C	-2.387781	-0.365851	0.709055
C	-3.432912	0.312400	0.063754
C	-4.754749	0.161481	0.487064
C	-5.044217	-0.654781	1.579614
C	-0.981895	-0.253790	0.236907
S	-3.052437	1.327050	-1.331586
C	-1.467942	1.942047	-0.810351
C	-0.556865	1.148693	-0.066663
C	0.662409	1.730305	0.273304
H	1.395144	1.195497	0.866789
C	1.009943	3.028224	-0.125044
C	0.113592	3.787627	-0.878952
C	-1.124582	3.233715	-1.201748
H	-4.231053	-1.912664	3.138732
H	-1.880590	-1.639266	2.369458
H	-5.557972	0.688875	-0.033356
H	-6.079490	-0.771530	1.907921
H	0.348190	4.802069	-1.201417
H	-1.840908	3.831853	-1.770375
C	-0.272165	-1.383379	-0.030888
C	1.171427	-1.542201	-0.330013

C	-0.873340	-2.724205	-0.488956
C	1.301737	-2.394561	-1.414335
H	-0.559916	-3.501527	0.239135
C	-0.043167	-2.952131	-1.779747
H	-0.520157	-2.382830	-2.596638
C	2.326378	-1.155268	0.414510
C	3.606886	-1.447588	-0.149679
C	3.692081	-2.176919	-1.369316
C	2.564076	-2.689898	-1.968153
C	4.778681	-1.066804	0.564522
C	4.691343	-0.491927	1.808579
C	3.423147	-0.288350	2.407416
C	2.272675	-0.609648	1.728447
H	-0.001406	-4.010780	-2.077340
H	4.680970	-2.378687	-1.789098
H	2.642433	-3.323770	-2.854687
H	5.753700	-1.263679	0.111032
H	5.598160	-0.215475	2.351302
H	3.361136	0.123969	3.417146
H	1.298459	-0.462270	2.200046
N	-2.285481	-2.759732	-0.798798
H	-2.479866	-3.624038	-1.303192
H	-2.847365	-2.798865	0.048708
O	2.224984	3.454184	0.274426
C	2.638815	4.753306	-0.071910
H	3.636246	4.891947	0.363818
H	2.708477	4.884307	-1.165320
H	1.961926	5.520988	0.340644

TS1

C	-4.436280	-1.907466	0.773900
C	-3.097787	-1.714395	0.466212
C	-2.544166	-0.445200	0.174723
C	-3.410311	0.649531	0.390900
C	-4.770681	0.460304	0.684927
C	-5.296835	-0.811178	0.847540
C	-1.103906	-0.303721	-0.174569
S	-2.891439	2.322689	0.483394
C	-1.210797	2.254571	-0.026706
C	-0.522809	1.062316	-0.339956
C	0.732335	1.223255	-0.950186
H	1.276198	0.361858	-1.329257
C	1.350469	2.460882	-1.116584
C	0.686840	3.622517	-0.705509
C	-0.597726	3.500545	-0.192866
H	-4.802698	-2.916507	0.973595
H	-2.448225	-2.586553	0.483905
H	-5.413918	1.335658	0.809657
H	-6.357432	-0.942263	1.071501
H	1.132272	4.611243	-0.814458
H	-1.148693	4.407778	0.069829
C	-0.316264	-1.418521	-0.387081
C	1.124010	-1.579718	-0.109788
C	-0.730063	-2.705196	-1.121122
C	1.650001	-2.571806	-0.922407
H	-0.951693	-3.499121	-0.375372
C	0.586157	-3.120843	-1.819729
H	0.618312	-2.633022	-2.809052
C	1.937129	-0.988539	0.915623
C	3.315252	-1.362527	0.967085
C	3.828019	-2.332005	0.055936
C	3.007380	-2.949051	-0.856377
C	4.157894	-0.777209	1.952091
C	3.659376	0.119300	2.866469
C	2.285209	0.454533	2.845604

C	1.447797	-0.083356	1.895553
H	0.664751	-4.206899	-1.975684
H	4.887256	-2.594771	0.116582
H	3.395866	-3.716797	-1.529651
H	5.213330	-1.061500	1.973443
H	4.316704	0.561362	3.618773
H	1.884936	1.143711	3.592916
H	0.389103	0.175058	1.904223
N	-1.772830	-2.531005	-2.116245
H	-1.886645	-3.408856	-2.622512
H	-2.675511	-2.349294	-1.682678
O	2.569278	2.441779	-1.693960
C	3.228967	3.662926	-1.923877
H	3.441275	4.196317	-0.981585
H	4.180955	3.419647	-2.412122
H	2.647202	4.323038	-2.589806

intermediate-Z

C	-4.908943	1.010012	0.658510
C	-3.529902	1.079417	0.844721
C	-2.649471	0.293065	0.085214
C	-3.219785	-0.626933	-0.823743
C	-4.602920	-0.691553	-1.014362
C	-5.449579	0.138500	-0.284822
C	-1.153398	0.354914	0.157938
S	-2.201216	-1.732319	-1.774062
C	-0.956534	-2.047823	-0.553210
C	-0.535384	-0.990646	0.273009
C	0.431676	-1.238670	1.244340
H	0.754549	-0.441111	1.916125
C	1.038067	-2.496235	1.354907
C	0.642482	-3.531275	0.498983
C	-0.363572	-3.301759	-0.441038
H	-5.564477	1.640917	1.263473
H	-3.098921	1.741802	1.597556
H	-5.016179	-1.410759	-1.725798
H	-6.529825	0.080437	-0.436213
H	1.092893	-4.521829	0.562587
H	-0.687178	-4.119458	-1.089401
C	-0.429198	1.511111	0.115229
C	1.016891	1.742106	-0.153942
C	-1.012542	2.861385	0.562013
C	1.315340	3.078936	0.088882
H	-1.955271	3.087467	0.039947
C	0.073908	3.900302	0.251569
H	0.144757	4.662372	1.041658
C	2.062717	0.903825	-0.690061
C	3.408789	1.386744	-0.623728
C	3.672879	2.715588	-0.183045
C	2.639107	3.570118	0.098952
C	4.475299	0.562163	-1.077575
C	4.229979	-0.655622	-1.663984
C	2.894212	-1.076051	-1.853210
C	1.846870	-0.319675	-1.379919
H	-0.120144	4.432690	-0.695289
H	4.709877	3.058147	-0.138403
H	2.827292	4.618213	0.343728
H	5.498070	0.935579	-0.979394
H	5.055743	-1.276041	-2.019627
H	2.686498	-2.005360	-2.388950
H	0.831453	-0.646221	-1.581820
N	-1.302314	2.780081	1.997546
H	-0.456001	2.512856	2.501916
H	-1.553134	3.707269	2.341404
O	1.985634	-2.615319	2.304383

C	2.628372	-3.855436	2.475427
H	3.171707	-4.162469	1.565571
H	3.351335	-3.725138	3.290376
H	1.915400	-4.649322	2.755322

TS2

C	-4.430886	-1.730701	-1.146194
C	-3.087363	-1.395442	-1.307474
C	-2.373363	-0.797157	-0.263426
C	-3.056609	-0.483401	0.928314
C	-4.399050	-0.829423	1.094581
C	-5.082523	-1.463506	0.057988
C	-0.916423	-0.437937	-0.307803
S	-2.186605	0.377505	2.229470
C	-1.316824	1.514137	1.171299
C	-0.799027	1.022553	-0.040636
C	-0.361707	1.927956	-1.004742
H	-0.022166	1.575300	-1.980716
C	-0.290141	3.298532	-0.721426
C	-0.704148	3.767962	0.531728
C	-1.244452	2.874829	1.457855
H	-4.970134	-2.208843	-1.967180
H	-2.557084	-1.634934	-2.231038
H	-4.913641	-0.585300	2.026996
H	-6.134771	-1.727047	0.186852
H	-0.653665	4.827572	0.782585
H	-1.639389	3.257762	2.401804
C	0.039314	-1.399074	-0.410932
C	1.515106	-1.497424	-0.110553
C	-0.390281	-2.821841	-0.802367
C	1.816069	-2.847425	0.062986
H	-1.401485	-3.041839	-0.440184
C	0.629293	-3.736939	-0.123674
H	0.856710	-4.629944	-0.725818
C	2.585197	-0.542747	0.083288
C	3.886196	-1.033583	0.441673
C	4.116892	-2.427115	0.603329
C	3.098440	-3.319562	0.416019
C	4.962391	-0.123940	0.636104
C	4.792030	1.229986	0.484191
C	3.520132	1.722348	0.122432
C	2.463876	0.861740	-0.068071
H	0.263537	-4.086565	0.857014
H	5.118877	-2.767339	0.876896
H	3.260423	-4.393001	0.539148
H	5.938559	-0.532619	0.910042
H	5.627462	1.916943	0.636587
H	3.365294	2.795539	-0.013337
H	1.507793	1.276387	-0.347327
N	-0.417905	-2.916470	-2.262120
H	0.512573	-2.725173	-2.636875
H	-0.631846	-3.877398	-2.529909
O	0.201237	4.078695	-1.702450
C	0.313737	5.465295	-1.486567
H	0.990075	5.694522	-0.645639
H	0.736938	5.890962	-2.404993
H	-0.668209	5.931959	-1.299512

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C	-1.044563	3.061426	0.131670
C	-0.569140	1.833940	0.614483
C	0.505869	1.183462	0.019970
C	1.182639	1.841816	-1.033781
C	0.713371	3.061388	-1.513597

C	-0.412386	3.669049	-0.956386
C	1.039812	-0.158404	0.404280
S	2.649753	1.136821	-1.754362
C	3.360378	0.434898	-0.287006
C	2.505790	-0.143284	0.666059
C	3.064848	-0.703037	1.820615
H	2.400582	-1.132576	2.574870
C	4.446434	-0.727226	2.001307
C	5.286316	-0.176531	1.032150
C	4.745604	0.413643	-0.109324
H	-1.075297	1.406211	1.473762
H	1.238254	3.561724	-2.330994
H	-0.758247	4.620700	-1.359842
H	6.369643	-0.190984	1.171138
H	5.399983	0.864138	-0.859378
C	0.405122	-1.346970	0.253318
C	-0.983837	-1.637784	-0.181568
C	1.168571	-2.645611	-0.005414
C	-0.911083	-2.585321	-1.189368
H	2.238197	-2.442164	-0.173661
C	0.497746	-3.101857	-1.323181
H	0.536329	-4.193499	-1.459223
C	-2.252637	-1.196660	0.296133
C	-3.411046	-1.565996	-0.457288
C	-3.275954	-2.423199	-1.585812
C	-2.055940	-2.964968	-1.920061
C	-4.690396	-1.124974	-0.013258
C	-4.827877	-0.424389	1.160045
C	-3.690591	-0.153742	1.960956
C	-2.439268	-0.532545	1.539581
H	1.010921	-2.636188	-2.181427
H	-4.173823	-2.690825	-2.149065
H	-1.971920	-3.684571	-2.738224
H	-5.568933	-1.381952	-0.611268
H	-5.816418	-0.102380	1.495757
H	-3.813175	0.347062	2.924077
H	-1.570726	-0.362140	2.177760
H	4.869986	-1.175534	2.902716
N	0.928032	-3.621018	1.049846
H	1.416354	-4.487458	0.823515
H	1.347842	-3.285712	1.916454
O	-2.105407	3.574742	0.783980
C	-2.644070	4.802463	0.355442
H	-3.020921	4.743349	-0.679716
H	-3.483901	5.025935	1.025312
H	-1.906012	5.619410	0.426692

TS2'

C	1.250604	-2.047569	1.738581
C	0.520950	-0.880602	1.483796
C	-0.447909	-0.832303	0.480917
C	-0.735663	-2.014091	-0.223284
C	-0.028206	-3.183845	0.037556
C	0.977378	-3.207392	1.003320
C	-1.186543	0.441938	0.218813
S	-1.952356	-1.966147	-1.504312
C	-3.100360	-0.853334	-0.731226
C	-2.670180	0.228499	0.075258
C	-3.678492	0.999730	0.673516
H	-3.377681	1.849118	1.281594
C	-5.030176	0.755724	0.443508
C	-5.428542	-0.285259	-0.391006
C	-4.457159	-1.095789	-0.968030
H	0.746977	0.009133	2.074134
H	-0.256544	-4.096017	-0.519023

H	1.520079	-4.135376	1.183591
H	-6.486668	-0.481518	-0.577991
H	-4.748604	-1.941082	-1.596129
C	-0.468951	1.604389	0.111786
C	0.990878	1.669219	-0.195096
C	-0.869677	3.071975	0.367326
C	1.527327	2.843379	0.302947
H	-1.128862	3.527426	-0.604731
C	0.454356	3.710045	0.870275
H	0.463539	3.682831	1.974223
C	1.822728	0.807337	-0.990195
C	3.228343	1.068708	-1.011489
C	3.750245	2.221698	-0.355982
C	2.909985	3.124900	0.243686
C	4.088209	0.205925	-1.746231
C	3.581406	-0.833780	-2.487708
C	2.182046	-1.027348	-2.553746
C	1.330068	-0.228368	-1.827603
H	0.555925	4.764566	0.571989
H	4.828312	2.399132	-0.387873
H	3.299617	4.045631	0.684511
H	5.163597	0.401852	-1.727032
H	4.250114	-1.485987	-3.054109
H	1.771102	-1.809846	-3.196326
H	0.255490	-0.367039	-1.930753
H	-5.776663	1.393007	0.923666
N	-1.969183	3.315947	1.278636
H	-1.690780	3.059605	2.226665
H	-2.165422	4.315417	1.304565
O	2.183740	-1.962583	2.707282
C	2.955278	-3.098546	3.013247
H	3.544585	-3.438488	2.144616
H	3.645770	-2.802991	3.813042
H	2.330528	-3.933407	3.374035

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C	1.298099	-2.281452	1.352160
C	0.569019	-1.087326	1.275872
C	-0.430995	-0.923178	0.323204
C	-0.764389	-2.004486	-0.513096
C	-0.053062	-3.197154	-0.430653
C	0.990829	-3.337592	0.485692
C	-1.179543	0.357355	0.161770
S	-2.064129	-1.792787	-1.709501
C	-3.175732	-0.852146	-0.685245
C	-2.655619	0.114850	0.198128
C	-3.533491	0.700880	1.119631
H	-3.138170	1.408191	1.846256
C	-4.898774	0.426449	1.081031
C	-5.410855	-0.463555	0.136404
C	-4.545923	-1.121885	-0.734014
H	0.832518	-0.270624	1.950227
H	-0.310037	-4.034385	-1.083965
H	1.537742	-4.279491	0.526161
H	-6.481790	-0.676028	0.100488
H	-4.928307	-1.868977	-1.433520
C	-0.550289	1.536222	-0.063324
C	0.928123	1.752407	-0.132262
C	-1.090158	2.967490	-0.119093
C	1.209292	2.973360	0.457101
H	-0.895074	3.296647	-1.162129
C	-0.064729	3.706565	0.765913
H	-0.359151	3.594431	1.823892
C	1.979823	0.985616	-0.722721
C	3.324005	1.408229	-0.483284

C	3.573040	2.610191	0.240521
C	2.536773	3.406353	0.665185
C	4.396810	0.640246	-1.018432
C	4.154406	-0.461811	-1.801692
C	2.821640	-0.827206	-2.112160
C	1.765477	-0.121176	-1.589380
H	-0.002618	4.782447	0.542818
H	4.609836	2.911223	0.411559
H	2.730943	4.359357	1.163187
H	5.422210	0.955600	-0.807960
H	4.986240	-1.040302	-2.210199
H	2.631489	-1.671793	-2.778680
H	0.745870	-0.393005	-1.858435
H	-5.567026	0.909693	1.797424
N	-2.447633	3.238746	0.292715
H	-2.604244	4.244189	0.224887
H	-3.108576	2.815095	-0.356276
O	2.272910	-2.320046	2.281102
C	3.111200	-3.448590	2.345965
H	3.636988	-3.618562	1.391051
H	3.853586	-3.241581	3.126985
H	2.553935	-4.360323	2.621121

TS3

C	-1.177949	2.751075	-0.678212
C	-0.668533	1.455619	-0.602903
C	0.656043	1.155310	-0.247474
C	1.508959	2.276548	-0.104658
C	1.002104	3.579216	-0.168379
C	-0.337078	3.838463	-0.425764
C	1.141009	-0.261287	-0.151589
S	3.261524	2.205108	-0.003757
C	3.578295	0.495174	0.195096
C	2.585099	-0.506331	0.161604
C	3.012187	-1.796700	0.552489
H	2.277073	-2.595912	0.661161
C	4.339445	-2.103066	0.816536
C	5.315640	-1.109028	0.740449
C	4.923951	0.189093	0.456850
H	-1.370497	0.670113	-0.854949
H	1.684933	4.421761	-0.029215
H	-0.693134	4.868169	-0.458745
H	6.366003	-1.332739	0.939378
H	5.663662	0.994350	0.454546
C	0.310418	-1.336438	-0.384319
C	-1.167021	-1.447532	-0.321443
C	0.719892	-2.655332	-1.061897
C	-1.602205	-2.278154	-1.342433
H	1.702170	-2.567444	-1.546216
C	-0.416244	-2.788119	-2.113219
H	-0.537496	-3.823395	-2.465573
C	-2.086293	-0.985876	0.673216
C	-3.468204	-1.302400	0.500057
C	-3.882817	-2.088384	-0.614221
C	-2.967631	-2.587132	-1.511520
C	-4.408668	-0.833482	1.459425
C	-4.000829	-0.100462	2.547669
C	-2.626797	0.187039	2.733097
C	-1.694062	-0.242698	1.818753
H	-0.208112	-2.150727	-2.989783
H	-4.946787	-2.311576	-0.728287
H	-3.288995	-3.222801	-2.340136
H	-5.466036	-1.070612	1.315280
H	-4.732444	0.254125	3.277292
H	-2.306636	0.752790	3.611178

H	-0.636731	-0.020270	1.971666
H	4.607422	-3.123755	1.098902
N	0.760590	-3.784643	-0.138051
H	-0.143521	-3.889312	0.324031
H	0.916482	-4.646864	-0.659259
O	-2.483131	2.851016	-1.003249
C	-3.059953	4.129598	-1.110369
H	-4.112885	3.976699	-1.377820
H	-3.014926	4.679101	-0.154717
H	-2.575568	4.732672	-1.897316

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C	-1.189875	-2.541730	1.188646
C	-0.531770	-1.305468	1.215379
C	0.501599	-1.028415	0.326026
C	0.937719	-2.033505	-0.556209
C	0.293560	-3.267249	-0.577144
C	-0.779289	-3.523461	0.278128
C	1.169563	0.298544	0.283965
S	2.270758	-1.685875	-1.679504
C	3.272530	-0.687832	-0.600047
C	2.658623	0.188647	0.316110
C	3.478339	0.860755	1.233363
H	3.020345	1.474361	2.010822
C	4.865696	0.749686	1.173438
C	5.461007	-0.061573	0.207212
C	4.664216	-0.798590	-0.665281
H	-0.872781	-0.544630	1.919771
H	0.626787	-4.047361	-1.265697
H	-1.270487	-4.495564	0.235062
H	6.548264	-0.151420	0.153805
H	5.121801	-1.480467	-1.386035
C	0.501904	1.469320	0.158278
C	-0.961474	1.715615	0.058994
C	1.117392	2.861794	0.265657
C	-1.230631	2.923843	0.681118
H	2.075822	2.852952	0.801553
C	0.045550	3.616494	1.078608
H	0.028519	4.693153	0.850064
C	-2.014762	0.990238	-0.581160
C	-3.354554	1.444954	-0.375629
C	-3.595293	2.632207	0.374478
C	-2.552812	3.384129	0.859999
C	-4.429720	0.730481	-0.975475
C	-4.193026	-0.354663	-1.783852
C	-2.862006	-0.756230	-2.051995
C	-1.804150	-0.100796	-1.468763
H	0.238278	3.508003	2.159306
H	-4.628447	2.959337	0.517563
H	-2.739342	4.326623	1.380615
H	-5.451664	1.074438	-0.794957
H	-5.026729	-0.890386	-2.243710
H	-2.672973	-1.586691	-2.736363
H	-0.785556	-0.400163	-1.710775
H	5.483582	1.293996	1.890962
N	1.225384	3.434420	-1.073548
H	1.642101	4.363026	-1.008134
H	1.877434	2.876312	-1.624314
O	-2.200331	-2.692702	2.065809
C	-2.964169	-3.874250	2.033844
H	-3.745595	-3.764139	2.796230
H	-3.444550	-4.021468	1.051483
H	-2.356965	-4.762910	2.277045

*anti-(M)-stable-Z**

C	-1.771155	-1.738376	1.380757
C	-0.807300	-0.737496	1.340979
C	0.426385	-0.903694	0.669008
C	0.711707	-2.214180	0.182754
C	-0.237625	-3.223973	0.260925
C	-1.500062	-2.990153	0.812039
C	1.270211	0.237345	0.370075
S	2.165744	-2.543174	-0.730770
C	3.217917	-1.228751	-0.247653
C	2.710691	0.019587	0.205695
C	3.685680	1.010967	0.480539
H	3.376471	1.970870	0.881103
C	5.042928	0.794016	0.292437
C	5.506107	-0.435527	-0.177211
C	4.587560	-1.444269	-0.435321
H	-1.056617	0.220189	1.795678
H	-0.008417	-4.210145	-0.149839
H	-2.236952	-3.792536	0.821437
H	6.572720	-0.612126	-0.326955
H	4.927190	-2.420286	-0.790404
C	0.633272	1.513650	0.240399
C	-0.701018	1.725992	-0.208818
C	1.192848	2.885560	0.614392
C	-1.174925	2.976416	0.271114
H	1.836978	2.804300	1.510304
C	-0.062776	3.708552	0.958982
H	0.031109	4.750231	0.617299
C	-1.616486	0.853620	-0.926790
C	-3.014175	1.176183	-0.873250
C	-3.435203	2.394579	-0.305027
C	-2.519922	3.308194	0.224016
C	-3.948684	0.255366	-1.435557
C	-3.523208	-0.880263	-2.080270
C	-2.140312	-1.132368	-2.228756
C	-1.213056	-0.262972	-1.683535
H	-0.237348	3.725514	2.048789
H	-4.503038	2.628523	-0.298952
H	-2.868839	4.254696	0.643649
H	-5.015507	0.479017	-1.354006
H	-4.251192	-1.577782	-2.501329
H	-1.799538	-2.010712	-2.780461
H	-0.148406	-0.458008	-1.818308
H	5.749941	1.591790	0.529971
N	1.861668	3.488372	-0.538026
H	2.407232	4.299572	-0.251892
H	2.502777	2.832055	-0.977705
O	-2.944068	-1.407815	1.961300
C	-4.044301	-2.256332	1.786041
H	-4.906368	-1.753073	2.240864
H	-4.251960	-2.426751	0.714823
H	-3.901859	-3.230668	2.286251

syn-(*P*)-unstable-*E*

C	3.851721	-1.169922	-0.990538
C	2.462445	-1.013308	-0.905010
C	1.903431	-0.000066	-0.132932
C	2.753009	0.907346	0.521404
C	4.134167	0.760881	0.435729
C	4.691280	-0.280796	-0.308357
C	0.426815	0.155642	-0.023842
S	2.023210	2.197768	1.494141
C	0.646957	2.579509	0.433800
C	-0.029185	1.561611	-0.280000
C	-1.065090	1.963061	-1.130984

H	-1.574537	1.226092	-1.743150
C	-1.466672	3.294813	-1.221628
C	-0.823469	4.274274	-0.470011
C	0.246609	3.914979	0.345258
H	1.819937	-1.720934	-1.432277
H	4.793286	1.465714	0.948257
H	5.776142	-0.374880	-0.360365
H	-1.131197	5.320186	-0.536031
H	0.788966	4.678448	0.908192
C	-0.351196	-0.843437	0.471653
C	-1.831820	-0.893409	0.567397
C	0.097914	-1.924149	1.469532
C	-2.174674	-1.279423	1.852870
H	-0.152338	-2.913853	1.048099
C	-0.931088	-1.639007	2.611007
H	-0.554769	-0.789284	3.208056
C	-2.835302	-0.799799	-0.442977
C	-4.202033	-0.872331	-0.029210
C	-4.514735	-1.115408	1.338248
C	-3.522910	-1.365754	2.258569
C	-5.226719	-0.770365	-1.013228
C	-4.917432	-0.686742	-2.348634
C	-3.563116	-0.722015	-2.765295
C	-2.551157	-0.775374	-1.837695
H	-1.064652	-2.497928	3.285766
H	-5.566588	-1.160573	1.632580
H	-3.771972	-1.631413	3.288872
H	-6.269743	-0.790438	-0.686161
H	-5.712279	-0.624394	-3.095371
H	-3.324918	-0.714177	-3.831518
H	-1.509847	-0.822041	-2.163970
H	-2.286491	3.562214	-1.892029
N	1.477754	-1.949742	1.876483
H	1.736603	-1.065234	2.313677
H	1.599120	-2.669816	2.586613
O	4.287153	-2.200339	-1.743199
C	5.671436	-2.414486	-1.873603
H	6.149807	-2.610805	-0.898893
H	5.793295	-3.299768	-2.510204
H	6.174200	-1.558443	-2.355344

TS4

C	2.178082	2.908463	-1.266448
C	1.526067	1.696618	-1.106797
C	0.205852	1.583064	-0.612817
C	-0.470134	2.808772	-0.427440
C	0.189281	4.041673	-0.572743
C	1.515790	4.099867	-0.965162
C	-0.441526	0.246562	-0.441608
S	-2.194134	2.967365	-0.144283
C	-2.727763	1.304690	0.048171
C	-1.880968	0.179242	-0.059137
C	-2.433125	-1.042907	0.357828
H	-1.817929	-1.935636	0.417440
C	-3.767514	-1.193975	0.729016
C	-4.610889	-0.077768	0.734801
C	-4.068471	1.161021	0.418354
H	3.203329	2.921334	-1.642026
H	2.063344	0.797743	-1.396192
H	-0.366136	4.966036	-0.391946
H	2.015371	5.065000	-1.071789
H	-5.662059	-0.149255	1.013830
H	-4.704922	2.048058	0.478496
C	0.273477	-0.920468	-0.635346
C	1.701767	-1.181751	-0.366217

C	-0.223878	-2.197486	-1.339332
C	2.161995	-2.194099	-1.194714
H	-0.430794	-2.984268	-0.590421
C	1.059444	-2.646896	-2.097391
H	1.097887	-2.118480	-3.066359
C	2.540616	-0.680332	0.685187
C	3.880732	-1.170851	0.758176
C	4.330000	-2.162382	-0.162624
C	3.481169	-2.686048	-1.107602
C	4.746275	-0.677197	1.773551
C	4.303744	0.242892	2.693409
C	2.964140	0.695490	2.648145
C	2.106253	0.246201	1.670892
H	1.072537	-3.727467	-2.303262
H	5.360267	-2.518944	-0.083649
H	3.818831	-3.471562	-1.787833
H	5.772204	-1.052705	1.814182
H	4.978296	0.614141	3.468390
H	2.606422	1.404382	3.398477
H	1.073627	0.594960	1.659962
O	-4.150085	-2.442545	1.075097
C	-5.484107	-2.659058	1.462657
H	-6.192301	-2.405370	0.655254
H	-5.577534	-3.729145	1.687155
H	-5.749552	-2.083152	2.366176
N	-1.394421	-2.035444	-2.163506
H	-1.215229	-1.349865	-2.896712
H	-1.615747	-2.915178	-2.625726

intermediate-*E*

C	1.534161	-2.389540	2.298255
C	0.939352	-1.225470	1.820233
C	0.109921	-1.253361	0.691876
C	-0.162081	-2.494776	0.093653
C	0.433518	-3.665596	0.566981
C	1.293202	-3.608254	1.662415
C	-0.512043	-0.005152	0.179653
S	-1.223982	-2.535010	-1.323260
C	-2.393750	-1.301157	-0.799881
C	-1.981502	-0.160831	-0.068833
C	-2.965819	0.729326	0.360802
H	-2.673906	1.579220	0.980476
C	-4.314648	0.548963	0.026878
C	-4.702861	-0.555149	-0.737044
C	-3.734665	-1.479821	-1.128543
H	2.191789	-2.345885	3.169110
H	1.129163	-0.268895	2.312382
H	0.218253	-4.621056	0.082784
H	1.758878	-4.523996	2.033393
H	-5.744339	-0.726413	-1.009103
H	-4.040072	-2.365420	-1.691161
C	0.182696	1.147782	-0.045835
C	1.645185	1.389861	-0.179970
C	-0.489288	2.529754	-0.009830
C	1.877008	2.760854	-0.220969
H	-1.353042	2.575110	-0.691404
C	0.605242	3.528130	-0.411596
H	0.549496	4.452766	0.181818
C	2.770368	0.508002	-0.375165
C	4.084784	1.063478	-0.259632
C	4.257692	2.469873	-0.110870
C	3.176184	3.310658	-0.163060
C	5.219595	0.214131	-0.377987
C	5.079528	-1.116380	-0.690301
C	3.789711	-1.639008	-0.934894

C	2.673021	-0.850088	-0.781418
H	0.527775	3.820144	-1.472800
H	5.271424	2.868615	-0.021811
H	3.307580	4.395220	-0.145843
H	6.212494	0.652664	-0.247420
H	5.958705	-1.756936	-0.790084
H	3.674048	-2.675779	-1.259505
H	1.699607	-1.265377	-1.022581
N	-0.979564	2.763163	1.352229
H	-0.210372	2.658189	2.014951
H	-1.293797	3.730193	1.434541
O	-5.163857	1.489721	0.489814
C	-6.533674	1.379192	0.189879
H	-7.027156	2.242873	0.653186
H	-6.718219	1.406526	-0.897751
H	-6.971821	0.455941	0.606083

TS5

C	0.601109	3.523456	-1.628984
C	0.328770	2.159576	-1.551116
C	-0.114702	1.587029	-0.352057
C	-0.427862	2.441499	0.719195
C	-0.134073	3.805523	0.655046
C	0.406610	4.339337	-0.512956
C	-0.459570	0.142574	-0.216574
S	-1.333494	1.758254	2.091354
C	-2.447399	0.760809	1.113830
C	-1.940324	0.046963	0.007820
C	-2.819776	-0.663382	-0.802866
H	-2.437668	-1.228243	-1.654533
C	-4.186486	-0.725105	-0.495045
C	-4.677090	-0.052298	0.630067
C	-3.803289	0.697540	1.420069
H	0.970413	3.950662	-2.563712
H	0.488574	1.516794	-2.419808
H	-0.368272	4.454833	1.501836
H	0.629068	5.407357	-0.566982
H	-5.734683	-0.083530	0.892151
H	-4.197467	1.248406	2.277323
C	0.330543	-0.957558	-0.106851
C	1.802363	-1.227985	0.084648
C	-0.340756	-2.337977	-0.024710
C	1.924791	-2.503605	0.633691
H	-1.330158	-2.269272	0.441580
C	0.603140	-3.170117	0.843890
H	0.609195	-4.233159	0.558607
C	3.016923	-0.478561	-0.143616
C	4.273832	-1.092267	0.179445
C	4.320851	-2.398852	0.737919
C	3.163679	-3.090662	0.966860
C	5.489501	-0.392300	-0.056284
C	5.494584	0.874285	-0.586407
C	4.263834	1.489527	-0.900578
C	3.075899	0.830506	-0.684765
H	0.319060	-3.113950	1.908765
H	5.293671	-2.836584	0.975616
H	3.183723	-4.093989	1.398764
H	6.428601	-0.891105	0.197112
H	6.436111	1.399741	-0.761132
H	4.246686	2.497989	-1.321209
H	2.154231	1.334088	-0.932876
N	-0.528602	-2.850705	-1.381206
H	0.378268	-2.949648	-1.840076
H	-0.919679	-3.791626	-1.332076
O	-4.946024	-1.459794	-1.331536

C	-6.322560	-1.590914	-1.070456
H	-6.730236	-2.237324	-1.857849
H	-6.508851	-2.064423	-0.091323
H	-6.841536	-0.618050	-1.106407

syn-(M)-stable-E

C	4.116550	-0.755246	0.870572
C	2.723441	-0.675095	1.012483
C	1.966345	0.119481	0.156636
C	2.614702	0.883645	-0.830448
C	3.997525	0.809491	-0.969982
C	4.752865	-0.014487	-0.133120
C	0.479188	0.182596	0.222097
S	1.632475	1.890977	-1.917340
C	0.424398	2.453769	-0.738090
C	-0.029855	1.587324	0.280087
C	-0.877673	2.119434	1.255670
H	-1.169117	1.506716	2.104264
C	-1.352454	3.426864	1.166749
C	-0.960343	4.243125	0.107779
C	-0.050650	3.763862	-0.832067
H	2.238920	-1.260776	1.796508
H	4.504329	1.400271	-1.736819
H	5.834148	-0.055235	-0.265051
H	-1.334122	5.266385	0.028392
H	0.308914	4.416187	-1.631433
C	-0.245738	-0.920500	-0.084110
C	-1.703297	-1.065132	-0.331910
C	0.380118	-2.142866	-0.754716
C	-1.851014	-1.753695	-1.524737
H	1.421587	-1.938754	-1.049367
C	-0.518037	-2.262027	-2.007952
H	-0.572957	-3.292458	-2.391316
C	-2.851955	-0.706549	0.432821
C	-4.135657	-0.866740	-0.178086
C	-4.233804	-1.446047	-1.474725
C	-3.117808	-1.926749	-2.119607
C	-5.299836	-0.506924	0.558761
C	-5.207864	-0.084575	1.862608
C	-3.944309	-0.030870	2.501389
C	-2.800130	-0.333965	1.803751
H	-0.117693	-1.622660	-2.812611
H	-5.223432	-1.555215	-1.925956
H	-3.207837	-2.437060	-3.081698
H	-6.274917	-0.601859	0.073658
H	-6.110271	0.175229	2.420997
H	-3.882298	0.236983	3.558850
H	-1.834538	-0.340648	2.310247
H	-2.030828	3.806378	1.933975
N	0.242326	-3.326554	0.083678
H	0.637687	-4.130752	-0.403430
H	0.806223	-3.208321	0.924947
O	4.754672	-1.564255	1.737794
C	6.153608	-1.695608	1.649291
H	6.452950	-2.393985	2.440626
H	6.464827	-2.109146	0.674902
H	6.665254	-0.732105	1.812807

TSS'

C	-4.381063	0.349185	-0.097093
C	-3.066564	0.707757	0.227157
C	-1.979602	-0.124387	-0.037843
C	-2.266863	-1.394249	-0.602157
C	-3.573854	-1.750478	-0.926543

C	-4.641579	-0.885672	-0.694370
C	-0.535240	0.192888	0.240992
S	-0.997819	-2.595689	-0.924484
C	0.027152	-2.269493	0.477203
C	0.178313	-0.941505	0.905832
C	0.996889	-0.704942	2.020424
H	1.096886	0.315156	2.397307
C	1.695319	-1.738892	2.635737
C	1.566651	-3.046316	2.163673
C	0.718878	-3.315303	1.093029
H	-2.891159	1.701578	0.629732
H	-3.770263	-2.734115	-1.359905
H	-5.651578	-1.197075	-0.961467
H	2.109982	-3.863398	2.643543
H	0.589253	-4.338821	0.733326
C	0.171303	1.326823	-0.059773
C	1.660223	1.390775	-0.156280
C	-0.281125	2.787901	-0.256612
C	2.096083	2.676579	0.110846
H	-0.371092	2.965420	-1.342860
C	0.934489	3.598852	0.271641
H	0.761922	3.842378	1.334930
C	2.616370	0.407695	-0.586030
C	4.004802	0.726883	-0.463146
C	4.402634	2.026682	-0.033912
C	3.467272	3.004271	0.193516
C	4.978882	-0.239477	-0.838569
C	4.605791	-1.447695	-1.375979
C	3.235732	-1.722351	-1.594586
C	2.271619	-0.819786	-1.211473
H	1.069903	4.552220	-0.261308
H	5.470013	2.244807	0.055385
H	3.770309	4.022783	0.448007
H	6.036048	0.007556	-0.709874
H	5.362339	-2.179907	-1.666972
H	2.939051	-2.654305	-2.081866
H	1.226376	-1.032539	-1.428780
H	2.339277	-1.523625	3.491228
N	-1.523541	3.200618	0.361588
H	-1.408492	3.229171	1.375292
H	-1.737072	4.155221	0.076891
O	-5.325614	1.265006	0.204276
C	-6.668867	0.987136	-0.105977
H	-7.250960	1.863676	0.205995
H	-6.816413	0.830978	-1.188428
H	-7.041394	0.102196	0.437986

anti-(P)-unstable-E

C	-4.321459	0.412361	0.290017
C	-2.960126	0.685032	0.483380
C	-1.976990	-0.111902	-0.097466
C	-2.377328	-1.276064	-0.789292
C	-3.728610	-1.551670	-0.977798
C	-4.708047	-0.700936	-0.464151
C	-0.506497	0.111380	0.065350
S	-1.148463	-2.435235	-1.352021
C	-0.078793	-2.347040	0.066562
C	0.146479	-1.092797	0.657902
C	0.963920	-1.024461	1.790917
H	1.121363	-0.057946	2.274859
C	1.598748	-2.163977	2.278383
C	1.406624	-3.395162	1.649564
C	0.553861	-3.493008	0.551431
H	-2.682205	1.567906	1.055025
H	-4.031104	-2.454405	-1.513816

H	-5.758949	-0.938983	-0.629363
H	1.904389	-4.290188	2.029361
H	0.374869	-4.459541	0.074596
C	0.204607	1.201912	-0.311285
C	1.682123	1.382176	-0.169030
C	-0.244998	2.587157	-0.782849
C	1.921879	2.703094	0.170227
H	0.144884	2.666313	-1.820348
C	0.650782	3.498295	0.082968
H	0.176693	3.630458	1.071126
C	2.776687	0.487606	-0.378412
C	4.081566	0.939480	-0.008566
C	4.266941	2.274073	0.454931
C	3.216221	3.158485	0.501293
C	5.187965	0.056152	-0.159809
C	5.024644	-1.192961	-0.706879
C	3.746622	-1.604308	-1.158270
C	2.654774	-0.785655	-1.000267
H	0.799270	4.495021	-0.359272
H	5.274883	2.596018	0.729654
H	3.373752	4.199391	0.793795
H	6.177841	0.400474	0.151483
H	5.881742	-1.860658	-0.821192
H	3.628994	-2.576421	-1.642773
H	1.683676	-1.099380	-1.380329
H	2.249830	-2.090853	3.152206
N	-1.636090	2.962746	-0.691354
H	-1.727311	3.923524	-1.020696
H	-2.201249	2.399899	-1.324776
O	-5.180981	1.275005	0.868497
C	-6.564251	1.060797	0.727645
H	-7.064303	1.875371	1.266662
H	-6.878452	1.091364	-0.329806
H	-6.876799	0.098785	1.168449

TS6

C	3.813535	-1.304852	0.566598
C	2.460234	-1.073310	0.315628
C	1.956410	0.178562	-0.077266
C	2.886329	1.241698	-0.088538
C	4.240489	1.015263	0.172735
C	4.726310	-0.249736	0.477590
C	0.490076	0.334960	-0.351067
S	2.458922	2.921223	-0.359540
C	0.705337	2.889344	-0.329557
C	-0.086290	1.719482	-0.406925
C	-1.454126	1.951382	-0.674899
H	-2.106215	1.111990	-0.882904
C	-2.024527	3.214290	-0.721656
C	-1.231679	4.344027	-0.523544
C	0.131645	4.172157	-0.353277
H	1.797182	-1.932956	0.434947
H	4.937255	1.857726	0.151771
H	5.789901	-0.385312	0.673045
H	-1.663918	5.346684	-0.535036
H	0.783084	5.044943	-0.256809
C	-0.269020	-0.792629	-0.575262
C	-1.731831	-1.013124	-0.476404
C	0.215207	-2.072976	-1.276562
C	-2.132764	-1.855148	-1.502443
H	1.179626	-1.916039	-1.778616
C	-0.931485	-2.269873	-2.306773
H	-0.988758	-3.306559	-2.670953
C	-2.650525	-0.648668	0.557678
C	-4.009447	-1.065592	0.417154

C	-4.398436	-1.852590	-0.705679
C	-3.475975	-2.261909	-1.640262
C	-4.949869	-0.697653	1.419766
C	-4.561610	0.031019	2.518144
C	-3.207412	0.416263	2.670705
C	-2.276106	0.086910	1.714371
H	-0.785239	-1.608049	-3.177517
H	-5.445557	-2.153479	-0.794657
H	-3.773998	-2.903241	-2.473208
H	-5.990677	-1.010660	1.301916
H	-5.292876	0.307300	3.281068
H	-2.901834	0.976888	3.557201
H	-1.233257	0.382231	1.842389
H	-3.093506	3.311387	-0.921712
N	0.350573	-3.202531	-0.363801
H	-0.534728	-3.377271	0.112556
H	0.565581	-4.047709	-0.891490
O	4.143663	-2.571018	0.899779
C	5.482302	-2.863828	1.215721
H	5.831250	-2.290363	2.091861
H	5.521504	-3.933944	1.455605
H	6.158483	-2.668109	0.365710

motor 9

anti-(M)-stable-E

C	1.560231	2.510988	2.161048
C	0.952363	1.323563	1.763088
C	0.091194	1.296796	0.660644
C	-0.200363	2.502817	0.001439
C	0.411436	3.695614	0.394481
C	1.301744	3.693749	1.466479
C	-0.533136	0.038756	0.171849
S	-1.316179	2.484426	-1.381270
C	-2.469276	1.275421	-0.767413
C	-2.006444	0.174043	-0.018491
C	-2.942621	-0.686243	0.552636
H	-2.626225	-1.498507	1.208284
C	-4.759194	0.528433	-0.488737
C	-3.832368	1.434864	-1.003511
H	2.244082	2.512719	3.012536
H	1.161378	0.393356	2.295689
H	0.183585	4.625868	-0.131290
H	1.780339	4.626731	1.772308
H	-5.819405	0.680871	-0.690670
H	-4.188461	2.288911	-1.584491
C	0.166093	-1.082275	-0.118096
C	1.625705	-1.342764	-0.004097
C	-0.427406	-2.443767	-0.455529
C	1.791869	-2.667347	0.368876
H	-1.485131	-2.540332	-0.181316
C	0.467442	-3.384936	0.377567
H	0.526642	-4.393975	-0.058793
C	2.766455	-0.524044	-0.271492
C	4.055327	-1.061320	0.035870
C	4.172785	-2.395010	0.522695
C	3.066891	-3.200681	0.652107
C	5.212270	-0.266364	-0.200900
C	5.107769	0.983508	-0.760972
C	3.837350	1.485392	-1.134067
C	2.699826	0.751622	-0.897068
H	0.065531	-3.485565	1.400199
H	5.169616	-2.782322	0.748916
H	3.169001	-4.241519	0.968698
H	6.191585	-0.679688	0.054638

H	6.004145	1.580386	-0.944543
H	3.760366	2.459663	-1.622323
H	1.733501	1.136902	-1.218655
C	-4.314701	-0.528649	0.313549
O	-5.123578	-1.431941	0.899952
O	-0.259954	-2.643926	-1.842629
H	-0.576414	-3.531418	-2.049530
C	-6.515082	-1.326517	0.712455
H	-6.970331	-2.151975	1.273667
H	-6.908970	-0.372009	1.101026
H	-6.791224	-1.426330	-0.350881

anti-(M)-stable-*E**

C	2.240913	1.995796	2.589682
C	1.449171	0.998980	2.046130
C	0.249020	1.279552	1.331866
C	-0.118822	2.652848	1.260409
C	0.685546	3.655184	1.811418
C	1.871409	3.336149	2.462625
C	-0.525839	0.209384	0.725659
S	-1.561783	3.206500	0.452328
C	-2.450256	1.735464	0.131872
C	-1.871463	0.437233	0.223753
C	-2.657559	-0.640842	-0.234573
H	-2.255321	-1.654707	-0.234717
C	-4.521871	0.815873	-0.744349
C	-3.752799	1.901443	-0.333882
H	3.156256	1.724133	3.119151
H	1.747012	-0.039665	2.177389
H	0.365012	4.697012	1.733608
H	2.491941	4.129348	2.884281
H	-5.538630	0.987900	-1.096592
H	-4.175871	2.907489	-0.390463
C	0.082679	-1.092795	0.679310
C	1.393061	-1.363228	0.209882
C	-0.426957	-2.369927	1.342614
C	1.900016	-2.535640	0.822692
H	-1.092980	-2.134385	2.191947
C	0.874982	-3.070084	1.781373
H	0.778136	-4.166056	1.756878
C	2.232090	-0.605489	-0.690473
C	3.581220	-1.052282	-0.876837
C	4.040391	-2.220262	-0.222299
C	3.207888	-2.957671	0.613286
C	4.430950	-0.310587	-1.746190
C	3.967849	0.795212	-2.418356
C	2.626516	1.209124	-2.260532
C	1.780117	0.516579	-1.418888
H	1.139734	-2.776867	2.813526
H	5.072026	-2.541304	-0.387784
H	3.586579	-3.849876	1.118304
H	5.464168	-0.642481	-1.877102
H	4.633079	1.350668	-3.083221
H	2.256419	2.078813	-2.807511
H	0.739828	0.831043	-1.318507
C	-3.958542	-0.465851	-0.701970
O	-4.601461	-1.588266	-1.093038
O	-1.109992	-3.179505	0.392484
H	-1.572510	-3.876455	0.868763
C	-5.896569	-1.485559	-1.613780
H	-6.204736	-2.500651	-1.892803
H	-6.610694	-1.089480	-0.869962
H	-5.929299	-0.845839	-2.513474

syn-(P)-unstable-*Z*

C	-4.069221	-1.450163	2.131655
C	-2.742171	-1.241583	1.758688
C	-2.418828	-0.432616	0.659293
C	-3.461663	0.220922	-0.015308
C	-4.792922	0.017798	0.355454
C	-5.096332	-0.828911	1.420005
C	-1.001300	-0.268880	0.236771
S	-3.070133	1.266992	-1.384420
C	-1.520790	1.921705	-0.809636
C	-0.611060	1.146944	-0.046473
C	0.580625	1.756765	0.337930
H	1.308112	1.234301	0.948981
C	0.904285	3.067807	-0.036815
C	0.010136	3.810013	-0.810649
C	-1.201743	3.226462	-1.177628
H	-4.300930	-2.094362	2.982663
H	-1.933371	-1.722151	2.315445
H	-5.593280	0.527635	-0.186386
H	-6.138824	-0.986853	1.704910
H	0.226217	4.833896	-1.115753
H	-1.916179	3.811112	-1.762403
C	-0.252864	-1.374758	-0.017438
C	1.189434	-1.508783	-0.322555
C	-0.825409	-2.731371	-0.484540
C	1.327119	-2.353295	-1.413625
H	-0.525082	-3.513980	0.239800
C	-0.008175	-2.931921	-1.781345
H	-0.505442	-2.358216	-2.582302
C	2.342204	-1.103527	0.415873
C	3.623688	-1.369513	-0.158419
C	3.713991	-2.094688	-1.380494
C	2.591947	-2.625976	-1.973846
C	4.792855	-0.968875	0.548775
C	4.703380	-0.399138	1.795175
C	3.436005	-0.222654	2.403827
C	2.287146	-0.564642	1.732087
H	0.045820	-3.985091	-2.092181
H	4.703588	-2.276984	-1.807443
H	2.675984	-3.256150	-2.862466
H	5.768367	-1.146019	0.088425
H	5.608396	-0.107129	2.332645
H	3.373439	0.184452	3.415591
H	1.313919	-0.441762	2.212452
O	2.093919	3.522934	0.403576
O	-2.177840	-2.814984	-0.790974
H	-2.691200	-2.824583	0.025017
C	2.481920	4.836741	0.082821
H	3.462708	4.996800	0.547939
H	2.578635	4.981973	-1.006677
H	1.773201	5.580958	0.484611

TS1

C	-3.769466	-2.652467	1.129081
C	-2.526162	-2.176400	0.737935
C	-2.277610	-0.818159	0.427041
C	-3.338718	0.066315	0.724639
C	-4.603912	-0.410545	1.104423
C	-4.836732	-1.765873	1.276019
C	-0.937111	-0.363373	-0.032849
S	-3.173219	1.810476	0.837001
C	-1.600850	2.110459	0.111173
C	-0.706415	1.091790	-0.279920
C	0.397540	1.504490	-1.043607
H	1.070844	0.772107	-1.482032

C	0.697901	2.842502	-1.292063
C	-0.154290	3.840932	-0.806316
C	-1.308019	3.455117	-0.136525
H	-3.896941	-3.716335	1.338927
H	-1.703706	-2.888859	0.724582
H	-5.407984	0.307142	1.288267
H	-5.827515	-2.121135	1.565965
H	0.042121	4.899651	-0.975278
H	-2.013031	4.225638	0.187126
C	0.066147	-1.271741	-0.296515
C	1.524913	-1.087500	-0.196417
C	-0.109754	-2.651883	-0.963479
C	2.166779	-1.957246	-1.065177
H	-0.065549	-3.458519	-0.203935
C	1.162235	-2.762066	-1.827945
H	0.943942	-2.298687	-2.805101
C	2.291606	-0.284507	0.712947
C	3.714826	-0.328977	0.597514
C	4.328165	-1.188547	-0.360779
C	3.572870	-2.009500	-1.162192
C	4.507034	0.473955	1.463820
C	3.923049	1.269216	2.420358
C	2.515698	1.279932	2.563859
C	1.721483	0.524445	1.732225
H	1.470171	-3.801968	-2.005905
H	5.419044	-1.197973	-0.428751
H	4.048054	-2.689194	-1.873338
H	5.594704	0.441114	1.358726
H	4.542368	1.881255	3.080144
H	2.056063	1.890667	3.344460
H	0.640079	0.532991	1.867506
O	1.810990	3.074448	-2.016949
O	-1.217103	-2.790509	-1.800346
H	-2.019939	-2.861519	-1.270683
C	2.150465	4.402760	-2.332998
H	3.068842	4.358520	-2.931779
H	1.362532	4.895578	-2.927927
H	2.347720	5.000893	-1.427113

intermediate-Z

C	4.889425	-1.148519	0.660118
C	3.508974	-1.167942	0.847223
C	2.653922	-0.374081	0.067139
C	3.252984	0.505580	-0.862740
C	4.637284	0.520737	-1.054201
C	5.456852	-0.318189	-0.304196
C	1.157801	-0.384140	0.140768
S	2.268279	1.620666	-1.836970
C	1.036525	2.004541	-0.621974
C	0.585109	0.982592	0.231538
C	-0.367303	1.282432	1.202339
H	-0.710188	0.509937	1.893166
C	-0.930839	2.561837	1.286525
C	-0.507404	3.562581	0.403235
C	0.484544	3.279172	-0.536997
H	5.524152	-1.785028	1.280910
H	3.069866	-1.802501	1.615070
H	5.073518	1.208811	-1.782450
H	6.538312	-0.298695	-0.456224
H	-0.925263	4.568413	0.445769
H	0.830272	4.070831	-1.205897
C	0.397933	-1.515607	0.120158
C	-1.057343	-1.713991	-0.111344
C	0.958146	-2.866558	0.572952
C	-1.387417	-3.031114	0.187826

H	1.878770	-3.137015	0.027162
C	-0.165935	-3.881458	0.359955
H	-0.230959	-4.590354	1.198660
C	-2.087176	-0.862399	-0.653759
C	-3.444452	-1.305722	-0.552415
C	-3.737182	-2.611438	-0.063786
C	-2.723247	-3.484144	0.235544
C	-4.494616	-0.465514	-1.015829
C	-4.224489	0.728068	-1.639827
C	-2.880725	1.108111	-1.857130
C	-1.847293	0.336736	-1.377790
H	-0.011858	-4.474227	-0.557030
H	-4.782219	-2.923713	0.007201
H	-2.937192	-4.516727	0.521386
H	-5.525744	-0.807135	-0.892671
H	-5.038202	1.360649	-2.001785
H	-2.656295	2.018064	-2.418714
H	-0.825781	0.631594	-1.598586
O	-1.867213	2.735255	2.238270
O	1.222845	-2.729128	1.963837
C	-2.466426	4.000104	2.384287
H	-3.187476	3.913384	3.206679
H	-1.724962	4.775552	2.640878
H	-3.005641	4.304207	1.471006
H	1.530833	-3.585007	2.288937

TS2

C	4.328114	-1.797482	1.102860
C	3.003799	-1.399631	1.279406
C	2.328713	-0.708991	0.267340
C	3.032029	-0.367331	-0.904177
C	4.354781	-0.775134	-1.086357
C	4.998063	-1.500253	-0.084158
C	0.892466	-0.280377	0.331504
S	2.209893	0.604755	-2.156460
C	1.391654	1.723647	-1.039213
C	0.848563	1.197258	0.147357
C	0.461128	2.073155	1.158248
H	0.112588	1.689654	2.119189
C	0.456947	3.458149	0.945026
C	0.892714	3.969789	-0.283861
C	1.388194	3.099264	-1.255279
H	4.837618	-2.347158	1.897519
H	2.461128	-1.657419	2.190252
H	4.886461	-0.509177	-2.003060
H	6.035382	-1.812182	-0.225143
H	0.894591	5.041990	-0.480483
H	1.803018	3.509601	-2.178956
C	-0.105416	-1.201941	0.370452
C	-1.584673	-1.218501	0.088779
C	0.280804	-2.664129	0.616682
C	-1.945503	-2.535341	-0.186566
H	1.267630	-2.892176	0.189167
C	-0.803863	-3.492057	-0.061363
H	-1.063741	-4.386061	0.525847
C	-2.611717	-0.206217	-0.014859
C	-3.925256	-0.601915	-0.437814
C	-4.214469	-1.964487	-0.722647
C	-3.243123	-2.917378	-0.588430
C	-4.955504	0.370867	-0.563309
C	-4.730118	1.693555	-0.271348
C	-3.450580	2.087676	0.174809
C	-2.436901	1.165712	0.295807
H	-0.477883	-3.834685	-1.057541
H	-5.224469	-2.233738	-1.041885

H	-3.453524	-3.969009	-0.796701
H	-5.941778	0.036829	-0.896007
H	-5.530731	2.429760	-0.371953
H	-3.256401	3.131725	0.432516
H	-1.474332	1.502260	0.648685
O	0.005516	4.210046	1.966359
O	0.296575	-2.848294	2.021572
H	0.582198	-3.754418	2.192652
C	-0.032334	5.610342	1.824351
H	-0.430191	6.008819	2.765983
H	0.973261	6.032118	1.657651
H	-0.696889	5.919723	0.999899

syn-(*M*)-stable-*Z*

C	0.989725	3.097464	-0.116015
C	0.491987	1.879754	-0.600410
C	-0.590382	1.244125	-0.003075
C	-1.250903	1.908917	1.056578
C	-0.758436	3.118343	1.539191
C	0.373811	3.710184	0.978458
C	-1.142443	-0.087592	-0.395434
S	-2.727173	1.228830	1.780379
C	-3.451396	0.535745	0.315853
C	-2.611189	-0.058016	-0.640245
C	-3.185561	-0.622673	-1.785160
H	-2.532535	-1.083941	-2.529390
C	-4.567974	-0.625942	-1.958004
C	-5.393921	-0.053136	-0.989464
C	-4.838003	0.533952	0.145965
H	0.984678	1.448586	-1.465486
H	-1.271012	3.623888	2.361177
H	0.736964	4.654562	1.383813
H	-6.478075	-0.051109	-1.122748
H	-5.481107	0.997536	0.897784
C	-0.509161	-1.281738	-0.291485
C	0.882689	-1.601959	0.114578
C	-1.276335	-2.577119	-0.059061
C	0.812802	-2.574633	1.099567
H	-2.349849	-2.396278	0.099730
C	-0.600839	-3.075911	1.241107
H	-0.657548	-4.170338	1.347313
C	2.151211	-1.168187	-0.371817
C	3.314681	-1.570253	0.356724
C	3.184412	-2.452568	1.466269
C	1.962496	-2.987584	1.803790
C	4.593855	-1.136860	-0.095036
C	4.725151	-0.412735	-1.254611
C	3.581114	-0.110367	-2.034038
C	2.330418	-0.481216	-1.603713
H	-1.102041	-2.624632	2.114162
H	4.086455	-2.744712	2.010278
H	1.879987	-3.725933	2.605165
H	5.476607	-1.419149	0.485028
H	5.713365	-0.096800	-1.596940
H	3.697504	0.408080	-2.988498
H	1.456502	-0.287781	-2.227740
H	-5.003389	-1.076897	-2.852369
O	2.054395	3.596550	-0.772862
O	-1.068193	-3.445381	-1.147726
H	-1.524450	-4.273622	-0.956405
C	2.614771	4.814065	-0.343278
H	2.994291	4.746330	0.690352
H	3.455546	5.025610	-1.015819
H	1.890041	5.643405	-0.409448

TS2'

C	0.749874	-2.264438	2.101522
C	0.289664	-1.004985	1.697809
C	-0.579115	-0.866244	0.616909
C	-1.047581	-2.027325	-0.022502
C	-0.610974	-3.283114	0.387058
C	0.297865	-3.411486	1.437864
C	-1.034655	0.488158	0.189442
S	-2.121788	-1.852845	-1.418059
C	-3.089165	-0.482875	-0.832490
C	-2.517135	0.549622	-0.051168
C	-3.396049	1.529481	0.436176
H	-2.991230	2.308132	1.074617
C	-4.748058	1.536357	0.101359
C	-5.276098	0.546666	-0.723629
C	-4.444419	-0.473063	-1.174771
H	0.647773	-0.123480	2.232617
H	-0.977493	-4.180618	-0.117081
H	0.628048	-4.406299	1.736881
H	-6.334961	0.546522	-0.991546
H	-4.850849	-1.285524	-1.781801
C	-0.127038	1.496230	0.019702
C	1.342234	1.349870	-0.158740
C	-0.390890	3.006365	0.074506
C	1.974736	2.543179	0.147534
H	-0.770517	3.348828	-0.906964
C	0.986989	3.640213	0.376641
H	0.984603	3.974293	1.426456
C	2.130228	0.264779	-0.679114
C	3.552108	0.357542	-0.567815
C	4.152132	1.557161	-0.084572
C	3.381931	2.654419	0.205049
C	4.359010	-0.725957	-1.012592
C	3.797362	-1.824552	-1.617486
C	2.401422	-1.860504	-1.840404
C	1.594229	-0.843686	-1.386147
H	1.204693	4.518381	-0.250094
H	5.241465	1.604253	-0.006930
H	3.842085	3.601557	0.496526
H	5.442630	-0.655600	-0.886342
H	4.427070	-2.648074	-1.961926
H	1.959588	-2.694933	-2.390343
H	0.531192	-0.864437	-1.615434
H	-5.392587	2.324423	0.497833
O	1.614695	-2.273634	3.134335
O	-1.296634	3.343899	1.100583
H	-1.507144	4.281422	1.008951
C	2.117897	-3.504004	3.595355
H	2.797371	-3.272431	4.425166
H	1.314275	-4.162068	3.967628
H	2.684210	-4.033651	2.810314

anti-(P)-unstable-Z

C	1.153797	-2.287141	1.492323
C	0.434856	-1.091744	1.363103
C	-0.528662	-0.943054	0.370711
C	-0.837677	-2.040576	-0.453322
C	-0.136291	-3.234613	-0.318654
C	0.872575	-3.360310	0.638066
C	-1.257115	0.341017	0.155534
S	-2.090071	-1.848973	-1.700972
C	-3.228632	-0.866413	-0.747658
C	-2.736797	0.122678	0.126453
C	-3.649832	0.756274	0.979491
H	-3.280322	1.481733	1.701604

C	-5.014022	0.493947	0.889876
C	-5.493982	-0.425818	-0.043708
C	-4.599034	-1.122743	-0.850269
H	0.677796	-0.262252	2.029500
H	-0.373877	-4.084753	-0.962603
H	1.412294	-4.303737	0.719303
H	-6.564678	-0.628499	-0.120614
H	-4.958201	-1.888433	-1.541940
C	-0.598984	1.507529	-0.047336
C	0.879837	1.713619	-0.062115
C	-1.123139	2.938373	-0.110288
C	1.152884	2.934490	0.532933
H	-0.940032	3.287695	-1.146269
C	-0.123577	3.673664	0.812507
H	-0.455080	3.548296	1.857471
C	1.941957	0.935306	-0.618459
C	3.281667	1.350986	-0.345754
C	3.519159	2.556942	0.375724
C	2.477726	3.361674	0.769472
C	4.363288	0.571785	-0.845247
C	4.134391	-0.536253	-1.624272
C	2.808168	-0.896691	-1.966138
C	1.742834	-0.178877	-1.478849
H	-0.052946	4.751011	0.600280
H	4.553009	2.852631	0.571958
H	2.664823	4.315864	1.267776
H	5.384670	0.882500	-0.610001
H	4.972987	-1.123973	-2.004783
H	2.630212	-1.747289	-2.628333
H	0.729118	-0.447684	-1.772078
H	-5.708276	1.011962	1.555468
O	2.093293	-2.310060	2.457633
O	-2.459599	3.119721	0.230646
H	-2.696231	4.031643	0.024744
C	2.928113	-3.437188	2.572531
H	3.488054	-3.623511	1.640326
H	3.641729	-3.216336	3.376242
H	2.361040	-4.344182	2.843153

TS3

C	-1.130672	2.754683	-0.801801
C	-0.618796	1.462295	-0.702053
C	0.695150	1.172486	-0.300408
C	1.538325	2.296813	-0.133546
C	1.027437	3.596865	-0.219087
C	-0.303530	3.846961	-0.523039
C	1.179672	-0.240572	-0.188382
S	3.285957	2.230243	0.030187
C	3.606650	0.518316	0.201486
C	2.617643	-0.486392	0.142145
C	3.042673	-1.778918	0.529880
H	2.306609	-2.573937	0.634285
C	4.366532	-2.085829	0.807375
C	5.340668	-1.088180	0.751290
C	4.949618	0.211968	0.476774
H	-1.306950	0.669846	-0.972802
H	1.700060	4.444049	-0.059837
H	-0.663814	4.874546	-0.571651
H	6.388840	-1.311348	0.961602
H	5.687824	1.018420	0.492971
C	0.349582	-1.316088	-0.423646
C	-1.123333	-1.441027	-0.349970
C	0.776457	-2.615018	-1.111244
C	-1.556599	-2.299380	-1.348088
H	1.751801	-2.508059	-1.612672

C	-0.373690	-2.808615	-2.123957
H	-0.475021	-3.858363	-2.438271
C	-2.044004	-0.954312	0.630896
C	-3.424900	-1.280771	0.467007
C	-3.836959	-2.099075	-0.624463
C	-2.919979	-2.618463	-1.508374
C	-4.367529	-0.788454	1.412507
C	-3.963101	-0.024227	2.480323
C	-2.590084	0.272235	2.658457
C	-1.655464	-0.179521	1.756608
H	-0.192305	-2.199961	-3.025974
H	-4.900148	-2.329051	-0.732018
H	-3.239361	-3.276959	-2.319698
H	-5.423893	-1.033684	1.274574
H	-4.696419	0.347575	3.199647
H	-2.271717	0.861799	3.521431
H	-0.599150	0.048661	1.907233
H	4.633055	-3.107167	1.087997
O	-2.422628	2.848103	-1.176311
O	0.791867	-3.689058	-0.188833
H	1.037815	-4.489303	-0.669844
C	-2.996923	4.123600	-1.327249
H	-4.034140	3.963859	-1.647055
H	-3.002699	4.684534	-0.377230
H	-2.475098	4.719225	-2.095709

anti-(M)-stable-Z

C	1.030856	-2.539454	-1.334846
C	0.390155	-1.294337	-1.310055
C	-0.618685	-1.029471	-0.389210
C	-1.050862	-2.053911	0.472105
C	-0.422933	-3.296113	0.442515
C	0.627273	-3.541257	-0.443271
C	-1.261504	0.307063	-0.291222
S	-2.357152	-1.725698	1.631347
C	-3.360521	-0.670124	0.610178
C	-2.751494	0.226990	-0.288853
C	-3.577945	0.948622	-1.161000
H	-3.125896	1.580889	-1.927142
C	-4.965422	0.862470	-1.072201
C	-5.553933	0.028478	-0.121430
C	-4.752256	-0.754688	0.705111
H	0.726271	-0.517735	-1.999327
H	-0.751937	-4.091977	1.114870
H	1.105879	-4.520539	-0.439207
H	-6.641223	-0.041954	-0.044784
H	-5.207175	-1.451795	1.412825
C	-0.563097	1.457477	-0.154603
C	0.908420	1.665956	-0.105874
C	-1.135821	2.867005	-0.223123
C	1.187563	2.867025	-0.738069
H	-2.135831	2.910921	-0.672684
C	-0.087056	3.583492	-1.100106
H	-0.043202	4.664393	-0.895318
C	1.961104	0.911101	0.498161
C	3.304724	1.333946	0.254798
C	3.551923	2.517500	-0.499139
C	2.514569	3.294870	-0.955614
C	4.378683	0.589281	0.819158
C	4.137994	-0.495936	1.626239
C	2.805701	-0.868734	1.928368
C	1.747933	-0.183049	1.381141
H	-0.332658	3.454889	-2.168056
H	4.588105	2.819898	-0.671514
H	2.709495	4.232392	-1.482051

H	5.403366	0.908726	0.611411
H	4.970993	-1.055346	2.058324
H	2.616407	-1.701295	2.610057
H	0.728956	-0.460690	1.647254
H	-5.588806	1.444672	-1.754298
O	2.018717	-2.678726	-2.239292
O	-1.164506	3.375615	1.092555
H	-1.462940	4.291914	1.047279
C	2.772247	-3.867324	-2.252273
H	3.537963	-3.745609	-3.028714
H	3.272437	-4.041808	-1.284353
H	2.152070	-4.744812	-2.503256

*anti-(M)-stable-Z**

C	1.260960	-2.484189	-1.894826
C	0.678654	-1.287207	-1.481191
C	-0.617541	-1.229466	-0.925933
C	-1.327945	-2.458671	-0.817406
C	-0.737226	-3.649473	-1.228884
C	0.550440	-3.682732	-1.764127
C	-1.168806	0.035264	-0.481783
S	-2.978552	-2.576051	-0.229164
C	-3.346806	-0.957376	0.328161
C	-2.462292	0.140932	0.156910
C	-2.882258	1.387931	0.691931
H	-2.203310	2.237466	0.588272
C	-4.107846	1.544588	1.317135
C	-4.969324	0.452432	1.449943
C	-4.581528	-0.791113	0.961994
H	1.272060	-0.380105	-1.590977
H	-1.296761	-4.583803	-1.136393
H	0.973958	-4.638655	-2.070768
H	-5.937278	0.564428	1.942399
H	-5.241290	-1.654642	1.079405
C	-0.415505	1.233924	-0.721405
C	0.808127	1.650392	-0.154212
C	-0.749553	2.154049	-1.899578
C	1.282801	2.811149	-0.813241
H	-0.543542	1.560225	-2.818807
C	0.256584	3.307000	-1.786616
H	-0.280814	4.177489	-1.371831
C	1.587291	1.054749	0.907290
C	2.873826	1.621250	1.182323
C	3.324427	2.749691	0.452623
C	2.534362	3.346856	-0.519692
C	3.670750	1.039038	2.207546
C	3.212855	-0.030185	2.939850
C	1.932305	-0.568192	2.682516
C	1.140873	-0.035502	1.685973
H	0.679825	3.611978	-2.754765
H	4.311436	3.159382	0.682024
H	2.891837	4.231902	-1.051724
H	4.657375	1.463837	2.409471
H	3.835520	-0.462143	3.726474
H	1.566570	-1.410287	3.273929
H	0.148102	-0.447944	1.498716
H	-4.394111	2.522286	1.709816
O	2.507547	-2.389238	-2.403615
O	-2.057868	2.654533	-1.946875
H	-2.669731	1.911405	-1.996265
C	3.165944	-3.554937	-2.813218
H	4.154326	-3.247814	-3.176263
H	3.298596	-4.266526	-1.979310
H	2.629481	-4.064724	-3.633016

syn-(P)-unstable-E

C	3.751214	-1.316221	-0.884022
C	2.371753	-1.075199	-0.795711
C	1.876635	0.037013	-0.112518
C	2.784913	0.951910	0.443902
C	4.154487	0.721479	0.350045
C	4.646049	-0.412773	-0.297816
C	0.408788	0.258266	-0.007254
S	2.159579	2.363436	1.306761
C	0.735205	2.701536	0.299621
C	-0.013975	1.663646	-0.304802
C	-1.110278	2.046726	-1.087314
H	-1.690239	1.291090	-1.605813
C	-1.486505	3.380975	-1.226854
C	-0.759367	4.383887	-0.592154
C	0.360355	4.040804	0.159954
H	1.684803	-1.781548	-1.267413
H	4.859492	1.434412	0.784343
H	5.723548	-0.565877	-0.355875
H	-1.044658	5.432936	-0.697185
H	0.960471	4.819509	0.636907
C	-0.376828	-0.728696	0.498861
C	-1.850680	-0.832494	0.594391
C	0.107969	-1.796511	1.505085
C	-2.175699	-1.254033	1.874882
H	-0.054734	-2.802078	1.069062
C	-0.924390	-1.583007	2.635467
H	-0.575664	-0.734687	3.249187
C	-2.861430	-0.765304	-0.412165
C	-4.222842	-0.894877	0.004967
C	-4.521368	-1.168768	1.369831
C	-3.517886	-1.395544	2.283408
C	-5.254613	-0.818373	-0.973777
C	-4.954468	-0.702536	-2.308835
C	-3.601622	-0.679870	-2.730374
C	-2.584338	-0.709670	-1.807204
H	-1.029737	-2.461340	3.287978
H	-5.569658	-1.257983	1.666525
H	-3.753028	-1.686804	3.309878
H	-6.294542	-0.883822	-0.643058
H	-5.753961	-0.659264	-3.051920
H	-3.367940	-0.645209	-3.796973
H	-1.543851	-0.711716	-2.139126
H	-2.354544	3.630427	-1.841168
O	4.117145	-2.428699	-1.547115
O	1.385169	-1.675356	2.037949
H	2.033972	-1.902373	1.361337
C	5.486019	-2.739945	-1.661554
H	5.958330	-2.872729	-0.673517
H	5.546758	-3.686853	-2.212218
H	6.034784	-1.965042	-2.223237

TS4

C	1.432875	2.759384	-1.825604
C	0.937694	1.519364	-1.455182
C	-0.256357	1.356062	-0.717100
C	-1.004468	2.531932	-0.509126
C	-0.507684	3.793539	-0.875765
C	0.719991	3.916606	-1.505625
C	-0.707307	-0.009544	-0.315887
S	-2.634578	2.553884	0.136395
C	-3.048149	0.846847	0.237831
C	-2.118169	-0.211313	0.115886
C	-2.569272	-1.467415	0.564149

H	-1.881567	-2.300666	0.689714
C	-3.886236	-1.720281	0.952071
C	-4.817890	-0.676977	0.942839
C	-4.372092	0.596097	0.613885
H	2.370807	2.820168	-2.381184
H	1.496006	0.636982	-1.760558
H	-1.113912	4.682211	-0.680394
H	1.096301	4.903604	-1.782671
H	-5.859821	-0.828510	1.224199
H	-5.075468	1.431138	0.670710
C	0.163385	-1.075906	-0.396627
C	1.625954	-1.091919	-0.210807
C	-0.182695	-2.496211	-0.891328
C	2.173104	-2.162078	-0.903606
H	-0.296305	-3.187731	-0.032237
C	1.102161	-2.903662	-1.638970
H	1.014805	-2.543562	-2.678295
C	2.453400	-0.298679	0.653140
C	3.853948	-0.582503	0.675977
C	4.379036	-1.652911	-0.106202
C	3.553882	-2.446390	-0.865543
C	4.707123	0.194393	1.507861
C	4.199670	1.193602	2.303316
C	2.808021	1.447057	2.312717
C	1.958634	0.721662	1.509411
H	1.252752	-3.991916	-1.667552
H	5.453709	-1.848481	-0.068546
H	3.956265	-3.286594	-1.436387
H	5.777776	-0.026496	1.510406
H	4.864545	1.781740	2.940092
H	2.403088	2.221619	2.968105
H	0.888212	0.923201	1.540887
O	-4.156688	-2.984226	1.329703
O	-1.254854	-2.594166	-1.777506
H	-2.081579	-2.464291	-1.296910
C	-5.457931	-3.304300	1.762496
H	-6.204828	-3.144088	0.966775
H	-5.446679	-4.369491	2.024753
H	-5.747550	-2.721882	2.653503

intermediate-*E*

C	1.601090	-2.321506	2.332335
C	0.975541	-1.184399	1.829712
C	0.136588	-1.262499	0.710699
C	-0.113520	-2.524747	0.148943
C	0.512593	-3.668905	0.647509
C	1.381529	-3.562156	1.731763
C	-0.514529	-0.041266	0.171111
S	-1.186136	-2.626810	-1.256324
C	-2.373536	-1.396534	-0.766587
C	-1.980387	-0.227899	-0.070321
C	-2.981663	0.657200	0.330437
H	-2.720773	1.532724	0.921455
C	-4.326979	0.446006	-0.000196
C	-4.695221	-0.687567	-0.729717
C	-3.711024	-1.607133	-1.090751
H	2.265386	-2.239669	3.195287
H	1.144885	-0.210591	2.294585
H	0.314350	-4.641760	0.191559
H	1.871254	-4.456879	2.122525
H	-5.733331	-0.884440	-0.997068
H	-4.000670	-2.514658	-1.626026
C	0.161960	1.116270	-0.078475
C	1.617731	1.378014	-0.212017
C	-0.533300	2.479914	-0.063215

C	1.835822	2.750280	-0.218262
H	-1.366007	2.524279	-0.787131
C	0.555559	3.514083	-0.366006
H	0.478724	4.377643	0.311373
C	2.745200	0.507255	-0.431844
C	4.056480	1.070358	-0.325371
C	4.219869	2.475088	-0.151140
C	3.131283	3.308673	-0.165302
C	5.194520	0.230029	-0.473635
C	5.057330	-1.097306	-0.800667
C	3.767157	-1.626886	-1.029596
C	2.648045	-0.847044	-0.850380
H	0.482574	3.901163	-1.395726
H	5.231538	2.880562	-0.069417
H	3.255343	4.393279	-0.121542
H	6.186823	0.672434	-0.352042
H	5.938871	-1.730769	-0.922438
H	3.653916	-2.661255	-1.362688
H	1.672456	-1.265774	-1.078307
O	-5.190640	1.387137	0.431960
O	-1.012559	2.661643	1.263253
H	-1.420090	3.536373	1.308833
C	-6.558915	1.245958	0.135296
H	-7.065694	2.115489	0.572366
H	-6.742897	1.237787	-0.952616
H	-6.982152	0.328939	0.579377

TS5

C	-0.681268	3.593600	1.542821
C	-0.370494	2.236774	1.489840
C	0.072342	1.651188	0.297182
C	0.352066	2.492371	-0.794391
C	0.021103	3.848842	-0.754170
C	-0.522965	4.391097	0.408174
C	0.457976	0.214996	0.177013
S	1.267455	1.812254	-2.162478
C	2.417771	0.863748	-1.179106
C	1.937972	0.157501	-0.057241
C	2.838371	-0.517465	0.760361
H	2.478689	-1.071054	1.628525
C	4.203896	-0.552926	0.442613
C	4.668683	0.110390	-0.699235
C	3.772208	0.826031	-1.495579
H	-1.049851	4.029417	2.473827
H	-0.493562	1.611154	2.376805
H	0.229330	4.487264	-1.615906
H	-0.775128	5.453324	0.442589
H	5.724649	0.098279	-0.969247
H	4.147539	1.369042	-2.366178
C	-0.294752	-0.910589	0.070474
C	-1.755310	-1.240558	-0.084343
C	0.435984	-2.250006	-0.071383
C	-1.842825	-2.510102	-0.650909
H	1.400662	-2.127518	-0.583241
C	-0.502800	-3.129759	-0.887739
H	-0.458340	-4.184156	-0.574773
C	-2.988683	-0.542731	0.191535
C	-4.229262	-1.181618	-0.143214
C	-4.241255	-2.472922	-0.738130
C	-3.066033	-3.127869	-0.985016
C	-5.462116	-0.525282	0.126337
C	-5.498053	0.716266	0.711869
C	-4.283197	1.347859	1.055180
C	-3.079147	0.733051	0.802356
H	-0.245774	-3.090288	-1.959572

H	-5.202289	-2.931932	-0.983540
H	-3.060344	-4.122856	-1.436137
H	-6.388938	-1.038900	-0.142119
H	-6.452462	1.207858	0.913302
H	-4.292323	2.332324	1.529332
H	-2.169326	1.243019	1.080011
O	4.987724	-1.253132	1.285457
O	0.632314	-2.746291	1.240296
H	1.131591	-3.569438	1.169857
C	6.366055	-1.351568	1.017348
H	6.797784	-1.963910	1.818836
H	6.558885	-1.845644	0.049738
H	6.856372	-0.363414	1.022361

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C	4.118694	-0.662133	0.860179
C	2.721415	-0.610237	0.966032
C	1.975979	0.229520	0.142859
C	2.640560	1.059479	-0.777872
C	4.027873	1.012344	-0.881740
C	4.772318	0.149740	-0.075198
C	0.487218	0.269577	0.188716
S	1.681489	2.113969	-1.837552
C	0.417461	2.583383	-0.678670
C	-0.052617	1.660828	0.281541
C	-0.960102	2.126904	1.237362
H	-1.273930	1.468130	2.041366
C	-1.467714	3.423585	1.185103
C	-1.053332	4.296781	0.181728
C	-0.091747	3.882897	-0.736871
H	2.220994	-1.261897	1.684597
H	4.546412	1.656452	-1.595973
H	5.857383	0.132429	-0.177994
H	-1.451790	5.312458	0.130140
H	0.281368	4.578269	-1.492592
C	-0.218119	-0.845446	-0.121703
C	-1.673164	-1.028788	-0.359260
C	0.428141	-2.034662	-0.821542
C	-1.812754	-1.690158	-1.569248
H	1.473563	-1.833733	-1.098242
C	-0.468627	-2.141372	-2.077814
H	-0.489220	-3.161195	-2.492464
C	-2.824119	-0.733248	0.429257
C	-4.108531	-0.916268	-0.173571
C	-4.202882	-1.461463	-1.485145
C	-3.079737	-1.888612	-2.155015
C	-5.275698	-0.614802	0.584657
C	-5.183291	-0.231799	1.900446
C	-3.915638	-0.162460	2.529647
C	-2.769692	-0.407216	1.812375
H	-0.086944	-1.464702	-2.861086
H	-5.193537	-1.589772	-1.928940
H	-3.164396	-2.376232	-3.129215
H	-6.252238	-0.724263	0.105731
H	-6.087340	-0.016731	2.474950
H	-3.851149	0.070531	3.595132
H	-1.799713	-0.403278	2.311360
H	-2.189236	3.749486	1.937387
O	4.744472	-1.516886	1.691617
O	0.337746	-3.168587	0.008098
H	0.694312	-3.920453	-0.480171
C	6.147272	-1.619471	1.638531
H	6.435633	-2.361802	2.393024
H	6.495563	-1.964794	0.650091
H	6.636648	-0.660448	1.878870

TS5'

C	-4.562149	0.804355	-0.202858
C	-3.231882	0.998228	0.191237
C	-2.228617	0.075109	-0.102679
C	-2.622824	-1.121039	-0.754827
C	-3.945591	-1.314063	-1.145567
C	-4.924071	-0.353707	-0.894164
C	-0.768978	0.226055	0.219670
S	-1.470145	-2.430683	-1.093268
C	-0.468287	-2.280402	0.355732
C	-0.187562	-0.995827	0.847804
C	0.628496	-0.889740	1.982987
H	0.828683	0.099493	2.400582
C	1.196787	-2.017689	2.567155
C	0.936747	-3.283501	2.039534
C	0.091554	-3.418013	0.941019
H	-2.977384	1.913353	0.715998
H	-4.228135	-2.243501	-1.645894
H	-5.950072	-0.537723	-1.213436
H	1.376650	-4.172836	2.496265
H	-0.134975	-4.406902	0.535373
C	0.028082	1.306927	-0.036727
C	1.512784	1.308689	-0.131133
C	-0.394272	2.773989	-0.187732
C	1.995248	2.591631	0.066811
H	-0.707720	2.957278	-1.233469
C	0.881402	3.583231	0.144775
H	0.767062	3.989124	1.162958
C	2.437075	0.271327	-0.501811
C	3.834393	0.539001	-0.361255
C	4.276103	1.843613	0.006012
C	3.377364	2.869075	0.155585
C	4.774844	-0.484449	-0.663043
C	4.364031	-1.698870	-1.157626
C	2.990513	-1.921092	-1.410492
C	2.056889	-0.962580	-1.092675
H	1.042374	4.433115	-0.535608
H	5.349418	2.023469	0.108526
H	3.716205	3.888145	0.356592
H	5.837954	-0.276073	-0.516674
H	5.095139	-2.475655	-1.392799
H	2.667575	-2.855999	-1.874735
H	1.012036	-1.132022	-1.343759
H	1.842374	-1.908454	3.441219
O	-5.418687	1.791196	0.132186
O	-1.421703	3.129673	0.707241
H	-1.732705	4.010685	0.465555
C	-6.772990	1.671203	-0.228871
H	-7.274499	2.578228	0.131464
H	-6.901778	1.605657	-1.322890
H	-7.246474	0.792971	0.242304

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C	-4.316232	0.300223	0.279546
C	-2.960635	0.594562	0.474192
C	-1.964046	-0.191597	-0.097112
C	-2.344839	-1.360604	-0.790790
C	-3.691448	-1.656301	-0.984125
C	-4.684474	-0.820645	-0.473013
C	-0.497862	0.049138	0.076414
S	-1.099964	-2.498869	-1.361406
C	-0.027454	-2.402370	0.053400
C	0.176567	-1.149539	0.655320

C	0.997083	-1.075975	1.785930
H	1.137947	-0.111203	2.278413
C	1.654511	-2.207591	2.261578
C	1.483212	-3.436430	1.622283
C	0.628736	-3.540278	0.526119
H	-2.699222	1.479650	1.049880
H	-3.978643	-2.562839	-1.522107
H	-5.731280	-1.074537	-0.640442
H	1.998699	-4.325450	1.992421
H	0.466307	-4.505682	0.041132
C	0.196874	1.157501	-0.275492
C	1.667203	1.374687	-0.136263
C	-0.290395	2.537725	-0.705998
C	1.878687	2.696536	0.221481
H	0.038986	2.663453	-1.756929
C	0.587724	3.460737	0.170839
H	0.117693	3.549855	1.165271
C	2.780716	0.509706	-0.371474
C	4.078964	0.989632	-0.015044
C	4.238555	2.323645	0.460110
C	3.167390	3.180739	0.534043
C	5.204291	0.135400	-0.190342
C	5.063671	-1.111975	-0.747710
C	3.790028	-1.549817	-1.185828
C	2.680745	-0.759708	-1.004618
H	0.701058	4.471524	-0.248792
H	5.242464	2.667325	0.722897
H	3.303467	4.221506	0.837381
H	6.189693	0.500736	0.110921
H	5.935064	-1.757346	-0.880480
H	3.689319	-2.519580	-1.678737
H	1.712629	-1.093680	-1.374727
H	2.306813	-2.130032	3.134084
O	-5.191480	1.150374	0.855016
O	-1.656781	2.773695	-0.597660
H	-1.850697	3.601814	-1.051962
C	-6.570366	0.917281	0.704952
H	-7.085425	1.725564	1.239441
H	-6.877621	0.941988	-0.354731
H	-6.873634	-0.048195	1.144978

TS6

C	3.870641	-1.130050	0.522373
C	2.508758	-0.945906	0.281204
C	1.958694	0.283230	-0.122487
C	2.849322	1.379135	-0.145384
C	4.212743	1.201241	0.106588
C	4.744626	-0.043772	0.415727
C	0.488519	0.384617	-0.390329
S	2.359115	3.042510	-0.407434
C	0.608289	2.943662	-0.405269
C	-0.136572	1.743663	-0.474062
C	-1.508791	1.914624	-0.766040
H	-2.122471	1.044765	-0.968736
C	-2.127261	3.152700	-0.841301
C	-1.381705	4.315936	-0.649831
C	-0.015259	4.202279	-0.458620
H	1.874527	-1.818792	0.427472
H	4.879704	2.067173	0.075333
H	5.813664	-0.140773	0.604136
H	-1.853062	5.300266	-0.684228
H	0.598948	5.102266	-0.368352
C	-0.232464	-0.773957	-0.584854
C	-1.677899	-1.058080	-0.446448
C	0.301060	-2.026371	-1.284156

C	-2.060334	-1.957139	-1.429503
H	1.240314	-1.824497	-1.823321
C	-0.861709	-2.346675	-2.250065
H	-0.865596	-3.404587	-2.553232
C	-2.597328	-0.680067	0.581666
C	-3.942665	-1.147965	0.475143
C	-4.315907	-1.996545	-0.607310
C	-3.389145	-2.415630	-1.533564
C	-4.885777	-0.765876	1.469878
C	-4.511959	0.022915	2.531138
C	-3.169597	0.457060	2.652931
C	-2.236786	0.115926	1.702103
H	-0.778731	-1.732121	-3.162209
H	-5.353112	-2.335738	-0.671207
H	-3.673948	-3.101962	-2.334584
H	-5.916511	-1.118200	1.377024
H	-5.245070	0.309014	3.288676
H	-2.873817	1.064414	3.511581
H	-1.202813	0.448432	1.808721
H	-3.196120	3.205220	-1.057888
O	4.246121	-2.379874	0.865824
O	0.461971	-3.083606	-0.356876
H	0.801834	-3.850196	-0.835363
C	5.594993	-2.621299	1.184615
H	5.923081	-2.024663	2.053184
H	5.671746	-3.686179	1.437969
H	6.263131	-2.412517	0.331518