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Computational Insight to Improve the Thermal Isomerization Performance of Overcrowded Alkene-Based Molecular Motors through Structural Redesign

Baswanth Oruganti, Jun Wang, and Bo Durbeej*^[a]

[a] *B. Oruganti, Dr. J. Wang, Prof. B. Durbeej*
Division of Theoretical Chemistry, IFM
Linköping University
581 83 Linköping (Sweden)
E-mail: bodur@ifm.liu.se

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Abstract

Synthetic overcrowded alkene-based molecular motors achieve 360° unidirectional rotary motion of one motor half (rotator) relative to the other (stator) through sequential photochemical and thermal isomerization steps. In order to facilitate and expand the use of these motors for various applications, it is important to investigate ways to increase the rates and efficiencies of the reactions governing the rotary motion. Here, we use computational methods to explore whether the thermal isomerization performance of some of the fastest available motors of this type can be further improved by reducing the sizes of the motor halves. Presenting three new redesigned motors that combine an indanylidene rotator with a cyclohexadiene, pyran or thiopyran stator, we first use multiconfigurational quantum chemical methods to verify that the photoisomerizations of these motors sustain unidirectional rotary motion. Then, by performing density functional calculations, we identify both stepwise and concerted mechanisms for the thermal isomerizations of the motors and show that the rate-determining free-energy barriers of these processes are up to 25 kJ mol⁻¹ smaller than those of the original motors. Furthermore, the thermal isomerizations of the redesigned motors proceed in fewer steps. Altogether, the results suggest that the redesigned motors are useful templates for improving the thermal isomerization performance of existing overcrowded alkene-based motors.

1. Introduction

The design and synthesis of molecules that can perform useful mechanical work by consuming energy is a major research field^[1–4] with potential applications in nanotechnology.^[5–7] Light is a clean and readily available source of energy for executing such work. Light-driven rotary molecular motors are molecules that exhibit repetitive unidirectional rotary motion about a carbon-carbon^[8–24] or carbon-nitrogen^[25, 26] double bond through the absorption of UV or visible light. Motors of this type based on sterically overcrowded alkenes were first synthesized by Feringa and coworkers in the late nineties,^[8, 9] and have subsequently attracted considerable interest.^[10–23] These motors contain two identical or distinct halves connected by a carbon-carbon double bond (axle) and achieve 360° unidirectional rotation of one motor half (rotator) relative to the other half (stator) by means of consecutive photochemical and thermal isomerization steps.

An essential feature of overcrowded alkene-based molecular motors is the presence of at least one stereocenter, whose configuration (*R* or *S*) determines the direction of rotation (clockwise or counterclockwise). Another distinguishing chiral feature is the *P* (right-handed) or *M* (left-handed) helicity(ies) adopted by the motor half(ves) because of steric interactions between the rotator and stator in the so-called *fford* regions (see Scheme 1).^[8, 9] These interactions determine the rates of the thermal isomerizations, which are believed to limit the rotational frequencies that the motors can attain.^[14, 15, 27, 28] Accordingly, a major experimental effort has been invested in optimizing the steric interactions between the motor halves in such a way that the thermal isomerizations are accelerated.^[10–17, 19–21] Motors **1a–1c** shown in Scheme 1, which have

been found capable of achieving MHz rotational frequencies under suitable irradiation conditions^[15, 19] are key achievements of this work.

Scheme 1. Chemical structures of molecular motors **1a–1c**.

Each 360° rotation of motors of the type shown in Scheme 1 comprises two photoisomerizations and two thermal isomerizations that connect the *E* and *Z* isomers (with respect to the central olefinic bond) along the rotary cycle. This is illustrated in Scheme 2 for motor **1c**, which has a cyclopentanaphthalynidene rotator and a thioxanthene stator. Each of the *E* and *Z* isomers of motor **1c** has four possible conformations that differ in two ways. First, the stereogenic methyl substituent can adopt either a favorable pseudo-axial orientation, as in the “stable” isomers, or a strained (due to steric interactions) pseudo-equatorial orientation, as in the “unstable” isomers. Second, relative to the plane containing the central olefinic bond and the stereocenter (hereafter referred to as the olefinic plane), the rotator and stator can either fold toward the same side (*syn*-folded) or toward opposite sides (*anti*-folded). In a recent computational study, the relative stabilities of these conformations and their roles in the rotary cycle of motor **1c** were investigated by density functional theory (DFT) methods.^[29]

Scheme 2. Overall rotary cycle of molecular motor **1c**.

As shown in Scheme 2, the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations in the rotary cycle of motor **1c** produce a strained unstable isomer, whereas the thermal isomerizations conversely release the strain and produce stable isomers. Further, each process involves a change in the rotator helicity ($M \rightarrow P$ or $P \rightarrow M$) and a change in the relative rotator-stator folding ($anti \rightarrow syn$ or $syn \rightarrow anti$). Overall, the rotary motion is governed by steric interactions between the rotator and stator in the *fford* regions, which render the photoisomerizations unidirectional and the thermal isomerizations exergonic. Importantly, this exergonicity prevents photo-induced back rotations of the unstable isomers.^[9, 14]

A key requirement for the possibility to efficiently use synthetic rotary molecular motors for applications (in, *e.g.*, molecular transport^[30] or viscosity sensing,^[31, 32]) is that they can achieve high rotational frequencies under ambient conditions.^[14, 33] Therefore, many experimental studies have investigated how conformational, steric and electronic motor properties influence the rates of both the thermal isomerizations^[10–17, 19–21] and photoisomerizations^[27, 28] of overcrowded alkene-based motors. These studies have been complemented by several computational studies exploring the mechanisms of the rotary cycles of overcrowded alkenes,^[21, 29, 34–42] or proposing alternative light-driven motor designs with potentially more efficient rotary cycles.^[43–47]

In our own computational work, we have established a three-step mechanism for the thermal isomerizations of motor **1c** and several variants thereof, and also outlined systematic strategies for accelerating these processes by modulating the steric bulkiness of the rotator substituent.^[29, 42] From a dynamical point of view, however, it would seem advantageous to develop motors whose thermal isomerizations occur in fewer than three steps. Furthermore, it would also be advantageous to eliminate the undesirable side reaction that was identified in both rotary half cycles of motor **1c**, and which is likely to impact the thermal isomerization rates negatively.^[29] In this paper, we present a computational study focused on these goals.

Specifically, we present a structural redesign of motors **1a–1c**, wherein the sizes of the rotator and stator are reduced to obtain motors **2a–2c** shown in Scheme 3. In these motors, the cyclopentanaphthalynidene rotator (3-ring system) of motors **1a–1c** is replaced with a synthetically viable indanylidene rotator^[16, 24] (2-ring system), and the phenanthrylidene, xanthene and thioxanthene stators (3-ring systems) of motors **1a–1c**

are replaced, respectively, with cyclohexadiene, pyran and thiopyran stators (1-ring systems).

Scheme 3. Chemical structures, atom numbering and definition of dihedral angles in redesigned molecular motors **2a–2c** considered in this work.

The paper is organized as follows. First, by performing multiconfigurational quantum chemical calculations, we show that the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of motors **2a–2c** occur in a unidirectional fashion and thus produce rotary motion. Then, by performing DFT calculations, we identify two possible mechanisms for the thermal isomerizations of these motors. Through the identified mechanisms, we find that the thermal isomerizations proceed in fewer steps than those of motor **1c** and other overcrowded alkene-based motors,^[21, 41] and furthermore have free-energy barriers that are up to 25 kJ mol⁻¹ smaller. Furthermore, unlike motor **1c**, the thermal isomerizations are not impeded by a side reaction.^[29] Thus, through this work, we propose that motors **2a–2c** are members of a new family of overcrowded alkene-based rotary molecular motors capable of improving the thermal isomerization performance of some of the fastest motors of this type known to date (*i.e.*, motors **1a–1c**).

Computational Details

The rotary cycles of motors **2a–2c** were explored in the following way. First, the stationary points on the ground-state potential energy surfaces (PESs) corresponding to the stable and unstable *E* and *Z* isomers of the motors were located by performing geometry optimizations using the ω B97X-D range-separated hybrid density functional^[48] in combination with the SVP basis set. Frequency calculations were then performed at the same level of theory to ensure that the resulting geometries are potential-energy minima, and to derive Gibbs free energies at room temperature. Single point calculations, in turn, were carried out with ω B97X-D and Dunning's correlation-consistent polarized valence triple- ζ (cc-pVTZ) basis set. All calculations were performed with the SMD^[49] continuum solvation model to describe the dichloromethane solvent used in the experimental reference study of motor **1c**.^[15]

Although it has been found that the calculated thermal barriers of motor **1c** and several variants thereof are not very sensitive to the choice of density functional,^[29] there are at least three good reasons for using ω B97X-D in the calculations. First, the merits of ω B97X-D in organocatalytic modeling have been firmly established in an extensive benchmark study by Clark and coworkers.^[50] Second, it has been found that ω B97X-D yields thermal free-energy barriers for reference motor **1c**^[29] that are in good agreement with available experimental data.^[15] Third, because of its inclusion of empirical atom-atom dispersion corrections,^[51, 52] ω B97X-D is well-suited to describe the critical intramolecular interactions between the motor halves during the rotary cycles.

From the calculations on the stable and unstable *E* and *Z* isomers of motors **2a–2c**, it was observed that, for each of the three motors, the two lowest-energy isomers are

anti-(M)-stable-*E* and *anti-(M)*-stable-*Z*. As further discussed in section 2.1 below, these isomers show a sterically favorable *anti* folding of the rotator and stator substituents relative to the olefinic plane. Also, these are the light-absorbing isomers of the rotary cycles.

As the main focus of this work is to offer guidelines for improving the thermal isomerization performance of overcrowded alkene-based motors, the photochemical modeling of motors **2a–2c** was limited to demonstrating the unidirectionality of the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of the light-absorbing isomers. This was done by performing multiconfigurational quantum chemical calculations using the complete active space self-consistent field (CASSCF)^[53] and second-order perturbation theory (CASPT2)^[54, 55] methods, as further described in the Supplementary Computational Details section of the Supporting Information. Furthermore, from these calculations, it was also established that the $E \rightarrow Z$ photoisomerization of *anti-(M)*-stable-*E* produces the (*P*)-unstable-*Z* ground-state isomer, and that the $Z \rightarrow E$ photoisomerization of *anti-(M)*-stable-*Z*, analogously, yields the (*P*)-unstable-*E* ground-state isomer. Notably, these photoisomerization products lack the type of rotator and stator folding manifested in the parent light-absorbing isomers. Below, we will return to this issue and its mechanistic implications.

Having found the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerization products of motors **2a–2c**, the mechanisms for the subsequent thermal (*P*)-unstable-*Z* $\rightarrow$ *anti-(M)*-stable-*Z* and (*P*)-unstable-*E* $\rightarrow$ *anti-(M)*-stable-*E* isomerizations that complete the rotary cycles were explored by locating all the relevant transition structures (TSs) and intermediates through ω B97X-D calculations as detailed above. The corresponding frequency calculations

showed that all the resulting stationary points have either zero (for minima) or one (for TSs) imaginary vibrational frequency. In addition, intrinsic reaction coordinate (IRC)^[56] calculations were carried out to verify that the TSs do indeed mediate relevant chemical transformations.

All DFT calculations were performed with the Gaussian 09 suite of programs,^[57] and all CASSCF and CASPT2 calculations were performed with the MOLCAS 8.0 suite of programs.^[58]

2. Results and Discussion

2.1. Ground-State Minima of Motors **2a–2c**

Each ground-state minimum (*E* or *Z*) of motors **2a–2c** was found to have three possible conformations that differ in two ways. First, analogous to the situation for motor **1c**,^[29] the rotator methyl substituent can either adopt a pseudo-axial (“stable”) or a pseudo-equatorial (“unstable”) orientation. Second, as illustrated in Scheme 4, the stable isomers have two different conformations with respect to the orientation of the rotator and stator substituents relative to the olefinic plane. In the *syn*-folded conformations, these substituents are oriented toward the same side of the olefinic plane, whereas they are oriented toward opposite sides in the *anti*-folded conformations. As a result, the *anti*-folded conformations exhibit less steric overcrowding in the *fford* regions than the *syn*-folded conformations. For the unstable isomers, such folding is not manifested because the stator substituents are nearly co-planar with the central olefinic bond. This is a key structural feature that distinguishes motors **2a–2c** from reference motor **1c**^[29] and other overcrowded alkene-based motors,^[21, 59] whose unstable isomers can be both *anti*-folded

and *syn*-folded. As we will see, this feature has a significant impact on the mechanisms for the thermal isomerizations of motors **2a–2c**.

Scheme 4. Structures of the ground-state minima of motors **2a–2c** and their relative ω B97X-D free energies (ΔG , in kJ mol⁻¹). Shown also are the corresponding optimized structures of motor **2a** (without hydrogen atoms).

Scheme 4 also shows the relative ω B97X-D free energies of the ground-state minima of motors **2a–2c**. As can be seen, the parent light-absorbing *anti-(M)*-stable-*E* and *anti-(M)*-stable-*Z* species are by some margin the most stable isomers. Comparing their energies with those of the (*P*)-unstable-*Z* and (*P*)-unstable-*E* isomers produced (see Section 2.2) by the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations, these energy differences vary considerably between the motors; from 15–17 kJ mol⁻¹ for motor **2b** (with X = O) to ~25 and ~38 kJ mol⁻¹ for motors **2a** (X = CH₂) and **2c** (X = S), respectively. This is because the increase in the size of stator bridging atom X from oxygen in motor **2b** to sulphur in motor **2c** increases the steric repulsion in the *fford* regions of the photoisomerization products. Thus, these results, which are corroborated by complementary CASPT2//CASSCF energies in Table S1 of the Supporting Information, suggest that the stator bridging atom is a suitable element for exerting control of the rotary cycle.

2.2. Unidirectionality and Products of the Photoisomerizations of Motors 2a–2c

Although this work focuses on improving the thermal isomerization performance of overcrowded alkene-based motors through structural redesign of existing motors, it is important to first verify that the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of motor candidates **2a–2c** actually produce unidirectional rotary motion. This was done by modeling, using CASSCF and CASPT2 as described in the Supplementary Computational Details section of the Supporting Information, the geometric relaxation of the light-absorbing *anti-(M)*-stable-*E* and *anti-(M)*-stable-*Z* isomers from the vertically excited Franck-Condon (FC) points in the lowest excited singlet state (*S*₁) populated by

light absorption. Producing S_1 minima henceforth labeled *anti-(M)-stable-E** and *anti-(M)-stable-Z**, the results of these calculations are presented in Figure 1.

Figure 1. FC relaxation of the light-absorbing *anti-(M)-stable-E* and *anti-(M)-stable-Z* isomers of motors **2a–2c**.

Notably, Figure 1 shows that the FC relaxation processes of all three motors involve appreciable torsional motion along the α photoisomerization coordinate (see Scheme 3). Specifically, the torsional motion amounts to 76–83° for the FC relaxation of the *anti*-(*M*)-stable-*E* isomers, and to 84–91° for the FC relaxation of the *anti*-(*M*)-stable-*Z* isomers. This motion is facilitated by the concurrent elongation of the central olefinic bond by 0.12–0.14 Å in the excited state, details of which are given in Table S2 of the Supporting Information. More importantly, however, for each of the three motors, the direction of photoinduced torsional motion is the *same* – toward decreasing α – for the *anti*-(*M*)-stable-*E* and *anti*-(*M*)-stable-*Z* isomers. Thus, the associated $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations occur in a *unidirectional* fashion and produce *rotary* motion.

From previous computational studies of overcrowded alkene-based motors, the formation of the ground-state (S_0) photoisomerization products is likely to be mediated by S_1/S_0 conical intersections at highly twisted molecular geometries along the α coordinate.^[36, 37] Here, rather than firstly trying to locate such intersections, the photoproducts were located directly by performing CASSCF S_0 geometry optimizations starting from the (already highly twisted) *anti*-(*M*)-stable-*E** and *anti*-(*M*)-stable-*Z** S_1 minima. These calculations yielded (*P*)-unstable-*Z* as the photoproduct of the $E \rightarrow Z$ isomerization and (*P*)-unstable-*E* as the photoproduct of the $Z \rightarrow E$ isomerization. Thus, the photoisomerizations invert the rotator helicity from *M* to *P*.

2.3. The Thermal Isomerizations of Motors **2a–2c**

In the (*P*)-unstable-*Z* and (*P*)-unstable-*E* photoproducts of motors **2a–2c**, the stereogenic rotator methyl substituent adopts a strained pseudo-equatorial orientation because of

steric interactions with the stator. During the subsequent thermal (*P*)-unstable-*Z* $\rightarrow$ *anti*-(*M*)-stable-*Z* and (*P*)-unstable-*E* $\rightarrow$ *anti*-(*M*)-stable-*E* isomerizations that complete the rotary cycles, the methyl regains its preferred pseudo-axial orientation as the rotator helicity changes from *P* to *M*. As a result, the thermal isomerizations are exergonic, which introduces a “forward” driving force in the rotary cycles and depletes the photoproducts, thereby preventing undesirable photo-induced back reactions.^[9, 14]

Two possible mechanisms were identified for the thermal isomerizations, one being concerted and occurring without any intermediate(s), and the other occurring through two separate steps. The calculated free-energy profiles for these mechanisms are presented in Figure 2. Associated changes in the β , γ , δ and δ' (see Scheme 3) dihedral angles, which respectively reflect rotator helicity and orientations of the rotator methyl, stator methyl, and stator ethyl group, are given in Tables S3–S5 of the Supporting Information. Figure 3, finally, shows optimized TSs for the case of motor **2a**.

Figure 2. Free-energy profiles for stepwise and concerted mechanisms for the thermal isomerizations of motors **2a–2c**.

Figure 3. Optimized TSs for the thermal isomerizations of motor **2a** (hydrogen atoms not shown).

Starting with the stepwise mechanism, for each of the motors, the TS for the first step is denoted TS1 for the isomerization of (*P*)-unstable-*Z* and TS4 for the isomerization of (*P*)-unstable-*E*. This step involves a $P \rightarrow M$ change in rotator helicity that releases the conformational strain of the pseudo-equatorial stereogenic methyl in the initial species. Furthermore, while the rotator and stator substituents are neither *syn*- nor *anti*-folded in the initial species, the intermediates produced by this step are *syn*-folded: *syn*-(*M*)-stable-*Z* and *syn*-(*M*)-stable-*E*. As can be seen from Figure 2, the TS1/TS4 free-energy barriers increase with decreasing size of the stator bridging atom X of the motor; from virtually zero for motor **2c** (X = S) to 13–18 and 35–41 kJ mol⁻¹ for motors **2a** (X = CH₂) and **2b** (X = O), respectively. Qualitatively, this can be understood by noting, in Table S6 of the Supporting Information, that the appreciable *fford*-region steric repulsion in the (*P*)-unstable-*Z* and (*P*)-unstable-*E* reactant isomers of motor **2c**, is much reduced in TS1/TS4

of this motor. Thereby, decreasing the size of the bridging atom from sulphur (motor **2c**) to oxygen (motor **2b**) has a stabilizing effect on (*P*)-unstable-*Z* and (*P*)-unstable-*E*, which is *not* fully countered by a corresponding effect on TS1/TS4.

Continuing with the second step that proceeds *via* TS2/TS5 along the *Z/E* pathway, this step completes the thermal isomerizations by accomplishing a stator ring flip that changes the relative rotator-stator folding from *syn* in the intermediates to *anti* in the final *anti*-(*M*)-stable-*Z* and *anti*-(*M*)-stable-*E* isomers. By light absorption of these isomers, the rotary cycles are then continued photochemically. Notably, the TS2/TS5 barriers show a contrasting trend to the TS1/TS4 barriers; decreasing from 19–24 kJ mol⁻¹ for motor **2c** to 10 and 3–4 kJ mol⁻¹ for motors **2a** and **2b**, respectively. This, too, can be understood in terms of how the steric repulsion in motor **2c** is different in the TSs than in the associated reactant species.

Overall, the rate-determining step of the stepwise mechanism is the first step for motors **2a** ($\Delta G^\ddagger = 13\text{--}18$ kJ mol⁻¹) and **2b** ($\Delta G^\ddagger = 35\text{--}41$ kJ mol⁻¹), and the second step for motor **2c** ($\Delta G^\ddagger = 19\text{--}24$ kJ mol⁻¹). For motors **2a** and **2b**, one potential caveat of this mechanism is the slight (5–10 kJ mol⁻¹) endergonicity of the first step of the isomerization of (*P*)-unstable-*Z*, which means that the reverse isomerization of the *syn*-(*M*)-stable-*Z* intermediate back to (*P*)-unstable-*Z* is predicted to have a smaller barrier than the forward reaction. However, the negative impact of this scenario seems to be nullified by the 29–32 kJ mol⁻¹ exergonicity of the subsequent second step.

Turning to the concerted mechanism, for each of the motors, the corresponding TS is denoted TS3 for the isomerization of (*P*)-unstable-*Z* and TS6 for the isomerization of (*P*)-unstable-*E*. In these TSs, the *P* rotator helicity and the strained pseudo-equatorial

orientation of the stereogenic methyl shown by the initial (*P*)-unstable-*Z* and (*P*)-unstable-*E* species are retained, contrary to the situation in TS1/TS4 of the stepwise mechanism. In this regard, TS3 and TS6 can be described as being highly asynchronous. This description is reminiscent of the way that organic pericyclic reactions oftentimes occur in a perfectly concerted fashion (*i.e.*, without intermediates), despite that the corresponding TSs are asynchronous with respect to how far the bond formation processes mediated by the TSs have progressed.^[60–62] Notwithstanding, in TS3/TS6, the stator substituents are no longer co-planar with the olefinic bond, as they are in the initial species (*e.g.*, for motor **2a**, the δ dihedral angle changes from 9° in (*P*)-unstable-*Z* to 75° in TS3, see Table S3). This facilitates the *P* → *M* change in rotator helicity that releases the stereogenic methyl strain and, without any further barrier, completes the isomerizations by producing the *anti*-(*M*)-stable-*Z* and *anti*-(*M*)-stable-*E* isomers. Comparing the different motors, the TS3/TS6 barriers increase from 22–23 kJ mol⁻¹ for motor **2c** to 46–49 and 66–71 kJ mol⁻¹ for motors **2a** and **2b**, respectively. The overall exergonicities of the isomerizations, in turn, decrease from 37–39 kJ mol⁻¹ for motor **2c** to 24–27 and 13–19 kJ mol⁻¹ for motors **2a** and **2b**, respectively. This can be explained in terms of how the different sizes of the stator bridging atom of the motors introduce different amounts of steric repulsion in the (*P*)-unstable-*Z* and (*P*)-unstable-*E* reactants.

Comparing the calculated free-energy barriers of the stepwise and concerted mechanisms, the stepwise mechanism has a rate-determining barrier that – for motors **2a** and **2b** – is ~30 kJ mol⁻¹ smaller than the concerted barrier. For motor **2c**, an analogous comparison reveals that the two mechanisms are equally favorable in this respect. As explained above, a key difference between the mechanisms is that the conformational

strain of the stereogenic methyl is already released in TS1/TS4 (stepwise), which is not the case in TS3/TS6 (concerted). For example, using motor **2a** to illustrate this, Table S3 shows that the γ dihedral angle changes from 40° in (*P*)-unstable-*Z* to 112° in TS1, but only to 24° in TS3. This difference may explain why the stepwise mechanism is preferred over the concerted ditto, at least as far as motors **2a** and **2b** are concerned.

Overall, for motors **2a** and **2b**, the rate-determining barriers of the preferred stepwise mechanism are 18 (**2a**) and 41 kJ mol⁻¹ (**2b**). For motor **2c**, in turn, the rate-determining barrier of the stepwise mechanism is 24 kJ mol⁻¹, which is very similar to the barrier of 23 kJ mol⁻¹ for the concerted process. Comparing these values with the calculated – using the same exact methodology – rate-determining barrier of 43 kJ mol⁻¹ for reference motor **1c**,^[29] which is close to the corresponding experimental estimate,^[15] no rate acceleration is observed for motor **2b**. For motors **2a** and **2c**, on the other hand, the thermal isomerizations are kinetically favored by 25 and 19–20 kJ mol⁻¹, respectively. From a dynamical point of view, it is also encouraging that the thermal isomerizations of motors **2a–2c** proceed in fewer steps than those of motor **1c**^[29] and other overcrowded alkene-based motors.^[21, 41] Furthermore, as a consequence of the absence of *syn*- or *anti*-folded conformations for the photoproduct isomers of motors **2a–2c**, there are no *syn* → *anti* equilibration side reactions to hamper the performance of these motors, which is a key advantage over motor **1c**^[29] and related motors.^[21, 59] Altogether, based on the results of this study, we propose that motors **2a–2c** constitute a new family of overcrowded alkene-based motors with the potential to improve the thermal isomerization performance of existing motors of this type.

Finally, to solidify this proposal, the thermal isomerizations of motors **2a–2c** were also explored using the M06-2X global hybrid density functional,^[63] as a complement to the ω B97X-D calculations. All M06-2X calculations were performed in the same way as the ω B97X-D ones with respect to choice of basis set and treatment of solvent effects, as already described in the Computational Details section. The resulting free-energy profiles for both the stepwise and concerted mechanisms are shown in Figure S2 of the Supporting Information. Pleasingly, these profiles support the same mechanistic features as the ω B97X-D calculations summarized in Figure 2. For example, for motors **2a** and **2b**, the stepwise mechanism is favored over the concerted one by 29–31 kJ mol⁻¹, which is close to the value of 31 kJ mol⁻¹ predicted by ω B97X-D. Overall, at the M06-2X level, the rate-determining barriers of the preferred stepwise mechanism for motors **2a–2c** are 24, 44 and 13 kJ mol⁻¹, respectively, which are similar to (or even smaller than) the corresponding ω B97X-D estimates of 18, 41 and 24 kJ mol⁻¹. Given that M06-2X yields a rate-determining barrier of 39 kJ mol⁻¹ for reference motor **1c**,^[29] which is close to the 43 kJ mol⁻¹ predicted by ω B97X-D,^[29] our proposal that motors **2a** and **2c** achieve significant acceleration of the thermal isomerizations relative to reference motor **1c** is also supported by M06-2X.

3. Conclusions

We have reported a computational study aimed at improving the thermal isomerization performance of overcrowded alkene-based rotary molecular motors through a structural redesign of some of the fastest available motors of this type,^[15, 19] wherein the sizes of the rotator and stator motor halves are substantially reduced. To this end, we have designed

three new motors **2a–2c**, all featuring a synthetically viable indanylidene rotator^[16, 24] and a six-membered diene ring stator, but differing in the stator bridging atom ($X = \text{CH}_2$ or O or S).

First, by performing multiconfigurational quantum chemical calculations, it is demonstrated that the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of motors **2a–2c** occur in a unidirectional fashion and produce rotary motion. Then, by using DFT calculations to explore the mechanisms for the thermal isomerizations, one stepwise and one concerted mechanism are identified for these processes. The stepwise mechanism occurs in two steps *via* a *syn*-folded intermediate, where the first step involves a $P \rightarrow M$ rotator helicity inversion and the second step a *syn* $\rightarrow$ *anti* change in relative rotator-stator folding. The concerted mechanism, in turn, proceeds without any intermediate(s) but through a highly asynchronous TS in which no change in rotator helicity is yet manifested.

From the calculations, it is observed that the free-energy barriers of the two thermal mechanisms vary considerably between the motors. Further, it is found that this variation can be explained in terms of how a change in the size of the stator bridging atom contributes differently to steric repulsion in reactants and TSs. For motors **2a** and **2b**, the stepwise mechanism is kinetically preferred with a rate-determining barrier of 18 and 41 kJ mol⁻¹, respectively. For motor **2c**, the two mechanisms show similarly favorable kinetics with barriers of 23–24 kJ mol⁻¹.

Additionally, it is also observed that the calculated rate-determining thermal isomerization barriers for the newly designed motors **2a–2c** are up to 25 kJ mol⁻¹ smaller than the corresponding barrier previously calculated for reference motor **1c**.^[29] Also, the motors isomerize through fewer steps than motor **1c**^[29] (and other overcrowded alkene-

based motors)^[21, 41] and without the negative impact of a competing side reaction.^[29] These mechanistic differences can be attributed to the lack of *syn*- or *anti*-folded conformations of the photoisomerization products of motors **2a–2c**. Taken together, the results of this work suggest a conformational approach to the design of overcrowded alkene-based motors with better thermal isomerization performance than existing motors of this type.

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Keywords: density functional calculations • isomerization • molecular motors • rotary rates • stepwise or concerted

References

- [1] G. S. Kottas, L. I. Clarke, D. Horinek, J. Michl, *Chem. Rev.* **2005**, *105*, 1281–1376.
- [2] J. Michl, E. C. H. Sykes, *ACS Nano* **2009**, *3*, 1042–1048.
- [3] S. Erbas-Cakmak, D. A. Leigh, C. T. McTernan, A. L. Nussbaumer, *Chem. Rev.* **2015**, *115*, 10081–10206.
- [4] C. Cheng, J. F. Stoddart, *ChemPhysChem* **2016**, *17*, 1780–1793.
- [5] W. R. Browne, B. L. Feringa, *Nat. Nanotechnol.* **2006**, *1*, 25–35.
- [6] E. R. Kay, D. A. Leigh, F. Zerbetto, *Angew. Chem. Int. Ed.* **2007**, *46*, 72–191.
- [7] V. Balzani, A. Credi, M. Venturi, *Chem. Soc. Rev.* **2009**, *38*, 1542–1550.
- [8] N. Harada, N. Koumura, B. L. Feringa, *J. Am. Chem. Soc.* **1997**, *119*, 7256–7264.
- [9] N. Koumura, R. W. J. Zijlstra, R. A. van Delden, N. Harada, B. L. Feringa, *Nature* **1999**, *401*, 152–155.
- [10] N. Koumura, E. M. Geertsema, M. B. van Gelder, A. Meetsma, B. L. Feringa, *J. Am. Chem. Soc.* **2002**, *124*, 5037–5051.
- [11] M. K. J. ter Wiel, R. A. van Delden, A. Meetsma, B. L. Feringa, *J. Am. Chem. Soc.* **2003**, *125*, 15076–15086.
- [12] D. Pijper, R. A. van Delden, A. Meetsma, B. L. Feringa, *J. Am. Chem. Soc.* **2005**, *127*, 17612–17613.
- [13] J. Vicario, M. Walko, A. Meetsma, B. L. Feringa, *J. Am. Chem. Soc.* **2006**, *128*, 5127–5135.
- [14] M. M. Pollard, M. Klok, D. Pijper, B. L. Feringa, *Adv. Funct. Mater.* **2007**, *17*, 718–729.
- [15] M. Klok, N. Boyle, M. T. Pryce, A. Meetsma, W. R. Browne, B. L. Feringa, *J. Am. Chem. Soc.* **2008**, *130*, 10484–10485.
- [16] M. M. Pollard, A. Meetsma, B. L. Feringa, *Org. Biomol. Chem.* **2008**, *6*, 507–512.
- [17] M. M. Pollard, P. V. Wesenhagen, D. Pijper, B. L. Feringa, *Org. Biomol. Chem.* **2008**, *6*, 1605–1612.
- [18] N. Ruangsupapichat, M. M. Pollard, S. R. Harutyunyan, B. L. Feringa, *Nat. Chem.* **2010**, *3*, 53–60.
- [19] J. Vachon, G. T. Carroll, M. M. Pollard, E. M. Mes, A. M. Brouwer, B. L. Feringa, *Photochem. Photobiol. Sci.* **2014**, *13*, 241–246.
- [20] J. Bauer, L. Hou, J. C. M. Kistemaker, B. L. Feringa, *J. Org. Chem.* **2014**, *79*, 4446–4455.
- [21] A. Cnossen, J. C. M. Kistemaker, T. Kojima, B. L. Feringa, *J. Org. Chem.* **2014**, *79*, 927–935.
- [22] J. Conyard, A. Cnossen, W. R. Browne, B. L. Feringa, S. R. Meech, *J. Am. Chem. Soc.* **2014**, *136*, 9692–9700.
- [23] J. C. M. Kistemaker, P. Štacko, J. Visser, B. L. Feringa, *Nat. Chem.* **2015**, *7*, 890–896.
- [24] M. Guentner, M. Schildhauer, S. Thumser, P. Mayer, D. Stephenson, P. J. Mayer, H. Dube, *Nat. Commun.* **2015**, *6*, 8406.

- [25] L. Greb, J.-M. Lehn, *J. Am. Chem. Soc.* **2014**, *136*, 13114–13117.
- [26] L. Greb, A. Eichöfer, J.-M. Lehn, *Angew. Chem. Int. Ed.* **2015**, *54*, 14345–14348.
- [27] R. Augulis, M. Klok, B. L. Feringa, P. H. M. van Loosdrecht, *Phys. Status Solidi C* **2009**, *6*, 181–184.
- [28] J. Conyard, K. Addison, I. A. Heisler, A. Cnossen, W. R. Browne, B. L. Feringa, S. R. Meech, *Nat. Chem.* **2012**, *4*, 547–551.
- [29] B. Oruganti, C. Fang, B. Durbeej, *Phys. Chem. Chem. Phys.* **2015**, *17*, 21740–21751.
- [30] P.-T. Chiang, J. Mielke, J. Godoy, J. M. Guerrero, L. B. Alemany, C. J. Villagómez, A. Saywell, L. Grill, J. M. Tour, *ACS Nano* **2012**, *6*, 592–597.
- [31] J. Chen, J. C. M. Kistemaker, J. Robertus, B. L. Feringa, *J. Am. Chem. Soc.* **2014**, *136*, 14924–14932.
- [32] K. Gavvala, S. Satpathi, P. Hazra, *RSC Adv.* **2015**, *5*, 72793–72800.
- [33] M. Klok, W. R. Browne, B. L. Feringa, *Phys. Chem. Chem. Phys.* **2009**, *11*, 9124–9131.
- [34] S. Grimm, C. Bräuchle, I. Frank, *ChemPhysChem* **2005**, *6*, 1943–1947.
- [35] A. Kazaryan, M. Filatov, *J. Phys. Chem. A* **2009**, *113*, 11630–11634.
- [36] A. Kazaryan, J. C. M. Kistemaker, L. V Schäfer, W. R. Browne, B. L. Feringa, M. Filatov, *J. Phys. Chem. A* **2010**, *114*, 5058–5067.
- [37] A. Kazaryan, Z. Lan, L. V. Schäfer, W. Thiel, M. Filatov, *J. Chem. Theory Comput.* **2011**, *7*, 2189–2199.
- [38] F. Liu, K. Morokuma, *J. Am. Chem. Soc.* **2012**, *134*, 4864–4876.
- [39] M. Filatov, M. Olivucci, *J. Org. Chem.* **2014**, *79*, 3587–3600.
- [40] R. W. J. Zijlstra, W. F. Jager, B. de Lange, P. Th. van Duijnen, B. L. Feringa, H. Goto, A. Saito, N. Koumura, N. Harada, *J. Org. Chem.* **1999**, *64*, 1667–1674.
- [41] G. Pérez-Hernández, L. González, *Phys. Chem. Chem. Phys.* **2010**, *12*, 12279–12289.
- [42] C. Fang, B. Oruganti, B. Durbeej, *RSC Adv.* **2014**, *4*, 10240–10251.
- [43] Y. Amatatsu, *J. Phys. Chem. A* **2011**, *115*, 13611–13618.
- [44] Y. Amatatsu, *J. Phys. Chem. A* **2012**, *116*, 10182–10193.
- [45] C. García-Iriepa, M. Marazzi, F. Zapata, A. Valentini, D. Sampedro, L. M. Frutos, *J. Phys. Chem. Lett.* **2013**, *4*, 1389–1396.
- [46] G. Marchand, J. Eng, I. Schapiro, A. Valentini, L. M. Frutos, M. Olivucci, J. Léonard, E. Gindensperger, *J. Phys. Chem. Lett.* **2015**, *6*, 599–604.
- [47] A. Nikiforov, J. A. Gamez, W. Thiel, M. Filatov, *J. Phys. Chem. Lett.* **2016**, *7*, 105–110.
- [48] J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615–6620.
- [49] A. V Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378–6396.
- [50] S. Schenker, C. Schneider, S. B. Tsogoeva, T. Clark, *J Chem. Theory Comput.* **2011**, *7*, 3586–3595.
- [51] S. Grimme, *J. Comput. Chem.* **2004**, *25*, 1463–1473.
- [52] J. Antony, S. Grimme, *Phys. Chem. Chem. Phys.* **2006**, *8*, 5287–5293.

- [53] B. O. Roos, P. R. Taylor, P. E. M. Siegbahn, *Chem. Phys.* **1980**, *48*, 157–173.
- [54] K. Andersson, P.-Å. Malmqvist, B. O. Roos, A. J. Sadlej, K. Wolinski, *J. Phys. Chem.* **1990**, *94*, 5483–5488.
- [55] K. Andersson, P.-Å. Malmqvist, B. O. Roos, *J. Chem. Phys.* **1992**, *96*, 1218–1226.
- [56] H. P. Hratchian, H. B. Schlegel, *J. Chem. Phys.* **2004**, *120*, 9918–9924.
- [57] Gaussian 09 (Revision D.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, USA, **2009**.
- [58] F. Aquilante, J. Autschbach, R. K. Carlson, L. F. Chibotaru, M. G. Delcey, L. De Vico, I. Fdez. Galván, N. Ferré, L. M. Frutos, L. Gagliardi, M. Garavelli, A. Giussani, C. E. Hoyer, G. Li Manni, H. Lischka, D. Ma, P.-Å. Malmqvist, T. Müller, A. Nenov, M. Olivucci, T. B. Pedersen, D. Peng, F. Plasser, B. Pritchard, M. Reiher, I. Rivalta, I. Schapiro, J. Segarra-Martí, M. Stenrup, D. G. Truhlar, L. Ungur, A. Valentini, S. Vancoillie, V. Veryazov, V. P. Vysotskiy, O. Weingart, F. Zapata, R. Lindh, *J. Comput. Chem.* **2016**, *37*, 506–541.
- [59] M. Klok, M. Walko, E. M. Geertsema, N. Ruangsapapichat, J. C. M. Kistemaker, A. Meetsma, B. L. Feringa, *Chem. Eur. J.* **2008**, *14*, 11183–11193.
- [60] B. A. Hess Jr., L. Smentak, *Org. Biomol. Chem.* **2012**, *10*, 7503–7509.
- [61] M. G. Memeo, P. Quadrelli, *Chem. Eur. J.* **2012**, *18*, 12554–12582.
- [62] E. H. Krenske, S. He, J. Huang, Y. Du, K. N. Houk, R. P. Hsung, *J. Am. Chem. Soc.* **2013**, *135*, 5242–5245.
- [63] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215–241.

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Smaller but faster: Reducing the sizes of the rotator and stator halves (see picture) of some of the fastest available overcrowded alkene-based molecular motors is found to lower the thermal isomerization barriers by up to 25 kJ mol^{-1} and facilitate the isomerization process by reducing the number of steps involved.

Computational Insight to Improve the Thermal Isomerization Performance of Overcrowded Alkene-Based Molecular Motors through Structural Redesign

Baswanth Oruganti, Jun Wang, and Bo Durbeej*[a]

Supporting Information

[a] *B. Oruganti, Dr. J. Wang, Prof. B. Durbeej*
Division of Theoretical Chemistry, IFM
Linköping University
581 83 Linköping (Sweden)
E-mail: bodur@ifm.liu.se

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Supplementary Computational Details

To verify that the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of motors **2a–2c** produce unidirectional rotary motion, the geometric relaxation of the light-absorbing *anti-(M)*-stable-*E* and *anti-(M)*-stable-*Z* isomers from the vertically excited Franck-Condon (FC) points in the lowest excited singlet state (S_1) populated by light absorption was modeled using CASSCF^[1] and CASPT2^[2–4] in combination with the SVP basis set. Throughout, active spaces comprising either 12 π -electrons in 12 orbitals (for motor **2a**, see Figure S1 below), or 14 electrons (12 π + one lone pair of the stator heteroatom) in 13 orbitals (for motors **2b** and **2c**), were employed. The procedure was as follows.

First, the ground-state (S_0) geometries of *anti-(M)*-stable-*E* and *anti-(M)*-stable-*Z* were optimized with CASSCF. Single point calculations were then performed to obtain the S_0 and S_1 energies at the resulting geometries. For the ground state, this was achieved by performing (single-state) CASPT2 calculations. For the excited state, this was achieved by first performing state-averaged CASSCF (SA-CASSCF) calculations with equal (0.5) weights for S_0 and S_1 , followed by multi-state CASPT2 (MS-CASPT2)^[4] calculations. Second, the FC relaxation processes were modeled by optimizing the S_1 geometries of *anti-(M)*-stable-*E* and *anti-(M)*-stable-*Z* using SA-CASSCF, again with equal weights for S_0 and S_1 . Finally, the S_1 energies of the resulting minima, denoted *anti-(M)*-stable-*E** and *anti-(M)*-stable-*Z**, were obtained from MS-CASPT2 single point calculations.

Figure S1. Active molecular orbitals and their occupation numbers in different CASSCF-optimized species of motor **2a**.

anti-(M)-stable-Z

Figure S1. Continued

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

Figure S1. Continued

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

Figure S1. Continued

(P)-unstable-Z

Figure S1. Continued

(*P*)-unstable-*E*

Figure S1. Continued

Figure S2. M06-2X free-energy profiles for stepwise and concerted mechanisms for the thermal isomerizations of motors **2a–2c**.

Table S1. Relative CASPT2//CASSCF energies (in kJ mol ⁻¹) of the light-absorbing and photoproduct isomers of motors 2a–2c . ^[a]				
Motor	<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	(<i>P</i>)-unstable- <i>E</i>	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	(<i>P</i>)-unstable- <i>Z</i>
2a	1.2	24.3	0.0	27.0
2b	0.0	11.7	2.2	16.0
2c	0.0	36.1	9.6	38.0
[a] All calculations carried out using the SVP basis set.				

Table S2. CASSCF geometric parameters (in Å and degrees) of the light-absorbing isomers and the corresponding excited-state minima of motors **2a–2c**.^[a]

Motor	Stationary point	C4–C1'	α
2a	<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.365	167.6
	<i>anti</i> -(<i>M</i>)-stable- <i>E</i> *	1.496	89.1
	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.366	−6.1
	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i> *	1.496	−92.7
2b	<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.367	165.9
	<i>anti</i> -(<i>M</i>)-stable- <i>E</i> *	1.495	89.6
	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.367	−9.2
	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i> *	1.494	−93.5
2c	<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.362	172.6
	<i>anti</i> -(<i>M</i>)-stable- <i>E</i> *	1.499	89.4
	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.362	−2.2
	<i>anti</i> -(<i>M</i>)-stable- <i>Z</i> *	1.499	−93.2

[a] All calculations carried out using the SVP basis set.

Table S3. Geometric parameters (in Å and degrees) of stationary points relevant for the thermal isomerizations of motors 2a . ^[a]						
Stationary point	C4–C1'	α	β	γ	δ	δ'
(<i>P</i>)-unstable- <i>Z</i>	1.377	36.5	25.1	40.2	9.1	16.1
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.361	−9.1	−60.6	119.0	−51.9	51.0
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.362	−10.7	−29.3	90.6	38.4	−46.0
TS1	1.357	0.8	−47.3	112.0	−69.3	80.9
TS2	1.372	−20.7	−52.6	115.7	−25.4	10.5
TS3	1.359	9.0	28.9	24.0	75.1	−88.6
(<i>P</i>)-unstable- <i>E</i>	1.376	−144.0	29.3	34.8	6.0	17.7
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.358	−176.6	−59.5	119.2	52.1	−58.0
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.362	166.0	−28.8	90.1	−46.9	43.1
TS4	1.357	2.2	−42.2	109.4	79.0	−70.4
TS5	1.365	−177.4	−61.4	122.4	36.1	−44.7
TS6	1.360	172.9	26.5	27.3	−87.7	74.2
[a] All calculations performed at the ω B97X-D/SVP level of theory using an SMD description of the dichloromethane solvent.						

Table S4. Geometric parameters (in Å and degrees) of stationary points relevant for the thermal isomerizations of motor 2b . ^[a]						
Stationary point	C4–C1'	α	β	γ	δ	δ'
(<i>P</i>)-unstable- <i>Z</i>	1.378	34.3	25.3	41.6	8.2	16.5
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.368	−12.7	−57.2	116.6	−34.4	28.2
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.365	−14.0	−34.8	97.7	23.9	−36.0
TS1	1.359	2.3	−37.4	104.0	−64.1	73.7
TS2	1.369	−14.4	−56.0	116.0	−30.9	22.4
TS3	1.364	15.2	19.6	37.2	65.5	−76.6
(<i>P</i>)-unstable- <i>E</i>	1.378	−145.4	27.5	37.7	8.1	16.3
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.373	161.8	−44.6	109.7	−10.0	−12.6
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.364	165.1	−31.1	92.7	−39.5	32.3
TS4	1.358	−158.1	−30.7	99.6	76.1	−66.3
TS5	1.369	159.5	−31.7	92.4	−33.7	21.7
TS6	1.365	179.3	15.4	40.9	−74.4	65.0
[a] All calculations performed at the ω B97X-D/SVP level of theory using an SMD description of the dichloromethane solvent.						

Table S5. Geometric parameters (in Å and degrees) of stationary points relevant for the thermal isomerizations of motor 2c . ^[a]						
Stationary point	C4–C1'	α	β	γ	δ	δ'
(<i>P</i>)-unstable- <i>Z</i>	1.384	36.5	22.3	42.3	6.1	20.1
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	1.356	−5.2	−58.7	119.1	−64.4	65.0
<i>anti</i> -(<i>M</i>)-stable- <i>Z</i>	1.361	−9.1	−27.2	88.3	44.9	−50.8
TS1	1.355	−2.6	−53.5	115.7	−67.1	69.5
TS2	1.377	−20.2	−54.2	117.6	−22.9	6.8
TS3	1.356	10.8	42.4	12.2	74.7	−83.8
(<i>P</i>)-unstable- <i>E</i>	1.382	−143	29.5	32.8	5.7	19.6
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	1.358	−176.6	−59.5	119.2	52.1	−58.0
<i>anti</i> -(<i>M</i>)-stable- <i>E</i>	1.360	170.6	−26.5	87.1	−51.3	49.2
TS4	1.374	−157.1	9.9	72.3	45.4	−33.7
TS5	1.375	165.2	−55.8	118.5	11.4	−27.2
TS6	1.355	172.6	38.1	15.1	−87.2	76.9
[a] All calculations performed at the ω B97X-D/SVP level of theory using an SMD description of the dichloromethane solvent.						

Table S6. Possible pair-wise *fford*-region steric interactions between the rotator and stator in different stationary points relevant for the thermal isomerizations of motor **2c**.^[a]

Stationary point	Steric interactions	Total ^[b]
(<i>P</i>)-unstable- <i>Z</i>	C9'-C9, C9'-C4, C2'-C9, C2'-C5, O8'-C7, O8'-C3, C1'-C7, C7'-C7, C7'a-C3	9
<i>syn</i> -(<i>M</i>)-stable- <i>Z</i>	C2'-C9, C2'-C5, O8'-C7, O8'-C8, C7'a-C3	5
TS1	C2'-C9, C2'-C5, O8'-C7, C7'a-C3	4
TS2	C9'-C9, C2'-C9, C2'-C5, O8'-C7, O8'-C3, C1'-C7, C7'a-C3, C7'-C7	8
TS3	C9'-C9, C9'-C5, C9'-C4, C2'-C5, O8'-C7, C7'a-C3	6
(<i>P</i>)-unstable- <i>E</i>	C9'-C3, C9'-C7, C9'-C4, C2'-C7, C2'-C3, O8'-C9, C7'-C9, C1'-C7, C7'a-C5, C1'-C9	10
<i>syn</i> -(<i>M</i>)-stable- <i>E</i>	C2'-C7, C2'-C3, O8'-C9, C7'-C9, C1'-C7, C7'a-C5, C1'-C9	7
TS4	C2'-C7, C2'-C3, O8'-C9, C7'a-C5, C1'-C9	5
TS5	C9'-C7, C2'-C7, C2'-C3, O8'-C9, C7'-C9, C1'-C7, C7'a-C5, C1'-C9	8
TS6	C9'-C3, C9'-C7, C9'-C4, C2'-C3, O8'-C9, C7'a-C5	6

[a] Interactions listed are those involving any heavy atom of the rotator that resides within the nominal van der Waals distance (taken from Ref. 5) of any heavy atom of the stator. [b] Total number of possible interactions.

References for this document

- [1] B. O. Roos, P. R. Taylor, P. E. M. Siegbahn, *Chem. Phys.* **1980**, *48*, 157–173.
- [2] K. Andersson, P.-Å. Malmqvist, B. O. Roos, A. J. Sadlej, K. Wolinski, *J. Phys. Chem.* **1990**, *94*, 5483–5488.
- [3] K. Andersson, P.-Å. Malmqvist, B. O. Roos, *J. Chem. Phys.* **1992**, *96*, 1218–1226.
- [4] J. Finley, P.-Å. Malmqvist, B. O. Roos, L. Serrano-Andrés, *Chem. Phys. Lett.* **1998**, *288*, 299–306.
- [5] A. Bondi, *J. Phys. Chem.* **1964**, *68*, 441–451.

Cartesian coordinates for stationary points of motors 2a–2c

CASSCF geometries of stationary points relevant for the photoisomerizations of motors 2a–2c

motor 2a - *anti*-(*M*)-stable-*E*

C	-1.80655483	2.50038437	0.19913850
C	-1.18814040	0.13480678	0.18124522
C	-3.29995827	0.81649868	-0.80807371
C	-2.60825665	-0.18836433	-0.22843553
C	-0.11703182	-0.67629595	-0.06062023
C	1.34920601	-0.39083917	0.05451239
C	-0.17702135	-2.15928985	-0.45298752
C	2.03982224	-1.59607372	0.24856870
H	-1.06022488	-2.64000537	-0.05356154
C	1.07410265	-2.75302109	0.22907573
H	1.47171813	-3.62011828	-0.30118892
C	2.09427874	0.79042234	-0.14671296
C	3.48769450	0.74936719	-0.01822691
C	4.14731252	-0.45576866	0.25698656
C	3.42935730	-1.64418565	0.37358557
H	0.83843173	-3.07587149	1.24740591
H	5.22596321	-0.45803339	0.34523696
H	3.93918120	-2.58504959	0.53544459
H	4.07390886	1.64512813	-0.15403572
C	-1.07375852	1.51904156	0.75669909
C	-3.30651333	-1.50912259	0.04678631
H	-2.90391597	-2.31313847	-0.56840813
C	-0.29795677	1.72950819	2.03349459
H	0.71003464	1.32652372	1.99322048
H	-0.23097310	2.79116143	2.27364281
H	-0.80860918	1.23214102	2.86283680
H	-1.76831267	3.50876170	0.59562490
C	-0.15724242	-2.35679281	-1.97206985
H	-0.17848492	-3.41985787	-2.22395233
H	-1.02112156	-1.88106780	-2.43866344
H	0.74084474	-1.92373030	-2.41693169
O	1.42188773	1.90277031	-0.49048106
C	2.07230521	3.11550795	-0.68332916
H	2.59269320	3.44652894	0.21857092
H	2.78704389	3.06670216	-1.50810261
H	1.30388036	3.84337204	-0.92981782
C	-2.74090110	2.21004981	-0.94613093
H	-3.55879735	2.93329456	-0.95615501
H	-2.22537812	2.32533813	-1.90751832
H	-4.31520897	0.64414885	-1.14675535
C	-3.28626949	-1.92050507	1.51923442
H	-3.75656887	-1.15582396	2.14064630
H	-3.83195261	-2.85493885	1.66699198
H	-2.27028919	-2.06493989	1.88953737
H	-4.34511555	-1.39849371	-0.26820535

motor 2a - *anti*-(*M*)-stable-*Z*

C	2.42990384	-1.82085433	-0.14163690
C	1.25694549	0.30703867	0.15312587
C	3.50518700	0.30462258	-0.78094114
C	2.56304834	1.01249587	-0.12194954
C	0.03047801	0.88602489	-0.00619804
C	-1.33212798	0.26464726	-0.00856591

C	-0.24761945	2.38906860	-0.15352247
C	-2.28195661	1.23401738	0.34480870
H	0.50087872	2.98375078	0.35341438
C	-1.60509789	2.56347207	0.56080807
H	-2.18610866	3.39787336	0.16416323
C	-1.78366308	-1.00230257	-0.43463297
C	-3.15057307	-1.29688996	-0.37057357
C	-4.07176379	-0.33422915	0.06351362
C	-3.64686458	0.94747525	0.40732643
H	-1.45465255	2.75095703	1.62804593
H	-5.12313108	-0.58869672	0.09761007
H	-4.36071406	1.70847519	0.69479797
H	-3.51444739	-2.26518142	-0.67799286
C	1.46035671	-1.14182580	0.49987711
H	4.45254594	0.77153837	-1.02623446
C	2.87612014	2.42228995	0.33455850
H	2.45509546	3.18585764	-0.31902456
H	2.50577856	2.60525150	1.34429383
H	3.95577815	2.56896565	0.34830019
C	0.72585865	-1.74602339	1.67912979
H	-0.33112735	-1.49420737	1.65387087
C	-0.30894253	2.82407866	-1.62144005
H	-1.08604607	2.28188177	-2.16373350
H	-0.52701122	3.89196255	-1.69944451
H	0.63980541	2.63465851	-2.12573327
O	-0.86879690	-1.86105516	-0.91756248
C	-1.22196177	-3.13586320	-1.34318292
H	-0.30402622	-3.62044642	-1.66505455
H	-1.66624881	-3.72561784	-0.53789627
H	-1.91667732	-3.10474900	-2.18575328
C	3.31982489	-1.14465312	-1.15037871
H	2.90229750	-1.23381622	-2.16092693
H	4.29154187	-1.64176685	-1.18398267
H	0.78662760	-2.83421044	1.60940890
C	1.30377238	-1.29496532	3.02284206
H	0.75068465	-1.74172756	3.85232695
H	2.35142981	-1.58604601	3.12013649
H	1.24775773	-0.21021217	3.13473255
H	2.61706853	-2.86227851	0.09612803

motor 2a - anti-(M)-stable-E*

C	-2.99102396	-0.81751753	-1.75679703
C	-1.15070918	0.11912722	-0.36761600
C	-3.24317584	-0.66718306	0.71909237
C	-1.92744648	-0.06680691	0.80817820
C	0.20483560	0.74785893	-0.29020328
C	1.45082548	0.10499933	-0.08348880
C	0.45126855	2.20507288	-0.67497857
C	2.51858254	1.03954594	-0.18494808
H	0.26955199	2.29622415	-1.75181907
C	1.96102849	2.42482192	-0.40944852
H	2.11068803	3.03666357	0.48499532
C	1.75564591	-1.26292287	0.19025083
C	3.08557393	-1.64470163	0.33481400
C	4.12607059	-0.69940239	0.21889467
C	3.84377485	0.64915288	-0.03748951
H	2.45493406	2.94537279	-1.23196588
H	5.15002973	-1.02882370	0.33383126
H	4.64720924	1.37036655	-0.11701748
H	3.34095388	-2.67404147	0.53634451
C	-1.65316783	-0.27936019	-1.63365662
C	-1.40513208	0.23408383	2.19747029
H	-1.37257307	-0.70412736	2.76169089
H	-0.37556445	0.58060220	2.13984566
C	-0.85532320	-0.14815100	-2.90820692

H	0.21488353	-0.09142238	-2.72315889
H	-1.03305663	-1.00822007	-3.55652399
H	-1.14573848	0.74357240	-3.47313991
H	-3.36067503	-1.08004219	-2.73915202
C	-0.44539518	3.22751185	0.02032998
H	-0.21465173	4.23633935	-0.32990003
H	-1.49945846	3.03701003	-0.18519213
H	-0.30195314	3.20940725	1.10239026
O	0.70792854	-2.10354730	0.29105306
C	0.89956715	-3.45716844	0.54212246
H	1.48408832	-3.93715335	-0.24642833
H	1.39328711	-3.62608006	1.50214252
H	-0.08694568	-3.91213423	0.57178839
H	-3.79812797	-0.85336263	1.62827353
C	-2.23148652	1.25367162	2.98621210
H	-3.25699257	0.91544200	3.14249561
H	-1.78936758	1.42385022	3.97044520
H	-2.27728544	2.21334974	2.46918696
C	-3.90120312	-1.00130646	-0.58339389
H	-4.80205776	-0.38582771	-0.71225122
H	-4.26770815	-2.03467371	-0.55758689

motor 2a - *anti*-(M)-stable-Z*

C	3.18162496	-0.05654587	-1.57780429
C	1.21075327	0.45625000	-0.14711505
C	3.38472278	-0.13754226	0.90549737
C	1.98400284	0.21288471	1.01850203
C	-0.21114442	0.89956194	-0.01116307
C	-1.38375762	0.10816093	0.01521429
C	-0.57304843	2.35664102	0.27130738
C	-2.53153950	0.92161116	0.23132597
H	-0.18793478	2.61049220	1.26481657
C	-2.12271318	2.37346614	0.31135555
H	-2.52902420	2.92788148	-0.53906467
C	-1.55924266	-1.30083484	-0.14341429
C	-2.83979888	-1.83784768	-0.06937967
C	-3.95945768	-1.00956156	0.15615523
C	-3.80694156	0.37573317	0.30415283
H	-2.50541789	2.85822709	1.21156755
H	-4.94227138	-1.45812648	0.21099067
H	-4.67153714	1.00594419	0.46953394
H	-2.99545407	-2.90018056	-0.18168528
C	1.78942600	0.31601953	-1.43632931
C	1.39432409	0.21154988	2.41314564
H	2.06735543	0.75517629	3.08324346
H	0.44889150	0.74957307	2.42829720
C	1.00170977	0.45544358	-2.71424904
H	-0.02121495	0.77828560	-2.54295533
H	1.47542088	1.17303710	-3.38956290
H	0.95959580	-0.50252076	-3.24042025
H	3.59701369	-0.15100246	-2.57258842
C	0.01983584	3.37229713	-0.70641859
H	-0.26580467	4.38664295	-0.41817198
H	1.10932255	3.32410138	-0.71786023
H	-0.33743705	3.20222036	-1.72391965
O	-0.44200937	-2.02509618	-0.35369971
C	-0.51035727	-3.39718389	-0.56824206
H	-0.91977348	-3.92360168	0.29716530
H	-1.11136241	-3.63951090	-1.44790125
H	0.50789821	-3.73849295	-0.73462484
H	3.96155432	-0.27921692	1.80996342
C	1.16369774	-1.19643988	2.97098896
H	2.09778297	-1.75753202	3.03889963
H	0.72927185	-1.14987111	3.97225015
H	0.48467996	-1.75745576	2.32879150

C	4.09903802	-0.22577109	-0.40721354
H	4.62188309	-1.18704694	-0.48097988
H	4.89396803	0.53142591	-0.44730032

motor 2a - (P)-unstable-Z

C	-3.24258246	-0.38187910	-1.63767214
C	-1.13559469	0.15820421	-0.45520730
C	-2.92070572	-1.11269805	0.70663621
C	-1.70068560	-0.52952801	0.74475386
C	0.15381314	0.67921816	-0.47688532
C	1.37753396	0.11903356	0.14466916
C	0.57567957	2.00699351	-1.14397287
C	2.42905259	1.04211560	0.08258379
H	0.71310517	1.87739992	-2.21754737
C	1.96007071	2.33331937	-0.52723059
H	1.86663813	3.10672130	0.24012384
C	1.66668043	-1.21032774	0.53917135
C	2.95827910	-1.53308534	0.96201989
C	3.97664675	-0.56751084	0.95722454
C	3.72343320	0.72334768	0.50141581
H	2.66275140	2.71301049	-1.27091797
H	4.96940947	-0.84676357	1.28508196
H	4.51647621	1.45833525	0.45401815
H	3.19331744	-2.53716273	1.28000496
C	-2.04247032	0.24790682	-1.64076198
C	-1.08995587	-0.32995138	2.12641149
H	-1.31458285	-1.21017906	2.73192001
H	-0.01123281	-0.25921370	2.09275293
C	-1.55089292	0.76506912	-2.98071830
H	-0.60959375	0.28648611	-3.25416937
H	-2.27755193	0.52339284	-3.75454146
H	-1.39631789	1.84001036	-3.01181714
H	-3.81722498	-0.40117362	-2.55635522
C	-0.40118193	3.16003389	-0.89233648
H	-0.03959842	4.07371065	-1.37122590
H	-1.40368835	2.96220568	-1.26340664
H	-0.48481726	3.35723477	0.17802090
O	0.66836355	-2.10856692	0.46533315
C	0.87067640	-3.44671742	0.78294256
H	1.62868784	-3.90475308	0.14341700
H	1.16092852	-3.57723132	1.82805246
H	-0.07783143	-3.95098843	0.61884535
H	-3.33264284	-1.51026904	1.62820118
C	-1.63231688	0.91498134	2.83362730
H	-2.71077537	0.84822625	2.98821898
H	-1.15981226	1.04047782	3.81089424
H	-1.43743527	1.81806310	2.25238330
C	-3.80982047	-1.15449342	-0.49219070
H	-4.79868441	-0.76343712	-0.22578934
H	-3.98903892	-2.18949791	-0.80849325

motor 2a - (P)-unstable-E

C	2.91028285	-0.16411549	-1.72559822
C	1.13162806	0.37885725	-0.11183917
C	3.51403913	0.62398578	0.54704678
C	2.20726830	0.66171876	0.88964801
C	-0.18650347	0.71426945	0.14913250
C	-1.42440780	0.03134129	-0.30020832
C	-0.68045967	1.98529561	0.87344144
C	-2.50236366	0.92551024	-0.28846988
H	-0.93648302	1.75211808	1.91194494
C	-2.01415789	2.28303297	0.13927511
H	-1.82752192	2.91832945	-0.73220628
C	-1.67938215	-1.34728917	-0.45490982

C	-2.98215225	-1.76778381	-0.74304314
C	-4.03116230	-0.84009916	-0.82179793
C	-3.80504075	0.51358801	-0.57249183
H	-2.72663068	2.80971590	0.77605869
H	-5.02983173	-1.19370429	-1.04286073
H	-4.62499445	1.21996247	-0.57466581
H	-3.20111341	-2.81509999	-0.88467582
C	1.59055381	-0.18399058	-1.41686225
C	1.86836306	0.66468089	2.37443333
H	2.69172204	1.13374152	2.91708089
H	0.98860618	1.26021110	2.59295475
C	0.62539579	-0.51961156	-2.53511843
H	-0.10170919	0.27899637	-2.68283439
H	1.17463946	-0.63944097	-3.46807163
H	0.07902418	-1.43819166	-2.35217865
H	3.20864605	-0.44837373	-2.72802061
C	0.23807180	3.20548131	0.83512997
H	-0.28833537	4.07333163	1.23998031
H	1.15094838	3.07962333	1.41111690
H	0.52488280	3.43774751	-0.19215240
O	-0.64633811	-2.19640041	-0.27561166
C	-0.83659723	-3.57441700	-0.29174788
H	-1.55578974	-3.89231530	0.46643953
H	-1.17205290	-3.92757121	-1.26975804
H	0.12765506	-4.02441308	-0.07149151
H	4.26262797	0.73800361	1.32358973
C	1.64725982	-0.74842222	2.92145066
H	2.55001212	-1.35358627	2.81863287
H	1.38324722	-0.71539083	3.98120649
H	0.84338292	-1.25720402	2.38799293
C	4.00725008	0.31975802	-0.82996573
H	4.80184957	-0.43208662	-0.77045948
H	4.48220206	1.20145181	-1.27841519

motor 2b - *anti*-(M)-stable-E

C	-1.91592790	2.44979105	0.27244668
C	-1.16299175	0.13856288	0.15584247
C	-3.29150868	0.90209811	-0.70663060
C	-2.57097750	-0.15465420	-0.27627244
C	-0.08645008	-0.68001834	-0.03804358
C	1.36992465	-0.36940757	0.09069641
C	-0.11599563	-2.18098423	-0.35876612
C	2.07336435	-1.55022473	0.36912628
H	-1.00858790	-2.65619459	0.02882064
C	1.11695903	-2.71581430	0.40436592
H	1.53558531	-3.61561527	-0.04962042
C	2.09689246	0.80499477	-0.19189186
C	3.49011018	0.79404816	-0.05260001
C	4.16353270	-0.37988316	0.31057452
C	3.46208416	-1.56914393	0.50515009
H	0.84943731	-2.96554901	1.43532425
H	5.24149021	-0.36068490	0.40499532
H	3.98569588	-2.48877013	0.73201097
H	4.06513381	1.68636908	-0.24701972
C	-1.07489845	1.51258444	0.74155144
C	-3.26610926	-1.50149163	-0.23132766
H	-2.75223572	-2.23698462	-0.84686935
C	-0.23866884	1.80261656	1.96289460
H	0.80609981	1.53680574	1.84558453
H	-0.28931548	2.86201784	2.21792385
H	-0.62333454	1.23890071	2.81665376
H	-1.94968164	3.47163146	0.62026408
C	-0.02071741	-2.45899251	-1.86279153
H	-0.02865449	-3.53408845	-2.05822085
H	-0.85776898	-2.01104926	-2.40005435

H	0.89868731	-2.04779449	-2.28363943
O	1.40511359	1.87934838	-0.61281520
C	2.04508348	3.06203414	-0.96511246
H	2.57770667	3.50477990	-0.11995687
H	2.74710821	2.91329308	-1.78867216
H	1.26868852	3.75057493	-1.28772537
H	-4.28990507	0.81919195	-1.10977051
C	-3.45225733	-2.04144886	1.18763059
H	-4.05818542	-1.35637776	1.78341351
H	-3.95644056	-3.01013588	1.17122643
H	-2.49942656	-2.16859839	1.70362185
H	-4.25084179	-1.38131766	-0.68661497
O	-2.86810769	2.18232869	-0.65303876

motor 2b - *anti*-(*M*)-stable-*Z*

C	2.51636833	-1.75315213	0.05811284
C	1.23450819	0.31706358	0.12998321
C	3.54042999	0.18481397	-0.60607441
C	2.55115916	0.97825270	-0.14588334
C	0.00924730	0.89774842	-0.04100465
C	-1.34279032	0.26190425	-0.05437327
C	-0.29015744	2.39901856	-0.16285885
C	-2.30426507	1.20795029	0.32856261
H	0.46090108	2.99998264	0.33533155
C	-1.63556110	2.53546212	0.58592308
H	-2.22986002	3.38033512	0.23380250
C	-1.77293086	-0.99046078	-0.53761533
C	-3.13679247	-1.30394998	-0.49726235
C	-4.07176958	-0.36946060	-0.03169648
C	-3.66565103	0.90329226	0.36774470
H	-1.46404195	2.68121754	1.65650064
H	-5.12040044	-0.63676152	-0.01709095
H	-4.39222321	1.64331705	0.67726776
H	-3.48732043	-2.26311408	-0.84634816
C	1.44000366	-1.10754047	0.54021881
H	4.51015579	0.55370972	-0.90536518
C	2.86110207	2.44612011	0.03999332
H	2.35055637	3.08462835	-0.67849512
H	2.58933283	2.78242269	1.04155241
H	3.93142656	2.61391377	-0.07873993
C	0.62716317	-1.75891845	1.63996859
H	-0.43712209	-1.62547044	1.47851352
C	-0.40688783	2.85653506	-1.62111713
H	-1.20293986	2.32033576	-2.14096825
H	-0.63113488	3.92471565	-1.67388847
H	0.51991838	2.67785525	-2.16765102
O	-0.83791518	-1.81679239	-1.04057520
C	-1.17720245	-3.05127805	-1.58223468
H	-0.25188725	-3.50195141	-1.93100318
H	-1.63085617	-3.71153396	-0.83916522
H	-1.85905286	-2.94845857	-2.42945193
H	0.80674829	-2.83624195	1.61148771
C	0.98421247	-1.22788087	3.03016404
H	0.37856151	-1.71601763	3.79707567
H	2.03517026	-1.40738553	3.26488884
H	0.80534472	-0.15340220	3.10148392
H	2.76582297	-2.77824318	0.28955803
O	3.44784738	-1.15628765	-0.72150164

motor 2b - *anti*-(*M*)-stable-*E**

C	-3.01070870	-0.74169055	-1.69581549
C	-1.13837071	0.08295717	-0.36921413
C	-3.23024978	-0.68544819	0.60965210
C	-1.91743347	-0.11446064	0.79373502

C	0.20107839	0.74031616	-0.28066285
C	1.45948178	0.12733618	-0.06883378
C	0.41029223	2.20137412	-0.67220342
C	2.50379782	1.08854681	-0.16633243
H	0.24077451	2.28278310	-1.75142189
C	1.91123762	2.45935171	-0.38967595
H	2.03439693	3.06939909	0.50995898
C	1.79438315	-1.23302101	0.20436239
C	3.13238877	-1.58358665	0.35244764
C	4.15001112	-0.61319201	0.24057817
C	3.83704992	0.72911441	-0.01494027
H	2.39842891	2.99819731	-1.20419637
H	5.18118270	-0.91818255	0.35804826
H	4.62375397	1.46881117	-0.09088617
H	3.41136226	-2.60686709	0.55356244
C	-1.64364791	-0.27601689	-1.63692065
C	-1.43765274	0.09881606	2.21003464
H	-1.45479633	-0.86263506	2.73593091
H	-0.39402586	0.40742369	2.19373680
C	-0.89697201	-0.13559876	-2.93596941
H	0.18024918	-0.12979227	-2.78011781
H	-1.12535806	-0.97267591	-3.60007419
H	-1.16090123	0.78096305	-3.47500139
H	-3.54593852	-1.00195327	-2.59274566
C	-0.52014949	3.20266645	0.00902059
H	-0.30798829	4.21610530	-0.33949404
H	-1.56650084	2.98737962	-0.21046353
H	-0.39102221	3.18786617	1.09287453
O	0.76434318	-2.09464025	0.30154418
C	0.98263416	-3.44660692	0.54239255
H	1.57849230	-3.90760749	-0.24886000
H	1.47756621	-3.61250184	1.50219986
H	0.00545203	-3.92136906	0.56607738
H	-3.94874935	-0.86159876	1.39140414
C	-2.24795835	1.11386486	3.02133167
H	-3.29378276	0.81550453	3.11818001
H	-1.84196853	1.21152566	4.03074328
H	-2.23067499	2.09971926	2.55444429
O	-3.70127698	-0.92588673	-0.59306139

motor 2b - anti-(M)-stable-Z*

C	3.30872279	-0.47646031	0.83818231
C	1.20980572	0.35838589	-0.08143594
C	3.21586495	0.01910626	-1.42274269
C	1.82718108	0.40518787	-1.35036903
C	-0.18241637	0.87434290	0.08849272
C	-1.40361687	0.17339216	-0.03686260
C	-0.45223169	2.28519388	0.60674953
C	-2.50074061	1.02715856	0.26980304
H	-0.12044206	2.32716759	1.64980460
C	-1.99580061	2.41903201	0.56721974
H	-2.30444263	3.10708328	-0.22483610
C	-1.66539794	-1.18090556	-0.40737083
C	-2.98069361	-1.63039874	-0.44694091
C	-4.04965553	-0.76595538	-0.12967151
C	-3.81115883	0.56865366	0.22695445
H	-2.39874660	2.81513637	1.50107234
H	-5.06149807	-1.14650785	-0.16722649
H	-4.63757741	1.22750780	0.46106835
H	-3.20238016	-2.65145101	-0.71839721
C	1.92814676	-0.09747539	1.04586237
C	1.16210261	0.83512839	-2.62961979
H	1.33276705	0.09868807	-3.41988038
H	0.08655910	0.93854837	-2.50823857
C	1.34453424	-0.32603203	2.41981236

H	0.42234325	0.24151929	2.53188578
H	2.03367815	0.06809642	3.17435339
H	4.00029679	-0.75755644	1.61416139
C	0.27552035	3.40265046	-0.14037438
H	0.03271483	4.37252901	0.29985613
H	1.35751785	3.27604701	-0.08988672
H	-0.01384560	3.43095192	-1.19262271
O	-0.59047851	-1.94186415	-0.69033932
C	-0.73793035	-3.25590152	-1.12189811
H	-1.21341962	-3.88121931	-0.36269585
H	-1.31873376	-3.31453717	-2.04534986
H	0.26210245	-3.63639744	-1.31145430
H	3.82406949	0.04282849	-2.31083492
H	1.55055351	1.79187099	-2.99356173
C	1.05686135	-1.79865538	2.72997869
H	1.96606543	-2.40166760	2.68059636
H	0.63733926	-1.91077254	3.73260576
H	0.34695842	-2.21011063	2.01220414
O	3.86358538	-0.37161119	-0.34876849

motor 2b - (P)-unstable-Z

C	-3.22622081	-0.47082236	-1.55584402
C	-1.12699232	0.12512699	-0.44385777
C	-2.92278556	-1.16726484	0.61182563
C	-1.70081049	-0.60383300	0.71641189
C	0.14525025	0.67746567	-0.45617766
C	1.37604340	0.14512917	0.16987706
C	0.53103721	2.01964598	-1.11376308
C	2.39968002	1.10166829	0.13246239
H	0.67823199	1.89952722	-2.18857177
C	1.90080046	2.38118840	-0.48098104
H	1.77761356	3.15085438	0.28585504
C	1.70443011	-1.18135532	0.53938164
C	2.99757220	-1.46794444	0.98529743
C	3.98231229	-0.46917243	1.01609745
C	3.69557666	0.81897543	0.56998911
H	2.60144324	2.78093902	-1.21599369
H	4.97719552	-0.71981922	1.36030115
H	4.46637145	1.57839143	0.54347805
H	3.26094133	-2.46947029	1.28902303
C	-2.05698725	0.20687547	-1.59903239
C	-1.14351261	-0.48464593	2.12547511
H	-1.53676585	-1.31223182	2.72003318
H	-0.06740670	-0.59681599	2.14072681
C	-1.64505133	0.73741328	-2.95568153
H	-0.70777421	0.27724999	-3.27174794
H	-2.40119591	0.48729611	-3.69928633
H	-1.51109300	1.81521433	-2.98465702
H	-3.88722134	-0.55729860	-2.40409241
C	-0.47706035	3.14624117	-0.86514383
H	-0.13991838	4.06853048	-1.34538999
H	-1.47385156	2.92212197	-1.23656525
H	-0.56795263	3.34362460	0.20447122
O	0.74268155	-2.11552317	0.41307567
C	0.98642481	-3.45148603	0.71062932
H	1.78124771	-3.86723667	0.08726540
H	1.24872714	-3.59279819	1.76184112
H	0.06398211	-3.98837637	0.50609829
H	-3.43448803	-1.62918430	1.44228450
C	-1.51419147	0.83481125	2.80676775
H	-2.59673282	0.94783371	2.89067382
H	-1.09222233	0.87812924	3.81345395
H	-1.13273581	1.69170850	2.25058892
O	-3.68236221	-1.16599314	-0.50123021

motor 2b - (*P*)-unstable-*E*

C	3.49098289	0.03139889	0.53433638
C	1.13566541	0.31591243	-0.08487510
C	2.90287181	-0.28089099	-1.66612400
C	1.58519138	-0.08524724	-1.44051834
C	-0.16008096	0.70696546	0.20821577
C	-1.42106523	0.15881487	-0.33865800
C	-0.57132329	1.86443348	1.13958451
C	-2.48402293	1.03762042	-0.08894959
H	-0.70311942	1.50514106	2.16508769
C	-1.97056939	2.27026090	0.60463178
H	-1.87627963	3.09689389	-0.10580377
C	-1.71063065	-1.14706189	-0.79206901
C	-3.02873876	-1.47683547	-1.12408378
C	-4.06310716	-0.54526857	-0.95354073
C	-3.80230293	0.71319609	-0.41193888
H	-2.63466410	2.60964932	1.40112489
H	-5.07475775	-0.82820603	-1.21371350
H	-4.60814356	1.41105631	-0.22467114
H	-3.27022787	-2.46276308	-1.49092995
C	2.23086426	0.32920870	0.91935866
C	0.69729593	0.01035613	-2.66034158
H	1.30263682	-0.02207072	-3.56632765
H	-0.02807774	-0.79320710	-2.71850824
C	1.97152393	0.32819163	2.41779580
H	1.35033882	1.16405323	2.72211962
H	2.92587385	0.47285967	2.92849398
H	4.31144032	-0.07442778	1.22761924
C	0.36566243	3.07404661	1.13623573
H	-0.05157281	3.87140443	1.75642340
H	1.36230345	2.85360630	1.50979791
H	0.47676592	3.46340424	0.12250428
O	-0.69072918	-2.02887279	-0.84194781
C	-0.91111615	-3.36969652	-1.13854527
H	-1.61059713	-3.82941349	-0.43671071
H	-1.28751849	-3.50618972	-2.15520444
H	0.05033377	-3.86918652	-1.05425501
H	3.31537119	-0.44911216	-2.64843552
H	0.15197504	0.95502528	-2.66176916
C	1.33638408	-0.97276718	2.91526845
H	1.98790484	-1.82569438	2.71646919
H	1.16181608	-0.92624131	3.99260296
H	0.38122007	-1.16563227	2.42661762
O	3.86830687	-0.23398714	-0.72708166

motor 2c - *anti*-(*M*)-stable-*E*

C	-1.96242481	2.08469356	0.31767752
C	-1.03091407	-0.18599124	0.23532431
S	-2.98294102	1.72761582	-1.08034995
C	-3.26288423	0.01756221	-0.74156874
C	-2.38261941	-0.77507978	-0.09253570
C	0.15037576	-0.77831531	-0.09455591
C	1.55609671	-0.27354391	0.01873316
C	0.30306825	-2.21390196	-0.61263653
C	2.43091197	-1.36896592	0.08214559
H	-0.47980392	-2.85776372	-0.23285491
C	1.66032866	-2.65957883	-0.03052093
H	2.16712471	-3.39424114	-0.65850913
C	2.10321527	1.02479929	-0.06083354
C	3.48954092	1.18947508	0.04443120
C	4.33584275	0.08156760	0.18043884
C	3.81410155	-1.21022025	0.18289104
H	1.52607240	-3.11440044	0.95528744
H	5.40390522	0.23978488	0.25386700

H	4.46756848	-2.07095388	0.24078660
H	3.92479007	2.17588417	0.00031663
C	-1.14514526	1.16880370	0.86920210
C	-2.84238243	-2.15189804	0.36696596
C	-0.46036876	1.42220022	2.18984411
H	0.59353914	1.15629783	2.16420458
H	-0.54193052	2.47057152	2.47747106
H	-0.92771962	0.82233250	2.97509107
H	-2.08501722	3.07636851	0.73291475
C	0.27839056	-2.27155409	-2.14353559
H	0.40689375	-3.29886543	-2.49261105
H	-0.66983320	-1.89701062	-2.53140333
H	1.07730092	-1.66637707	-2.57646002
O	1.25823794	2.04970860	-0.26325550
C	1.72027994	3.34296535	-0.47943244
H	2.24125715	3.74179750	0.39424822
H	2.38460274	3.39569839	-1.34474222
H	0.84428884	3.95601143	-0.67351584
H	-4.24463859	-0.33849827	-1.02500139
H	-2.40311818	-2.93880500	-0.24626651
C	-2.56788533	-2.43766584	1.84261247
H	-2.96286603	-3.41616026	2.12284260
H	-1.50009636	-2.43262414	2.06540676
H	-3.04327339	-1.68950873	2.48012175
H	-3.91712835	-2.21569429	0.19260347

motor 2c - anti-(M)-stable-Z

C	2.25464491	-1.32468516	-0.09745729
C	3.28013786	-0.82313890	0.62307161
C	1.02205000	-0.47205057	-0.25710446
S	3.31962466	0.82291376	1.25951107
C	2.33075183	1.58887270	0.01175807
C	1.35223678	0.93861699	-0.64585952
C	-0.23536481	-0.92350438	0.00809750
C	-1.54531119	-0.19913732	0.03414294
C	-0.60575376	-2.38699952	0.28110114
C	-2.58066398	-1.12040567	-0.18572481
H	0.06609426	-3.06907138	-0.22417555
C	-2.01908520	-2.51275602	-0.32420423
H	-2.63002642	-3.26127095	0.18316983
C	-1.88106613	1.13302325	0.35518844
C	-3.22528661	1.52318446	0.33057785
C	-4.23559112	0.59833906	0.03679315
C	-3.92273389	-0.73718913	-0.20723508
H	-1.96195832	-2.80127679	-1.37792415
H	-5.26641276	0.92784565	0.03102765
H	-4.70363117	-1.46421930	-0.38854470
H	-3.50060383	2.54108983	0.55962781
O	-0.88311103	1.96439003	0.69956536
C	-1.13330617	3.25905436	1.13997807
H	-1.59200784	3.87337339	0.36154583
H	-1.77380587	3.26858368	2.02459783
H	-0.16996385	3.68852457	1.40150585
H	4.18767992	-1.38951372	0.78827309
C	0.70062659	1.54894739	-1.86999066
H	-0.37428011	1.38169579	-1.84598679
C	2.42318724	-2.66986698	-0.78038849
H	1.87165589	-2.70584562	-1.72004708
H	3.47412818	-2.84653590	-1.00721570
H	2.08146128	-3.49909275	-0.16034611
C	-0.58400516	-2.70712348	1.77953447
H	0.41244564	-2.55242859	2.19573401
H	-1.27753435	-2.07033645	2.33214401
H	-0.86845355	-3.74726939	1.95546435
H	0.84717876	2.63058582	-1.84532302

C	1.25995061	0.99229178	-3.18090988
H	0.76089339	1.44929628	-4.03823062
H	2.33017906	1.18821574	-3.26932326
H	1.11113070	-0.08720390	-3.24983686
H	2.60863258	2.60702836	-0.22811868

motor 2c - anti-(M)-stable-E*

C	-2.25401028	1.23215768	2.24452200
C	-0.81509815	-0.10336822	0.69701851
S	-3.58724999	1.20920678	1.24289031
C	-3.12291643	0.36662268	-0.11983495
C	-1.81892970	-0.24741092	-0.29335738
C	0.48540547	-0.82528937	0.50997136
C	1.64887649	-0.36620909	-0.15495952
C	0.81196945	-2.11228513	1.26516210
C	2.70813422	-1.30420788	-0.01100661
H	0.89689593	-1.86067330	2.32773559
C	2.21335437	-2.51547613	0.74264212
H	2.14040580	-3.37142793	0.06528756
C	1.88225318	0.83291218	-0.89263739
C	3.14235154	1.05782629	-1.43766184
C	4.17922737	0.11606404	-1.27212514
C	3.96283096	-1.07205001	-0.56068314
H	2.88654196	-2.80985635	1.54976943
H	5.14876135	0.32121503	-1.70582181
H	4.76188704	-1.79318097	-0.44516228
H	3.34492482	1.95994992	-1.99495842
C	-0.97462120	0.63915980	1.89296365
C	-1.58966076	-0.92913349	-1.62753192
H	-1.71250650	-0.18408873	-2.42180174
H	-0.55814718	-1.26592603	-1.69666704
C	0.12953560	0.83819725	2.90342291
H	1.11385816	0.65699926	2.47879061
H	0.12024163	1.86568611	3.27463645
H	0.01477019	0.18318148	3.77400225
H	-2.40564223	1.72570977	3.19254110
C	-0.22593279	-3.22645282	1.14785332
H	0.08197260	-4.09454400	1.73539267
H	-1.20048995	-2.90387636	1.51609148
H	-0.34426814	-3.54966002	0.11210362
O	0.83938155	1.67666936	-1.00781683
C	0.96375693	2.87963214	-1.69385763
H	1.71602050	3.52890711	-1.23973279
H	1.21823741	2.72236159	-2.74472625
H	-0.00322191	3.37222563	-1.63783494
H	-3.88747383	0.29241725	-0.87752020
C	-2.51842639	-2.11110337	-1.91885046
H	-3.56823349	-1.81257032	-1.93755410
H	-2.28736071	-2.54767367	-2.89317381
H	-2.41486689	-2.89384207	-1.16623865

motor 2c - anti-(M)-stable-Z*

C	-2.34023347	1.18304721	2.33928163
C	-0.84942720	-0.08178879	0.78464483
S	-3.66673245	1.13386052	1.32938465
C	-3.16805372	0.32995286	-0.04428100
C	-1.83358077	-0.21030941	-0.22632269
C	0.46345465	-0.77485035	0.58030183
C	1.63579785	-0.28383542	-0.03905908
C	0.74641488	-2.14032007	1.20373873
C	2.68353006	-1.24305297	0.04618166
H	0.75913370	-2.01580599	2.29161904
C	2.17669667	-2.49494179	0.72204569
H	2.15244397	-3.32405732	0.00955400

C	1.88886583	0.95793231	-0.69761675
C	3.15253282	1.20078760	-1.22428139
C	4.17721589	0.23653872	-1.11751981
C	3.94297265	-0.99131511	-0.48359096
H	2.82130076	-2.80870301	1.54516702
H	5.15052752	0.45633347	-1.53518309
H	4.73223391	-1.72883657	-0.41262022
H	3.36873151	2.13453920	-1.72106271
C	-1.04910982	0.59973337	2.01031450
C	-1.59007153	-0.87978696	-1.55674090
H	-1.84629657	-0.20263679	-2.37652896
H	-0.55250424	-1.17220335	-1.68964055
C	0.05510928	0.86318989	3.01405015
H	0.89328387	0.19163756	2.84409071
H	-0.31441296	0.63618150	4.01961125
H	-2.51554616	1.66174961	3.29085416
C	-0.28583336	-3.22439526	0.89220092
H	-0.01432707	-4.15816567	1.39004607
H	-1.27949824	-2.93909064	1.23917050
H	-0.34472720	-3.42230950	-0.17961370
O	0.85940861	1.82506764	-0.75414697
C	0.97753696	3.03196630	-1.43520379
H	1.73529046	3.67856712	-0.98659018
H	1.22052815	2.87824892	-2.48920793
H	0.01190842	3.52544240	-1.36577213
H	-3.92561558	0.22358667	-0.80618162
H	-2.20807377	-1.77539284	-1.67516912
C	0.57293394	2.30477366	2.98689290
H	-0.22186461	3.02087598	3.20597806
H	1.36271752	2.44792768	3.72821467
H	0.97629862	2.54813552	2.00382949

motor 2c - (P)-unstable-Z

C	-2.50638832	0.93049604	2.22981408
C	-0.76617582	-0.11210308	0.76359508
S	-3.54197731	1.56212147	0.97973256
C	-2.73043757	0.91167621	-0.41995513
C	-1.56851179	0.21565207	-0.44956882
C	0.49303000	-0.70785086	0.65966511
C	1.54437564	-0.43147994	-0.34409963
C	1.04600709	-1.82621511	1.57069705
C	2.57852508	-1.37227452	-0.24953867
H	1.43336168	-1.41525498	2.50292538
C	2.24707203	-2.41163078	0.78429531
H	1.96853273	-3.35263710	0.30191122
C	1.73657244	0.70613933	-1.16545773
C	2.89901340	0.80774602	-1.93350943
C	3.89083305	-0.18269728	-1.86662671
C	3.74410586	-1.27332506	-1.01280709
H	3.09603859	-2.63121928	1.43376901
H	4.78372553	-0.07613824	-2.46861984
H	4.52481325	-2.01821544	-0.92906311
H	3.05639687	1.66145217	-2.57464047
C	-1.35823533	0.21840117	2.08954577
C	-1.28296552	-0.47706420	-1.77966919
H	-1.64566873	0.16341974	-2.58541131
H	-0.22320719	-0.60097171	-1.95541487
C	-0.55896170	0.04568301	3.37085164
H	0.42740691	0.49805447	3.26365546
H	-1.06307977	0.55040355	4.19267960
H	-0.42055833	-0.98932978	3.66840758
H	-2.81962859	1.25069041	3.21360399
C	0.03021916	-2.92831850	1.88755342
H	0.48524147	-3.68932882	2.52670729
H	-0.86135823	-2.56032259	2.38968857

H	-0.29529064	-3.41928435	0.96886716
O	0.77697918	1.64841928	-1.14750931
C	0.90536568	2.83068961	-1.86861060
H	1.78849321	3.39647755	-1.56369808
H	0.95432972	2.64692439	-2.94438092
H	0.01895021	3.42172169	-1.65488457
H	-3.31014533	1.02803987	-1.32620957
C	-1.95961963	-1.84594297	-1.88649151
H	-3.04545302	-1.76089545	-1.81565730
H	-1.72084794	-2.31818448	-2.84225185
H	-1.62834004	-2.51672835	-1.09260747

motor 2c - (P)-unstable-E

C	-2.72695602	0.03004118	2.31092160
C	-0.76917941	-0.12748407	0.73854714
S	-3.95578229	-0.18499207	1.08911167
C	-2.98575676	0.09981831	-0.34054439
C	-1.63350944	0.14972903	-0.44391315
C	0.52605463	-0.60918245	0.65790414
C	1.57363498	-0.36035478	-0.36580704
C	1.13628996	-1.70195548	1.56258168
C	2.43731534	-1.46107854	-0.44098152
H	1.84057621	-1.24857643	2.26865612
C	1.98488749	-2.50630456	0.54315512
H	1.36110102	-3.26049606	0.05310390
C	1.94030817	0.84205451	-1.00377852
C	3.06783319	0.85232774	-1.83263195
C	3.85862568	-0.29657815	-1.97740726
C	3.56565499	-1.45770589	-1.26141715
H	2.81503914	-3.02983852	1.01973106
H	4.72713412	-0.25875641	-2.62194262
H	4.21455948	-2.32175403	-1.32086175
H	3.35887886	1.75338274	-2.35049833
C	-1.39510537	0.05809961	2.08694343
C	-1.08731039	0.23363100	-1.85452399
H	-1.90913765	0.23998665	-2.56867558
H	-0.49882750	1.12992824	-2.01083424
C	-0.51617301	0.57142426	3.22143164
H	0.40890432	0.00695973	3.29294028
H	-1.03894190	0.41908304	4.16793644
H	-3.12477747	0.24220846	3.29472215
C	0.18329146	-2.62235108	2.32107369
H	0.74718874	-3.45795917	2.74247967
H	-0.32960574	-2.13107804	3.14367622
H	-0.57594361	-3.03330423	1.65345258
O	1.20158907	1.94173425	-0.74117138
C	1.58381118	3.19313301	-1.21619261
H	2.58474985	3.46590262	-0.87492390
H	1.55492604	3.24043424	-2.30726017
H	0.86982863	3.90908392	-0.81800613
H	-3.59451158	0.16276581	-1.23173371
H	-0.46048954	-0.62768963	-2.08305784
C	-0.17318153	2.05524998	3.06708511
H	-1.07552039	2.66952114	3.07854782
H	0.47066810	2.38711096	3.88487177
H	0.34881874	2.24210701	2.12812886

ω B97X-D geometries of stationary points relevant for the thermal isomerizations of motors 2a–2c

motor 2a - (*P*)-unstable-*Z*

C	-2.415223	0.663342	-0.890114
C	-3.568135	-0.037296	-0.879304
C	-1.231839	0.184888	-0.122409
C	-2.630546	-1.652283	0.747183
C	-1.440782	-1.017989	0.731445
C	-0.019042	0.834968	-0.184747
C	1.321391	0.233846	-0.145058
C	0.183994	2.360241	-0.221894
C	2.303986	1.217030	0.046084
H	0.079429	2.750451	-1.247181
C	1.658891	2.560182	0.217590
H	1.699744	2.868991	1.276749
C	1.728193	-1.072506	-0.507628
C	3.094687	-1.382311	-0.520036
C	4.046596	-0.397650	-0.242952
C	3.663132	0.916463	0.021193
H	2.174535	3.342907	-0.358586
H	5.106303	-0.664069	-0.266496
H	4.411131	1.695852	0.184191
H	3.428454	-2.389840	-0.769251
C	-0.460287	-1.373275	1.837213
H	0.555843	-1.530806	1.461999
H	-0.774712	-2.338184	2.264305
C	-2.276175	1.760270	-1.921859
H	-2.147161	2.763078	-1.494071
C	-0.759924	3.124218	0.708706
H	-0.568837	4.207485	0.646553
H	-1.821091	2.957014	0.482080
H	-0.598183	2.813759	1.753222
H	-2.782984	-2.459535	1.471535
O	0.766717	-1.945517	-0.850530
C	1.102493	-3.273649	-1.165951
H	1.750171	-3.333117	-2.057163
H	1.600203	-3.779296	-0.321205
H	0.157378	-3.788860	-1.378732
C	-3.806258	-1.272369	-0.083272
H	-4.090444	-2.096932	-0.766427
H	-4.692485	-1.149499	0.568588
H	-4.372119	0.268924	-1.556513
H	-3.170621	1.792315	-2.559832
H	-1.407659	1.568001	-2.571041
C	-0.409955	-0.332571	2.957360
H	-0.050437	0.640698	2.590659
H	-1.404647	-0.177244	3.404838
H	0.273260	-0.659265	3.756706

motor 2a - *syn*-(*M*)-stable-*Z*

C	2.590803	1.221294	-1.584383
C	1.354192	-0.014998	0.086240
C	3.708705	-0.558943	-0.296130
C	2.658477	-0.607979	0.537787
C	0.200655	-0.720021	0.241687
C	-1.197188	-0.418152	-0.175830
C	0.180574	-2.239484	0.450629
C	-1.709753	-1.548745	-0.831894
H	1.185917	-2.668916	0.351101
C	-0.701987	-2.667352	-0.751410
H	-1.176912	-3.649906	-0.608852

C	-2.072830	0.632468	0.149917
C	-3.371472	0.622555	-0.384873
C	-3.814229	-0.460259	-1.146497
C	-3.000959	-1.575534	-1.349586
H	-0.091955	-2.717560	-1.669475
H	-4.832105	-0.445496	-1.544125
H	-3.379157	-2.457815	-1.870968
H	-4.058144	1.444289	-0.180395
C	1.538196	1.222828	-0.745907
C	2.787873	-1.148189	1.938591
H	2.241247	-2.089271	2.090296
C	0.659943	2.445849	-0.666636
H	0.919614	3.102990	-1.511138
H	-0.396743	2.184156	-0.791454
H	2.735966	2.071785	-2.258788
C	-0.440917	-2.682187	1.776612
H	-0.452450	-3.780754	1.851737
H	0.119219	-2.287798	2.636928
H	-1.480041	-2.327253	1.867653
O	-1.634781	1.565302	1.015174
C	-2.468376	2.646317	1.353049
H	-2.718353	3.262764	0.472731
H	-3.401628	2.305552	1.832339
H	-1.909034	3.260505	2.069105
H	4.673730	-0.976144	0.009613
H	3.843367	-1.337110	2.183070
H	2.389466	-0.425471	2.668845
C	0.855897	3.209157	0.642494
H	1.895953	3.560477	0.736006
H	0.196480	4.089861	0.689132
H	0.630471	2.571989	1.510028
C	3.610032	0.120332	-1.628778
H	4.590192	0.524756	-1.926572
H	3.347327	-0.611790	-2.418681

motor 2a - anti-(M)-stable-Z

C	2.418866	-1.859601	-0.175618
C	1.266128	0.277961	0.110983
C	3.523331	0.256191	-0.786156
C	2.571060	0.969849	-0.157996
C	0.051194	0.887877	0.026029
C	-1.303638	0.279302	0.001065
C	-0.211750	2.395152	-0.045292
C	-2.256048	1.232114	0.393392
H	0.546041	2.960009	0.503396
C	-1.578488	2.548136	0.657438
H	-2.160127	3.402845	0.279804
C	-1.750857	-0.972645	-0.472105
C	-3.116776	-1.282322	-0.398211
C	-4.031884	-0.339020	0.074271
C	-3.615185	0.936023	0.454024
H	-1.439546	2.700081	1.741471
H	-5.092023	-0.602147	0.112589
H	-4.337867	1.689886	0.774296
H	-3.478920	-2.253151	-0.737960
C	1.437309	-1.174371	0.430622
H	4.475069	0.736306	-1.036356
C	2.862748	2.392624	0.252709
H	2.384458	3.136628	-0.401156
H	2.529170	2.590042	1.282999
H	3.946363	2.574322	0.211008
C	0.657318	-1.786055	1.572564
H	-0.419944	-1.599273	1.475371
C	-0.253012	2.895306	-1.491956
H	-1.046915	2.387792	-2.063736

H	-0.447913	3.978711	-1.527496
H	0.702428	2.703353	-2.004113
O	-0.835207	-1.795631	-1.005638
C	-1.177171	-3.120708	-1.322817
H	-0.249195	-3.614420	-1.638646
H	-1.587290	-3.655209	-0.449469
H	-1.905047	-3.170892	-2.150304
C	3.361563	-1.195073	-1.133005
H	2.997050	-1.299262	-2.175140
H	4.341081	-1.698643	-1.118829
H	0.789844	-2.879364	1.540576
C	1.119756	-1.251964	2.929772
H	0.555386	-1.721508	3.750661
H	2.190013	-1.453057	3.094714
H	0.967021	-0.163387	3.001822
H	2.575733	-2.917254	0.061330

motor 2a – TS1

C	-2.526415	-0.961157	-0.158341
C	-3.156165	-1.079570	1.020276
C	-1.266110	-0.136329	-0.115040
C	-2.128387	1.030131	1.780374
C	-1.515801	1.165063	0.592736
C	-0.066915	-0.724218	-0.353767
C	1.326324	-0.307954	0.001552
C	0.060156	-2.219520	-0.659167
C	1.998777	-1.442270	0.492024
H	-0.883556	-2.743986	-0.467033
C	1.127790	-2.662614	0.360362
H	1.693539	-3.550443	0.039254
C	2.046038	0.898472	-0.103617
C	3.348795	0.968471	0.415951
C	3.957120	-0.156936	0.970976
C	3.296459	-1.382800	0.991329
H	0.654674	-2.900907	1.328176
H	4.973821	-0.071687	1.362626
H	3.784630	-2.279614	1.379494
H	3.908208	1.902446	0.365882
C	-1.371775	2.502928	-0.088608
H	-0.469158	2.516099	-0.703117
H	-1.267355	3.290862	0.675291
C	-3.048410	-1.517122	-1.452240
H	-3.271211	-0.695147	-2.152938
C	0.502214	-2.488350	-2.099474
H	0.604045	-3.569832	-2.280191
H	-0.225546	-2.088286	-2.821829
H	1.475636	-2.017492	-2.311630
H	-2.379691	1.913055	2.378385
O	1.476016	1.925230	-0.758216
C	2.142767	3.161986	-0.847516
H	2.320185	3.603406	0.147416
H	3.101774	3.069961	-1.383645
H	1.483914	3.828591	-1.418643
C	-2.638623	-0.320757	2.222270
H	-1.829372	-0.900942	2.709130
H	-3.425042	-0.207281	2.982379
H	-4.073185	-1.670120	1.115248
H	-3.975542	-2.087013	-1.291972
H	-2.325784	-2.172340	-1.959882
C	-2.585735	2.803601	-0.972130
H	-2.710735	2.033120	-1.750230
H	-3.515556	2.836147	-0.382374
H	-2.469454	3.773222	-1.481790

motor 2a – TS2

C	0.579613	2.042617	-1.156361
C	1.639631	1.069992	-0.653365
C	2.909409	1.401671	-0.965118
C	1.355363	-0.263782	-0.031497
C	3.812342	-0.572446	0.196233
C	2.564829	-0.986320	0.484489
C	2.412007	-2.086870	1.508364
C	0.127195	-0.874735	-0.016926
C	-1.234063	-0.313183	-0.185656
C	-0.113667	-2.387849	-0.170380
C	-2.001005	-1.182257	-0.972558
H	0.799252	-2.907293	-0.488152
C	-1.153408	-2.376379	-1.326605
H	-1.731507	-3.310339	-1.390661
C	-1.861397	0.753202	0.483177
C	-3.217512	1.004445	0.227453
C	-3.938653	0.175905	-0.637025
C	-3.346542	-0.939194	-1.231642
H	-0.644655	-2.224935	-2.293822
H	-4.994976	0.392456	-0.815227
H	-3.932124	-1.617489	-1.856351
C	-0.723362	-3.090240	1.047701
H	-0.068626	-3.050082	1.927174
H	-1.684459	-2.629721	1.325968
H	-0.915106	-4.150069	0.818084
H	-3.727435	1.836840	0.712699
H	4.659754	-1.088840	0.658926
H	3.074687	2.326160	-1.529446
H	-0.420330	1.609619	-1.112066
H	3.372479	-2.270000	2.010441
H	1.678046	-1.800527	2.276524
H	2.082888	-3.043715	1.081224
O	-1.114676	1.456722	1.352978
C	-1.716538	2.482236	2.105741
H	-0.940651	2.879000	2.772393
H	-2.089075	3.299162	1.465354
H	-2.547886	2.098678	2.721313
H	0.767782	2.219875	-2.227753
C	0.595497	3.388878	-0.432788
H	1.540088	3.926839	-0.611069
H	-0.225206	4.034255	-0.784573
H	0.486698	3.258356	0.652469
C	4.124270	0.597061	-0.665095
H	4.889602	1.227153	-0.175476
H	4.604111	0.274328	-1.610642

motor 2a – TS3

C	2.460154	-0.847406	-0.324154
C	3.123823	-0.971557	0.833533
C	1.137169	-0.139681	-0.203111
C	1.984612	1.039276	1.672764
C	1.371770	1.179772	0.485353
C	-0.039643	-0.796515	-0.379778
C	-1.446498	-0.342783	-0.116304
C	-0.182911	-2.302454	-0.725419
C	-2.257940	-1.460133	0.141379
H	-0.390529	-2.356796	-1.810629
C	-1.469125	-2.719917	0.010730
H	-1.214648	-3.111226	1.012279
C	-2.075561	0.923583	-0.124091
C	-3.431697	1.030041	0.222453
C	-4.185883	-0.101810	0.528683
C	-3.607110	-1.364461	0.472840
H	-2.019003	-3.515361	-0.514502
H	-5.240906	0.014769	0.788436

H	-4.191255	-2.264971	0.675749
H	-3.915597	2.006161	0.235791
O	-1.357609	1.987067	-0.510725
C	-1.955359	3.257744	-0.574318
H	-2.811516	3.270716	-1.269333
H	-2.285684	3.606198	0.418589
H	-1.188686	3.945935	-0.952156
H	4.093952	-1.475373	0.892985
C	1.300416	2.520034	-0.221356
H	0.714225	2.421691	-1.139922
H	0.778992	3.256110	0.411038
C	2.989496	-1.214492	-1.680838
H	3.357587	-0.306278	-2.188064
H	3.826286	-1.925977	-1.616350
H	2.211464	-1.637627	-2.333212
C	0.909047	-3.317760	-0.391152
H	1.800711	-3.253700	-1.021629
H	1.221290	-3.238437	0.660349
H	0.488379	-4.326021	-0.536753
C	2.541089	-0.311645	2.068880
H	1.746806	-0.957172	2.493872
H	3.300407	-0.203231	2.856248
C	2.693272	3.051105	-0.570970
H	2.620094	4.003633	-1.120244
H	3.297419	3.227420	0.332162
H	3.244861	2.339756	-1.206183
H	2.261503	1.917605	2.266533

motor 2a - (P)-unstable-E

C	2.414070	0.455763	0.405019
C	3.570719	-0.217817	0.240200
C	1.174534	0.024967	-0.298893
C	2.477312	-1.790584	-1.332309
C	1.282411	-1.190786	-1.151595
C	0.004235	0.742068	-0.201314
C	-1.369725	0.221522	-0.155193
C	-0.120228	2.273416	-0.176637
C	-2.296008	1.247082	-0.398640
H	-0.073372	2.650010	0.861473
C	-1.561890	2.520793	-0.697751
H	-1.535871	2.699185	-1.787394
C	-1.836897	-1.014608	0.346404
C	-3.218837	-1.231829	0.438228
C	-4.119482	-0.218968	0.098965
C	-3.668417	1.039168	-0.300364
H	-2.036578	3.400955	-0.239717
H	-5.191282	-0.414078	0.185686
H	-4.374193	1.846860	-0.507550
H	-3.603528	-2.185885	0.799269
C	0.145510	-1.612368	-2.052838
H	-0.655127	-2.139134	-1.520298
H	-0.308797	-0.740244	-2.548063
H	0.518790	-2.287809	-2.835660
C	2.346619	1.448674	1.553965
H	1.952439	2.423139	1.240938
C	0.897763	3.013085	-1.042878
H	0.697458	4.096314	-1.027100
H	1.936816	2.862839	-0.721465
H	0.825549	2.671397	-2.087838
H	2.552002	-2.593827	-2.072620
O	-0.916735	-1.908055	0.751847
C	-1.327190	-3.152889	1.260558
H	-1.942453	-3.041422	2.169426
H	-1.889479	-3.736396	0.512046
H	-0.411141	-3.698928	1.518532

C	3.746506	-1.382864	-0.668552
H	4.178816	-2.228970	-0.100107
H	4.510434	-1.163789	-1.440098
H	4.430260	0.054052	0.862233
H	3.376995	1.642638	1.889951
C	1.528471	0.943671	2.744218
H	0.477981	0.758563	2.473650
H	1.941715	0.000872	3.136376
H	1.539582	1.683116	3.560002

motor 2a - syn-(M)-stable-E

C	2.419563	1.906553	-1.486813
C	1.271658	0.209205	-0.170855
C	3.693351	0.003746	-0.569085
C	2.618986	-0.371029	0.144810
C	0.155007	-0.568444	-0.077339
C	-1.282891	-0.239603	-0.259543
C	0.176707	-2.098103	-0.202006
C	-1.864161	-1.221395	-1.075205
H	1.169160	-2.458938	-0.502633
C	-0.834674	-2.284151	-1.366380
H	-1.269348	-3.294510	-1.401270
C	-2.111408	0.689468	0.393783
C	-3.469631	0.742885	0.043068
C	-4.000937	-0.171412	-0.870266
C	-3.213279	-1.185927	-1.415268
H	-0.335340	-2.097616	-2.332399
H	-5.063750	-0.111007	-1.117807
H	-3.649483	-1.947000	-2.066315
H	-4.130498	1.476799	0.504987
C	1.329436	1.586175	-0.762572
C	2.797047	-1.253587	1.364933
H	2.307753	-2.228561	1.230232
C	0.206705	2.583223	-0.674297
H	-0.023641	2.832742	0.368598
H	0.485963	3.506521	-1.201355
H	-0.718615	2.204829	-1.132004
H	2.443176	2.872521	-2.001520
C	-0.293777	-2.851298	1.045118
H	-0.272054	-3.937830	0.867361
H	0.339422	-2.638705	1.918208
H	-1.326825	-2.575384	1.310229
O	-1.561554	1.438100	1.367205
C	-2.333050	2.433462	1.994551
H	-2.691701	3.186220	1.272328
H	-3.197642	2.004219	2.528423
H	-1.676351	2.923824	2.723930
H	4.678861	-0.401428	-0.316247
H	3.871315	-1.472300	1.468272
C	2.287997	-0.615809	2.657547
H	2.475804	-1.277787	3.517024
H	2.793579	0.343556	2.851553
H	1.206255	-0.417719	2.614740
C	3.609959	1.016578	-1.663528
H	4.533660	1.618432	-1.691245
H	3.567078	0.521097	-2.654649

motor 2a - anti-(M)-stable-E

C	-1.773818	2.523813	0.197198
C	-1.179822	0.155695	0.151678
C	-3.301284	0.859596	-0.787720
C	-2.595458	-0.151740	-0.249874
C	-0.129967	-0.691114	-0.038002
C	1.327436	-0.410061	0.048795

C	-0.207237	-2.182447	-0.377226
C	2.026166	-1.608318	0.261351
H	-1.089751	-2.649040	0.068148
C	1.062427	-2.761760	0.284053
H	1.453657	-3.646990	-0.239851
C	2.062965	0.771959	-0.183108
C	3.458947	0.744964	-0.046872
C	4.119267	-0.450115	0.245131
C	3.413101	-1.644405	0.379941
H	0.851158	-3.063204	1.324374
H	5.208412	-0.444163	0.336271
H	3.934352	-2.587942	0.556852
H	4.042146	1.653578	-0.198594
C	-1.030766	1.534463	0.714873
C	-3.263677	-1.490937	-0.023973
H	-2.821303	-2.273883	-0.657831
C	-0.193210	1.742863	1.948504
H	0.800882	1.282443	1.890847
H	-0.064295	2.814726	2.159090
H	-0.696120	1.286563	2.818280
H	-1.695607	3.538868	0.600327
C	-0.229778	-2.424652	-1.888396
H	-0.272567	-3.502637	-2.110361
H	-1.105149	-1.945206	-2.352849
H	0.672520	-2.013380	-2.369177
O	1.380808	1.863594	-0.560916
C	2.022069	3.112051	-0.618852
H	2.491978	3.373849	0.344233
H	2.786643	3.144347	-1.413386
H	1.243618	3.851094	-0.847759
C	-2.763634	2.257499	-0.898109
H	-3.588814	2.985627	-0.859360
H	-2.291188	2.404549	-1.890611
H	-4.324825	0.677431	-1.131708
C	-3.246550	-1.931238	1.439425
H	-3.767463	-1.197487	2.074406
H	-3.748319	-2.903303	1.563244
H	-2.220624	-2.031294	1.827615
H	-4.308860	-1.399991	-0.357764

motor 2a - TS4

C	-2.528805	0.097516	0.016446
C	-3.052619	0.420524	1.208725
C	-1.074684	0.463742	-0.137357
C	-1.364645	2.205622	1.460876
C	-0.847342	1.893038	0.261795
C	-0.139843	-0.512402	-0.252836
C	1.330388	-0.494457	0.008677
C	-0.495403	-2.002010	-0.292076
C	1.674347	-1.696149	0.651776
H	-1.534457	-2.170774	0.016985
C	0.474943	-2.599925	0.745010
H	0.723768	-3.653933	0.548597
C	2.352032	0.432314	-0.272745
C	3.652881	0.182970	0.192628
C	3.948571	-0.992831	0.883084
C	2.965661	-1.955173	1.102602
H	0.036117	-2.546214	1.755877
H	4.971772	-1.162926	1.227226
H	3.200066	-2.894469	1.608711
H	4.450824	0.899427	-0.001840
C	-0.313242	2.942973	-0.685137
H	0.036014	2.502910	-1.624169
H	-1.115091	3.661199	-0.920801
H	0.518870	3.513010	-0.246561

C	-3.292644	-0.494874	-1.141755
H	-2.746220	-1.359528	-1.547105
C	-0.274703	-2.613047	-1.678927
H	-0.529613	-3.684469	-1.676225
H	-0.892249	-2.116119	-2.442227
H	0.778178	-2.517129	-1.990017
H	-1.283347	3.224239	1.856007
O	2.039078	1.498087	-1.026139
C	3.006264	2.484974	-1.283985
H	3.375422	2.948946	-0.353856
H	3.861665	2.081041	-1.851045
H	2.513771	3.253873	-1.892685
C	-2.216616	1.201692	2.199993
H	-1.579641	0.505625	2.781334
H	-2.857796	1.707584	2.936157
H	-4.090791	0.190662	1.463533
H	-3.276755	0.253508	-1.954561
C	-4.730177	-0.898111	-0.846638
H	-4.778738	-1.662577	-0.055183
H	-5.337344	-0.038403	-0.523218
H	-5.203239	-1.318500	-1.746752

motor 2a – TS5

C	-0.039296	-2.619167	-0.549746
C	-1.163754	-1.639222	-0.743391
C	-2.184715	-1.979159	-1.553813
C	-1.180175	-0.264266	-0.146427
C	-3.552962	-0.080739	-0.769415
C	-2.556435	0.294992	0.047974
C	-2.855620	1.191223	1.238887
C	-0.097171	0.549858	0.015528
C	1.355170	0.279603	-0.161676
C	-0.177240	2.080049	-0.097243
C	1.888601	1.283300	-0.983906
H	-1.187374	2.407698	-0.376719
C	0.813821	2.301991	-1.272770
H	1.207263	3.328754	-1.317756
C	2.225967	-0.619373	0.477803
C	3.582145	-0.616626	0.114220
C	4.068505	0.320967	-0.799943
C	3.234802	1.302892	-1.336158
H	0.314187	2.088158	-2.232942
H	5.130784	0.304914	-1.056488
H	3.633041	2.081284	-1.991074
C	0.288989	2.852254	1.139972
H	-0.331078	2.638121	2.021967
H	1.330418	2.602469	1.398012
H	0.241517	3.936173	0.951924
H	4.275953	-1.325593	0.566578
H	-4.556440	0.334992	-0.625902
H	-2.151759	-2.949646	-2.059534
H	0.128422	-2.832243	0.513209
H	-1.923161	1.466107	1.743777
H	-3.315521	2.132890	0.895772
O	1.716059	-1.398525	1.448859
C	2.526460	-2.381547	2.045377
H	1.895796	-2.906437	2.773834
H	2.897390	-3.109643	1.304053
H	3.385001	-1.937228	2.576673
H	0.909267	-2.242925	-0.959808
C	-3.773771	0.521430	2.262124
H	-3.953764	1.186733	3.121300
H	-4.750662	0.268091	1.822419
H	-3.326262	-0.410171	2.643481
H	-0.274333	-3.561590	-1.064529

C	-3.366703	-1.106471	-1.839616
H	-4.277808	-1.720753	-1.934650
H	-3.249060	-0.623892	-2.831166

motor 2a - TS6

C	2.452185	0.158072	-0.134065
C	3.076998	0.342001	1.037121
C	0.973286	0.439455	-0.097955
C	1.354342	1.978308	1.665758
C	0.774439	1.823669	0.463409
C	0.060284	-0.558069	-0.238364
C	-1.432965	-0.535860	-0.095664
C	0.410557	-2.058788	-0.427247
C	-1.898265	-1.828276	0.199046
H	0.358419	-2.263709	-1.513000
C	-0.763535	-2.795917	0.241809
H	-0.509399	-3.025384	1.292329
C	-2.405932	0.479057	-0.251644
C	-3.757947	0.191505	-0.007359
C	-4.168670	-1.095461	0.336692
C	-3.239514	-2.125290	0.426040
H	-0.998013	-3.753001	-0.247622
H	-5.229687	-1.287579	0.513923
H	-3.546747	-3.146758	0.661599
H	-4.507727	0.975851	-0.104658
O	-2.004141	1.685247	-0.675602
C	-2.945806	2.706671	-0.893787
H	-3.697518	2.413958	-1.645602
H	-3.457324	2.998783	0.038624
H	-2.387239	3.570820	-1.274543
H	1.339280	2.950583	2.170451
C	3.095452	-0.152160	-1.461195
H	2.974859	0.748518	-2.090316
H	2.513704	-0.931673	-1.980970
C	0.328037	3.012545	-0.356533
H	-0.094025	2.713774	-1.319917
H	-0.414992	3.627334	0.172234
H	1.201950	3.654526	-0.554538
C	1.712300	-2.646528	0.117182
H	2.609888	-2.365372	-0.441194
H	1.863041	-2.373830	1.172319
H	1.637284	-3.744917	0.066174
C	2.269508	0.896431	2.196125
H	2.926061	1.294120	2.982805
H	1.686728	0.078760	2.665170
C	4.565706	-0.540516	-1.408037
H	4.951311	-0.740434	-2.418984
H	5.179747	0.262268	-0.971383
H	4.722720	-1.447595	-0.802671
H	4.148040	0.163889	1.166586

motor 2b - (P)-unstable-Z

C	-2.448019	0.623517	-0.834626
C	-3.556842	-0.146228	-0.802014
C	-1.231017	0.174251	-0.129373
C	-2.633168	-1.664227	0.663113
C	-1.434822	-1.045840	0.681574
C	-0.030837	0.847727	-0.200870
C	1.315036	0.268239	-0.159941
C	0.135744	2.377788	-0.215852
C	2.284307	1.265154	0.034052
H	-0.023996	2.794822	-1.224380
C	1.622042	2.606040	0.176315
H	1.691257	2.958775	1.220116

C	1.745629	-1.032317	-0.513431
C	3.114845	-1.330174	-0.491958
C	4.051898	-0.334223	-0.204418
C	3.646562	0.978906	0.034881
H	2.113200	3.370667	-0.444388
H	5.114637	-0.589239	-0.202277
H	4.382972	1.769005	0.201000
H	3.462815	-2.336384	-0.727674
C	-0.485085	-1.474635	1.780984
H	-0.841272	-2.436057	2.183922
H	0.522794	-1.665715	1.397703
C	-2.435654	1.751872	-1.832150
H	-1.609973	1.609965	-2.547612
H	-3.376239	1.774667	-2.400726
H	-2.304964	2.742242	-1.376541
C	-0.789215	3.094803	0.770740
H	-0.626330	4.184095	0.733519
H	-1.854474	2.909713	0.577302
H	-0.583421	2.758177	1.799523
O	0.799327	-1.911801	-0.894938
C	1.155982	-3.237962	-1.190265
H	1.844369	-3.297618	-2.050557
H	1.619031	-3.739588	-0.323301
H	0.225537	-3.760955	-1.445456
H	-4.451825	0.060701	-1.391366
C	-0.395844	-0.460558	2.922726
H	-1.382474	-0.287959	3.381146
H	0.284311	-0.825490	3.707697
H	-0.010557	0.508887	2.573374
H	-2.883546	-2.515846	1.298577
O	-3.686966	-1.283157	-0.089626

motor 2b - syn-(M)-stable-Z

C	2.860786	1.287833	-1.216450
C	1.349164	-0.171394	0.004952
C	3.780077	-0.494442	-0.106018
C	2.608508	-0.828821	0.463544
C	0.146672	-0.815421	0.103826
C	-1.239683	-0.365097	-0.189535
C	0.021470	-2.347149	0.112252
C	-1.897621	-1.372354	-0.913547
H	0.980200	-2.825673	-0.125178
C	-0.973078	-2.552532	-1.060033
H	-1.503498	-3.515484	-1.010432
C	-1.994485	0.714748	0.305020
C	-3.332398	0.850775	-0.097477
C	-3.929936	-0.113321	-0.912368
C	-3.227140	-1.252011	-1.305926
H	-0.437076	-2.511998	-2.023786
H	-4.975876	0.014373	-1.202344
H	-3.715871	-2.042710	-1.880023
H	-3.927595	1.696860	0.246689
C	1.633788	1.117217	-0.682204
C	2.643329	-1.758563	1.650038
H	2.294577	-2.775706	1.425839
C	0.668150	2.261648	-0.897921
H	0.875307	2.713034	-1.881168
H	-0.361590	1.898171	-0.947360
H	3.124231	2.144268	-1.840647
C	-0.546012	-2.937513	1.405816
H	-0.651986	-4.030546	1.319486
H	0.099111	-2.724981	2.269354
H	-1.542209	-2.520082	1.623619
O	-1.394594	1.545298	1.179354
C	-2.123289	2.618040	1.723314

H	-2.449644	3.330380	0.947147
H	-3.007298	2.267180	2.282634
H	-1.449720	3.135246	2.417546
H	4.741454	-0.929305	0.174668
H	3.666534	-1.844227	2.043573
H	2.002918	-1.364930	2.454506
C	0.810270	3.337961	0.178917
H	1.797237	3.822896	0.110916
H	0.041290	4.118515	0.068724
H	0.715566	2.904149	1.184011
O	3.911157	0.450070	-1.061227

motor 2b - anti-(M)-stable-Z

C	2.551440	-1.806075	0.057992
C	1.284550	0.279503	0.067858
C	3.603852	0.118249	-0.620959
C	2.594260	0.918085	-0.221150
C	0.068323	0.893528	-0.015114
C	-1.268351	0.259550	-0.018896
C	-0.232563	2.396618	-0.019842
C	-2.224643	1.164800	0.465310
H	0.549708	2.969060	0.488305
C	-1.547352	2.468658	0.794487
H	-2.163117	3.344046	0.537020
C	-1.699366	-0.965494	-0.565754
C	-3.056506	-1.310422	-0.477069
C	-3.975947	-0.420380	0.083496
C	-3.574735	0.835748	0.540671
H	-1.328030	2.526557	1.874686
H	-5.029222	-0.708348	0.131766
H	-4.304958	1.548915	0.930338
H	-3.410742	-2.263573	-0.871182
C	1.457050	-1.143350	0.471551
H	4.574678	0.492650	-0.952040
C	2.872654	2.395920	-0.153566
H	2.271281	2.975474	-0.867423
H	2.670178	2.793648	0.852590
H	3.931511	2.590995	-0.376397
C	0.586678	-1.803581	1.517324
H	-0.468927	-1.831305	1.222513
C	-0.430357	2.957758	-1.431605
H	-1.270744	2.458795	-1.940867
H	-0.648023	4.037118	-1.396394
H	0.465812	2.809898	-2.052582
O	-0.772748	-1.725711	-1.176774
C	-1.099575	-3.028001	-1.590613
H	-0.175546	-3.471169	-1.983375
H	-1.461352	-3.644823	-0.750212
H	-1.859852	-3.027136	-2.389956
H	0.905531	-2.853537	1.615978
C	0.692286	-1.113849	2.878137
H	0.074378	-1.634088	3.626148
H	1.731807	-1.103543	3.242184
H	0.342966	-0.070931	2.825295
H	2.762486	-2.851372	0.294395
O	3.551498	-1.233154	-0.652520

motor 2b – TS1

C	2.401909	-1.210193	0.051386
C	3.105760	-1.131147	-1.090681
C	1.205788	-0.305527	0.092745
C	2.361902	0.995920	-1.527546
C	1.625928	1.040682	-0.402228
C	-0.047224	-0.805229	0.253517

C	-1.405274	-0.247389	-0.031472
C	-0.288469	-2.301329	0.476481
C	-2.225783	-1.299306	-0.481758
H	0.583387	-2.889565	0.165545
C	-1.481626	-2.603783	-0.445012
H	-2.107091	-3.435256	-0.085671
C	-1.981844	1.035610	0.077981
C	-3.305283	1.239487	-0.343422
C	-4.071353	0.181391	-0.831133
C	-3.541493	-1.104237	-0.891472
H	-1.131821	-2.867315	-1.457682
H	-5.101469	0.369600	-1.143511
H	-4.143163	-1.945881	-1.242144
H	-3.755945	2.228979	-0.270508
C	1.516996	2.335435	0.378796
H	0.824741	2.188775	1.211979
H	1.078964	3.125190	-0.253066
C	2.863037	-2.063511	1.200148
H	3.062328	-1.428210	2.078826
C	-0.616638	-2.614620	1.939420
H	-0.779311	-3.694573	2.081339
H	0.196010	-2.299183	2.610857
H	-1.532893	-2.090708	2.256821
H	2.710980	1.870604	-2.082923
O	-1.245892	2.011952	0.630633
C	-1.766995	3.311459	0.756419
H	-2.008279	3.752713	-0.225042
H	-2.665154	3.332497	1.396567
H	-0.983397	3.914441	1.232966
H	3.958970	-1.762300	-1.350760
H	3.797855	-2.585421	0.947264
H	2.127235	-2.816663	1.511955
C	2.869893	2.802450	0.919706
H	3.320144	2.036992	1.572078
H	3.584993	3.010839	0.108843
H	2.755193	3.724142	1.512695
O	2.857433	-0.171537	-2.029093

motor 2b – TS2

C	-0.656657	-2.204197	-0.976029
C	-1.645034	-1.096427	-0.671353
C	-2.895412	-1.309003	-1.131670
C	-1.350459	0.202863	-0.010521
C	-3.793077	0.488425	-0.029714
C	-2.599272	0.872384	0.457569
C	-2.602014	1.868582	1.588741
C	-0.139285	0.836265	0.069272
C	1.241154	0.352062	-0.190462
C	0.017007	2.365590	0.032624
C	1.933845	1.324605	-0.928571
H	-0.928007	2.856608	-0.232717
C	1.032065	2.514099	-1.131449
H	1.577031	3.469877	-1.107587
C	1.961066	-0.729179	0.350867
C	3.306666	-0.899237	-0.010218
C	3.942318	0.031062	-0.835874
C	3.270491	1.168808	-1.282989
H	0.509355	2.447992	-2.101084
H	4.993187	-0.122660	-1.093549
H	3.788378	1.931930	-1.868715
C	0.584262	2.986745	1.312286
H	-0.074917	2.822237	2.175242
H	1.566976	2.552375	1.556303
H	0.719536	4.072895	1.188326
H	3.877077	-1.745643	0.372868

H	-4.745102	0.922950	0.281397
H	-3.165022	-2.177287	-1.736452
H	0.363759	-1.814284	-1.003870
H	-3.614116	1.976442	2.004671
H	-1.939706	1.520189	2.396343
H	-2.260806	2.870952	1.296644
O	1.318489	-1.528457	1.224011
C	2.016419	-2.590351	1.826726
H	1.314859	-3.078370	2.514559
H	2.360835	-3.330348	1.085042
H	2.884796	-2.230108	2.404238
H	-0.857734	-2.581777	-1.991314
C	-0.764142	-3.367244	0.010593
H	-1.736828	-3.874470	-0.092630
H	0.025851	-4.114141	-0.165115
H	-0.678230	-3.013788	1.047049
O	-3.961091	-0.503627	-0.927588

motor 2b – TS3

C	2.367292	-0.992538	-0.440060
C	3.222135	-1.038888	0.592334
C	1.116793	-0.209723	-0.185072
C	2.427074	0.938691	1.422100
C	1.557356	1.099546	0.404578
C	-0.104636	-0.813542	-0.251151
C	-1.499897	-0.305530	-0.037233
C	-0.260646	-2.340897	-0.501446
C	-2.382749	-1.388223	0.125345
H	-0.274114	-2.500792	-1.595236
C	-1.658198	-2.687484	0.041256
H	-1.572925	-3.129018	1.049694
C	-2.079129	0.987100	-0.041543
C	-3.453547	1.143322	0.195950
C	-4.280699	0.040271	0.396955
C	-3.749544	-1.242324	0.347392
H	-2.184667	-3.425209	-0.582988
H	-5.347551	0.195651	0.574409
H	-4.383037	-2.123256	0.473342
H	-3.891668	2.140492	0.209530
O	-1.293392	2.037327	-0.313770
C	-1.851749	3.321350	-0.445196
H	-2.627832	3.348189	-1.227975
H	-2.279347	3.683260	0.504662
H	-1.033390	3.990799	-0.738812
H	4.141943	-1.626786	0.640143
C	1.359094	2.487937	-0.179793
H	0.759806	2.393438	-1.090405
H	0.773239	3.117661	0.506975
C	2.677433	-1.582866	-1.784939
H	2.913518	-0.775748	-2.498122
H	3.550936	-2.250462	-1.737280
H	1.832326	-2.142694	-2.210669
C	0.739079	-3.320157	0.123525
H	1.708739	-3.374366	-0.379407
H	0.914677	-3.080367	1.184004
H	0.303093	-4.331149	0.078708
C	2.674583	3.191708	-0.517322
H	2.480222	4.156749	-1.012736
H	3.276741	3.397761	0.380592
H	3.289768	2.580965	-1.197445
H	2.815589	1.748975	2.044332
O	3.032600	-0.252403	1.692596

motor 2b - (P)-unstable-E

C	2.429429	0.408456	0.338660
C	3.531830	-0.349918	0.162013
C	1.160522	0.008961	-0.302386
C	2.461018	-1.828789	-1.244633
C	1.262718	-1.223779	-1.109463
C	0.002321	0.747009	-0.198777
C	-1.374301	0.245036	-0.131298
C	-0.087565	2.279910	-0.186278
C	-2.293068	1.285236	-0.344772
H	0.039193	2.676893	0.838641
C	-1.550112	2.559309	-0.630194
H	-1.574197	2.777914	-1.712663
C	-1.853921	-0.991857	0.356032
C	-3.237230	-1.200571	0.446354
C	-4.131253	-0.173412	0.132151
C	-3.666614	1.088680	-0.240030
H	-1.993671	3.428059	-0.121228
H	-5.204606	-0.359724	0.218408
H	-4.364851	1.908625	-0.425047
H	-3.628005	-2.158131	0.791769
C	0.160936	-1.679244	-2.027796
H	-0.669827	-2.162992	-1.500869
H	-0.254741	-0.814988	-2.569986
H	0.547410	-2.393683	-2.768942
C	2.495777	1.444049	1.442133
H	2.133853	2.423511	1.103742
C	0.895994	2.978057	-1.125328
H	0.741821	4.068881	-1.102932
H	1.948645	2.786804	-0.876782
H	0.738948	2.635995	-2.161127
H	2.640418	-2.671468	-1.914343
O	-0.936987	-1.894661	0.759477
C	-1.356564	-3.147562	1.237043
H	-1.984563	-3.054637	2.139577
H	-1.910445	-3.714841	0.469443
H	-0.445797	-3.702009	1.496687
H	4.475925	-0.173771	0.681101
H	3.552938	1.595089	1.711431
C	1.714964	1.025290	2.689428
H	0.650257	0.860710	2.465804
H	2.116406	0.089232	3.108625
H	1.780576	1.802339	3.466536
O	3.596365	-1.442461	-0.623850

motor 2b - *syn*-(*M*)-stable-*E*

C	2.367959	2.133175	-1.044752
C	1.197527	0.070652	-0.410348
C	3.625546	0.379726	-0.263159
C	2.560831	-0.436920	-0.128070
C	0.054140	-0.679987	-0.293186
C	-1.333018	-0.187110	-0.188087
C	-0.113374	-2.190958	-0.529426
C	-2.204333	-1.074303	-0.835009
H	0.735422	-2.602662	-1.091488
C	-1.389827	-2.200938	-1.415983
H	-1.914877	-3.167761	-1.398162
C	-1.861178	0.858069	0.591015
C	-3.249210	1.060808	0.599108
C	-4.092297	0.206224	-0.117241
C	-3.582186	-0.882404	-0.827798
H	-1.126046	-1.980839	-2.465261
H	-5.170353	0.383902	-0.089905
H	-4.249997	-1.574377	-1.346433
H	-3.685355	1.875170	1.178704
C	1.201949	1.467631	-0.917580

C	2.842571	-1.745691	0.579424
H	2.257590	-2.569576	0.157325
C	0.002430	2.122148	-1.553156
H	-0.732636	2.479565	-0.823155
H	0.318363	2.986051	-2.155434
H	-0.512487	1.417322	-2.223453
H	2.446610	3.126197	-1.490585
C	-0.361777	-3.031929	0.727114
H	-0.568367	-4.079059	0.454664
H	0.495058	-3.029619	1.412517
H	-1.233579	-2.652783	1.284322
O	-0.987911	1.591873	1.311633
C	-1.464659	2.657258	2.095104
H	-1.958040	3.429425	1.480024
H	-2.168944	2.312314	2.871145
H	-0.589051	3.102099	2.584292
H	4.641665	0.086431	0.007877
H	3.896770	-2.014192	0.409231
C	2.594887	-1.637646	2.086452
H	2.726793	-2.611659	2.582813
H	3.300778	-0.925237	2.541379
H	1.577449	-1.278818	2.304020
O	3.580081	1.653286	-0.700503

motor 2b - *anti-(M)*-stable-*E*

C	-1.868728	2.486693	0.262674
C	-1.156546	0.162464	0.132288
C	-3.300456	0.950482	-0.665911
C	-2.563290	-0.107698	-0.271493
C	-0.107126	-0.696892	-0.016209
C	1.341227	-0.399340	0.075879
C	-0.163374	-2.203779	-0.286418
C	2.051214	-1.574748	0.366032
H	-1.059029	-2.661692	0.144573
C	1.089535	-2.729295	0.452414
H	1.495209	-3.650756	0.007630
C	2.061161	0.772086	-0.235896
C	3.457091	0.773129	-0.095775
C	4.130537	-0.392733	0.275303
C	3.437832	-1.585281	0.487709
H	0.849665	-2.949735	1.507065
H	5.219339	-0.368372	0.367352
H	3.971836	-2.508411	0.725052
H	4.029591	1.677037	-0.306960
C	-1.025855	1.533899	0.695523
C	-3.239009	-1.458742	-0.257092
H	-2.697708	-2.180100	-0.885205
C	-0.124132	1.836457	1.860805
H	0.907341	1.488876	1.732602
H	-0.098310	2.917405	2.063387
H	-0.515401	1.337032	2.763193
H	-1.843038	3.529122	0.587504
C	-0.110867	-2.525070	-1.782953
H	-0.141990	-3.612995	-1.952806
H	-0.959864	-2.071438	-2.316952
H	0.813852	-2.135428	-2.238363
O	1.359140	1.823778	-0.691651
C	1.980692	3.074877	-0.836007
H	2.440622	3.413463	0.108177
H	2.749944	3.064364	-1.626700
H	1.192254	3.783359	-1.120750
H	-4.309411	0.864173	-1.075071
C	-3.411730	-2.018145	1.155460
H	-4.051845	-1.358252	1.761555
H	-3.878266	-3.014758	1.128490

H	-2.447311	-2.111336	1.679251
H	-4.231853	-1.348214	-0.720504
O	-2.897225	2.239529	-0.587163

motor 2b – TS4

C	-2.503171	-0.015269	0.083898
C	-3.019223	0.501576	1.213078
C	-1.067543	0.368787	-0.137220
C	-1.539986	2.260013	1.217298
C	-0.946988	1.840446	0.086453
C	-0.081679	-0.563735	-0.196709
C	1.397507	-0.489617	0.016262
C	-0.399160	-2.062411	-0.220898
C	1.828059	-1.717196	0.556012
H	-1.391733	-2.254176	0.204299
C	0.683633	-2.681865	0.674827
H	0.960479	-3.703900	0.373791
C	2.370692	0.514831	-0.180685
C	3.699234	0.281000	0.206907
C	4.080629	-0.939602	0.762347
C	3.146360	-1.955559	0.934510
H	0.343609	-2.731039	1.723199
H	5.124401	-1.092782	1.047258
H	3.434619	-2.921672	1.354960
H	4.452869	1.054790	0.063254
C	-0.489596	2.832174	-0.955101
H	0.108060	2.353935	-1.734962
H	-1.371093	3.290306	-1.432994
H	0.103113	3.646806	-0.512983
C	-3.324572	-0.804048	-0.908862
H	-2.874855	-1.791418	-1.085788
C	-0.337669	-2.631626	-1.642320
H	-0.585906	-3.704818	-1.642317
H	-1.039810	-2.117026	-2.314701
H	0.672435	-2.518830	-2.068564
H	-1.528021	3.286604	1.593373
O	1.990620	1.658536	-0.770529
C	2.926222	2.683855	-0.992602
H	3.344082	3.068641	-0.047288
H	3.749804	2.352478	-1.647044
H	2.385820	3.495511	-1.496217
H	-4.009121	0.290508	1.620603
H	-3.248866	-0.278449	-1.877080
C	-4.792713	-0.987404	-0.546584
H	-4.912364	-1.554619	0.389872
H	-5.305817	-0.020752	-0.424044
H	-5.313142	-1.544730	-1.339664
O	-2.350466	1.440030	1.949200

motor 2b – TS5

C	0.095651	-1.771730	-1.904993
C	-0.901208	-1.493210	-0.812106
C	-1.765198	-2.466632	-0.476588
C	-1.080507	-0.129145	-0.241187
C	-3.227762	-0.982551	0.483586
C	-2.491929	0.102681	0.162300
C	-3.161763	1.454968	0.356314
C	-0.035830	0.747343	-0.115796
C	1.404928	0.411945	-0.109939
C	-0.065001	2.277574	0.003385
C	2.166255	1.536927	-0.461425
H	-0.912652	2.712143	-0.537273
C	1.243483	2.698487	-0.709552
H	1.648151	3.649072	-0.329496

C	2.071232	-0.741447	0.353827
C	3.472140	-0.790272	0.296737
C	4.201017	0.318444	-0.139919
C	3.556912	1.503009	-0.499568
H	1.066693	2.826018	-1.791438
H	5.292015	0.258163	-0.165279
H	4.130757	2.386860	-0.788306
C	-0.092533	2.757870	1.456422
H	-0.989782	2.394333	1.978567
H	0.787782	2.387066	2.005929
H	-0.087465	3.858266	1.509516
H	4.004660	-1.684690	0.621833
H	-4.226899	-0.923926	0.918622
H	-1.712326	-3.492580	-0.846640
H	1.143785	-1.717447	-1.586925
H	-3.264744	1.661009	1.435218
H	-2.522418	2.247343	-0.036078
O	1.312361	-1.728778	0.862380
C	1.892837	-2.970109	1.169163
H	1.074209	-3.627165	1.490101
H	2.385063	-3.419007	0.289452
H	2.626611	-2.892323	1.989591
H	-0.025210	-1.032475	-2.713796
C	-4.527385	1.581567	-0.319574
H	-4.933867	2.594988	-0.177317
H	-4.447855	1.397842	-1.402668
H	-5.265881	0.873527	0.085500
H	-0.071605	-2.770180	-2.334819
O	-2.841244	-2.266366	0.317518

motor 2b – TS6

C	2.430397	0.067322	-0.202464
C	3.172665	0.439956	0.851646
C	0.976096	0.420529	-0.103504
C	1.725836	2.138225	1.351232
C	0.925724	1.863935	0.302619
C	0.021382	-0.554464	-0.134922
C	-1.476870	-0.521019	-0.045267
C	0.400745	-2.062866	-0.187336
C	-1.972218	-1.822123	0.158539
H	0.602710	-2.324107	-1.241202
C	-0.866384	-2.816411	0.249023
H	-0.767511	-3.156193	1.294602
C	-2.444207	0.507864	-0.171792
C	-3.808841	0.212982	-0.027054
C	-4.247091	-1.088682	0.205930
C	-3.325447	-2.123491	0.289860
H	-1.055647	-3.715883	-0.356360
H	-5.317094	-1.283790	0.310358
H	-3.644145	-3.155298	0.454321
H	-4.547653	1.008779	-0.110026
O	-2.028474	1.749268	-0.457968
C	-2.969935	2.774942	-0.659690
H	-3.674060	2.528685	-1.471388
H	-3.535829	2.996779	0.260392
H	-2.404309	3.669480	-0.948682
H	1.792927	3.114673	1.838967
C	2.998485	-0.551239	-1.455411
H	2.843188	0.178743	-2.269452
H	2.405611	-1.431572	-1.747931
C	0.318348	3.023608	-0.455339
H	-0.152534	2.687625	-1.383446
H	-0.439012	3.557114	0.134990
H	1.106068	3.747188	-0.715168
C	1.568330	-2.558056	0.674175

H	2.561359	-2.331001	0.275742
H	1.505480	-2.141133	1.691947
H	1.501063	-3.654517	0.757011
C	4.472435	-0.929040	-1.393838
H	4.798295	-1.358206	-2.352900
H	5.108920	-0.054783	-1.186432
H	4.667014	-1.679472	-0.610747
H	4.223113	0.201257	1.025931
O	2.656642	1.258705	1.816847

motor 2c - (P)-unstable-Z

C	-3.345247	0.503371	-0.920580
C	-0.985984	0.401904	-0.114715
S	-3.917386	-0.950692	-0.170168
C	-2.509781	-1.392798	0.741922
C	-1.302214	-0.783940	0.724312
C	0.303055	0.901551	-0.186429
C	1.550721	0.129707	-0.183075
C	0.702021	2.389305	-0.190832
C	2.662518	0.970001	-0.016337
H	0.590619	2.833601	-1.192666
C	2.211953	2.389479	0.166888
H	2.355580	2.701409	1.215948
C	1.771560	-1.225611	-0.526607
C	3.081469	-1.721203	-0.555774
C	4.164505	-0.872405	-0.311656
C	3.966593	0.484797	-0.059786
H	2.796164	3.087819	-0.451062
H	5.176836	-1.282284	-0.348249
H	4.815640	1.156901	0.085221
H	3.267058	-2.769430	-0.791897
C	-2.103799	1.042390	-0.847590
C	-0.369960	-1.199730	1.852674
H	-0.693888	-2.185181	2.221090
H	0.663191	-1.329353	1.516187
C	-1.847154	2.183749	-1.806940
H	-1.015480	1.925047	-2.480772
H	-2.736273	2.368064	-2.424614
H	-1.591406	3.130864	-1.315432
H	-4.096177	0.948579	-1.578734
C	-0.086805	3.228359	0.817402
H	0.220959	4.285148	0.766070
H	-1.172849	3.186619	0.658797
H	0.104822	2.872500	1.841968
O	0.690518	-1.965122	-0.829968
C	0.820795	-3.350947	-1.021184
H	1.437023	-3.590210	-1.904392
H	1.253837	-3.843955	-0.134296
H	-0.192768	-3.739939	-1.182047
H	-2.706665	-2.205229	1.447495
C	-0.381127	-0.205824	3.015012
H	-1.390864	-0.098565	3.441715
H	0.292938	-0.544231	3.817046
H	-0.042983	0.790952	2.694811

motor 2c - syn-(M)-stable-Z

C	2.261110	1.151380	-1.569065
C	1.143106	0.074080	0.289135
S	3.353204	-0.216369	-1.745022
C	3.441974	-0.698815	-0.056390
C	2.439199	-0.469282	0.808043
C	0.010598	-0.656891	0.434233
C	-1.350795	-0.449830	-0.127195
C	0.030154	-2.142809	0.800729

C	-1.765933	-1.662819	-0.699604
H	1.057873	-2.529451	0.831474
C	-0.735572	-2.727892	-0.414711
H	-1.190127	-3.709120	-0.210796
C	-2.268397	0.608500	-0.023843
C	-3.503694	0.497742	-0.682472
C	-3.844951	-0.679573	-1.350732
C	-2.995252	-1.786455	-1.339197
H	-0.047062	-2.843566	-1.268941
H	-4.816059	-0.741703	-1.848052
H	-3.298251	-2.731254	-1.796018
H	-4.222161	1.317090	-0.651627
C	1.337722	1.268254	-0.594342
C	2.605098	-0.684262	2.287460
H	1.847273	-1.371065	2.691216
C	0.622938	2.584585	-0.408272
H	1.023856	3.299904	-1.142581
H	-0.444711	2.465507	-0.630019
H	2.432862	1.951877	-2.294877
C	-0.677376	-2.471478	2.116778
H	-0.654920	-3.555997	2.305522
H	-0.198350	-1.969148	2.970476
H	-1.732555	-2.155607	2.094440
O	-1.935677	1.647496	0.764669
C	-2.819250	2.734418	0.897630
H	-2.991212	3.242888	-0.066091
H	-3.788495	2.421361	1.320723
H	-2.343548	3.439070	1.590917
H	4.397724	-1.134325	0.249682
H	3.599951	-1.087381	2.525215
H	2.484064	0.272212	2.821999
C	0.779900	3.147502	1.001607
H	1.840572	3.319923	1.245002
H	0.251231	4.108218	1.099281
H	0.362717	2.454377	1.747299

motor 2c - anti-(M)-stable-Z

C	2.278321	1.252900	0.047144
C	3.323471	0.717314	-0.616512
C	1.033146	0.438457	0.207090
S	3.414697	-0.941203	-1.176124
C	2.302669	-1.663858	-0.030319
C	1.312921	-0.981453	0.571547
C	-0.221833	0.935420	0.033141
C	-1.519494	0.217368	-0.028186
C	-0.587550	2.414050	-0.119202
C	-2.566167	1.112107	0.244776
H	0.077777	3.052184	0.467700
C	-2.016130	2.494491	0.460405
H	-2.630979	3.269449	-0.022324
C	-1.838796	-1.100042	-0.421926
C	-3.177092	-1.518311	-0.387389
C	-4.189341	-0.623456	-0.034841
C	-3.898187	0.706874	0.262293
H	-1.982974	2.728532	1.538312
H	-5.224799	-0.973095	-0.025544
H	-4.695046	1.418332	0.490329
H	-3.439956	-2.539797	-0.663303
O	-0.833323	-1.878382	-0.848229
C	-1.052473	-3.242924	-1.100109
H	-1.458539	-3.760664	-0.214807
H	-1.734279	-3.398671	-1.953329
H	-0.073925	-3.674181	-1.347367
H	4.232626	1.295483	-0.806868
C	0.590227	-1.593435	1.751105

H	-0.491996	-1.416879	1.678062
C	2.435011	2.641239	0.623899
H	1.955108	2.718299	1.610806
H	3.500025	2.882624	0.747655
H	1.996605	3.416537	-0.022634
C	-0.527048	2.858868	-1.582472
H	0.486404	2.727970	-1.992363
H	-1.217534	2.267204	-2.205113
H	-0.801345	3.920722	-1.682582
H	0.736534	-2.684961	1.730945
C	1.090213	-1.031454	3.083004
H	0.554328	-1.491550	3.927712
H	2.166321	-1.222849	3.217642
H	0.931203	0.056982	3.141625
H	2.514675	-2.710294	0.208577

motor 2c – TS1

C	2.330397	-0.923212	0.756035
C	3.258068	-1.105804	-0.199114
C	1.093352	-0.155423	0.399784
C	2.272945	1.130115	-1.268233
C	1.420164	1.167005	-0.225658
C	-0.109110	-0.779672	0.420403
C	-1.437574	-0.351422	-0.097950
C	-0.249890	-2.294463	0.582537
C	-1.994172	-1.432887	-0.800675
H	0.728416	-2.790587	0.531863
C	-1.097276	-2.637699	-0.666563
H	-1.661551	-3.576664	-0.562806
C	-2.213402	0.802951	0.103939
C	-3.449301	0.913263	-0.554084
C	-3.932365	-0.138719	-1.333613
C	-3.224774	-1.335833	-1.442789
H	-0.443130	-2.733049	-1.549912
H	-4.900856	-0.028257	-1.827806
H	-3.636307	-2.182834	-1.996326
H	-4.057411	1.810212	-0.435268
C	0.912927	2.490383	0.314501
H	0.613344	2.335409	1.359785
H	-0.012678	2.765413	-0.212355
C	2.529866	-1.416098	2.162576
H	1.728806	-2.100837	2.476748
C	-0.963149	-2.704447	1.872987
H	-1.061097	-3.799665	1.930749
H	-0.412965	-2.365033	2.763271
H	-1.975171	-2.272427	1.925696
H	2.546226	2.024224	-1.834756
O	-1.759177	1.715129	0.979694
C	-2.459243	2.921210	1.159630
H	-2.579703	3.471436	0.211355
H	-3.453481	2.752997	1.607401
H	-1.861050	3.530594	1.848908
H	4.168526	-1.690601	-0.038529
H	2.517482	-0.569248	2.867909
S	3.146004	-0.314353	-1.766859
C	1.901806	3.649003	0.227521
H	2.133603	3.921960	-0.813178
H	1.477945	4.543984	0.708840
H	2.850824	3.409196	0.732526
H	3.491947	-1.937127	2.270679

motor 2c – TS2

C	-0.403969	-2.004433	-0.764608
C	-1.479558	-1.018298	-0.347381

C	-2.761616	-1.404153	-0.542936
C	-1.117062	0.372523	0.062204
S	-4.216546	-0.488855	-0.306344
C	-3.547254	0.940955	0.403469
C	-2.236925	1.243486	0.531976
C	-1.935063	2.467651	1.365894
C	0.153865	0.893847	-0.035897
C	1.468679	0.217360	-0.145409
C	0.482178	2.339285	-0.455674
C	2.251571	0.884290	-1.098837
H	-0.409877	2.858462	-0.829514
C	1.462843	2.053491	-1.627720
H	2.093296	2.919274	-1.880289
C	2.063030	-0.761816	0.670496
C	3.383711	-1.151891	0.404546
C	4.112460	-0.535065	-0.616124
C	3.563338	0.506421	-1.365555
H	0.899487	1.767922	-2.532809
H	5.141828	-0.854630	-0.796932
H	4.157025	1.028474	-2.119469
C	1.194708	3.202655	0.591597
H	0.585910	3.369752	1.488671
H	2.137053	2.731212	0.912740
H	1.443541	4.186733	0.164362
H	3.862877	-1.924691	1.006252
H	-4.309030	1.602670	0.825013
H	-2.985153	-2.391218	-0.949311
H	0.202580	-2.240938	0.117371
H	-2.833598	2.794108	1.907048
H	-1.154738	2.237722	2.106695
H	-1.585388	3.323894	0.774292
O	1.325981	-1.252494	1.688687
C	1.886507	-2.216081	2.547804
H	1.119309	-2.450697	3.296040
H	2.151957	-3.141352	2.008783
H	2.781394	-1.829207	3.063822
H	0.269612	-1.486269	-1.463413
C	-0.851490	-3.310474	-1.406942
H	-1.413526	-3.147628	-2.340099
H	0.036343	-3.909780	-1.659182
H	-1.473723	-3.920684	-0.733492

motor 2c – TS3

C	-2.335569	-0.526678	0.798569
C	-3.209597	-0.767133	-0.192226
C	-0.982368	-0.021098	0.409120
S	-2.819114	-0.341036	-1.859543
C	-1.853505	1.096723	-1.525950
C	-1.132327	1.239765	-0.395945
C	0.132255	-0.783104	0.530068
C	1.526153	-0.468516	0.095099
C	0.187880	-2.288910	0.866816
C	2.134168	-1.641100	-0.377109
H	0.663477	-2.380978	1.861261
C	1.209960	-2.801998	-0.174250
H	0.682262	-3.045272	-1.113964
C	2.306292	0.701995	0.179268
C	3.598051	0.704359	-0.370730
C	4.137369	-0.458069	-0.923142
C	3.422093	-1.653274	-0.905484
H	1.732411	-3.712185	0.155794
H	5.147288	-0.427676	-1.339597
H	3.863023	-2.578757	-1.282537
H	4.205142	1.609180	-0.341630
O	1.798697	1.746405	0.851574

C	2.517843	2.952493	0.925020
H	3.481906	2.822055	1.444606
H	2.699668	3.384038	-0.073750
H	1.898486	3.648511	1.505006
H	-4.209449	-1.180796	-0.031079
C	-0.736389	2.623528	0.091057
H	-0.353743	2.528995	1.113236
C	-2.685846	-0.636654	2.255902
H	-2.794189	0.370161	2.693173
H	-3.633726	-1.174066	2.405715
H	-1.891566	-1.142429	2.825683
C	-1.055696	-3.169114	0.840861
H	-1.772942	-2.948061	1.639241
H	-1.575829	-3.097673	-0.124776
H	-0.738006	-4.215886	0.973294
H	-2.014483	1.917393	-2.231084
H	0.101373	3.009700	-0.510242
C	-1.885433	3.631452	0.068253
H	-1.562693	4.591456	0.501366
H	-2.239528	3.832893	-0.954094
H	-2.744624	3.266732	0.653282

motor 2c - (P)-unstable-E

C	3.383646	0.297370	0.421859
C	0.971999	0.195326	-0.239090
S	3.945468	-1.014526	-0.561426
C	2.445964	-1.537798	-1.261096
C	1.214522	-1.006608	-1.072719
C	-0.272204	0.794056	-0.186852
C	-1.585700	0.140645	-0.165642
C	-0.552795	2.303814	-0.197508
C	-2.600466	1.057704	-0.480760
H	-0.616304	2.698324	0.834289
C	-1.979295	2.384778	-0.805816
H	-1.905069	2.511673	-1.900821
C	-1.944325	-1.123825	0.351831
C	-3.299618	-1.478657	0.402003
C	-4.284586	-0.571966	0.001338
C	-3.947185	0.714257	-0.422674
H	-2.560326	3.235724	-0.420909
H	-5.333966	-0.872097	0.057172
H	-4.721924	1.439033	-0.683185
H	-3.599679	-2.457182	0.777872
C	2.117190	0.767104	0.510852
C	0.136190	-1.534848	-1.989773
H	-0.638142	-2.102268	-1.461157
H	-0.362594	-0.701845	-2.509389
C	1.866499	1.718600	1.671741
H	1.320108	2.616966	1.363074
H	2.840246	2.076335	2.039330
H	4.164581	0.692977	1.077530
C	0.431029	3.143371	-1.008971
H	0.107911	4.196338	-1.029265
H	1.455589	3.119331	-0.613289
H	0.472662	2.781789	-2.048848
O	-0.949400	-1.908258	0.810504
C	-1.246074	-3.186296	1.315066
H	-1.903967	-3.136692	2.199452
H	-1.717180	-3.827966	0.551089
H	-0.289166	-3.633838	1.611245
H	2.590147	-2.343704	-1.985926
H	0.572089	-2.197551	-2.749675
C	1.115357	1.050377	2.824969
H	1.677790	0.187022	3.213475
H	0.969667	1.762306	3.651897

H	0.124360	0.689386	2.512287
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motor 2c - *syn*-(M)-stable-E

C	-2.175215	-1.624050	-1.511002
C	-1.073047	-0.138754	0.072955
S	-3.395766	-0.428088	-1.910597
C	-3.431273	0.433198	-0.383979
C	-2.388165	0.462802	0.463501
C	0.056395	0.610208	0.165800
C	1.458640	0.297335	-0.211657
C	0.038462	2.139518	0.232087
C	1.952920	1.369207	-0.970900
H	-0.979248	2.530624	0.096229
C	0.920469	2.470285	-1.002630
H	1.373426	3.471929	-0.953766
C	2.340363	-0.710145	0.212865
C	3.639734	-0.735589	-0.319304
C	4.070565	0.279141	-1.176586
C	3.245698	1.362029	-1.485765
H	0.315224	2.416463	-1.923494
H	5.089583	0.239714	-1.569715
H	3.615246	2.193313	-2.090511
H	4.336630	-1.525534	-0.037924
C	-1.207844	-1.477025	-0.582343
C	-2.560306	1.002254	1.866546
H	-1.854062	1.825051	2.047855
C	-0.321317	-2.656509	-0.286664
H	-0.211510	-2.810286	0.794781
H	-0.745827	-3.568158	-0.730172
H	0.686553	-2.517973	-0.701862
H	-2.279316	-2.555202	-2.075421
C	0.645617	2.719764	1.511476
H	0.622843	3.820351	1.484754
H	0.098733	2.391478	2.407686
H	1.695023	2.407383	1.632837
O	1.905915	-1.556988	1.163364
C	2.712600	-2.644208	1.543086
H	2.950176	-3.298000	0.686718
H	3.652952	-2.309783	2.012784
H	2.138181	-3.220006	2.279665
H	-4.395551	0.887575	-0.137813
H	-3.569967	1.431161	1.962322
C	-2.351339	-0.070612	2.935520
H	-2.476364	0.355253	3.942905
H	-3.076118	-0.891985	2.820833
H	-1.339416	-0.501136	2.875903

motor 2c - *anti*-(M)-stable-E

C	-1.912976	2.156684	0.325338
C	-1.022192	-0.136964	0.202243
S	-3.062614	1.836152	-0.961008
C	-3.287761	0.119212	-0.685779
C	-2.381356	-0.690711	-0.100855
C	0.140668	-0.790528	-0.064718
C	1.539739	-0.298255	0.005204
C	0.260561	-2.256279	-0.488632
C	2.418325	-1.389607	0.096017
H	-0.507586	-2.870395	-0.010809
C	1.647046	-2.678378	0.041836
H	2.136869	-3.431100	-0.594687
C	2.082725	0.998853	-0.123171
C	3.469475	1.174149	-0.007398
C	4.311274	0.072788	0.159823
C	3.797362	-1.222388	0.190474

H	1.557722	-3.114960	1.051228
H	5.388859	0.237148	0.237092
H	4.460508	-2.086634	0.272215
H	3.904522	2.171125	-0.080156
C	-1.082415	1.221292	0.817593
C	-2.817311	-2.089951	0.290275
C	-0.312302	1.479023	2.085415
H	0.732920	1.147767	2.023152
H	-0.325429	2.546639	2.347947
H	-0.772872	0.920426	2.917586
H	-1.967549	3.166311	0.742940
C	0.137579	-2.418896	-2.005285
H	0.224840	-3.478512	-2.292867
H	-0.834036	-2.045159	-2.364149
H	0.927518	-1.857686	-2.530150
O	1.233923	2.001774	-0.391124
C	1.681599	3.333300	-0.372501
H	2.138248	3.596408	0.596610
H	2.406489	3.534246	-1.179502
H	0.794557	3.959867	-0.531558
H	-4.275680	-0.248964	-0.978496
H	-2.346979	-2.844450	-0.358964
C	-2.538132	-2.418622	1.755180
H	-2.894629	-3.430148	2.001992
H	-1.462361	-2.375059	1.986116
H	-3.048656	-1.705633	2.421501
H	-3.898303	-2.172188	0.101710

motor 2c – TS4

C	2.387960	0.077683	-0.341954
C	3.142687	-0.134197	0.749788
C	0.956998	-0.367456	-0.280921
C	1.475219	-2.163462	1.237872
C	0.842442	-1.810071	0.102495
C	-0.027919	0.561466	-0.273011
C	-1.467727	0.436524	0.078367
C	0.245989	2.064170	-0.193027
C	-1.808552	1.526101	0.896007
H	1.306238	2.262487	0.013347
C	-0.630100	2.458247	1.018925
H	-0.926169	3.518247	1.014222
C	-2.473464	-0.458018	-0.325077
C	-3.759490	-0.325160	0.222817
C	-4.048917	0.717723	1.104473
C	-3.084470	1.670043	1.432775
H	-0.084276	2.264820	1.958138
H	-5.059714	0.801185	1.511605
H	-3.328985	2.517038	2.077796
H	-4.550721	-1.020663	-0.057690
C	0.184285	-2.867423	-0.753252
H	0.042420	-2.510809	-1.780542
H	0.805489	-3.774863	-0.779701
H	-0.803967	-3.148388	-0.364217
C	2.917665	0.682903	-1.620105
H	2.214905	1.457758	-1.962977
C	-0.176940	2.822248	-1.453561
H	0.019381	3.899593	-1.339358
H	0.368502	2.468260	-2.341164
H	-1.253160	2.693359	-1.651827
H	1.437041	-3.183841	1.632010
O	-2.158839	-1.360201	-1.269002
C	-3.126315	-2.281705	-1.706706
H	-3.493355	-2.916617	-0.882923
H	-3.983747	-1.776901	-2.183178
H	-2.635040	-2.919112	-2.452837

H	4.179125	0.198372	0.845337
H	2.873654	-0.101555	-2.396382
C	4.323826	1.259349	-1.551797
H	4.392947	2.062307	-0.801028
H	5.069164	0.490764	-1.294564
H	4.609525	1.685961	-2.524686
S	2.552025	-1.081223	2.115499

motor 2c – TS5

C	0.153939	-2.399776	-0.798206
C	-1.073404	-1.553238	-0.566173
C	-2.239929	-2.130520	-0.938365
C	-0.989979	-0.122329	-0.160937
S	-3.830005	-1.433063	-0.942124
C	-3.496842	0.048633	-0.106427
C	-2.280293	0.542681	0.205859
C	-2.228030	1.758796	1.118068
C	0.176028	0.606118	-0.183157
C	1.587958	0.155480	-0.219512
C	0.278780	2.082852	-0.605262
C	2.292837	0.932247	-1.150134
H	-0.668760	2.443712	-1.027292
C	1.349676	1.957241	-1.725813
H	1.843947	2.913441	-1.953786
C	2.297525	-0.700217	0.641707
C	3.673539	-0.876289	0.434608
C	4.335436	-0.164668	-0.569926
C	3.658378	0.767248	-1.358140
H	0.884070	1.584023	-2.653964
H	5.408790	-0.318581	-0.706047
H	4.192626	1.370415	-2.095879
C	0.780749	3.056629	0.466012
H	0.099794	3.126523	1.323882
H	1.766817	2.747424	0.847595
H	0.890249	4.065870	0.038892
H	4.246519	-1.551264	1.070844
H	-4.410416	0.551847	0.215636
H	-2.239129	-3.145982	-1.343402
H	0.694988	-2.593110	0.134310
H	-1.397362	1.592262	1.822107
H	-1.947625	2.652072	0.541241
O	1.609828	-1.280878	1.646559
C	2.283613	-2.125126	2.548112
H	1.536316	-2.460152	3.278243
H	2.707634	-3.009732	2.043405
H	3.089588	-1.593786	3.082054
H	0.847314	-1.907616	-1.494889
C	-3.489322	2.085417	1.908398
H	-3.285329	2.918997	2.597181
H	-4.322573	2.400827	1.261730
H	-3.829554	1.228143	2.510338
H	-0.130404	-3.366362	-1.234947

motor 2c – TS6

C	-2.314192	-0.112315	-0.386476
C	-3.043600	-0.121054	0.741583
C	-0.848180	-0.377156	-0.236041
S	-2.317710	-0.614202	2.277033
C	-1.203666	-1.825904	1.641384
C	-0.658132	-1.717567	0.413609
C	0.080349	0.598601	-0.387973
C	1.550325	0.536547	-0.127671
C	-0.189767	2.102277	-0.615861
C	1.990762	1.787656	0.330567

H	0.110014	2.321793	-1.658091
C	0.855817	2.762679	0.308315
H	0.426309	2.879377	1.319550
C	2.512347	-0.472725	-0.335097
C	3.841838	-0.244281	0.053397
C	4.228576	0.988013	0.581202
C	3.310123	2.027173	0.704430
H	1.157055	3.762757	-0.037629
H	5.272643	1.138740	0.866656
H	3.616608	3.010134	1.069147
H	4.592869	-1.022602	-0.080563
O	2.121115	-1.593735	-0.959075
C	3.049055	-2.623014	-1.196660
H	3.875461	-2.284963	-1.844152
H	3.465152	-3.026099	-0.258168
H	2.504498	-3.423018	-1.714194
H	-1.135911	-2.745018	2.232283
C	-2.883186	0.031483	-1.776600
H	-2.758737	-0.944146	-2.280125
H	-2.245379	0.724411	-2.350076
C	-0.160449	-2.956315	-0.299229
H	0.097189	-2.740453	-1.340907
H	0.726445	-3.384479	0.189386
H	-0.946864	-3.726443	-0.290644
C	-1.557285	2.727677	-0.366284
H	-2.321633	2.431546	-1.093077
H	-1.926324	2.497692	0.643104
H	-1.450575	3.821788	-0.442146
H	-4.112613	0.101381	0.785843
C	-4.339411	0.463920	-1.853533
H	-4.658405	0.558553	-2.902053
H	-5.004867	-0.266609	-1.367852
H	-4.496431	1.438590	-1.364601