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Excited-State Aromaticity Improves Molecular Motors: A Computational Analysis

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Supporting Information Placeholder

ABSTRACT: A new approach to the design of more efficient light-driven rotary molecular motors is presented and evaluated computationally based on molecular dynamics simulations. The approach involves enabling part of the motor to become aromatic in the photoactive excited state, and is found to sharply increase the rotary quantum yields of the photoisomerizations that underlie the motor function. Excited-state aromaticity thus holds promise as a guiding principle toward better-performing molecular motors.

Molecular motors are molecules that can perform net mechanical work using energy absorbed from an external source. Light-driven rotary molecular motors based on sterically overcrowded alkenes are the most developed class of synthetic molecular motors available today.¹ Fueled by UV light and heat, these motors produce 360° unidirectional rotary motion around a central olefinic bond connecting two molecular halves by means of consecutive photoisomerization and thermal isomerization steps. The rotary motion is controlled by the molecular chirality, which determines the preferred direction – clockwise (CW) or counterclockwise (CCW) – of the photoisomerizations.^{1a-d}

Although overcrowded-alkene motors have shown great potential for a wide variety of useful applications,^{2,3} their performance under ambient conditions is restrained in two different ways. First, the thermal isomerizations occur on much longer timescales than the photoisomerizations.^{1c,e} Second, the photoisomerization quantum yields (QYs) are limited (to ~20–30%) by the unwanted pyramidalization of one of the central olefinic carbon atoms that accompanies the desired torsional motion.^{4,5} While much effort has been invested in accelerating the thermal steps of the motors^{1b,c,e,6} and in developing alternative light-driven motor designs that complete a full 360° rotation without any thermal steps,⁷ successful attempts to address the second limitation and improve the photochemical efficiency are comparatively scarce.^{4,5,8}

Recently, however, it has been shown that a motor design that incorporates a protonated or alkylated nitrogen Schiff base offers a potential solution to this challenge.^{5,8} Specifically, it has been found that the electron-withdrawing effect of the cationic nitrogen center on the isomerizing bond hinders the aforementioned pyramidalization,⁵ whereby the associated photoisomerizations can attain both higher QYs and shorter excited-state lifetimes than overcrowded-alkene motors.⁸

In this work, we present a new motor design that, despite lacking a cationic moiety, is able to produce fast unidirectional rotary motion with similar efficiency as Schiff-base motors by rather exploiting cyclic electron delocalization in an excited state (i.e., excited-state aromaticity). In particular, by performing both minimum energy path (MEP) calculations and non-adiabatic molecular dynamics (NAMD) simulations⁹ based on multiconfigurational quantum chemistry,¹⁰ we demonstrate that the concept of excited-state aromaticity¹¹ holds substantial, yet hitherto unexplored, potential in the design of fast and efficient light-driven molecular motors. Indeed, although aromaticity is a well-established concept also for excited states,¹¹ it has in the past mostly been used to rationalize the photochemical reactivity of triplet excited states.¹²

The motor design, hereafter referred to as motor **1** and shown in Scheme 1, features a cyclopentadiene motif connected by an olefinic bond to an electron-donating chiral *N*-methyl pyrrolidine framework. As we will see, key to the performance of **1** is that the cyclopentadiene motif, which is not aromatic in its ground state, nonetheless exhibits cyclic electron delocalization in the bright second excited singlet state (S_2) of **1**.

Scheme 1. Photoinduced Cyclic Electron Delocalization in the *E* Isomer of Motor 1 and Definitions of Dihedral Angles and Cyclopentadiene Bond Length Alternation (BLA)

First, the ground-state (S_0) equilibrium geometries of the E and Z isomers of **1** with respect to the central olefinic bond were optimized with the complete active space self-consistent field (CASSCF) method.¹³ These and all other CASSCF-based calculations were performed with an active space of eight electrons (six π and the nitrogen lone pair) in seven orbitals and, unless otherwise noted, the cc-pVTZ basis set. By subsequently calculating the two lowest excited singlet states (S_1 and S_2) at the S_0 geometries using state-averaged CASSCF (SA-CASSCF), with energy corrections from complete active space second-order perturbation theory (CASPT2),¹⁴ it was found that S_1 is a dark state with negligible oscillator strength and S_2 a bright $\pi\pi^*$ state populated by a UV photon (see Table S2 of the Supporting Information (SI)). Starting from the vertical S_2 Franck-Condon (FC) points, the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of **1** were then first modeled by performing MEP calculations at the SA-CASSCF level, as further described in the SI. The resulting MEPs are given in Figure 1.

Figure 1. MEPs from the S_2 FC points of the E (a) and Z (b) isomers of motor **1**. Shown are also the motor geometries at the FC point and at two additional points along the respective path, as well as the corresponding ω dihedral angles (see Scheme 1). Encircled points are presumably close to conical intersection regions.

As illustrated by the MEPs, the geometric evolution in the S_2 state is dominated by torsional motion around the central olefinic bond, which is barrierless and (not shown) facilitated by a >0.1 Å elongation of this bond. Through this motion, the systems approach an assumed S_2/S_1 conical intersection (CI) region where they can decay to the S_1 state. With little further geometric distortion, the systems are then in a similar fashion funneled to the S_0 state through an assumed S_1/S_0 CI. Importantly, the direction of torsional motion is the same for the E and Z isomers – toward increasing values of the ω dihedral angle (see Scheme 1), which is here defined as CCW motion. Furthermore, starting CASSCF S_0 geometry optimizations

from the end points of the MEPs, the relaxation following the $S_1 \rightarrow S_0$ decay *continues* the CCW torsional motion and yields **1-Z** as the photoproduct of **1-E** and **1-E** as the photoproduct of **1-Z**, respectively. Altogether, then, the MEP results predict that consecutive $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of **1** produce a full 360° rotation, and thus that **1** is a light-driven rotary molecular motor that requires no thermal steps.

As for the character of the photoactive S_2 state of **1**, Table S4 of the SI gives the net charges of the cyclopentadiene motif in the S_0 , S_1 and S_2 states along the MEPs. Notably, despite that the motor is uncharged, in S_2 this motif acquires a sizable amount of negative charge (-0.4 – 0.5 e), which indicates the (partial) formation of a cyclopentadienyl anion. Given that this anion is well known to be aromatic, it appears that part of the motor exhibits cyclic electron delocalization in the S_2 state. Corroborating this conclusion are two observations from Figure S2 and Table S5 of the SI regarding the motor geometries along the MEPs. First, from Figure S2, it can be seen that the cyclopentadiene bond length alternation (BLA) is reduced by 0.08 – 0.12 Å in the S_2 state, compared to the situation for the FC geometries. Second, given that carbanions adopt distinctly pyramidal geometries in the absence of electron delocalization,¹⁵ it is notable from Table S5 that the C1' atom of the cyclopentadiene motif barely shows any pyramidalization at all.

With these results in mind and before probing the excited-state aromaticity of **1** in more detailed terms below, it is of interest to investigate how this feature influences the photoisomerization dynamics of the motor. To this end, the $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of **1** were modeled by performing NAMD simulations. For comparison, such simulations were also carried out for an isoelectronic analogue of **1** denoted motor **2** (see Figure 2), wherein the cyclopentadiene motif is replaced by cyclopentene and, consequently, the possibility of excited-state aromaticity is lost. Importantly, through MEP calculations analogous to those performed for **1**, but with the SA-CASSCF treatment adopted to the fact that the photoactive state of **2** is S_1 rather than S_2 (see Table S6 of the SI), it was first confirmed that also the UV-induced $E \rightarrow Z$ and $Z \rightarrow E$ photoisomerizations of **2** afford barrierless 360° unidirectional rotary motion (see Figure S3 of the SI).

Figure 2. Chemical structure of the E isomer of motor **2**.

As further described in the SI, the NAMD simulations were started in the photoactive state (S_2 for motor **1**; S_1 for motor **2**) and were run at the SA-CASSCF/6-31G(d) level for maximally 800 fs and with 200 different initial nuclear configurations and velocities for both the E and Z isomers. Hops between states were allowed based on the magnitudes of the energy gap and non-adiabatic coupling between the states.^{9a,10} To quantify the efficiency of the motors, the *rotary* QY of a photoisomerization is defined as the percentage of the 200 trajectories that form the Z (E) isomer from the E (Z) isomer by completing a

net CCW 180° rotation around the central olefinic bond relative to the starting nuclear configuration within 800 fs. Furthermore, the photoisomerization time (PIT) is defined as the time needed for one such rotation, and the excited-state lifetime (τ) as the time needed for any trajectory rotating in the CCW direction to first reach the S_0 state. The distributions of PIT and τ values from the NAMD simulations are presented in Figure 3 for motor **1** and in Figure S4 of the SI for motor **2**. Shown are also the corresponding rotary QYs and the percentages of trajectories that reach the S_0 state.

Figure 3. Distributions of τ (blue circles) and PIT (red circles) values for the $E \rightarrow Z$ (a) and $Z \rightarrow E$ (b) trajectories of motor **1** and the corresponding changes in the ω dihedral angle relative to the starting nuclear configurations (black circles). Shown are also the average τ and PIT values, the percentages of trajectories that reach the S_0 state, and the rotary QYs.

Starting with Figure 3, it is notable that the rotary QYs of **1** are much higher, 77 and 75%, than the QYs of ~20–30% typically achieved by overcrowded-alkene motors.^{4a,c} Accordingly, the net CCW directionality of the full 360° rotary cycle is a substantial 58% (77% $\times$ 75%). Another positive feature of **1** is that the average τ and PIT values are only ~200 and ~320 fs, respectively. As a comparison, overcrowded-alkene motors typically have excited-state lifetimes of ~1 ps or more.^{4a,c} Overall, it is also very encouraging that the performance data on **1** in Figure 3 compare very well with the corresponding data available for Schiff-base motors,⁸ despite that **1** lacks the ability of Schiff-base motors to favorably influence the efficiency of the rotary motion through a cationic nitrogen center.⁵

Continuing with the results for reference motor **2** in Figure S4, it is clear that replacing the cyclopentadiene motif of **1** with cyclopentene in **2** – and thereby foregoing the possibility of excited-state aromaticity – worsens the photochemical per-

formance. In fact, this reduces the rotary QYs from 77 and 75% to 40 and 49%, and increases the average τ and PIT values by ~250 fs. Thus, the presumed excited-state aromaticity of **1** has a major positive effect on the efficiency of this motor. This conclusion is corroborated by complementary NAMD results (summarized in the SI in connection to Figure S5) on a second isoelectronic reference motor, which, contrary to **2**, maintains a methyl group at the C5 position.

In order to further probe the aromaticity of the cyclopentadiene motif in the S_2 state of **1**, two different aromaticity indices were calculated based on the SA-CASSCF wave functions and geometries along the photoisomerization MEPs of **1**: the Shannon aromaticity (SA)¹⁶ index and the harmonic oscillator model of aromaticity (HOMA)¹⁷ index. As outlined in the SI, SA is an electronic index based on Bader’s theory of atoms in molecules¹⁸ that probes the electron density variation at bond critical points (BCPs).¹⁶ HOMA, in turn, is a geometric index based on the deviation of the carbon-carbon bond lengths from an ideal aromatic reference value.¹⁷ The results of the calculations are given in Figure 4.

Figure 4. SA and HOMA values for the cyclopentadiene motif along the photoisomerization MEPs of the E (a) and Z (b) isomers of motor **1**.

As can be seen from Figure 4, the SA values are ~0.007 at the S_2 FC points but drop into the range of 0.0001–0.001 as the photoisomerizations proceed in the S_2 state. Through a comparison with the previous BLA plots in Figure S2, it is clear that this effect is due to the pronounced cyclopentadiene bond length equalization in this state of the motor. The small SA values are reflective of small variations in electron density between different BCPs, as expected for an aromatic system.¹⁶ Moreover, the appreciable lowering of the SA values suggests that excited-state aromaticity may in fact provide the driving force for the photoisomerizations. The same picture emerges

from consideration of the HOMA values, which are close to 0 at the S₂ FC points but subsequently increase into a range (0.7–0.8) quite close to 1, as usually found for aromatic systems.^{17c} Finally, as a qualitative validation of the results in Figure 4, Table S7 of the SI gives nucleus-independent chemical shifts¹⁹ of the *E* and *Z* isomers of **1** calculated at the S₂ FC point and a subsequent S₂ MEP point.

In summary, we have discovered a new route to the design of fast and efficient light-driven rotary molecular motors along which excited-state aromaticity is exploited to both shorten the lifetimes and increase the rotary QYs of the *Z/E* photoisomerizations that underlie the motor function. Illustrating the potential of the route through comparative NAMD simulations of two motors with and without a moiety exhibiting such electron delocalization, the results attribute a key role to excited-state aromaticity in the future development of more powerful and efficient molecular motors.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website.

Computational details, complementary results (Figures S1–S5 and Tables S1–S7), description of multimedia files, and Cartesian coordinates and energies of different geometries of motors **1** and **2** (PDF). Two multimedia files are also supplied (AVI).

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Notes

The authors declare no competing financial interest.

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Excited-State Aromaticity Improves Molecular Motors: A Computational Analysis

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Computational details

MEP calculations. The minimum energy path (MEP) calculations on motor **1** were carried out with the complete active space self-consistent field (CASSCF) method¹ in combination with Dunning's correlation-consistent polarized valence triple- ζ (cc-pVTZ) basis set.² The active space included eight electrons (six π and the nitrogen lone pair) distributed in seven orbitals. First, following CASSCF optimization of the ground-state (S_0) equilibrium geometries of the *E* and *Z* isomers, the wave functions at the vertical Franck-Condon (FC) points in the first (S_1) and second (S_2) excited singlet states of the two isomers were calculated using state-averaged CASSCF (SA-CASSCF) with equal weights for the S_0 , S_1 and S_2 states and with energy corrections from complete active space second-order perturbation theory (CASPT2).³ Having found from these calculations that S_1 is a dark state with negligible oscillator strength and S_2 a bright $\pi\pi^*$ state populated by absorption of a UV photon (see Table S2), the actual SA-CASSCF MEP calculations were then started from the S_2 FC points.

With one exception, the protocol just described was also employed for the MEP calculations on motor **2**. Specifically, since the photoactive state of **2** is S_1 rather than S_2 (see Table S6), the corresponding SA-CASSCF treatment included only the S_0 and S_1 states, with equal weights.

NAMD simulations. Similar to the MEP calculations, the non-adiabatic molecular dynamics (NAMD) simulations of motor **1** were also carried out using three-state (S_0 , S_1 and S_2) SA-CASSCF with an active space of eight electrons in seven orbitals. For all simulations, Pople's 6-31G(d) split-valence double- ζ plus polarization basis set⁴ was used. First, following calculation of the S_0 vibrational normal modes of the *E* and *Z* isomers by means of Møller-Plesset second-order perturbation theory (MP2) with the def2-SVP basis set⁵ and within the resolution-of-the-identity (RI) approximation,⁶ 200 different initial nuclear configurations and velocities for the two isomers were generated from a harmonic-oscillator Wigner distribution.⁷ The use of MP2 for calculating the normal modes was validated through a favorable comparison of the geometries obtained with this method and those obtained with CASPT2 (see Tables S2 and S3). For both isomers, 200 photoisomerization trajectories were then initiated by promoting the systems to the S_2 state. Evaluating nuclear forces "on the fly", the trajectories were propagated classically using the velocity Verlet algorithm⁸ with a fixed integration time step of 0.5 fs.

Employing the algorithm by Robb and co-workers⁹ as implemented in the MOLCAS 8.0 suite of programs,¹⁰ the non-adiabatic coupling vectors $\langle \Psi_i | \frac{\partial}{\partial \mathbf{R}} \Psi_j \rangle$ between the S₂ and S₁ states and between the S₁ and S₀ states were evaluated in the framework of Landau-Zener theory,¹¹ wherein the couplings are large when $\langle \Psi_i | \frac{\partial}{\partial t} \Psi_j \rangle$ is large. Specifically, the $\langle \Psi_i | \frac{\partial}{\partial t} \Psi_j \rangle$ terms were computed at each step along the trajectories for which the energy gap between the states is smaller than 0.03 a.u., using the numerical approximation

$$\langle \Psi_i(t) | \frac{\partial}{\partial t} \Psi_j(t) \rangle \approx \frac{\langle \Psi_i(t) | \Psi_j(t + \Delta t) \rangle}{\Delta t}. \quad (1)$$

Based on this model, a trajectory was allowed to hop from one state to the other (and later possibly back again) when $\langle \Psi_i(t) | \Psi_j(t + \Delta t) \rangle$ is larger than 0.25, representing situations when the wave functions of the states in questions begin to deviate from orthogonality close to a conical intersection. Allowing maximally 20 hops in each trajectory, the simulations were run for up to 800 fs.

The NAMD simulations of motor **2**, in turn, were carried out with the same exact protocol as those of motor **1**, expect that the trajectories were started in the S₁ state and were run using two-state (S₀ and S₁) SA-CASSCF, to account for the fact that S₁ rather than S₂ is the photoactive state of this system (see Table S6).

Calculation of aromaticity indices. Below, the procedures to calculate Shannon aromaticity (SA)¹² and harmonic oscillator model of aromaticity (HOMA)¹³ indices are described. Based on SA-CASSCF wave functions and geometries along the photoisomerization MEPs of motor **1**, these indices were used to probe the aromaticity of the cyclopentadiene motif in the S₂ state of motor **1**.

Starting with SA, this electronic index is based on Bader's theory of atoms in molecules (AIM)¹⁴ and probes the variation in electron density between different bond critical points (BCPs) of the aromatic ring in question.¹² Specifically, this index is formulated in terms of the so-called Shannon entropy,¹⁵ defined as

$$S = - \sum_i^N p_i(\mathbf{r}_c) \ln p_i(\mathbf{r}_c), \quad (2)$$

where $\mathbf{r}_c$ is a BCP of the ring and N is the number of BCPs in the ring. Moreover, $p_i(\mathbf{r}_c)$ is the normalized probability electron density at a given BCP, defined as

$$p_i(\mathbf{r}_c) = \frac{\rho_i(\mathbf{r}_c)}{\sum_i \rho_i(\mathbf{r}_c)}, \quad (3)$$

where $\rho_i(\mathbf{r}_c)$ is the electron density at that BCP. By defining the SA index as the difference between the Shannon entropy that the system under consideration would have if it was perfectly aromatic and the Shannon entropy that it *actual* has, a small value for this difference then suggests that the electron density variation at BCPs is minor, as expected for an aromatic system.¹² Typically, aromatic compounds show SA values below 0.003.¹²

Continuing with HOMA, this geometric index probes the deviation of the carbon-carbon bond lengths R_i of the aromatic ring in question from the reference optimal bond length R_{opt} of the fully aromatic benzene molecule.¹³ Specifically,

$$\text{HOMA} = 1 - \frac{\alpha}{n} \sum_i^n (R_i - R_{\text{opt}})^2, \quad (4)$$

where n is the number of carbon-carbon bonds and α is an empirical normalization factor chosen in such a way that HOMA approaches 1 for an aromatic compound with all R_i close to R_{opt} , and approaches 0 for the corresponding (and hypothetical) non-aromatic Kekulé structures.¹³ In this work, the standard parameters $\alpha = 257.7 \text{ \AA}^{-2}$ and $R_{\text{opt}} = 1.388 \text{ \AA}$ were employed.¹³ Although these parameters have been defined for studies of ground-state compounds, this does not prevent them from being used for a balanced comparison of HOMA values for a series of different excited-state geometries of *one single compound*, for which the parameters are equally appropriate.

Finally, as a complement to the SA and HOMA indices, nucleus-independent chemical shifts (NICSs)¹⁶ of the *E* and *Z* isomers of motor **1** were calculated at the S_2 FC point and an arbitrarily chosen (the fifth) subsequent S_2 MEP point. Specifically, at these points, NICS(1)_{zz} values corresponding to the negative of the ZZ-component of the magnetic shielding tensor 1 Å above the cyclopentadiene ring center (as obtained from AIM theory) were calculated from state-specific CASSCF(8,7) wave functions obtained using gauge-including atomic orbitals and the 6-31G(d) basis set. For NICSs, negative values indicate aromaticity.^{16a} The reason for limiting the

NICS calculations to a single S_2 MEP point is the technical requirement that the S_2 CASSCF wave function is converged in a state-specific fashion, which becomes progressively more difficult as the S_2 and S_1 states come closer in energy.

Software used. The RI-MP2 calculations were done with TURBOMOLE 6.3.¹⁷ The SA and HOMA indices were calculated with Multiwfn.¹⁸ The NICS calculations were done with Dalton2013.¹⁹ All other calculations were done with MOLCAS 8.0.¹⁰

Figure S1. Active molecular orbitals at the CASSCF/cc-pVTZ S_0 equilibrium geometries of the *E* and *Z* isomers of motor **1**.

Figure S2. Bond length alternation (BLA) in the cyclopentadiene motif along the photoisomerization MEPs of the *E* (a) and *Z* (b) isomers of motor **1**. Only MEP points in the S_2 state are shown.

Figure S3. MEPs from the S_1 FC points of the *E* (a) and *Z* (b) isomers of motor **2**. Shown are also the motor geometries at the FC point and at two additional points along the respective path, as well as the corresponding ω dihedral angles (see Scheme 1). Encircled points are presumably close to conical intersection regions.

Figure S4. Distributions of excited-state lifetimes (τ , blue circles) and photoisomerization times (PITs, red circles) for the $E \rightarrow Z$ (a) and $Z \rightarrow E$ (b) trajectories of motor **2** and the corresponding changes in the ω dihedral angle relative to the starting nuclear configurations (black circles). Shown are also the average τ and PIT values, the percentages of trajectories that reach the S_0 state, and the rotary QYs.

Figure S5. Chemical structure of the *E* isomer of motor **3**.

Comments on Figure S5: Just like reference motor **2**, **3** is an isoelectronic analogue of motor **1**, that was studied to further solidify the conclusion that excited-state aromaticity is a key factor for the efficiency of **1**. Similar to **2**, **3** cannot exhibit excited-state aromaticity. However, in contrast to **2**, **3** carries a methyl group at the C5 position, which is also the situation for **1**. First, through CASSCF-based calculations identical to those summarized for **2** in Table S6, it was found that the photoactive state of **3** is S_1 , with oscillator strengths of ~ 0.4 – 0.5 . Second, in NAMD simulations of **3** identical to those performed for **2** but with much fewer initial nuclear configurations and velocities considered (10 instead of 200), it was observed that 4 out of the 10 trajectories run for both the *E* and *Z* isomers of **3** complete a 180° rotation within 800 fs, with the same preferred direction of rotation. Comparing with the 75/77% rotary QYs of **1** (see Figure 2), these results underline the positive influence of excited-state aromaticity on the motor efficiency. Moreover, comparing with the 40/49% rotary QYs of **2** (see Figure S4), they also suggest that the positions of methyl groups are not important in this regard.

Table S1. Occupation Numbers of Active Molecular Orbitals in the S₀, S₁ and S₂ States of the *E* and *Z* Isomers of Motor 1^a

isomer	state	active molecular orbital						
		1	2	3	4	5	6	7
<i>E</i>	S ₀	1.96	2.00	1.91	1.91	0.11	0.05	0.06
	S ₁	1.95	2.00	1.89	1.05	0.97	0.06	0.08
	S ₂	1.95	1.96	1.32	1.86	0.69	0.07	0.15
<i>Z</i>	S ₀	1.96	2.00	1.91	1.91	0.11	0.05	0.06
	S ₁	1.95	2.00	1.89	1.03	0.99	0.06	0.08
	S ₂	1.95	1.96	1.32	1.86	0.70	0.07	0.15

^aAll calculations performed based on SA-CASSCF/cc-pVTZ wave functions computed with equal weights for the S₀, S₁ and S₂ states at CASSCF/cc-pVTZ S₀ equilibrium geometries.

Table S2. Vertical CASPT2/cc-pVTZ Excitation Energies (eV) of the *E* and *Z* Isomers of Motor 1^a

isomer	excitation	CASPT2 treatment	S ₀ geometry			
			CASSCF/ cc-pVTZ	CASPT2/ cc-pVDZ ^b	RI-MP2/ cc-pVDZ	RI-MP2/ def2-SVP
<i>E</i>	S ₀ → S ₁	SS-CASPT2 ^c	4.03 (0.014)	3.74 (0.029)	3.75 (0.023)	3.74 (0.030)
		MS-CASPT2 ^d	4.14 (0.014)	3.87 (0.029)	3.87 (0.023)	3.87 (0.030)
	S ₀ → S ₂	SS-CASPT2 ^c	4.05 (0.691)	3.94 (0.535)	4.06 (0.529)	3.95 (0.541)
		MS-CASPT2 ^d	4.32 (0.691)	4.23 (0.535)	4.32 (0.529)	4.24 (0.541)
<i>Z</i>	S ₀ → S ₁	SS-CASPT2 ^c	4.05 (0.013)	3.75 (0.028)	3.75 (0.023)	3.75 (0.030)
		MS-CASPT2 ^d	4.16 (0.013)	3.88 (0.028)	3.88 (0.023)	3.88 (0.030)
	S ₀ → S ₂	SS-CASPT2 ^c	4.05 (0.696)	3.94 (0.537)	4.05 (0.530)	3.95 (0.542)
		MS-CASPT2 ^d	4.31 (0.696)	4.22 (0.537)	4.32 (0.530)	4.23 (0.542)

^aAll calculations performed based on SA-CASSCF wave functions computed with equal weights for the S₀, S₁ and S₂ states. Oscillator strengths in parentheses obtained with the complete active space state-interaction (CASSI) method (Ref. 20). ^bObtained with numerical CASPT2 gradients. ^cState-specific CASPT2.

^dMulti-state CASPT2.

Table S3. Optimized S_0 Geometric Parameters ($\text{\AA}$ and degrees) of the *E* and *Z* Isomers of Motor 1 at Different Levels of Theory

isomer	parameter ^a	CASSCF/ cc-pVTZ	CASPT2/ cc-pVDZ ^b	RI-MP2/ cc-pVDZ	RI-MP2/ def2-SVP
<i>E</i>	C1–C1'	1.36	1.39	1.39	1.38
	C1–N2	1.37	1.36	1.36	1.35
	θ	–178	–176	–173	–174
	θ'	–179	–171	–169	–168
	ω	–178	–173	–171	–171
<i>Z</i>	C1–C1'	1.36	1.39	1.39	1.38
	C1–N2	1.37	1.36	1.36	1.35
	θ	0	5	8	8
	θ'	2	7	10	10
	ω	1	6	9	9

^aParameters defined in Scheme 1. ^bObtained with numerical CASPT2 gradients.

Table S4. Sum of Mulliken Atomic Charges in the Cyclopentadiene Motif in the S₀, S₁ and S₂ States along the Photoisomerization MEPs of the *E* and *Z* Isomers of Motor 1^a

isomer	state	geometry/MEP point ^b										
		FC ^c	FC	1	2	3	4	5	6	7	8	9
<i>E</i>	S ₀	-0.16	-0.17	-0.22	-0.21	-0.21	-0.22	-0.23	-0.24	-0.25	-0.25	-0.25
	S ₁		0.02	0.08	0.08	0.08	0.08	0.07	0.07	0.07	0.07	0.07
	S ₂		-0.41	-0.37	-0.41	-0.43	-0.45	-0.46	-0.47	-0.47	-0.47	-0.47
<i>Z</i>	S ₀	-0.14	-0.15	-0.20	-0.20	-0.20	-0.20	-0.21	-0.22	-0.23	-0.23	-0.24
	S ₁		0.05	0.09	0.10	0.10	0.10	0.09	0.09	0.09	0.08	0.08
	S ₂		-0.39	-0.36	-0.39	-0.42	-0.43	-0.44	-0.45	-0.45	-0.45	-0.45

^aAll calculations except where otherwise indicated performed based on SA-CASSCF/cc-pVTZ wave functions computed with equal weights for the S₀, S₁ and S₂ states. ^bOnly MEP points in the S₂ state are shown. ^cCalculations performed based on state-specific CASSCF/cc-pVTZ wave functions.

Table S5. Pyramidalization Dihedral Angles (degrees) along the Photoisomerization MEPs of the *E* and *Z* Isomers of Motor 1^a

isomer	angle ^c	geometry/MEP point ^b									
		FC	1	2	3	4	5	6	7	8	9
<i>E</i>	α	0	-6	-12	-15	-16	-16	-16	-15	-14	-13
	α'	0	0	0	1	1	1	1	1	1	0
<i>Z</i>	α	0	-6	-13	-16	-17	-18	-18	-18	-17	-16
	α'	1	0	1	2	3	4	5	6	6	7

^aAll calculations performed based on SA-CASSCF/cc-pVTZ wave functions computed with equal weights for the S₀, S₁ and S₂ states. ^bOnly MEP points in the S₂ state are shown. ^cDihedral angles defined in Scheme 1.

Table S6. Vertical CASPT2/cc-pVTZ Excitation Energies (eV) of the *E* and *Z* Isomers of Motor 2^a

isomer	excitation	S ₀ geometry		
		CASSCF/ cc-pVTZ	RI-MP2/ cc-pVDZ	RI-MP2/ def2-SVP
<i>E</i>	S ₀ → S ₁	4.25 (0.293)	4.12 (0.243)	4.06 (0.227)
	S ₀ → S ₂	5.43 (0.050)	5.36 (0.032)	5.32 (0.031)
<i>Z</i>	S ₀ → S ₁	4.09 (0.298)	3.94 (0.239)	3.88 (0.226)
	S ₀ → S ₂	5.46 (0.031)	5.32 (0.025)	5.28 (0.024)

^aAll calculations performed using state-specific CASPT2, based on SA-CASSCF wave functions computed with equal weights for the S₀, S₁ and S₂ states. Oscillator strengths in parentheses obtained with the complete active space state-interaction (CASSI) method (Ref. 20).

Table S7. NICS(1)_{ZZ} Values (ppm) for the Cyclopentadiene Motif at Two Points along the Photoisomerization MEPs of the *E* and *Z* Isomers of Motor 1.^a

isomer	S ₂ FC point	S ₂ MEP point 5
<i>E</i>	−31	−82
<i>Z</i>	−35	−82

^aAll values calculated from state-specific CASSCF wave functions obtained using gauge-including atomic orbitals and the 6-31G(d) basis set.

Comment on Table S7: As a clear sign that the cyclopentadiene motif gains aromaticity during the photoisomerizations, the NICS(1)_{ZZ} values are much more negative at the fifth S₂ MEP points than at the S₂ FC points.

Description of multimedia files

1E-Z-E.avi This movie from the NAMD simulations of motor **1** shows two representative trajectories merged together to illustrate a full $360^\circ E \rightarrow Z \rightarrow E$ rotation around the central olefinic bond.

2E-Z-E.avi This movie from the NAMD simulations of motor **2** shows two representative trajectories merged together to illustrate a full $360^\circ E \rightarrow Z \rightarrow E$ rotation around the central olefinic bond.

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Cartesian coordinates (Å) and energies (a.u.) of different geometries of motors 1 and 2

1-*E*, S₀ geometry

CASSCF/cc-pVTZ S₀ energy: -518.96617911

C	-0.70961096	0.04538929	-0.14267191
C	0.62712810	0.28221913	-0.08052262
C	1.38252611	1.53489753	0.05711937
C	1.65428313	-0.76385311	-0.17239699
C	2.88325190	-0.20319303	-0.09920924
C	2.70352420	1.24501346	0.04611591
N	-1.74542353	0.94454595	-0.10787502
C	-3.04396237	0.30758001	-0.15944937
H	3.50304009	1.95501601	0.12754225
C	-1.31683303	-1.34602708	-0.26193028
C	-2.73238851	-1.05018967	-0.77166409
H	-2.72833176	-0.96572500	-1.85147653
H	-3.44956650	-1.81146443	-0.49552296
H	-3.48449265	0.21156146	0.83243180
H	-3.73009490	0.88933001	-0.76272180
H	-0.76757444	-1.94211545	-0.97539308
H	0.97319171	2.51528572	0.15074512
C	-1.64278234	2.31511402	0.31127943
H	-1.13636746	2.41072704	1.26659410
H	-1.11701016	2.91969401	-0.41742632
H	-2.63895578	2.72105466	0.41729056
C	-1.33279089	-2.07540993	1.08591288
H	-1.79995785	-3.04855087	0.98020735
H	-0.33120259	-2.21824514	1.46688796
H	-1.88995641	-1.51699265	1.83012818
H	1.45983655	-1.80976523	-0.29044185
C	4.21266196	-0.89009220	-0.15727088
H	4.80471128	-0.52919550	-0.99255379
H	4.78790745	-0.70880124	0.74535744
H	4.09605364	-1.96076373	-0.26898660

1-*E*, MEP point 1 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.93470749

SA-CASSCF/cc-pVTZ S₁ energy: -518.83174355

SA-CASSCF/cc-pVTZ S₂ energy: -518.78130766

C	-0.777366	0.021368	-0.044232
C	0.690352	0.295863	-0.048030
C	1.362454	1.528289	0.079874
C	1.640057	-0.740818	-0.198296
C	2.933890	-0.166793	-0.128563
C	2.760247	1.251023	0.037387
N	-1.741537	0.944018	-0.112075
C	-3.060338	0.333530	-0.211196
H	3.546388	1.970680	0.140151
C	-1.348466	-1.349777	-0.233149
C	-2.762381	-1.055579	-0.758294
H	-2.756034	-1.022975	-1.840273
H	-3.494492	-1.787731	-0.448225
H	-3.520568	0.299619	0.773812
H	-3.698037	0.924722	-0.853735
H	-0.769673	-1.896676	-0.967152
H	0.943766	2.498234	0.214283
C	-1.647896	2.336039	0.272715
H	-1.174332	2.441699	1.239553
H	-1.091558	2.905462	-0.455540
H	-2.648756	2.736326	0.330250
C	-1.343852	-2.143289	1.081736
H	-1.731274	-3.142933	0.917697
H	-0.342677	-2.226112	1.480078
H	-1.963001	-1.660907	1.830239
H	1.434945	-1.783422	-0.319186
C	4.238716	-0.897036	-0.168023
H	4.874662	-0.536498	-0.971836
H	4.796983	-0.777779	0.756746
H	4.086011	-1.958714	-0.322785

1-E, MEP point 2 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.92391335

SA-CASSCF/cc-pVTZ S₁ energy: -518.83276046

SA-CASSCF/cc-pVTZ S₂ energy: -518.78316126

C	-0.795225	0.019437	0.066775
C	0.695442	0.298779	0.003654
C	1.375166	1.520839	0.176120
C	1.640270	-0.719296	-0.261778
C	2.931179	-0.152499	-0.186617
C	2.761602	1.252040	0.061699
N	-1.730091	0.947409	-0.143250
C	-3.055795	0.356870	-0.279808
H	3.550922	1.965457	0.186340
C	-1.356826	-1.352243	-0.175545
C	-2.763828	-1.065982	-0.734080
H	-2.748138	-1.103802	-1.815355
H	-3.508240	-1.768396	-0.386974
H	-3.563339	0.389750	0.681643
H	-3.646028	0.925295	-0.984822
H	-0.754071	-1.855864	-0.921785
H	0.961647	2.479539	0.389916
C	-1.640280	2.354067	0.196185
H	-1.246996	2.484986	1.195714
H	-1.013029	2.883054	-0.502577
H	-2.634231	2.773002	0.156074
C	-1.355016	-2.204620	1.097860
H	-1.701613	-3.208054	0.877105
H	-0.359366	-2.272497	1.514053
H	-2.007567	-1.780790	1.853273
H	1.432878	-1.757041	-0.419564
C	4.234360	-0.890982	-0.216300
H	4.919426	-0.463536	-0.942893
H	4.736421	-0.866008	0.747457
H	4.085714	-1.931962	-0.479011

1-E, MEP point 3 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91603027

SA-CASSCF/cc-pVTZ S₁ energy: -518.83283303

SA-CASSCF/cc-pVTZ S₂ energy: -518.78616788

C	-0.804556	0.022089	0.120064
C	0.693942	0.298333	0.048355
C	1.383303	1.497898	0.312726
C	1.627507	-0.690194	-0.343997
C	2.917739	-0.135441	-0.241575
C	2.758126	1.242420	0.127186
N	-1.715120	0.945390	-0.184378
C	-3.043821	0.365431	-0.339041
H	3.553443	1.942124	0.287870
C	-1.357995	-1.354979	-0.120498
C	-2.758309	-1.083278	-0.706725
H	-2.735348	-1.185665	-1.783461
H	-3.512333	-1.757264	-0.325815
H	-3.583302	0.457449	0.600906
H	-3.600294	0.903594	-1.093301
H	-0.742318	-1.846046	-0.864259
H	0.975205	2.433134	0.623869
C	-1.623848	2.363205	0.110424
H	-1.342306	2.521445	1.144177
H	-0.906191	2.847297	-0.529468
H	-2.594681	2.804074	-0.056342
C	-1.358359	-2.221880	1.139910
H	-1.697097	-3.223963	0.902547
H	-0.363683	-2.290430	1.559157
H	-2.017450	-1.813385	1.897915
H	1.416046	-1.714187	-0.571390
C	4.217108	-0.880738	-0.288885
H	4.938643	-0.384107	-0.931047
H	4.670799	-0.963028	0.695613
H	4.077912	-1.886727	-0.667788

1-E, MEP point 4 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.90972695

SA-CASSCF/cc-pVTZ S₁ energy: -518.83316761

SA-CASSCF/cc-pVTZ S₂ energy: -518.79050879

C	-0.809663	0.024322	0.141087
C	0.691917	0.295076	0.078945
C	1.391447	1.459013	0.453177
C	1.616579	-0.648906	-0.431386
C	2.907674	-0.112498	-0.285680
C	2.757445	1.225691	0.212022
N	-1.701662	0.939464	-0.230256
C	-3.034158	0.368364	-0.386676
H	3.557503	1.907474	0.420087
C	-1.363350	-1.358560	-0.073039
C	-2.760998	-1.100975	-0.675050
H	-2.739295	-1.263226	-1.744272
H	-3.522237	-1.745243	-0.258711
H	-3.592421	0.514514	0.535056
H	-3.567137	0.874474	-1.179038
H	-0.744262	-1.854698	-0.810240
H	0.984208	2.359577	0.858205
C	-1.604843	2.364863	0.027239
H	-1.452700	2.550050	1.084831
H	-0.796024	2.805222	-0.528387
H	-2.532548	2.825833	-0.275900
C	-1.359796	-2.217505	1.190610
H	-1.694200	-3.221926	0.957401
H	-0.363636	-2.280944	1.607679
H	-2.019541	-1.809155	1.947953
H	1.399720	-1.649165	-0.744057
C	4.201566	-0.866651	-0.365153
H	4.946349	-0.321974	-0.937955
H	4.624422	-1.043354	0.620676
H	4.064483	-1.832345	-0.838160

1-E, MEP point 5 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.90378416

SA-CASSCF/cc-pVTZ S₁ energy: -518.83350211

SA-CASSCF/cc-pVTZ S₂ energy: -518.79614043

C	-0.810946	0.026463	0.147796
C	0.688510	0.289705	0.101205
C	1.397807	1.404877	0.589312
C	1.605793	-0.597048	-0.519096
C	2.897257	-0.085489	-0.322451
C	2.755711	1.199507	0.302959
N	-1.687106	0.931429	-0.278578
C	-3.023912	0.368785	-0.428162
H	3.559784	1.859467	0.560406
C	-1.369273	-1.360973	-0.028482
C	-2.765722	-1.116530	-0.640981
H	-2.749111	-1.335233	-1.700101
H	-3.532895	-1.729757	-0.190058
H	-3.593759	0.566126	0.476781
H	-3.539535	0.841789	-1.251801
H	-0.749908	-1.869596	-0.756961
H	0.989105	2.263058	1.079589
C	-1.583102	2.361800	-0.052982
H	-1.556711	2.574122	1.011227
H	-0.699669	2.762984	-0.515215
H	-2.453289	2.836549	-0.480288
C	-1.361657	-2.203078	1.244563
H	-1.695384	-3.210296	1.023424
H	-0.363603	-2.261219	1.658398
H	-2.019335	-1.787178	1.999549
H	1.382826	-1.564813	-0.918651
C	4.185675	-0.845702	-0.440482
H	4.947570	-0.264767	-0.951975
H	4.585693	-1.106119	0.536068
H	4.049141	-1.768414	-0.992810

1-E, MEP point 6 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89731635

SA-CASSCF/cc-pVTZ S₁ energy: -518.83361206

SA-CASSCF/cc-pVTZ S₂ energy: -518.80290761

C	-0.809277	0.028289	0.145710
C	0.683709	0.284159	0.117666
C	1.403244	1.336861	0.718922
C	1.595409	-0.534321	-0.602713
C	2.887205	-0.055392	-0.353095
C	2.753870	1.163864	0.395276
N	-1.672300	0.921415	-0.327721
C	-3.013542	0.367368	-0.465965
H	3.561559	1.797803	0.702238
C	-1.375911	-1.362369	0.014354
C	-2.771568	-1.130063	-0.606148
H	-2.761810	-1.402032	-1.652921
H	-3.544277	-1.710907	-0.122918
H	-3.590586	0.613040	0.422509
H	-3.515974	0.806588	-1.316075
H	-0.757565	-1.887493	-0.703473
H	0.992448	2.147891	1.284277
C	-1.560065	2.355369	-0.130519
H	-1.650220	2.595178	0.925400
H	-0.619404	2.722302	-0.497207
H	-2.363638	2.838455	-0.665892
C	-1.364401	-2.181892	1.300517
H	-1.699266	-3.192242	1.096282
H	-0.364370	-2.234522	1.710486
H	-2.018776	-1.754052	2.051520
H	1.364697	-1.460191	-1.088950
C	4.170050	-0.818833	-0.514704
H	4.945147	-0.209729	-0.970458
H	4.552959	-1.156120	0.445047
H	4.031686	-1.695810	-1.136530

1-E, MEP point 7 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.88998412

SA-CASSCF/cc-pVTZ S₁ energy: -518.83338678

SA-CASSCF/cc-pVTZ S₂ energy: -518.81080877

C	-0.805016	0.029755	0.138361
C	0.677686	0.279703	0.129643
C	1.407940	1.257029	0.839083
C	1.585632	-0.461564	-0.679792
C	2.877288	-0.023390	-0.377474
C	2.751737	1.117538	0.487286
N	-1.657473	0.909685	-0.376040
C	-3.002951	0.364116	-0.501781
H	3.563074	1.720026	0.843947
C	-1.382459	-1.362271	0.056039
C	-2.777869	-1.141519	-0.570593
H	-2.776638	-1.465164	-1.602540
H	-3.555334	-1.688410	-0.056380
H	-3.585532	0.656298	0.368800
H	-3.493752	0.768733	-1.375597
H	-0.766050	-1.905638	-0.650180
H	0.996447	2.012824	1.476878
C	-1.536933	2.346232	-0.206453
H	-1.731541	2.614637	0.829172
H	-0.555034	2.684093	-0.480875
H	-2.269694	2.832020	-0.833877
C	-1.367813	-2.155199	1.357296
H	-1.705550	-3.168457	1.173354
H	-0.366060	-2.202573	1.763820
H	-2.018218	-1.711970	2.102733
H	1.346264	-1.337264	-1.248652
C	4.154420	-0.785994	-0.588312
H	4.940364	-0.153445	-0.990371
H	4.524119	-1.197659	0.347140
H	4.012866	-1.612598	-1.274716

1-E, MEP point 8 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.88170354

SA-CASSCF/cc-pVTZ S₁ energy: -518.83280819

SA-CASSCF/cc-pVTZ S₂ energy: -518.81993201

C	-0.798506	0.030645	0.124905
C	0.670501	0.277446	0.136799
C	1.411769	1.165409	0.949828
C	1.577088	-0.379719	-0.749218
C	2.868480	0.009096	-0.395541
C	2.749733	1.060108	0.577804
N	-1.643767	0.896667	-0.423939
C	-2.993196	0.358905	-0.533975
H	3.563710	1.627247	0.983424
C	-1.389025	-1.360323	0.097253
C	-2.783645	-1.151263	-0.535812
H	-2.789153	-1.521822	-1.551864
H	-3.565691	-1.665659	0.004581
H	-3.577888	0.693785	0.319641
H	-3.476466	0.729142	-1.427209
H	-0.775337	-1.925285	-0.594525
H	1.000745	1.863239	1.651999
C	-1.514756	2.335427	-0.280863
H	-1.794627	2.630900	0.727657
H	-0.506119	2.648597	-0.475445
H	-2.180506	2.818773	-0.980923
C	-1.372404	-2.122692	1.415551
H	-1.713797	-3.138454	1.254044
H	-0.369005	-2.164981	1.818775
H	-2.018540	-1.662162	2.154215
H	1.329403	-1.196621	-1.397919
C	4.140045	-0.747329	-0.660751
H	4.933981	-0.094925	-1.012130
H	4.500546	-1.229484	0.243787
H	3.993556	-1.520197	-1.406243

1-E, MEP point 9 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.87216663

SA-CASSCF/cc-pVTZ S₁ energy: -518.83165974

SA-CASSCF/cc-pVTZ S₂ energy: -518.82995294

C	-0.790356	0.030646	0.108313
C	0.662875	0.276234	0.141887
C	1.414898	1.064305	1.049177
C	1.569513	-0.291000	-0.808153
C	2.860507	0.042472	-0.408401
C	2.747433	0.992058	0.664442
N	-1.630927	0.882590	-0.469589
C	-2.983764	0.352234	-0.564464
H	3.564272	1.516326	1.119273
C	-1.395476	-1.356655	0.137150
C	-2.789742	-1.159200	-0.500567
H	-2.803580	-1.575187	-1.498791
H	-3.575517	-1.640064	0.064853
H	-3.570419	0.728030	0.270522
H	-3.460020	0.687656	-1.475255
H	-0.785554	-1.943593	-0.539656
H	1.005537	1.695853	1.812852
C	-1.493286	2.323074	-0.355221
H	-1.842677	2.646706	0.622798
H	-0.467926	2.616462	-0.481498
H	-2.097712	2.799520	-1.113714
C	-1.377170	-2.085389	1.473370
H	-1.724058	-3.102923	1.336866
H	-0.372232	-2.123366	1.873200
H	-2.018214	-1.604936	2.203778
H	1.314399	-1.040724	-1.531719
C	4.126304	-0.702132	-0.731681
H	4.927334	-0.032851	-1.031258
H	4.479496	-1.254496	0.134588
H	3.974100	-1.414976	-1.533576

1-E, MEP point 10 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.85718028

SA-CASSCF/cc-pVTZ S₁ energy: -518.85672015

SA-CASSCF/cc-pVTZ S₂ energy: -518.81258442

C	-0.790905	0.022121	0.151007
C	0.648875	0.275565	0.145686
C	1.376357	1.061932	1.024541
C	1.554263	-0.304343	-0.780507
C	2.899080	0.067490	-0.377880
C	2.786894	0.967542	0.640362
N	-1.647510	0.901097	-0.505428
C	-2.981148	0.360139	-0.556996
H	3.590063	1.453728	1.154506
C	-1.385618	-1.362536	0.123837
C	-2.786962	-1.157730	-0.499508
H	-2.809618	-1.574261	-1.498207
H	-3.570745	-1.641641	0.069072
H	-3.587997	0.707558	0.283977
H	-3.480759	0.681123	-1.464885
H	-0.801165	-1.987114	-0.550709
H	0.987953	1.658718	1.822497
C	-1.501987	2.316714	-0.352909
H	-1.833676	2.675743	0.626822
H	-0.472305	2.614462	-0.489134
H	-2.094799	2.818552	-1.108904
C	-1.379018	-2.082374	1.473373
H	-1.730017	-3.102838	1.353922
H	-0.375227	-2.121941	1.881188
H	-2.015406	-1.588043	2.199345
H	1.305246	-0.996180	-1.557952
C	4.135686	-0.694673	-0.743867
H	4.943820	-0.037853	-1.040832
H	4.476280	-1.266101	0.111445
H	3.962829	-1.393560	-1.552501

1-Z, S₀ geometry

CASSCF/cc-pVTZ S₀ energy: -518.96623394

C	-0.71575957	-0.01383721	-0.13881212
C	0.62987589	-0.20097539	-0.11160125
C	1.27655587	-1.51326034	-0.22938278
C	1.74132571	0.75387457	0.00382530
C	2.91583922	0.08115815	-0.04108589
C	2.61682211	-1.34715808	-0.18710798
N	-1.42060552	1.16055816	-0.06503045
C	-2.85324578	0.96301281	-0.11906797
H	3.35372380	-2.12305684	-0.25380308
C	-1.72761733	-1.14540431	-0.25671208
C	-2.98398344	-0.41662202	-0.74814950
H	-2.96089148	-0.32427167	-1.82709098
H	-3.90090036	-0.91996011	-0.47235843
H	-3.30069204	0.99827813	0.87362989
H	-3.32366198	1.73737853	-0.71281268
H	-1.40051857	-1.87770478	-0.97959545
H	0.76651852	-2.44707410	-0.33854150
C	-0.89255480	2.42256144	0.37554766
H	-0.33692741	2.32581701	1.30228392
H	-0.24426237	2.87117667	-0.36752716
H	-1.71550899	3.10220044	0.54719433
C	-1.95734465	-1.84367379	1.08809106
H	-2.70819107	-2.61953456	0.98465343
H	-1.04729533	-2.29778327	1.45494219
H	-2.30166491	-1.14450401	1.84218241
H	1.65554339	1.81331763	0.10146355
C	4.29851060	0.65142732	0.03559290
H	4.27344861	1.72901641	0.13866823
H	4.84317401	0.24685683	0.88303772
H	4.87053087	0.41394133	-0.85595130

1-Z, MEP point 1 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.93503375

SA-CASSCF/cc-pVTZ S₁ energy: -518.83176850

SA-CASSCF/cc-pVTZ S₂ energy: -518.78141210

C	-0.786141	-0.019295	-0.037771
C	0.692863	-0.217417	-0.077746
C	1.263920	-1.495746	-0.251673
C	1.722376	0.744918	0.021622
C	2.965182	0.059832	-0.060505
C	2.676768	-1.339018	-0.225635
N	-1.415401	1.159085	-0.069692
C	-2.859479	0.994593	-0.165279
H	3.401571	-2.125451	-0.275264
C	-1.760716	-1.139108	-0.231053
C	-3.015469	-0.409021	-0.734412
H	-3.007508	-0.362650	-1.815895
H	-3.937702	-0.880146	-0.424898
H	-3.303081	1.091372	0.823082
H	-3.282357	1.766298	-0.793789
H	-1.391109	-1.831700	-0.976737
H	0.741630	-2.421605	-0.359858
C	-0.887177	2.442814	0.339984
H	-0.344877	2.359862	1.271374
H	-0.232156	2.854779	-0.412912
H	-1.717537	3.118649	0.479701
C	-1.991559	-1.907348	1.078775
H	-2.676503	-2.732191	0.914642
H	-1.062961	-2.305872	1.462022
H	-2.417597	-1.261963	1.839246
H	1.629036	1.798875	0.151512
C	4.326471	0.670647	0.040293
H	4.265646	1.750398	0.113022
H	4.865979	0.314387	0.914108
H	4.936130	0.434056	-0.827407

1-Z, MEP point 2 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.92359391

SA-CASSCF/cc-pVTZ S₁ energy: -518.83285755

SA-CASSCF/cc-pVTZ S₂ energy: -518.78322949

C	-0.803144	-0.019837	0.081169
C	0.699247	-0.220471	-0.024136
C	1.268103	-1.474406	-0.327466
C	1.733592	0.733318	0.108027
C	2.966759	0.065650	-0.065693
C	2.674384	-1.317637	-0.318300
N	-1.402693	1.158763	-0.093698
C	-2.847198	1.017900	-0.229049
H	3.396947	-2.103767	-0.403896
C	-1.770417	-1.139766	-0.175008
C	-3.019660	-0.415236	-0.711436
H	-3.022903	-0.434623	-1.793295
H	-3.945038	-0.855148	-0.367623
H	-3.315487	1.189900	0.737421
H	-3.230885	1.757292	-0.918172
H	-1.363059	-1.794965	-0.935310
H	0.745632	-2.395225	-0.476240
C	-0.873423	2.457853	0.273513
H	-0.376918	2.413291	1.232540
H	-0.178680	2.819519	-0.468103
H	-1.699238	3.150040	0.341331
C	-2.025747	-1.968545	1.088346
H	-2.673955	-2.807730	0.861870
H	-1.098308	-2.353633	1.489505
H	-2.502830	-1.371716	1.857993
H	1.643738	1.773554	0.325911
C	4.330485	0.673535	0.053590
H	4.272034	1.755417	0.090854
H	4.846118	0.344672	0.952509
H	4.960238	0.407226	-0.789968

1-Z, MEP point 3 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91459364

SA-CASSCF/cc-pVTZ S₁ energy: -518.83294476

SA-CASSCF/cc-pVTZ S₂ energy: -518.78622038

C	-0.811643	-0.017048	0.147038
C	0.698422	-0.222285	0.021825
C	1.257213	-1.433990	-0.435997
C	1.739882	0.710094	0.232116
C	2.960178	0.068812	-0.047810
C	2.658560	-1.280626	-0.431106
N	-1.389292	1.152154	-0.123624
C	-2.832560	1.023775	-0.285667
H	3.376789	-2.059907	-0.588839
C	-1.772058	-1.143674	-0.117172
C	-3.017649	-0.432834	-0.684579
H	-3.030744	-0.514280	-1.763228
H	-3.944458	-0.843688	-0.310095
H	-3.317776	1.261842	0.658018
H	-3.188858	1.725880	-1.026335
H	-1.345528	-1.786994	-0.876410
H	0.732735	-2.337969	-0.661183
C	-0.855971	2.462711	0.200255
H	-0.435530	2.467671	1.196655
H	-0.097541	2.760131	-0.505177
H	-1.667091	3.174173	0.162162
C	-2.038836	-1.991822	1.127281
H	-2.678737	-2.830423	0.877338
H	-1.113908	-2.380054	1.532172
H	-2.529373	-1.411837	1.901113
H	1.655225	1.721498	0.563220
C	4.328892	0.663736	0.081895
H	4.281248	1.746294	0.120355
H	4.836874	0.329318	0.983233
H	4.958767	0.391734	-0.759063

1-Z, MEP point 4 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.90700704

SA-CASSCF/cc-pVTZ S₁ energy: -518.83318629

SA-CASSCF/cc-pVTZ S₂ energy: -518.79057436

C	-0.816221	-0.016415	0.180428
C	0.696049	-0.228667	0.052083
C	1.246876	-1.379244	-0.553409
C	1.745445	0.669388	0.356182
C	2.956259	0.068073	-0.018872
C	2.645018	-1.232119	-0.540368
N	-1.378217	1.141544	-0.157773
C	-2.821392	1.023590	-0.330847
H	3.358954	-1.996358	-0.774541
C	-1.778630	-1.148285	-0.064931
C	-3.024055	-0.450182	-0.651474
H	-3.054680	-0.587937	-1.723850
H	-3.949422	-0.831053	-0.243332
H	-3.313411	1.320495	0.592213
H	-3.159689	1.688543	-1.113048
H	-1.347800	-1.794333	-0.818590
H	0.718920	-2.255355	-0.864524
C	-0.836393	2.458766	0.127496
H	-0.505620	2.517790	1.156421
H	-0.009701	2.689891	-0.522428
H	-1.619628	3.185110	-0.027651
C	-2.043401	-1.994741	1.178475
H	-2.678370	-2.836729	0.927513
H	-1.116527	-2.379326	1.583147
H	-2.537572	-1.417699	1.952153
H	1.659906	1.640902	0.793589
C	4.329155	0.652663	0.122696
H	4.287259	1.733902	0.194134
H	4.841874	0.289352	1.010033
H	4.950904	0.403371	-0.730785

1-Z, MEP point 5 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.90022295

SA-CASSCF/cc-pVTZ S₁ energy: -518.83354347

SA-CASSCF/cc-pVTZ S₂ energy: -518.79632526

C	-0.816461	-0.017786	0.196789
C	0.691839	-0.238256	0.071914
C	1.236880	-1.311426	-0.670532
C	1.748248	0.615164	0.471146
C	2.950839	0.064215	0.012655
C	2.631573	-1.172443	-0.642248
N	-1.366493	1.127869	-0.195285
C	-2.810499	1.019519	-0.367458
H	3.341939	-1.913297	-0.951306
C	-1.785206	-1.152865	-0.015415
C	-3.032012	-0.466047	-0.614823
H	-3.082627	-0.654789	-1.678603
H	-3.954564	-0.816530	-0.174162
H	-3.301452	1.368833	0.537608
H	-3.138453	1.648234	-1.183228
H	-1.357140	-1.810002	-0.760650
H	0.705216	-2.149166	-1.069271
C	-0.814477	2.448391	0.056205
H	-0.576229	2.563323	1.107143
H	0.074349	2.617202	-0.526210
H	-1.558827	3.182225	-0.213675
C	-2.044803	-1.987307	1.235070
H	-2.680117	-2.831223	0.992437
H	-1.115970	-2.369472	1.637898
H	-2.536156	-1.405261	2.006594
H	1.659722	1.538757	1.004768
C	4.326698	0.639460	0.170733
H	4.288773	1.716712	0.289846
H	4.846361	0.236653	1.036601
H	4.939235	0.426526	-0.698712

1-Z, MEP point 6 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89352592

SA-CASSCF/cc-pVTZ S₁ energy: -518.83404196

SA-CASSCF/cc-pVTZ S₂ energy: -518.80348543

C	-0.813468	-0.021273	0.203084
C	0.686212	-0.248374	0.082897
C	1.227383	-1.230041	-0.783238
C	1.749420	0.548680	0.574922
C	2.945067	0.056209	0.044818
C	2.618709	-1.103248	-0.736770
N	-1.355095	1.111593	-0.233116
C	-2.800156	1.012656	-0.398979
H	3.326529	-1.811484	-1.119931
C	-1.791772	-1.157494	0.032062
C	-3.040741	-0.480660	-0.576278
H	-3.113958	-0.716650	-1.629151
H	-3.958635	-0.800070	-0.103542
H	-3.286556	1.410304	0.488283
H	-3.122041	1.605712	-1.243467
H	-1.369227	-1.829858	-0.702546
H	0.689682	-2.018486	-1.266890
C	-0.791771	2.433329	-0.013910
H	-0.642267	2.605514	1.046262
H	0.148141	2.545592	-0.523948
H	-1.489517	3.165662	-0.390463
C	-2.044236	-1.973055	1.294569
H	-2.682025	-2.819260	1.066435
H	-1.113203	-2.352119	1.695630
H	-2.529869	-1.381038	2.062144
H	1.656223	1.416545	1.196216
C	4.322774	0.623120	0.223542
H	4.286550	1.693499	0.394235
H	4.848778	0.179583	1.065149
H	4.928075	0.452459	-0.659912

1-Z, MEP point 7 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.88626346

SA-CASSCF/cc-pVTZ S₁ energy: -518.83433626

SA-CASSCF/cc-pVTZ S₂ energy: -518.81176606

C	-0.808214	-0.026947	0.200460
C	0.679672	-0.257081	0.085545
C	1.219065	-1.135749	-0.889816
C	1.749781	0.471639	0.667233
C	2.939384	0.042615	0.077334
C	2.607234	-1.025696	-0.823259
N	-1.344977	1.093050	-0.272311
C	-2.791535	1.002868	-0.424352
H	3.312376	-1.692215	-1.279678
C	-1.797959	-1.161938	0.078472
C	-3.048755	-0.494524	-0.538100
H	-3.140430	-0.771892	-1.579439
H	-3.962791	-0.785095	-0.039704
H	-3.268693	1.441802	0.448405
H	-3.114012	1.563156	-1.290761
H	-1.383387	-1.853193	-0.643435
H	0.674936	-1.865400	-1.453307
C	-0.769961	2.414548	-0.082807
H	-0.699421	2.641705	0.976259
H	0.209182	2.478592	-0.521806
H	-1.418201	3.139624	-0.551784
C	-2.042577	-1.952297	1.357119
H	-2.685131	-2.799640	1.148226
H	-1.109549	-2.328674	1.756268
H	-2.519660	-1.345803	2.118645
H	1.653519	1.278091	1.367291
C	4.317772	0.602737	0.279345
H	4.281307	1.663859	0.500918
H	4.848980	0.120683	1.095933
H	4.917954	0.475928	-0.614638

1-Z, MEP point 8 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.87804944

SA-CASSCF/cc-pVTZ S₁ energy: -518.83425120

SA-CASSCF/cc-pVTZ S₂ energy: -518.82109710

C	-0.801287	-0.034885	0.192362
C	0.672775	-0.264339	0.081612
C	1.212056	-1.029868	-0.987480
C	1.749765	0.385816	0.745832
C	2.934114	0.024933	0.107234
C	2.597349	-0.940443	-0.901340
N	-1.336586	1.072863	-0.310109
C	-2.784302	0.991104	-0.446264
H	3.300680	-1.556500	-1.426297
C	-1.803476	-1.166004	0.122869
C	-3.057197	-0.507602	-0.498715
H	-3.169704	-0.824036	-1.526622
H	-3.965359	-0.769170	0.025773
H	-3.251051	1.468909	0.411390
H	-3.109497	1.518975	-1.332025
H	-1.398599	-1.876997	-0.585370
H	0.661397	-1.694600	-1.622411
C	-0.750779	2.393278	-0.151254
H	-0.759535	2.678854	0.896407
H	0.261043	2.413274	-0.513318
H	-1.343128	3.102572	-0.710329
C	-2.038642	-1.926912	1.419933
H	-2.687235	-2.775350	1.234982
H	-1.103480	-2.300130	1.817445
H	-2.505439	-1.302876	2.174033
H	1.650968	1.123809	1.517749
C	4.312409	0.576713	0.337908
H	4.274789	1.626178	0.609350
H	4.845269	0.057696	1.130356
H	4.911694	0.494017	-0.561496

1-Z, MEP point 9 (S₂)

SA-CASSCF/cc-pVTZ S₀ energy: -518.86865256

SA-CASSCF/cc-pVTZ S₁ energy: -518.83339412

SA-CASSCF/cc-pVTZ S₂ energy: -518.83118638

C	-0.793379	-0.045121	0.177760
C	0.665891	-0.271342	0.071987
C	1.207646	-0.914584	-1.074479
C	1.749273	0.293521	0.810790
C	2.928393	0.004152	0.134322
C	2.590410	-0.848179	-0.970460
N	-1.330747	1.051540	-0.346740
C	-2.779246	0.977648	-0.464590
H	3.293266	-1.403111	-1.560206
C	-1.808580	-1.169510	0.166175
C	-3.065785	-0.519986	-0.458637
H	-3.198614	-0.872279	-1.472473
H	-3.967517	-0.753726	0.089555
H	-3.234208	1.491094	0.378884
H	-3.110257	1.474353	-1.366196
H	-1.415791	-1.901575	-0.527841
H	0.652287	-1.503996	-1.776842
C	-0.734230	2.370267	-0.219938
H	-0.810603	2.711973	0.808758
H	0.299778	2.353128	-0.511113
H	-1.271987	3.058502	-0.855481
C	-2.032522	-1.897166	1.483257
H	-2.688626	-2.745036	1.324543
H	-1.095312	-2.267892	1.878180
H	-2.486725	-1.253455	2.228039
H	1.648272	0.954599	1.649785
C	4.306828	0.544255	0.398393
H	4.268283	1.580837	0.715672
H	4.837254	-0.009489	1.167954
H	4.908493	0.503042	-0.502262

1-Z, MEP point 10 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.83822920

SA-CASSCF/cc-pVTZ S₁ energy: -518.83419944

SA-CASSCF/cc-pVTZ S₂ energy: -518.79558534

C	-0.791976	-0.057909	0.219246
C	0.648641	-0.268375	0.055898
C	1.189785	-0.931548	-1.043189
C	1.719201	0.299056	0.793070
C	2.957797	-0.021286	0.101191
C	2.633674	-0.828529	-0.955200
N	-1.341109	1.074484	-0.373485
C	-2.775758	0.983772	-0.453772
H	3.321349	-1.301613	-1.625545
C	-1.802294	-1.178292	0.152154
C	-3.063217	-0.519996	-0.456816
H	-3.207289	-0.868114	-1.472383
H	-3.965067	-0.758767	0.093357
H	-3.263290	1.474618	0.392815
H	-3.132341	1.474941	-1.353201
H	-1.442879	-1.935190	-0.539753
H	0.645415	-1.465132	-1.791157
C	-0.743211	2.365885	-0.216964
H	-0.801740	2.740733	0.809065
H	0.296352	2.346953	-0.511086
H	-1.257465	3.071849	-0.857744
C	-2.033515	-1.894035	1.483465
H	-2.695312	-2.741247	1.340162
H	-1.096692	-2.264218	1.884143
H	-2.477496	-1.236779	2.222713
H	1.634609	0.918444	1.662671
C	4.312571	0.539031	0.405912
H	4.251616	1.576207	0.714651
H	4.827481	-0.003307	1.191453
H	4.932293	0.499610	-0.481759

2-*E*, S₀ geometry

CASSCF/cc-pVTZ S₀ energy: -518.96072038

C	-0.99383791	-0.39280169	0.02344371
C	0.32583112	-0.11057166	-0.03904560
C	1.02291189	1.24924852	-0.06235021
C	1.38950427	-1.12137353	-0.00581271
C	2.60601994	-0.58212598	-0.16059197
C	2.50568663	0.91053124	-0.35079658
N	-2.09236447	0.49902195	0.00914270
C	-3.33745901	-0.25841902	0.01772843
H	2.78875832	1.18066285	-1.36515818
C	-1.56192358	-1.73287163	0.22396359
C	-2.89445957	-1.66889709	0.25374614
H	-3.86414100	-0.17177625	-0.93315167
H	-4.01111945	0.10519719	0.78858191
H	0.63955665	1.87940525	-0.85137625
C	-2.10381655	1.66052736	-0.84541000
H	-1.92972307	1.41306467	-1.89308910
H	-1.37043843	2.38908979	-0.54072187
H	-3.07289087	2.13582306	-0.76945693
H	1.21423871	-2.17220105	0.11307945
H	3.17716373	1.45104046	0.30942802
H	-0.97504151	-2.61559347	0.35981521
H	-3.57220212	-2.48423662	0.40482322
C	0.86306955	1.97957410	1.27414680
H	-0.17915224	2.14383831	1.51589377
H	1.36421664	2.94191508	1.24994830
H	1.29760421	1.39532989	2.07814990
C	3.91820333	-1.29943287	-0.20567416
H	3.79314966	-2.36680709	-0.07424001
H	4.41909478	-1.13316598	-1.15509436
H	4.58549238	-0.93973177	0.57188047

2-E, MEP point 1 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91948028

SA-CASSCF/cc-pVTZ S₁ energy: -518.79493142

C	-1.043223	-0.446356	0.034692
C	0.365993	-0.105818	-0.085571
C	1.036807	1.262557	-0.053832
C	1.339653	-1.089948	-0.055247
C	2.647510	-0.552761	-0.134553
C	2.525594	0.930641	-0.339152
N	-2.077818	0.447722	-0.051950
C	-3.349374	-0.258249	-0.001991
H	2.785633	1.186185	-1.365522
C	-1.535732	-1.748612	0.251112
C	-2.990685	-1.660888	0.328829
H	-3.840403	-0.189829	-0.972441
H	-4.009603	0.204742	0.726282
H	0.667364	1.911843	-0.835963
C	-2.076095	1.668272	-0.826715
H	-1.909033	1.476730	-1.883921
H	-1.336088	2.366625	-0.478155
H	-3.043689	2.137557	-0.717182
H	1.143327	-2.140966	0.005558
H	3.196678	1.499343	0.297524
H	-0.951845	-2.577001	0.579871
H	-3.680481	-2.473362	0.237165
C	0.866568	1.977502	1.289959
H	-0.176944	2.136130	1.533480
H	1.360537	2.943967	1.276898
H	1.301550	1.388335	2.089930
C	3.932580	-1.302250	-0.211649
H	3.781736	-2.364882	-0.066005
H	4.417754	-1.165330	-1.176309
H	4.635682	-0.960082	0.543290

2-E, MEP point 2 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91336875

SA-CASSCF/cc-pVTZ S₁ energy: -518.79704023

C	-1.044358	-0.450136	0.039961
C	0.359496	-0.098732	-0.136201
C	1.035451	1.269888	-0.031609
C	1.342297	-1.080152	-0.125091
C	2.641571	-0.546118	-0.147189
C	2.528407	0.945069	-0.306267
N	-2.072174	0.415177	-0.143830
C	-3.348113	-0.268052	-0.045484
H	2.800521	1.227887	-1.322285
C	-1.543684	-1.731552	0.377281
C	-3.002331	-1.645925	0.396616
H	-3.832528	-0.268352	-1.020605
H	-4.004023	0.258803	0.642512
H	0.681798	1.955245	-0.790137
C	-2.044421	1.677465	-0.841694
H	-1.789526	1.554448	-1.890034
H	-1.352806	2.369585	-0.394246
H	-3.030581	2.115423	-0.781653
H	1.138556	-2.132326	-0.106251
H	3.192167	1.495346	0.353766
H	-0.963097	-2.508388	0.820578
H	-3.680645	-2.464866	0.260978
C	0.853726	1.932110	1.337880
H	-0.191186	2.088473	1.578455
H	1.352147	2.895910	1.366421
H	1.277550	1.311132	2.119468
C	3.928540	-1.295765	-0.236732
H	3.777825	-2.358363	-0.090596
H	4.404376	-1.158630	-1.206101
H	4.638168	-0.954064	0.511741

2-E, MEP point 3 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.90903187

SA-CASSCF/cc-pVTZ S₁ energy: -518.79844470

C	-1.042972	-0.433465	0.058984
C	0.353585	-0.089384	-0.170382
C	1.031074	1.270625	0.006426
C	1.341139	-1.075376	-0.188534
C	2.629187	-0.545824	-0.187560
C	2.525658	0.953670	-0.266571
N	-2.068028	0.395799	-0.224490
C	-3.342777	-0.280367	-0.080451
H	2.814100	1.291552	-1.260783
C	-1.539010	-1.671137	0.534198
C	-2.992292	-1.631350	0.439909
H	-3.833991	-0.330085	-1.049359
H	-3.991966	0.282382	0.586001
H	0.685166	1.993788	-0.720636
C	-2.019261	1.667061	-0.904542
H	-1.598093	1.573728	-1.898802
H	-1.449444	2.396595	-0.351589
H	-3.029593	2.038238	-0.995848
H	1.132540	-2.127325	-0.205247
H	3.183305	1.461802	0.432640
H	-0.951307	-2.424869	1.004538
H	-3.641635	-2.471790	0.292459
C	0.832895	1.867064	1.403269
H	-0.215135	2.021220	1.633432
H	1.337273	2.824554	1.486205
H	1.238630	1.206104	2.161335
C	3.919685	-1.289313	-0.281127
H	3.768694	-2.357238	-0.181809
H	4.415354	-1.111328	-1.233604
H	4.612336	-0.976882	0.495656

2-E, MEP point 4 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.90069033

SA-CASSCF/cc-pVTZ S₁ energy: -518.80010101

C	-1.042171	-0.410907	0.079573
C	0.347068	-0.079045	-0.192316
C	1.028894	1.268938	0.049834
C	1.340008	-1.069468	-0.246227
C	2.618160	-0.545191	-0.225702
C	2.523921	0.958407	-0.227230
N	-2.064563	0.374387	-0.299011
C	-3.337989	-0.291810	-0.103443
H	2.824537	1.347932	-1.198485
C	-1.541554	-1.587033	0.696250
C	-2.975215	-1.622300	0.463997
H	-3.853153	-0.369819	-1.055845
H	-3.966931	0.293085	0.564462
H	0.686806	2.025607	-0.645243
C	-2.001940	1.644571	-0.979441
H	-1.404984	1.578179	-1.878762
H	-1.596017	2.421352	-0.346463
H	-3.006117	1.930666	-1.255689
H	1.128116	-2.120196	-0.299947
H	3.177903	1.423465	0.504905
H	-0.937915	-2.364796	1.102969
H	-3.577184	-2.491027	0.281268
C	0.817245	1.804623	1.468700
H	-0.233050	1.962378	1.687605
H	1.330390	2.751772	1.600951
H	1.202339	1.106813	2.204001
C	3.910656	-1.284847	-0.332493
H	3.756657	-2.356488	-0.300063
H	4.429254	-1.051486	-1.260199
H	4.584447	-1.020217	0.478123

2-E, MEP point 5 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89289658

SA-CASSCF/cc-pVTZ S₁ energy: -518.80159983

C	-1.042212	-0.384698	0.089858
C	0.342280	-0.064658	-0.202789
C	1.030497	1.266613	0.102875
C	1.336973	-1.060547	-0.295308
C	2.608952	-0.543165	-0.256517
C	2.524705	0.960482	-0.181893
N	-2.063640	0.351476	-0.369826
C	-3.333758	-0.304664	-0.124600
H	2.834855	1.398544	-1.129112
C	-1.541499	-1.505946	0.809293
C	-2.955263	-1.599872	0.511214
H	-3.862769	-0.430115	-1.063059
H	-3.952858	0.310376	0.525792
H	0.692084	2.056683	-0.557334
C	-1.997622	1.609834	-1.070616
H	-1.242250	1.577748	-1.840761
H	-1.782730	2.433852	-0.400822
H	-2.954871	1.795128	-1.536388
H	1.119756	-2.107517	-0.393007
H	3.177268	1.381504	0.577896
H	-0.928159	-2.261629	1.244530
H	-3.531478	-2.491636	0.361490
C	0.809569	1.739181	1.542489
H	-0.241901	1.900110	1.754947
H	1.331173	2.673613	1.723198
H	1.177815	1.004735	2.250428
C	3.900794	-1.279988	-0.393675
H	3.743419	-2.351199	-0.427044
H	4.429895	-0.993286	-1.300207
H	4.566683	-1.066629	0.438387

2-E, MEP point 6 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.88779015

SA-CASSCF/cc-pVTZ S₁ energy: -518.80259896

C	-1.043073	-0.356691	0.093971
C	0.338724	-0.044053	-0.209027
C	1.035660	1.264854	0.164260
C	1.331366	-1.044913	-0.340939
C	2.601551	-0.538230	-0.280107
C	2.527664	0.962005	-0.135442
N	-2.064827	0.330829	-0.427114
C	-3.330496	-0.317856	-0.144020
H	2.840307	1.442452	-1.061181
C	-1.539215	-1.432478	0.884218
C	-2.939472	-1.565634	0.574283
H	-3.856877	-0.506062	-1.073080
H	-3.955102	0.331493	0.466557
H	0.700223	2.090604	-0.454358
C	-2.002286	1.558678	-1.180184
H	-1.136703	1.556648	-1.821790
H	-1.959953	2.424957	-0.529290
H	-2.888290	1.638116	-1.794485
H	1.106926	-2.085446	-0.484823
H	3.183102	1.342791	0.643005
H	-0.919453	-2.143304	1.381729
H	-3.514935	-2.466976	0.504667
C	0.813980	1.668088	1.624860
H	-0.237169	1.829749	1.839674
H	1.343166	2.587936	1.852632
H	1.171842	0.897160	2.298340
C	3.889897	-1.273445	-0.457041
H	3.726539	-2.340502	-0.548052
H	4.420455	-0.941694	-1.347304
H	4.557845	-1.109369	0.384669

2-E, MEP point 7 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.88343154

SA-CASSCF/cc-pVTZ S₁ energy: -518.80362049

C	-1.045800	-0.327110	0.093955
C	0.334418	-0.017973	-0.220464
C	1.041506	1.261641	0.225386
C	1.324283	-1.023683	-0.388914
C	2.594042	-0.531846	-0.297362
C	2.529626	0.963571	-0.098004
N	-2.066864	0.308061	-0.478532
C	-3.328470	-0.333055	-0.160954
H	2.834364	1.475938	-1.009459
C	-1.538455	-1.360567	0.942179
C	-2.922209	-1.526810	0.635339
H	-3.849954	-0.583570	-1.077749
H	-3.959167	0.349009	0.405524
H	0.708024	2.124036	-0.344589
C	-2.012510	1.502264	-1.284727
H	-1.064319	1.554543	-1.791221
H	-2.145289	2.390766	-0.676331
H	-2.802780	1.471111	-2.022187
H	1.092912	-2.056287	-0.576633
H	3.193859	1.314984	0.687101
H	-0.911246	-2.026582	1.490595
H	-3.513677	-2.417135	0.688755
C	0.830822	1.590991	1.706419
H	-0.218114	1.747117	1.937026
H	1.365817	2.495676	1.976310
H	1.189915	0.785764	2.338267
C	3.878733	-1.265856	-0.505425
H	3.709589	-2.328125	-0.635211
H	4.409396	-0.905276	-1.384617
H	4.550798	-1.137232	0.339484

2-E, MEP point 8 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.87569692

SA-CASSCF/cc-pVTZ S₁ energy: -518.80614393

C	-1.049324	-0.295069	0.090549
C	0.331864	0.020200	-0.244920
C	1.052147	1.252696	0.293758
C	1.313961	-0.988781	-0.471220
C	2.586994	-0.530358	-0.314477
C	2.534743	0.958034	-0.059431
N	-2.065519	0.266270	-0.536856
C	-3.325922	-0.361543	-0.182282
H	2.818051	1.500918	-0.961355
C	-1.551805	-1.289376	0.992118
C	-2.895314	-1.482897	0.704038
H	-3.843806	-0.684236	-1.078037
H	-3.960633	0.358401	0.329248
H	0.728862	2.150209	-0.230684
C	-2.025594	1.451457	-1.365087
H	-1.026817	1.587433	-1.735460
H	-2.330838	2.316530	-0.786904
H	-2.705355	1.334307	-2.197760
H	1.073181	-2.006333	-0.724650
H	3.216014	1.285861	0.722067
H	-0.916789	-1.904689	1.589899
H	-3.519085	-2.315791	0.948393
C	0.846472	1.529779	1.784753
H	-0.202289	1.685148	2.022726
H	1.382341	2.424980	2.084222
H	1.203883	0.704666	2.391142
C	3.868769	-1.266963	-0.533655
H	3.693814	-2.325466	-0.689374
H	4.410569	-0.892880	-1.401749
H	4.538383	-1.164864	0.317483

2-E, MEP point 9 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.86308218

SA-CASSCF/cc-pVTZ S₁ energy: -518.81347691

C	-1.044326	-0.264372	0.082075
C	0.330004	0.061322	-0.259300
C	1.067649	1.242741	0.361499
C	1.305591	-0.945164	-0.564811
C	2.579017	-0.525785	-0.342839
C	2.546155	0.948858	-0.013335
N	-2.067039	0.216150	-0.599444
C	-3.323117	-0.397075	-0.207591
H	2.824432	1.531471	-0.891712
C	-1.563343	-1.215153	1.048586
C	-2.879120	-1.431867	0.776621
H	-3.833151	-0.802855	-1.073303
H	-3.969871	0.353197	0.239905
H	0.758971	2.166375	-0.126371
C	-2.044722	1.397931	-1.436208
H	-1.025939	1.607864	-1.703418
H	-2.475189	2.229764	-0.888117
H	-2.629206	1.230383	-2.330303
H	1.052494	-1.942278	-0.881742
H	3.238605	1.233442	0.775549
H	-0.930204	-1.774274	1.702363
H	-3.516526	-2.204728	1.150555
C	0.860759	1.474331	1.858474
H	-0.187452	1.632741	2.099055
H	1.402133	2.356936	2.184208
H	1.211809	0.630221	2.443171
C	3.856948	-1.272106	-0.558019
H	3.674139	-2.324765	-0.743413
H	4.422531	-0.883988	-1.404630
H	4.509415	-1.199583	0.309663

2-E, MEP point 10 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.85132344

SA-CASSCF/cc-pVTZ S₁ energy: -518.82135944

C	-1.035774	-0.232162	0.067501
C	0.323814	0.109580	-0.274098
C	1.082773	1.236644	0.423950
C	1.295693	-0.900019	-0.633306
C	2.568294	-0.515854	-0.375918
C	2.558339	0.936977	0.040564
N	-2.067623	0.173764	-0.647453
C	-3.315480	-0.434885	-0.227923
H	2.854302	1.565810	-0.798923
C	-1.563454	-1.135284	1.101636
C	-2.867464	-1.371459	0.848811
H	-3.796592	-0.930647	-1.062834
H	-3.990887	0.331127	0.140123
H	0.796385	2.190762	-0.016247
C	-2.066700	1.331380	-1.520207
H	-1.045825	1.599936	-1.717699
H	-2.588908	2.142592	-1.024787
H	-2.572665	1.105113	-2.448000
H	1.031071	-1.870004	-1.018483
H	3.250245	1.160191	0.849839
H	-0.929544	-1.640544	1.797421
H	-3.504409	-2.109344	1.289662
C	0.874163	1.404617	1.929548
H	-0.172357	1.569998	2.173722
H	1.427588	2.263968	2.295132
H	1.209950	0.531813	2.480445
C	3.839015	-1.276139	-0.591430
H	3.643971	-2.317188	-0.823776
H	4.433573	-0.864384	-1.406132
H	4.468658	-1.249751	0.295455

2-E, MEP point 11 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.84316541

SA-CASSCF/cc-pVTZ S₁ energy: -518.82845758

C	-1.027566	-0.196992	0.050719
C	0.318160	0.168037	-0.295551
C	1.095676	1.236044	0.479759
C	1.282117	-0.853326	-0.675833
C	2.556013	-0.504610	-0.394494
C	2.569069	0.925282	0.095612
N	-2.069728	0.153426	-0.671552
C	-3.305391	-0.464763	-0.233418
H	2.888368	1.590586	-0.706139
C	-1.550369	-1.067260	1.133881
C	-2.851707	-1.310840	0.913455
H	-3.746018	-1.036407	-1.041141
H	-4.015090	0.299327	0.063822
H	0.839699	2.223259	0.099046
C	-2.088064	1.247377	-1.623060
H	-1.071331	1.560355	-1.777164
H	-2.686333	2.051166	-1.210320
H	-2.523897	0.929082	-2.559083
H	1.005271	-1.802085	-1.104274
H	3.255532	1.091451	0.923291
H	-0.913449	-1.514343	1.865624
H	-3.490845	-2.002993	1.420554
C	0.883341	1.317727	1.993852
H	-0.159392	1.496917	2.245066
H	1.456394	2.140171	2.410865
H	1.195855	0.406452	2.494603
C	3.815570	-1.278008	-0.631844
H	3.604155	-2.299905	-0.926347
H	4.433820	-0.833304	-1.410494
H	4.427831	-1.314884	0.266709

2-E, MEP point 12 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.83722842

SA-CASSCF/cc-pVTZ S₁ energy: -518.83384297

C	-1.020489	-0.156361	0.031770
C	0.314706	0.235786	-0.324343
C	1.106436	1.240642	0.527631
C	1.266201	-0.811118	-0.690315
C	2.541633	-0.497395	-0.385514
C	2.576148	0.918357	0.143322
N	-2.074922	0.149715	-0.685240
C	-3.296429	-0.477008	-0.220549
H	2.910850	1.598351	-0.640078
C	-1.524130	-1.013173	1.147327
C	-2.827577	-1.256799	0.966133
H	-3.714826	-1.099405	-1.002900
H	-4.028002	0.280606	0.034925
H	0.878097	2.257581	0.217440
C	-2.110293	1.150669	-1.734352
H	-1.103038	1.499132	-1.876019
H	-2.764934	1.954798	-1.420421
H	-2.490859	0.722441	-2.651304
H	0.979091	-1.737201	-1.161100
H	3.259659	1.052091	0.979379
H	-0.876642	-1.420047	1.892382
H	-3.465299	-1.905692	1.529470
C	0.890433	1.213664	2.045682
H	-0.146550	1.405202	2.310430
H	1.487433	1.983822	2.524872
H	1.175636	0.258438	2.476037
C	3.788514	-1.275587	-0.671691
H	3.559318	-2.274121	-1.027474
H	4.411555	-0.793448	-1.423889
H	4.402391	-1.377315	0.220817

2-Z, S₀ geometry

CASSCF/cc-pVTZ S₀ energy: -518.95982731

C	1.05736544	-0.11452398	-0.21194142
C	-0.28945738	-0.11145527	-0.11095564
C	-1.14437542	-1.38076373	-0.18133528
C	-1.23197987	1.00719437	0.01608278
C	-2.49926342	0.61676187	-0.18347416
C	-2.56030538	-0.85474031	-0.50861837
N	1.96520455	0.96227261	-0.17713207
C	3.32804817	0.46427287	-0.10489621
H	-2.80781192	-0.99541967	-1.55801060
C	1.87961456	-1.31309438	-0.43434766
C	3.17580028	-0.99639394	-0.39685970
H	3.76591044	0.61946389	0.88304641
H	3.96875452	0.97198776	-0.82049420
H	-0.80271067	-2.04084345	-0.96810440
C	1.69315975	2.18888314	0.52378635
H	1.33575360	2.02422925	1.53968553
H	0.96953591	2.79546257	-0.00112421
H	2.60631077	2.76604652	0.57976550
H	-0.95648246	2.01846664	0.22558256
H	-3.32651473	-1.37047737	0.06189001
H	1.47672955	-2.28733863	-0.60973738
H	4.00341478	-1.66324379	-0.52772192
C	-1.13574562	-2.15254439	1.14111100
H	-1.50050300	-1.52807641	1.94973657
H	-0.13745331	-2.48031220	1.40349554
H	-1.77308308	-3.02902933	1.08043208
C	-3.72357850	1.47645911	-0.16839028
H	-3.48313994	2.50842527	0.05404412
H	-4.22933759	1.44776091	-1.12926278
H	-4.43487203	1.12784605	0.57447878

2-Z, MEP point 1 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91956796

SA-CASSCF/cc-pVTZ S₁ energy: -518.79659049

C	1.112629	-0.151739	-0.198133
C	-0.333173	-0.082735	-0.105181
C	-1.158512	-1.362558	-0.179854
C	-1.194780	1.001314	-0.028239
C	-2.543235	0.610157	-0.159565
C	-2.583385	-0.855023	-0.495201
N	1.957357	0.910452	-0.087927
C	3.340274	0.469175	-0.104852
H	-2.820183	-0.988152	-1.550344
C	1.850931	-1.334408	-0.426629
C	3.268012	-0.969581	-0.472900
H	3.775363	0.606751	0.884848
H	3.921844	1.066557	-0.801117
H	-0.803521	-2.006747	-0.976211
C	1.667901	2.195853	0.498095
H	1.219510	2.100379	1.481278
H	1.016307	2.786048	-0.128765
H	2.596997	2.737340	0.600616
H	-0.912985	2.023351	0.107569
H	-3.342206	-1.395330	0.061693
H	1.438945	-2.274724	-0.708478
H	4.090639	-1.637997	-0.322049
C	-1.121991	-2.148403	1.136372
H	-1.527936	-1.547431	1.943478
H	-0.113443	-2.433108	1.406426
H	-1.717915	-3.051991	1.059002
C	-3.741958	1.495023	-0.170578
H	-3.482404	2.521362	0.060384
H	-4.233058	1.488278	-1.141941
H	-4.482330	1.169595	0.555681

2-Z, MEP point 2 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91533772

SA-CASSCF/cc-pVTZ S₁ energy: -518.79831259

C	1.114663	-0.170812	-0.186540
C	-0.333390	-0.092209	-0.103134
C	-1.169113	-1.364339	-0.160683
C	-1.190075	1.004819	-0.081049
C	-2.535879	0.627350	-0.179521
C	-2.603943	-0.853758	-0.436941
N	1.948497	0.868230	0.036834
C	3.336350	0.474103	-0.092426
H	-2.894138	-1.039327	-1.470126
C	1.868700	-1.336422	-0.479567
C	3.279877	-0.947468	-0.530494
H	3.834730	0.583367	0.868917
H	3.845454	1.124136	-0.799400
H	-0.837282	-2.002543	-0.972538
C	1.628894	2.199171	0.481864
H	0.965796	2.179523	1.335481
H	1.175489	2.792822	-0.302635
H	2.546188	2.686628	0.778576
H	-0.895317	2.030055	-0.006472
H	-3.340516	-1.355347	0.182982
H	1.459781	-2.240432	-0.868854
H	4.108208	-1.609030	-0.369080
C	-1.091419	-2.163004	1.144618
H	-1.489639	-1.577649	1.967040
H	-0.071764	-2.432726	1.387102
H	-1.672991	-3.076303	1.070972
C	-3.728305	1.524275	-0.199213
H	-3.455721	2.553812	0.000222
H	-4.232808	1.495885	-1.163100
H	-4.461227	1.225630	0.545713

2-Z, MEP point 3 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.91344892

SA-CASSCF/cc-pVTZ S₁ energy: -518.79924133

C	1.109134	-0.168606	-0.201774
C	-0.335904	-0.095809	-0.077969
C	-1.174866	-1.366322	-0.116116
C	-1.185691	1.008550	-0.147856
C	-2.528583	0.641130	-0.233193
C	-2.621569	-0.856860	-0.346356
N	1.941953	0.848813	0.100633
C	3.329940	0.473415	-0.078712
H	-2.989856	-1.141927	-1.329889
C	1.862856	-1.298395	-0.606623
C	3.277181	-0.940874	-0.543644
H	3.859747	0.580677	0.864212
H	3.803977	1.138699	-0.797136
H	-0.869983	-1.989415	-0.951128
C	1.616543	2.182451	0.531299
H	0.843328	2.167586	1.283797
H	1.295755	2.810845	-0.292767
H	2.501513	2.626038	0.965174
H	-0.878876	2.033578	-0.148006
H	-3.316680	-1.281307	0.372465
H	1.456121	-2.216220	-0.961030
H	4.083209	-1.619623	-0.343312
C	-1.051176	-2.192250	1.166801
H	-1.407450	-1.621626	2.018010
H	-0.024572	-2.476775	1.359641
H	-1.643739	-3.099022	1.099601
C	-3.715589	1.545005	-0.257152
H	-3.426483	2.584413	-0.156570
H	-4.274958	1.444575	-1.184804
H	-4.406325	1.313834	0.550367

2-Z, MEP point 4 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89513412

SA-CASSCF/cc-pVTZ S₁ energy: -518.79411325

C	1.101978	-0.154511	-0.226837
C	-0.337332	-0.091357	-0.049871
C	-1.177142	-1.362041	-0.067951
C	-1.185511	1.010522	-0.217427
C	-2.522530	0.648008	-0.287153
C	-2.633724	-0.852630	-0.237734
N	1.937152	0.837112	0.137191
C	3.323819	0.463761	-0.062608
H	-3.089303	-1.240548	-1.145451
C	1.851373	-1.243088	-0.750813
C	3.261301	-0.947734	-0.535724
H	3.867834	0.573900	0.870053
H	3.783731	1.127903	-0.792292
H	-0.907416	-1.961341	-0.933245
C	1.612150	2.160184	0.600004
H	0.785175	2.130400	1.291845
H	1.365017	2.829241	-0.217717
H	2.472107	2.563978	1.115379
H	-0.866410	2.030465	-0.292566
H	-3.268373	-1.179638	0.582272
H	1.443624	-2.193430	-1.005071
H	4.024375	-1.656303	-0.278676
C	-1.002035	-2.225349	1.182133
H	-1.310013	-1.677284	2.066208
H	0.029602	-2.526109	1.317744
H	-1.606549	-3.124576	1.118016
C	-3.707666	1.554842	-0.328016
H	-3.410931	2.596695	-0.348459
H	-4.322425	1.367064	-1.204886
H	-4.347256	1.409138	0.539352

2-Z, MEP point 5 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89957076

SA-CASSCF/cc-pVTZ S₁ energy: -518.80216958

C	1.095091	-0.141108	-0.243979
C	-0.339045	-0.084467	-0.030766
C	-1.181708	-1.353886	-0.022183
C	-1.184497	1.007877	-0.291800
C	-2.518177	0.649548	-0.336837
C	-2.640922	-0.834876	-0.111522
N	1.932411	0.827958	0.164813
C	3.316916	0.452072	-0.045810
H	-3.194076	-1.319881	-0.911133
C	1.838091	-1.198786	-0.838713
C	3.239360	-0.945560	-0.556745
H	3.863005	0.537610	0.887596
H	3.779405	1.128496	-0.762799
H	-0.963322	-1.927276	-0.920815
C	1.606607	2.132685	0.677863
H	0.726832	2.085829	1.298484
H	1.439271	2.850710	-0.119189
H	2.433058	2.485084	1.279643
H	-0.853401	2.016244	-0.445757
H	-3.188898	-1.043014	0.805321
H	1.421932	-2.135923	-1.129598
H	3.989158	-1.675084	-0.322430
C	-0.947905	-2.259320	1.185854
H	-1.190219	-1.736460	2.104629
H	0.083463	-2.584110	1.247745
H	-1.572808	-3.145130	1.129869
C	-3.700008	1.559306	-0.413479
H	-3.400098	2.591181	-0.552090
H	-4.356807	1.289699	-1.236156
H	-4.297366	1.506365	0.494510

2-Z, MEP point 6 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89529079

SA-CASSCF/cc-pVTZ S₁ energy: -518.80354019

C	1.088410	-0.129375	-0.252637
C	-0.341688	-0.075440	-0.011871
C	-1.188850	-1.341131	0.025093
C	-1.182786	0.998073	-0.367244
C	-2.516422	0.644382	-0.383069
C	-2.640840	-0.803903	0.016282
N	1.928606	0.816511	0.192870
C	3.310599	0.442426	-0.035983
H	-3.280369	-1.369015	-0.655300
C	1.823277	-1.162332	-0.895209
C	3.220822	-0.930683	-0.609943
H	3.857071	0.479910	0.900266
H	3.778134	1.147935	-0.720612
H	-1.029629	-1.890216	-0.902838
C	1.603184	2.096466	0.766243
H	0.679559	2.034754	1.316670
H	1.511358	2.864694	0.004520
H	2.392941	2.387853	1.445553
H	-0.840408	1.989651	-0.595757
H	-3.089763	-0.883528	1.005893
H	1.396467	-2.073101	-1.248049
H	3.975169	-1.670442	-0.428948
C	-0.902107	-2.286744	1.188349
H	-1.075939	-1.789350	2.136303
H	0.123749	-2.634539	1.176170
H	-1.547630	-3.158418	1.143990
C	-3.693815	1.554615	-0.509982
H	-3.391238	2.562732	-0.767202
H	-4.383420	1.208419	-1.274717
H	-4.256228	1.603748	0.420440

2-Z, MEP point 7 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.89089774

SA-CASSCF/cc-pVTZ S₁ energy: -518.80465940

C	1.082854	-0.116139	-0.256438
C	-0.343897	-0.064527	0.009242
C	-1.192764	-1.327876	0.075981
C	-1.182451	0.982788	-0.430497
C	-2.515737	0.630502	-0.426953
C	-2.635589	-0.774347	0.110554
N	1.929456	0.797990	0.229607
C	3.307167	0.430170	-0.032076
H	-3.324645	-1.391849	-0.456916
C	1.805759	-1.118227	-0.955592
C	3.198940	-0.908292	-0.680377
H	3.862255	0.411057	0.899660
H	3.772771	1.170695	-0.679746
H	-1.076028	-1.869782	-0.864374
C	1.610766	2.054461	0.858268
H	0.641376	1.998388	1.321880
H	1.615860	2.866659	0.138058
H	2.350606	2.270223	1.617904
H	-0.832793	1.955208	-0.725124
H	-3.012763	-0.748523	1.133840
H	1.366085	-1.994438	-1.374296
H	3.966658	-1.650127	-0.593101
C	-0.874365	-2.290430	1.214569
H	-1.001972	-1.805127	2.175584
H	0.145842	-2.651572	1.154902
H	-1.530998	-3.154382	1.184220
C	-3.690621	1.536922	-0.602724
H	-3.387201	2.516103	-0.953894
H	-4.401869	1.132640	-1.317631
H	-4.229421	1.672098	0.333562

2-Z, MEP point 8 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.88555047

SA-CASSCF/cc-pVTZ S₁ energy: -518.80615993

C	1.079576	-0.096450	-0.261328
C	-0.347146	-0.045632	0.028915
C	-1.191661	-1.311485	0.130118
C	-1.183499	0.956721	-0.507111
C	-2.518565	0.604837	-0.483349
C	-2.627661	-0.749315	0.174337
N	1.934650	0.774773	0.268606
C	3.307527	0.412723	-0.028474
H	-3.341426	-1.409984	-0.306847
C	1.790528	-1.064070	-1.017411
C	3.168808	-0.884437	-0.750494
H	3.874848	0.336440	0.892933
H	3.769858	1.186450	-0.638590
H	-1.097506	-1.862307	-0.809990
C	1.628361	2.004935	0.956486
H	0.616940	1.973357	1.319269
H	1.748446	2.853528	0.290669
H	2.303202	2.129310	1.793396
H	-0.832604	1.911049	-0.857256
H	-2.957662	-0.630185	1.208252
H	1.333446	-1.897304	-1.501175
H	3.960749	-1.597742	-0.835862
C	-0.860113	-2.273838	1.263068
H	-0.969549	-1.789036	2.226455
H	0.157791	-2.640352	1.186400
H	-1.520236	-3.135671	1.242086
C	-3.690924	1.512131	-0.671542
H	-3.392708	2.461126	-1.101607
H	-4.437078	1.071031	-1.326305
H	-4.188316	1.719670	0.275036

2-Z, MEP point 9 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.87404533

SA-CASSCF/cc-pVTZ S₁ energy: -518.80995691

C	1.074894	-0.072986	-0.262694
C	-0.355256	-0.016620	0.043586
C	-1.187629	-1.288351	0.190849
C	-1.190180	0.917538	-0.600060
C	-2.527387	0.568479	-0.548849
C	-2.623107	-0.730630	0.217027
N	1.943318	0.735498	0.325068
C	3.310758	0.384951	-0.011072
H	-3.340094	-1.432060	-0.198396
C	1.789278	-1.000608	-1.083596
C	3.137175	-0.851926	-0.830491
H	3.891104	0.231000	0.892116
H	3.772976	1.198329	-0.566732
H	-1.100737	-1.853472	-0.745188
C	1.651158	1.958910	1.037064
H	0.609338	1.974341	1.297910
H	1.892937	2.812017	0.410959
H	2.249271	2.012280	1.937016
H	-0.842311	1.851897	-1.007591
H	-2.933895	-0.529499	1.246292
H	1.317459	-1.787354	-1.629672
H	3.935258	-1.520945	-1.070167
C	-0.850821	-2.247913	1.321693
H	-0.955431	-1.766507	2.287321
H	0.168239	-2.612968	1.239299
H	-1.506284	-3.113485	1.300930
C	-3.693101	1.491822	-0.712764
H	-3.399335	2.418097	-1.193819
H	-4.480059	1.043356	-1.313330
H	-4.139110	1.745838	0.248915

2-Z, MEP point 10 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.86092218

SA-CASSCF/cc-pVTZ S₁ energy: -518.81628911

C	1.066568	-0.051468	-0.266007
C	-0.358748	0.007751	0.033207
C	-1.184884	-1.264778	0.246045
C	-1.207299	0.876648	-0.695421
C	-2.536893	0.534058	-0.595513
C	-2.619196	-0.710756	0.258529
N	1.953320	0.688643	0.384145
C	3.314478	0.348806	0.015577
H	-3.339408	-1.440973	-0.096704
C	1.785442	-0.927075	-1.163396
C	3.117514	-0.811613	-0.907348
H	3.900240	0.108579	0.895839
H	3.785546	1.198064	-0.473348
H	-1.104391	-1.855748	-0.675523
C	1.676280	1.905308	1.116596
H	0.619373	1.965161	1.298686
H	2.008557	2.757754	0.531641
H	2.207468	1.905347	2.059327
H	-0.869806	1.786738	-1.160853
H	-2.912093	-0.439569	1.276657
H	1.303232	-1.662531	-1.769830
H	3.912090	-1.444637	-1.242012
C	-0.839404	-2.205536	1.388144
H	-0.942012	-1.716141	2.350175
H	0.180684	-2.569204	1.305349
H	-1.492258	-3.073142	1.377148
C	-3.697608	1.466623	-0.753377
H	-3.412457	2.366585	-1.286383
H	-4.519595	1.007526	-1.295656
H	-4.092245	1.769606	0.216604

2-Z, MEP point 11 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.84933515

SA-CASSCF/cc-pVTZ S₁ energy: -518.82334835

C	1.057789	-0.031967	-0.273962
C	-0.357985	0.027859	0.015065
C	-1.178334	-1.240113	0.292373
C	-1.226771	0.842931	-0.773389
C	-2.544519	0.507437	-0.625647
C	-2.612974	-0.687616	0.299233
N	1.958409	0.640020	0.427038
C	3.315413	0.307348	0.038466
H	-3.336861	-1.437699	-0.004898
C	1.781114	-0.852496	-1.241676
C	3.104064	-0.765933	-0.982339
H	3.890296	-0.020874	0.897197
H	3.806028	1.184833	-0.373823
H	-1.111168	-1.866167	-0.607843
C	1.697429	1.834197	1.205988
H	0.634788	1.929869	1.331866
H	2.098844	2.692328	0.676114
H	2.175261	1.768574	2.173568
H	-0.901422	1.729948	-1.290914
H	-2.889515	-0.360973	1.305546
H	1.290686	-1.529810	-1.906735
H	3.895014	-1.367221	-1.377890
C	-0.821977	-2.145106	1.459757
H	-0.917519	-1.630075	2.409078
H	0.197793	-2.510940	1.379436
H	-1.473216	-3.014243	1.477864
C	-3.708770	1.432841	-0.806882
H	-3.435484	2.301099	-1.396072
H	-4.547596	0.948821	-1.299332
H	-4.073541	1.790291	0.156051

2-Z, MEP point 12 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.84101031

SA-CASSCF/cc-pVTZ S₁ energy: -518.83008766

C	1.048678	-0.016523	-0.279840
C	-0.358235	0.053352	0.008387
C	-1.168165	-1.212792	0.329812
C	-1.243416	0.822277	-0.826731
C	-2.550426	0.485071	-0.651483
C	-2.603310	-0.662798	0.333069
N	1.961727	0.601093	0.445901
C	3.314288	0.267704	0.046350
H	-3.332321	-1.427203	0.081494
C	1.773549	-0.791883	-1.303760
C	3.091603	-0.718972	-1.055338
H	3.866401	-0.142921	0.883162
H	3.831388	1.159839	-0.290074
H	-1.110631	-1.874387	-0.546298
C	1.716580	1.741750	1.308272
H	0.652796	1.861628	1.401180
H	2.166477	2.618061	0.854527
H	2.158038	1.586303	2.282513
H	-0.931461	1.691594	-1.381102
H	-2.859709	-0.284390	1.326779
H	1.274077	-1.412140	-2.016164
H	3.882750	-1.271621	-1.517771
C	-0.800071	-2.070488	1.529515
H	-0.887642	-1.517557	2.457985
H	0.219621	-2.439311	1.455650
H	-1.449353	-2.939250	1.588756
C	-3.725754	1.387294	-0.874898
H	-3.467286	2.220823	-1.518418
H	-4.567570	0.868939	-1.325369
H	-4.080264	1.799966	0.069788

2-Z, MEP point 13 (S₁)

SA-CASSCF/cc-pVTZ S₀ energy: -518.83700760

SA-CASSCF/cc-pVTZ S₁ energy: -518.83544199

C	1.040662	-0.001693	-0.280680
C	-0.359754	0.084757	0.014912
C	-1.155468	-1.183146	0.359347
C	-1.256431	0.823309	-0.848263
C	-2.553856	0.467344	-0.674719
C	-2.594722	-0.642794	0.353444
N	1.967784	0.579771	0.445848
C	3.314310	0.240557	0.031973
H	-3.323389	-1.419336	0.139735
C	1.756606	-0.754963	-1.343183
C	3.075595	-0.678793	-1.123481
H	3.846827	-0.232494	0.848813
H	3.855647	1.137161	-0.247691
H	-1.096461	-1.876732	-0.492931
C	1.741356	1.632869	1.418440
H	0.678846	1.773382	1.501370
H	2.228674	2.534314	1.066115
H	2.157877	1.358584	2.377610
H	-0.954601	1.679096	-1.429877
H	-2.841104	-0.226811	1.334737
H	1.243623	-1.330494	-2.082699
H	3.863286	-1.182941	-1.643171
C	-0.777794	-1.990129	1.592653
H	-0.865870	-1.398090	2.496882
H	0.244335	-2.355777	1.531585
H	-1.420936	-2.860178	1.691942
C	-3.747119	1.329358	-0.955651
H	-3.502119	2.129331	-1.645778
H	-4.575512	0.768086	-1.379420
H	-4.115858	1.789269	-0.038828