Supplementary Materials for

Conformer-specific photochemistry imaged in real space and time

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The PDF file includes:

Other Supplementary Material for this manuscript includes the following:

Materials and Methods

Ultrafast electron diffraction experiments: The experimental apparatus is described in detail elsewhere.(*31*) In short, we use the 800 nm output of a Ti:Sapphire laser system and separate two beam paths. Pulses in both beam paths are frequency-tripled. The pulses of the probe beam path are directed onto the photocathode of an RF gun and eject an ultrashort pulse containing ~10^4 electrons. 3.7 MeV electrons are generated using a S-band photocathode radio frequency (RF) gun(*32*) and focused through a holey mirror to a spot size of 200 µm FWHM in the interaction region of a gas phase experimental chamber. The pump pulses (7 µJ) are focused into the experimental chamber to a diameter of 240 µm FWHM and overlapped with the electron pulses at a 2° angle. The experimental response function including effects of the optical and electron pulse length as well as relative arrival time jitter is estimated to be 150 fs.(*22*) αPH is purchased from Sigma-Aldrich and used without further purification. We use a static-filled 3 mm flow cell (550 µm orifices, sample at room temperature) in combination with a repetition rate of 360 Hz. Diffracted electrons are detected by a combination of a phosphor screen and an EMCCD camera. Based on the relative static and dynamic signal levels, we estimate to excite about 2.5 % of the molecules (see **Fig. S4**). Time-dependent diffraction is measured at a series of time delay points between -2 ps and +1 ps in each scan. The separation between time delay points is 50 fs, except for the earliest and latest delay points, where it was considerably larger. At each time delay point, we integrate diffraction signal for 10 seconds. The full data set includes 88 such scans. The sequence of delay steps is randomized for every scan to avoid systematic errors.

Generation of modified molecular diffraction and pair distribution functions from experimental data: Determination of modified molecular diffraction (sM(s), see **Fig. S5**) from 2-dimensional molecular diffraction data is described in detail in the supplementary information of Ref. (*22*). Similar to Ref. (*22*), generation of static atomic pair distribution functions (PDFs, see **Fig. 2a**) requires extrapolating the experimental sM(s) for $s \leq 0.8$ Å^{-1} with simulated sM(s) signal (see **Fig. S5**). As evident from **Fig. S5**, the extrapolated range (dashed black line) does not show conformer-dependence in the simulations. Thus, our mode of extrapolation does not bias the shape of the PDF towards a specific conformer.

ΔsM(s, t) is generated by subtracting sM(s) before time zero (before the onset of transient features) from sM(s) of all pump-probe delays. As for PDFs, extrapolation of these traces to s=0 Å^{-1} is required to avoid artifacts in ΔPDF(r,t). In this low s region, the traces are set to $\Delta sM_{hole}(s,t) = \Delta sM_{eq}(s,t=1ps) \times (1 + \mathrm{erf}[(t-t0)/\tau])$. The first term is the average of the simulated ΔsM(s,t) traces for the three equatorial conformers at a delay of 1 ps. The second term sets the time-dependence, which is assumed to follow a simple error function with the onset time t0 and width τ found by curve-fitting to ΔsMeq(s,t). As described in detail in the supplementary material of Ref.(*22*), for the generation of ΔPDF(r,t), the high s contributions of ΔsMeq(s,t) are smoothly damped using a Gaussian function e^{-ks^2} with k=0.028 Å^2. To ensure that the low s extrapolation of the experimental data does not bias the ΔPDF(r,t), we generate ΔPDF(r,t) for both the simulated averaged eq conformers and the experimental data, where we set the low s range to zero (see **Fig. S6**).

Theoretical Method: AIMS simulations interfaced with GPU-accelerated α-CASSCF(*23, 33-35*) are used to model the photodynamics of isolated ax and eq rotamers of αPH. The α-CASSCF has shown to be well-suited for this system based on our previous CHD work and single-point

XMSPT2 calculations (**Fig. S7-9**).(*22*) Our active space consists of six electrons in four orbitals determined to minimize the average energy of the lowest two singlet states, within the 6-31G* basis set, i.e. α-SA-2-CASSCF(6,4)/6-31G*. Electronic structure calculations are performed with TeraChem.(*36-38*) Following previous work, we use an α value of 0.82. A total of 90 initial conditions (15 sets of positions and momenta for each conformer) were selected from the computed electronic absorption spectrum (**Fig. S10**) and used to initiate the AIMS dynamics. The active-space molecular orbitals (MO) for all isomers were nearly identical to CHD (**Fig. S11**). These ICs are then placed on the S_1 surface and propagated with AIMS.

The first two singlet states (S_0 and S_1) are included in the dynamics. All required electronic structure quantities (energies, gradients, and nonadiabatic couplings) are calculated as needed with α-SA-2-CASSCF(6,4)/6-31G*. An adaptive timestep of 0.48 fs (20 au) (reduced to 0.12 fs (5 au) in regions with large nonadiabatic coupling) is used to propagate the centers of the trajectory basis functions (TBFs). A coupling threshold of 0.01 au (scalar product of nonadiabatic coupling and velocity vectors) demarcates spawning events generating new TBFs on different electronic states. Population transfer between TBFs is described by solving the time-dependent Schrödinger equation in the time-evolving TBF basis set.

We simulate the ultrafast dynamics for the first 1 ps of all six equatorial and axial conformational isomers of α-PH by: 1) using AIMS to propagate the initial wavepacket for the first 500 fs or until all population has returned to the ground state, 2) stopping TBFs on the ground state when they are decoupled from other TBFs (off-diagonal elements of the Hamiltonian become small), and 3) adiabatically continuing these stopped TBFs using the positions and momenta from the last frame in AIMS as initial conditions for adiabatic molecular dynamics with unrestricted DFT using the Perdew-Burke-Ernzerof hybrid exchange-correlation functional,(*39*) i.e uPBE0/6-31G*. A total of 398 TBFs are propagated, with 306 of these being adiabatically continued on the ground state with DFT. The level of convergence of the simulations is benchmarked for the equatorial and axial T conformers (see **Fig. 2**) in comparison to simulations with twice the initial conditions (**Fig. S12**)

Simulation of modified molecular diffraction and pair distribution functions: The sM(s) simulations within the independent atom model (IAM) are generated from molecular geometries using a publicly available python code(*40*) and atomic scattering functions from the elsepa program.(*41*) PDFs are generated from the simulated sM(s) using the same code as for the experimental data.

For the creation of ΔPDFs from the AIMS simulations, sM(s) functions are evaluated for each time step of the simulation and each trajectory basis function (TBF) of a given initial condition separately both for the portion of the simulation using α-CASSCF and the extension on the ground state surface with DFT. The sM(s) functions of different TBFs are averaged for each time step according to their population weights. The resulting averaged time-dependent sM(s) functions are rebinned to 2 fs time steps. ΔsM(s, t) of a specific conformer are created by averaging the sM(s, t) from all initial conditions of this conformer and subtracting the initial sM(s, t=0) function from the average. The ΔPDF(r, t) functions are created from ΔsM(s, t) functions using the same code as for the experimental ΔPDFs. To account for the experimental response function, the ΔPDFs are convolved with a 150 fs FWHM Gaussian in time.

Supplementary Text

Supplementary text 1: We investigate the ground state potential energy surface using a number of different methods. A summary of our results can be found in **Fig. S13**. Our quantum chemical calculations find six possible αPH minimum geometries, three different rotamers for eq and ax geometries, which we label according to the C_3-C_1-C_2-H_{ISO} dihedral angle of the isopropyl group shown in **Fig. 2** (i.e. gauche- (G-), trans (T), and gauche+ (G+)). Their S_0 minima are at -58.5°/-70.7° (G-), -172.9°/179.4° (T), and 57.0°/48.9° (G+) for ax/eq conformers, respectively. Our calculations find the eq-αPH minimum geometries to be in general more stable than ax-αPH and the thermal equilibrium, thus, dominated by similar fractions of the three eq-αPH rotamers. This is confirmed by a recent study on matrix isolated αPH which could only identify vibrational signatures of equatorial conformers.(*21*)

To quantify the possible amount of axial conformers in our gas phase sample, we fit a linear combination of the simulated sM(s) functions of all six conformers to the experimental sM(s). The coefficients of the axial conformer sM(s) functions are always negative or zero if forced to be positive semidefinite. Thus, we cannot find any direct evidence for the presence of axial conformers in the static diffraction. We estimate the uncertainty of this assessment to be on the order of 10 %,

To quantify the contribution of ax-αPH ring-opening to the experimental signal, we create linear combinations of the averaged eq-αPH and ax-αPH and compare the time-dependence of the integrated α, β, and γ regions to the experimental data, analogous to **Fig. 3d**. A comparison using a linear combination with 20% ax-αPH contribution is plotted in **Fig. S14**. The α and β regions are only moderately sensitive to the fraction of ax-αPH contribution, since both ax- αPH and eq-αPH open the ring. As expected from **Fig. S3**, the γ-region is significantly more sensitive to the fraction of ax-αPH contribution. In **Fig. S14**, the intensity of the γ-signature is reduced far enough to be outside the error bars (68% confidence interval) of the experiment. Therefore, we estimate the contribution of ax-αPH to the time-dependent experimental signal to be <20%.

Supplementary text 2: In the AIMS simulations, we observe an additional photoproduct, 2-ladderane (5-isopropyl-2-methylbicyclo[2.2.0]hex-2-ene), which is formed in the electronic ground state exclusively by population having undergone internal conversion through the conical intersection CI-1. Since we do not observe internal conversion through CI-1 for the eq-G+ and ax-G- rotamers, the product is exclusively observed for the eq-T, eq-G-, ax-T, and ax-G+ rotamers (see **supplementary movies 1-4**). The ΔPDF signatures of 2-ladderane and ZEDOT are quite similar (see **Fig. S15**), especially in the γ-region. Additionally, the simulations predict only 5 % of the eq-α-phellandrene population undergoing internal conversion through CI-1 (see **Fig. 4** and **Table S1**). Therefore, a direct signature from the 2-ladderane contribution would be difficult to extract from the experimental data. However, it is included in the simulations and, therefore contributes to the quantitative agreement with experiment.

Supplementary Figures

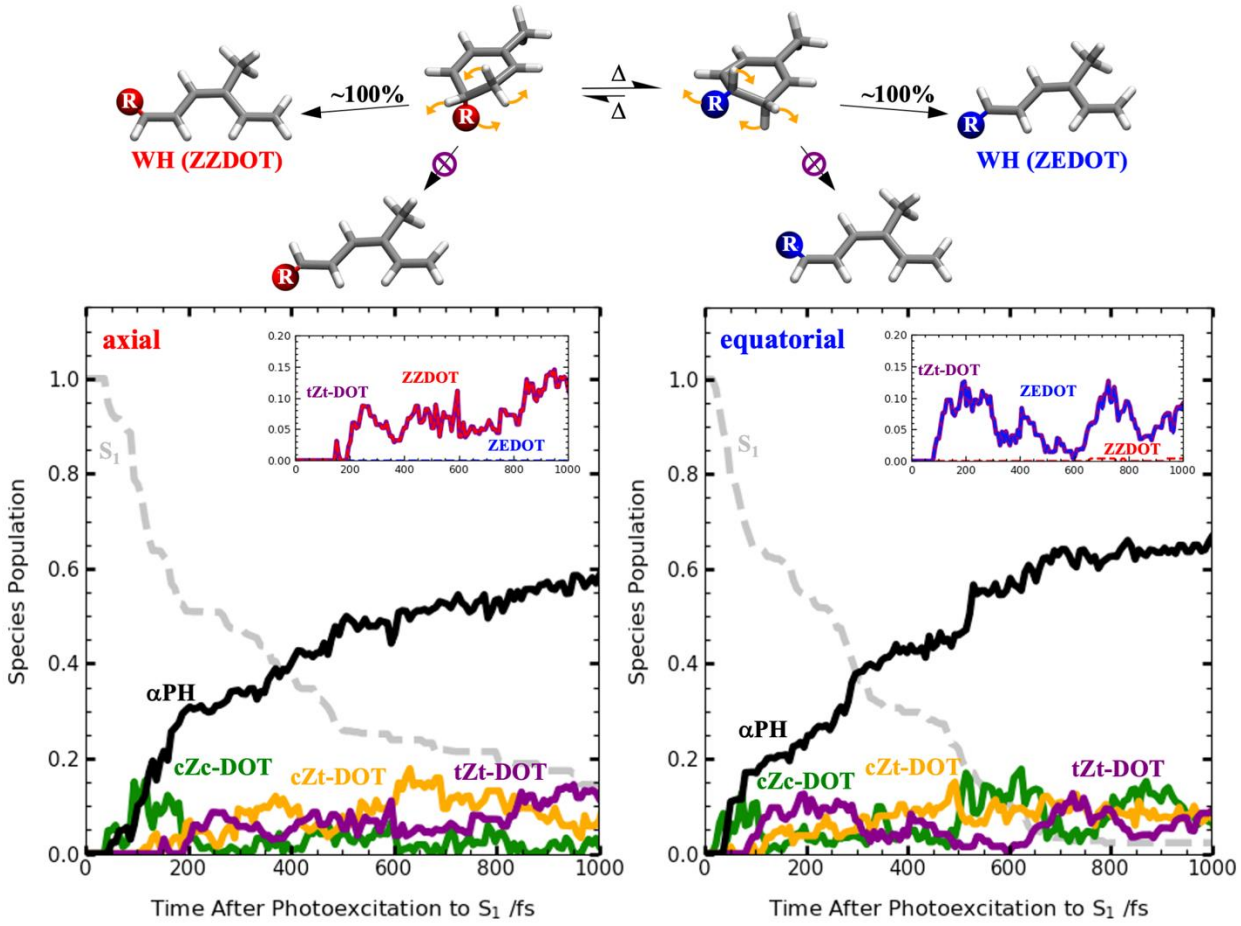


Fig. S1. AIMS Wavepacket Population for Axial and Equatorial Conformers. (Top) The Woodward-Hoffman allowed photoproducts from ax and eq αPH (the isopropyl group is represented as the R group). (Bottom) The wavepacket population from the axial (left) and equatorial (right) AIMS dynamics for the first picosecond after photoexcitation for all 90 ICs (45 each for ax and eq) considered. Snapshots every 5fs were binned based on the αPH, cZc, cZt, and tZt configurations and weighted according to their amplitudes. The insets show the tZt-DOT population decomposed into ZZDOT and ZEDOT contributions for ax (left) and eq (right) photoproducts. Conrotatory ring-opening in the ax and eq ICs leads almost exclusively to the WH predicted ZZDOT (red) and ZEDOT (blue) photoproducts, respectively.

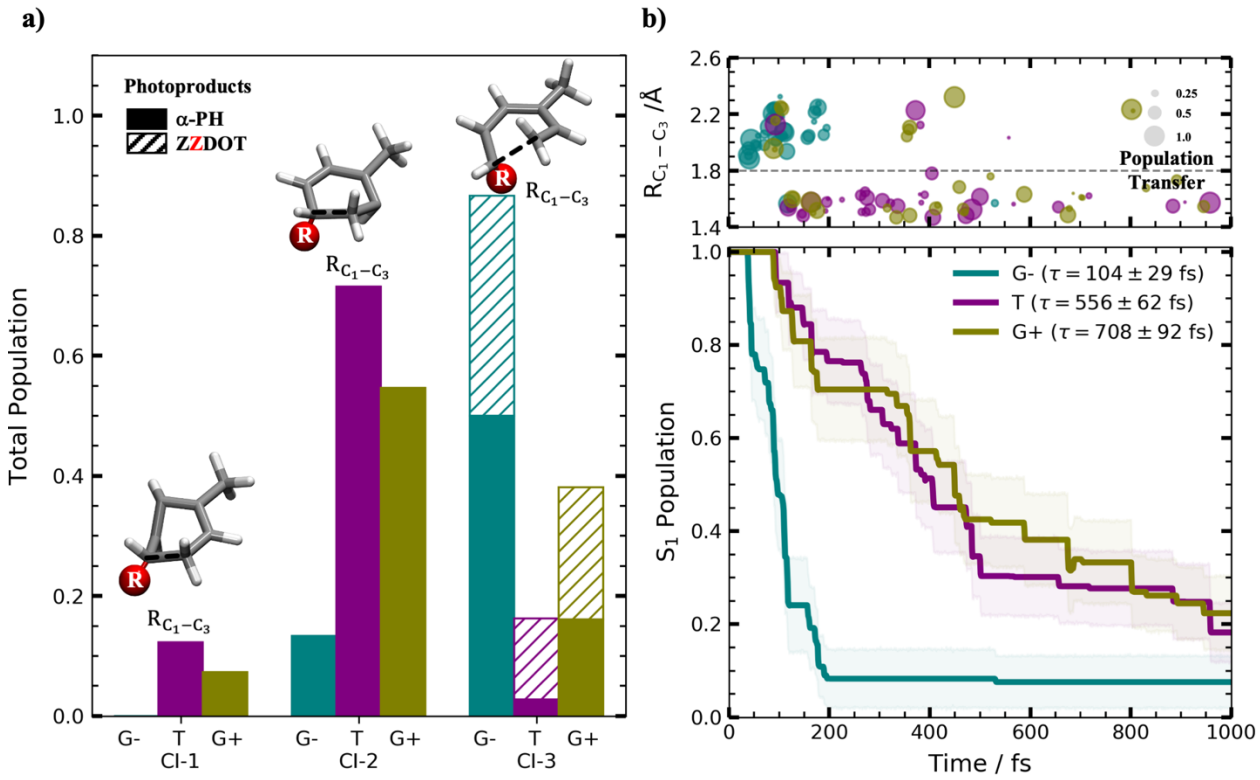


Fig. S2. Characterization of the Closed- and Open-Ring Nonradiative Relaxation Pathways for ax-Rotamers. a) A histogram of the branching ratio between the closed and open pathways from AIMS dynamics. Solid and striped bars represent fractional population that reformed ⟨PH or cZc-ZDOT, respectively. b) (top) The C_1-C_3 distance vs spawning time for all 45 ax initial conditions. The black dashed line corresponds to the threshold used to determine if open or closed. The circle radius is proportional to the population transferred during the spawning event and separated into eq-G- (teal), eq-T (purple), and eq-G+ (olive). (bottom) The S_1 population decay for eq-G-, eq-T, and eq-G+ for the first ps after photoexcitation.

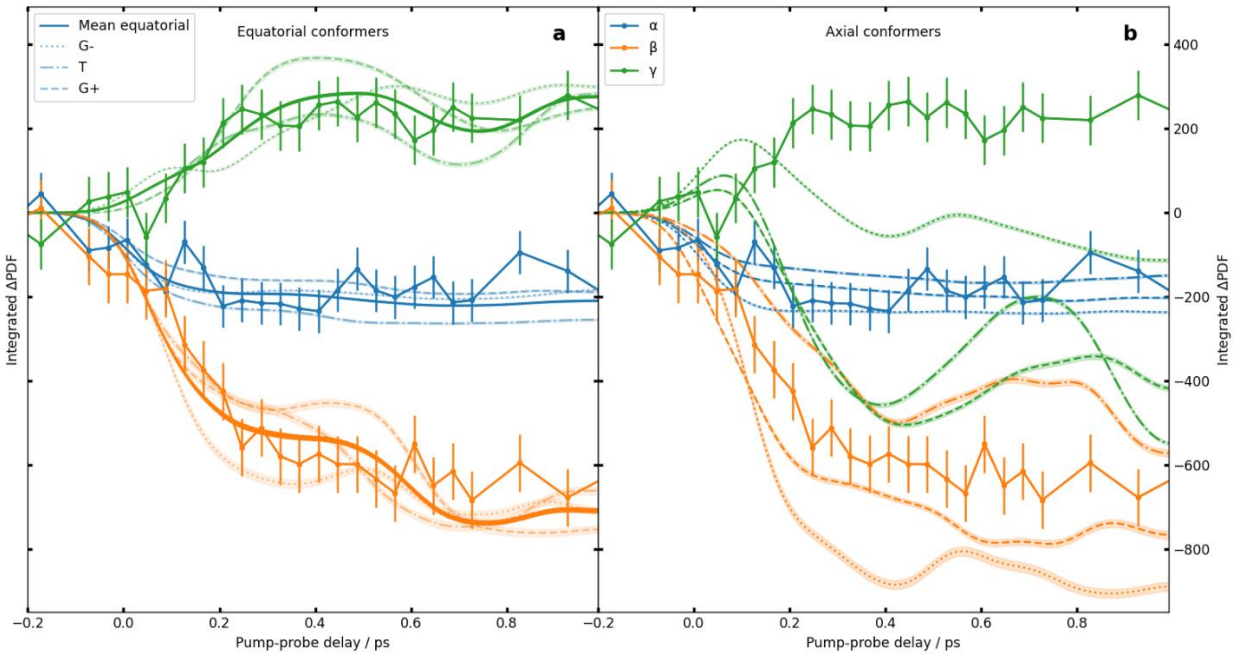


Fig. S3. Experimental and Simulated Signal Rise-Times Along Coordination Shells. (a) Temporal evolution of the integrated regions of the first (α, blue), second (β, orange) and third (γ, green) coordination shells of the experimental (connected points with error bars) and simulated ΔPDF averaged over the three equatorial rotamers (continuous lines). Simulated ΔPDF signals of the individual equatorial rotamers are shown as dotted (G-), dash-dotted (T), and dashed (G+) lines. The experimental data show quantitative agreement with the average of the simulated equatorial rotamer signals. (b) Analogous comparison between the experimental and simulated ΔPDF signals of the individual axial rotamers. Error bars represent a 68% confidence interval obtained from bootstrap analysis. The error bars of the simulations are visualized by the width of the lines and reflect convergence with respect to initial condition sampling.

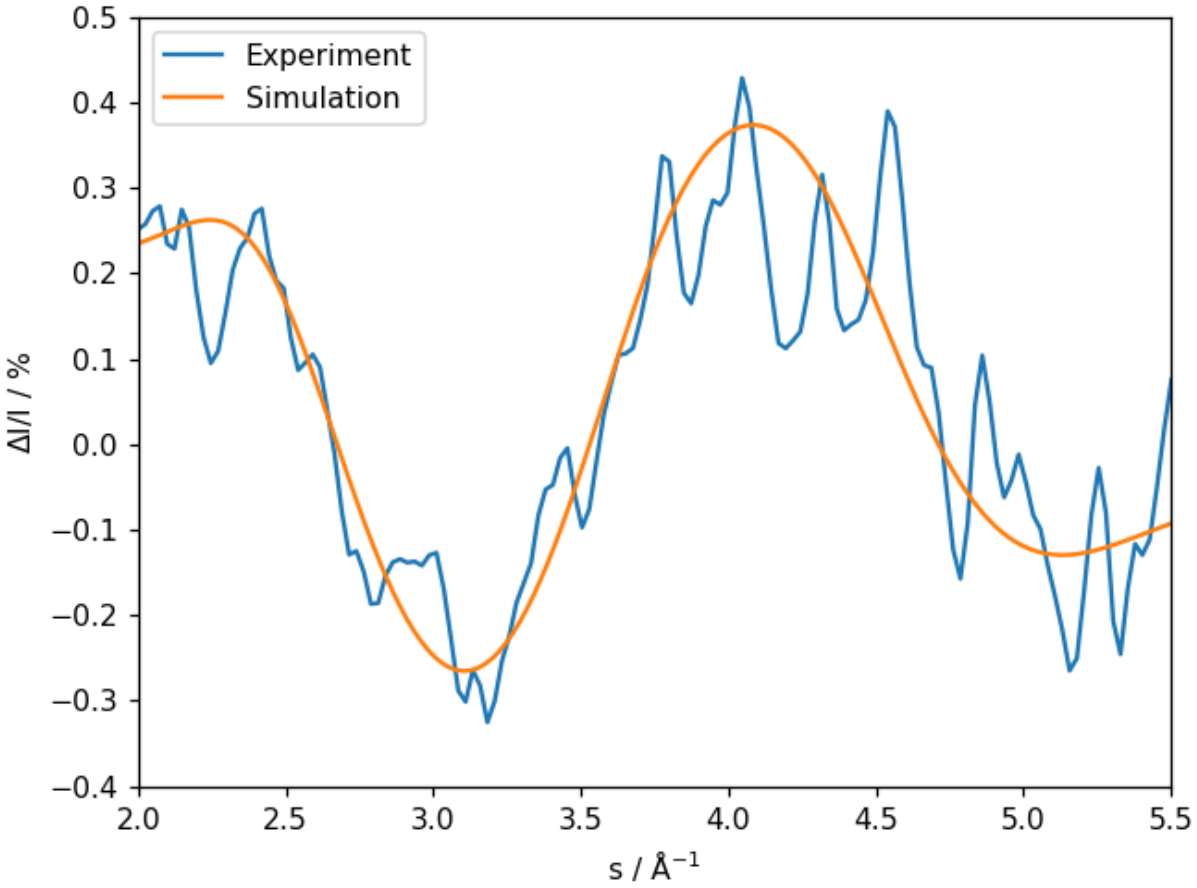


Fig. S4. Experimental and Simulated Relative Difference Diffraction Signals. Comparison between experimental and simulated relative difference diffraction signals (I(1 ps)-I(steady-state))/I(steady-state). The simulation is scaled by a factor of 0.025 to match the amplitude of the experiment. This suggests an excitation ratio of 2.5 %.

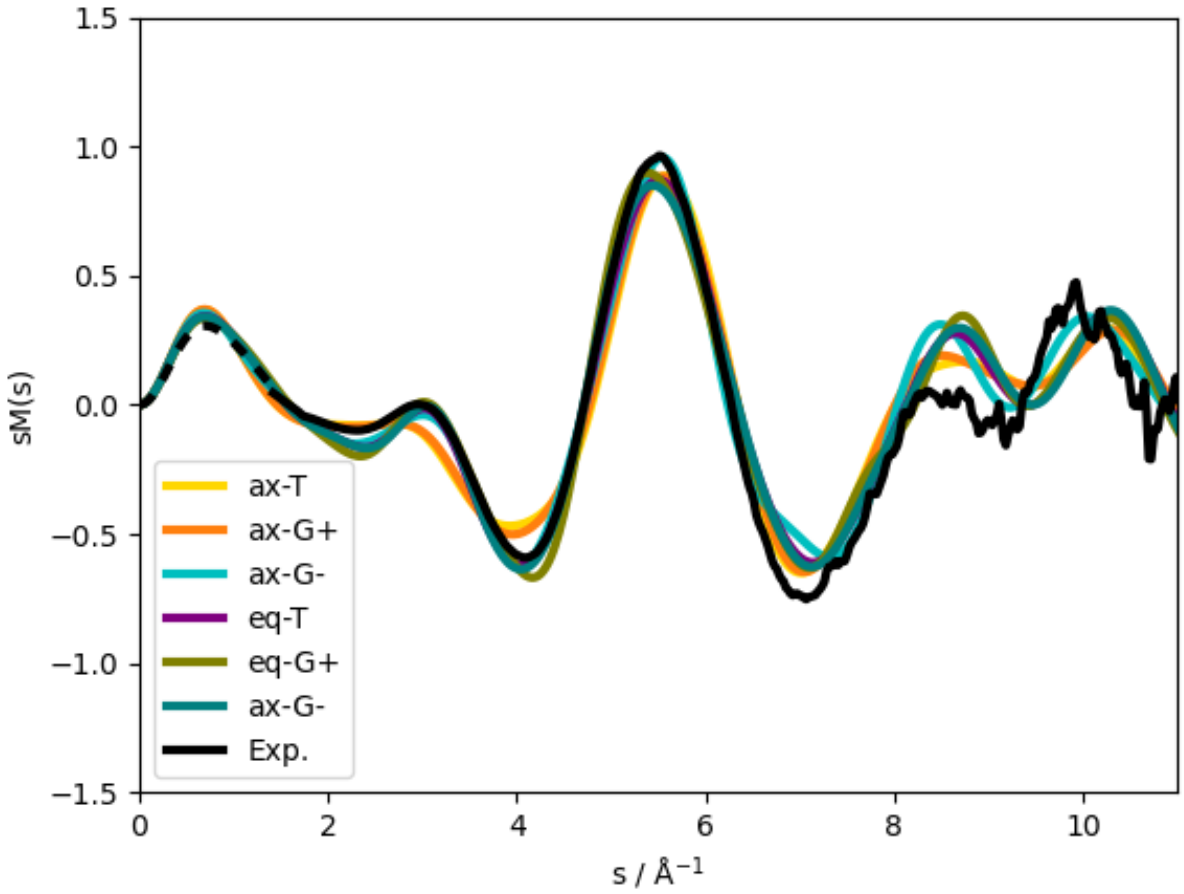


Fig. S5. Comparison of the experimental modified molecular diffraction sM(s) with simulations of all six phellandrene conformers. The experimental sM(s) is replaced by the average of the simulated sM(s) below 1.5 Å^{-1} to avoid artifacts from the hole in the detector in the experimental PDF (see Fig. 2a). As in Fig. 2a, we find good agreement between the experimental sM(s) and four of the six possible conformers, all three equatorial and the ax-G- conformer, in a wide range from 1.5 Å^{-1} to 8 Å^{-1}. The agreement in Fig. 2a is worse in the range >8 Å^{-1}, which might be due to shortcomings in the subtraction of the atomic scattering background and limited signal-to-noise levels. The ax-T and ax-G+ conformers show significantly worse agreement with the experimental data in the region between 2 Å^{-1} and 4.5 Å^{-1}.

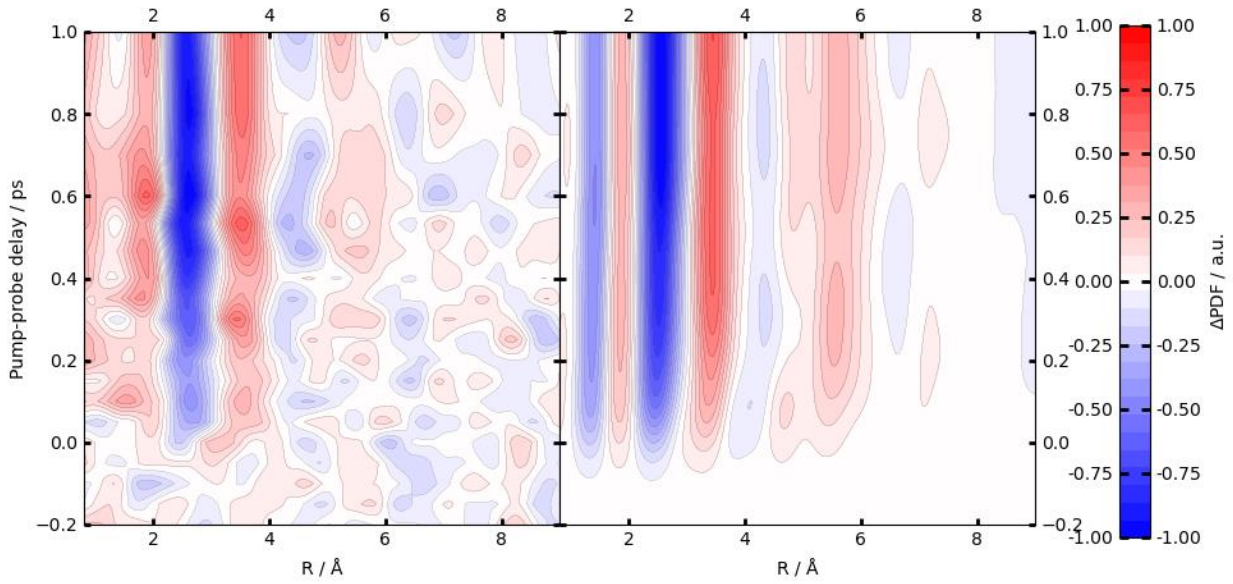


Fig. S6. Experimental ΔPDF(r,t) (left) and the average of the simulated ΔPDF(r,t) of equatorial rotamers (right) . Both ΔPDF(r,t) are generated while setting the s range <0.6 $Å^{-1}$ to zero to assess the bias to the experimental ΔPDF(r,t) by treatment of the s<0.6 $Å^{-1}$ for Fig. 3 (see supplementary note 4). The main artifacts introduced by setting s<0.6 $Å^{-1}$ to zero are a smooth positive contribution to distances <2 Å and a negative contribution to distances > 4 Å.

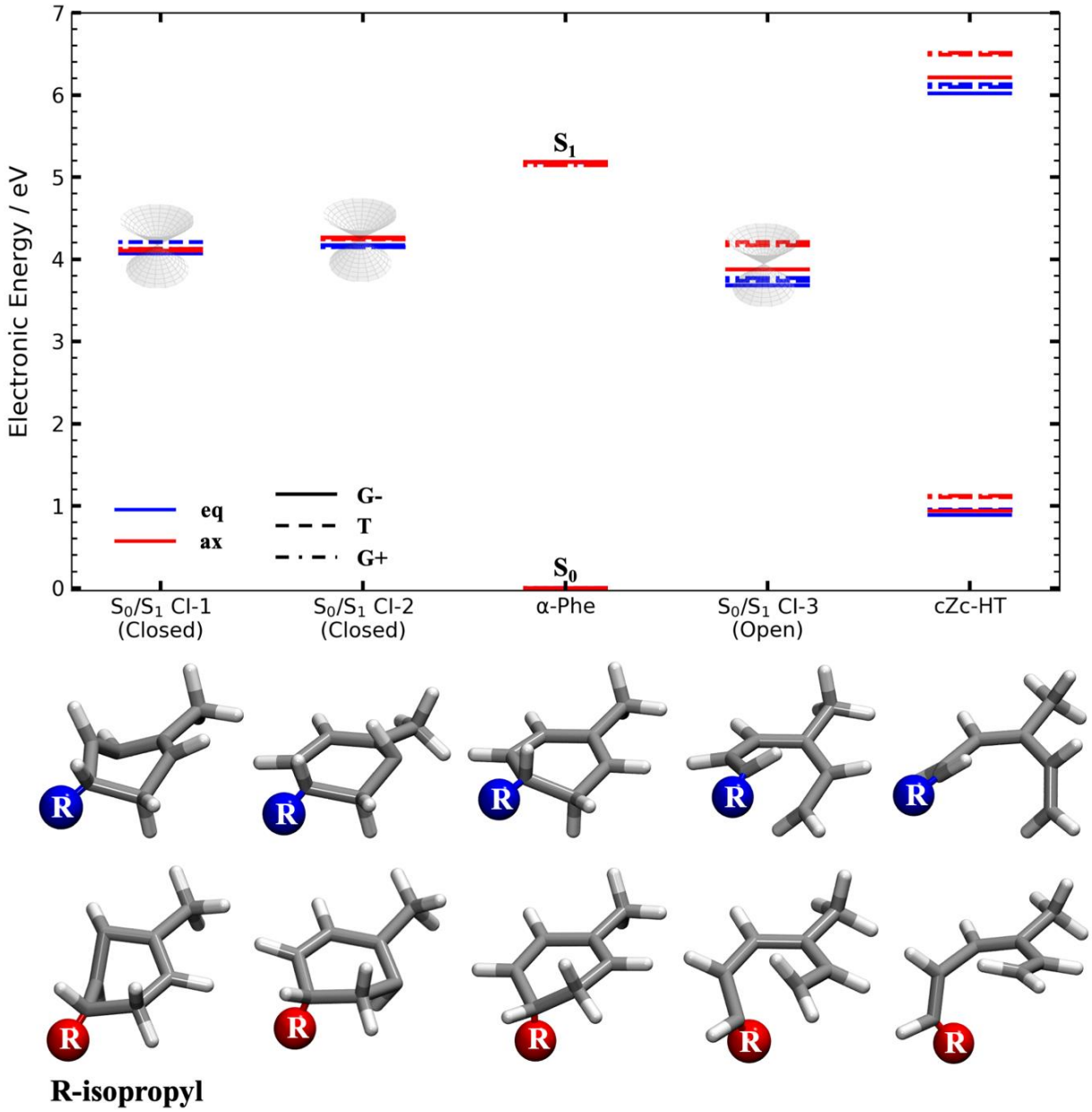
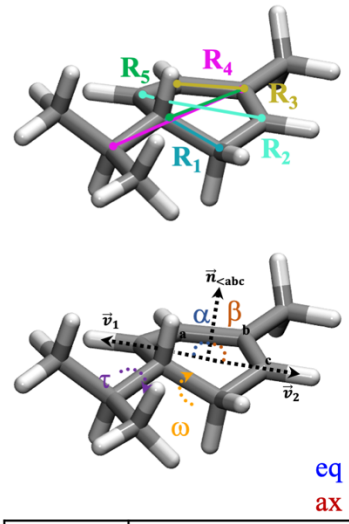


Fig. S7. Critical Points Along Nonradiative Relaxation Pathways in Ax and Eq αPH. The computed ax (red) and eq(blue) PESs at critical points along the OOP and ring-opening reaction coordinates in αPH. The energies are relative to each isomer's respective S_0 minimum ground-state energy. Geometries are shown in the bottom of the figure with the red (ax) and blue (eq) spheres representing the location of the ISO. Computed at the α(0.82)-SA2-CAS(6,4)-SCF/6-31G* level of theory. See **Table S2** for coordinates, energies, and CI vectors.



		G-		T		G+			G-		T		G+	
S_0 min	R_1 (Å)	1.53	1.54	1.53	1.54	1.53	1.54	cZc-DOT	3.51	3.63	3.52	3.73	3.49	3.72
	R_2 (Å)	2.82	2.82	2.82	2.83	2.82	2.83		3.18	3.15	3.18	3.15	3.18	3.15
	R_3 (Å)	1.47	1.47	1.47	1.47	1.47	1.47		1.36	1.34	1.36	1.34	1.36	1.34
	R_4 (Å)	4.36	3.59	4.36	3.85	4.36	3.81		4.71	3.67	4.70	4.04	4.70	4.09
	R_5 (Å)	2.89	2.9	2.88	2.9	2.9	2.9		3.22	3.38	3.21	3.50	3.21	3.52
	ω (°)	44.2	-46.7	43.4	-32.9	45.2	-35.2		71.7	-70.2	73.2	-61.2	72.7	-57.7
	τ (°)	-70.7	-58.5	179.4	-172.9	48.9	57.0		-104.8	-52.3	133.2	168.1	17.2	53.5
	α (°)	89.6	90.4	88.1	91.8	88.2	90.7		119.0	33.4	120.7	23.1	121.2	21.4
	β (°)	92.3	88.4	92.2	89.8	92.0	88.9		47.5	114.0	46.7	106.1	48.4	103.4

		G-		T		G+			G-		T		G+	
S_1/S_0 CI_1	R_1 (Å)	1.54	1.55	1.53	1.54	1.54	1.54	S_1/S_0 CI_2	1.55	1.55	1.55	1.56	1.55	1.56	S_1/S_0 CI_3	2.28	2.13	2.27	2.15	2.23	2.12
	R_2 (Å)	2.27	2.28	2.26	2.27	2.27	2.27		2.90	2.90	2.90	2.90	2.91	2.90		2.89	2.85	2.89	2.84	2.89	2.85
	R_3 (Å)	1.39	1.40	1.38	1.39	1.39	1.39		1.46	1.46	1.46	1.47	1.46	1.47		1.41	1.38	1.41	1.39	1.41	1.39
	R_4 (Å)	4.05	4.27	4.19	4.24	4.06	4.25		4.28	3.82	4.28	4.08	4.28	4.08		4.57	3.42	4.56	3.74	4.56	3.69
	R_5 (Å)	2.96	2.9	2.96	2.9	3.0	2.9		2.90	2.9	2.89	2.9	2.9	2.9		3.06	3.0	3.06	3.1	3.1	3.08
	ω (°)	20.3	-0.5	25.4	-13.8	20.6	-13.8		38.7	-42.3	36.6	-22.4	37.6	-23.3		65.8	-66.9	65.4	-61.3	65.9	-62.0
	τ (°)	-57.1	-53.9	179.1	-171.5	-52.01	57.3		-74.3	-66.4	176.8	-175.0	40.1	53.3		-73.3	-52.6	-167.4	-164.4	14.6	63.1
	α (°)	9.5	178.4	12.8	169.9	10.4	171.3		96.7	81.2	96.5	84.3	96.0	84.0		104.2	56.7	104.2	52.4	106.9	51.4
	β (°)	79.0	97.5	78.1	99.2	79.4	98.6		-31.4	-148.5	-31.6	-146.9	-31.6	-147.2		69.7	117.1	69.2	118.0	68.9	117.4

Fig. S8. The Structural Properties of the Critical Points. Computed structural properties of the critical points for all eq and ax isomers at the α(0.82)-SA2-CAS(6,4)-SCF/6-31G* level of theory. See **Table S2** for coordinates, energies, and CI vectors.

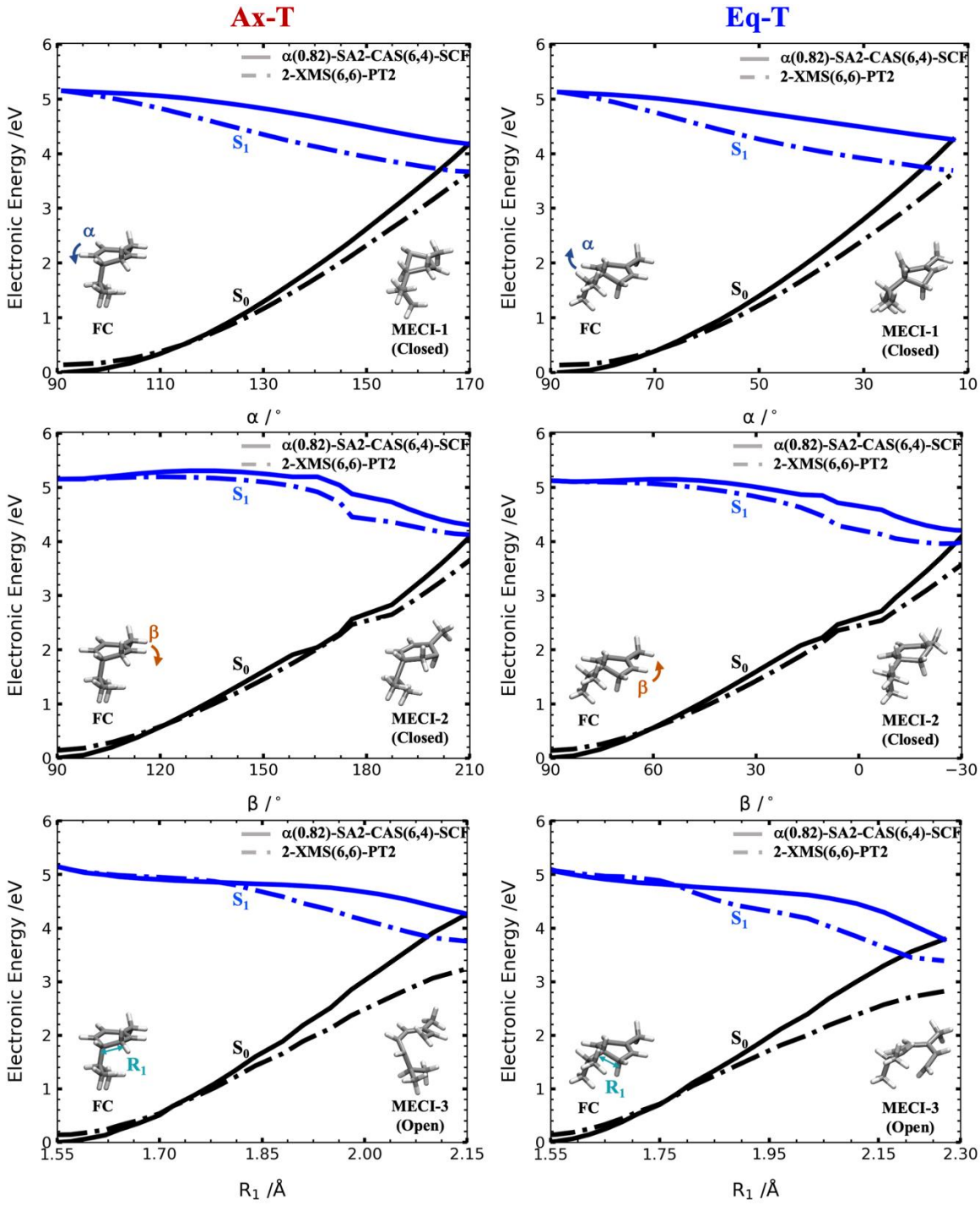


Fig. S9. Benchmarking α-SA-CASSCF Against XMSPT2 on S_1 with the G- Ax and Eq Conformers. Potential energy surface scans along the OOP (CI-1 and CI-2) and ring-opening (CI-3) coordinates on the S_1 electronic state. The pathways were generated from geodesic interpolation between the FC point and CI-1, CI-2, and CI-3 MECI structures, respectively, optimized at the α(0.82)-SA2-CAS(6,4)SCF/6-31G* level of theory and compared against single-point energy calculations with SA2-XMS-CAS(6,6)-PT2/6-31G*.

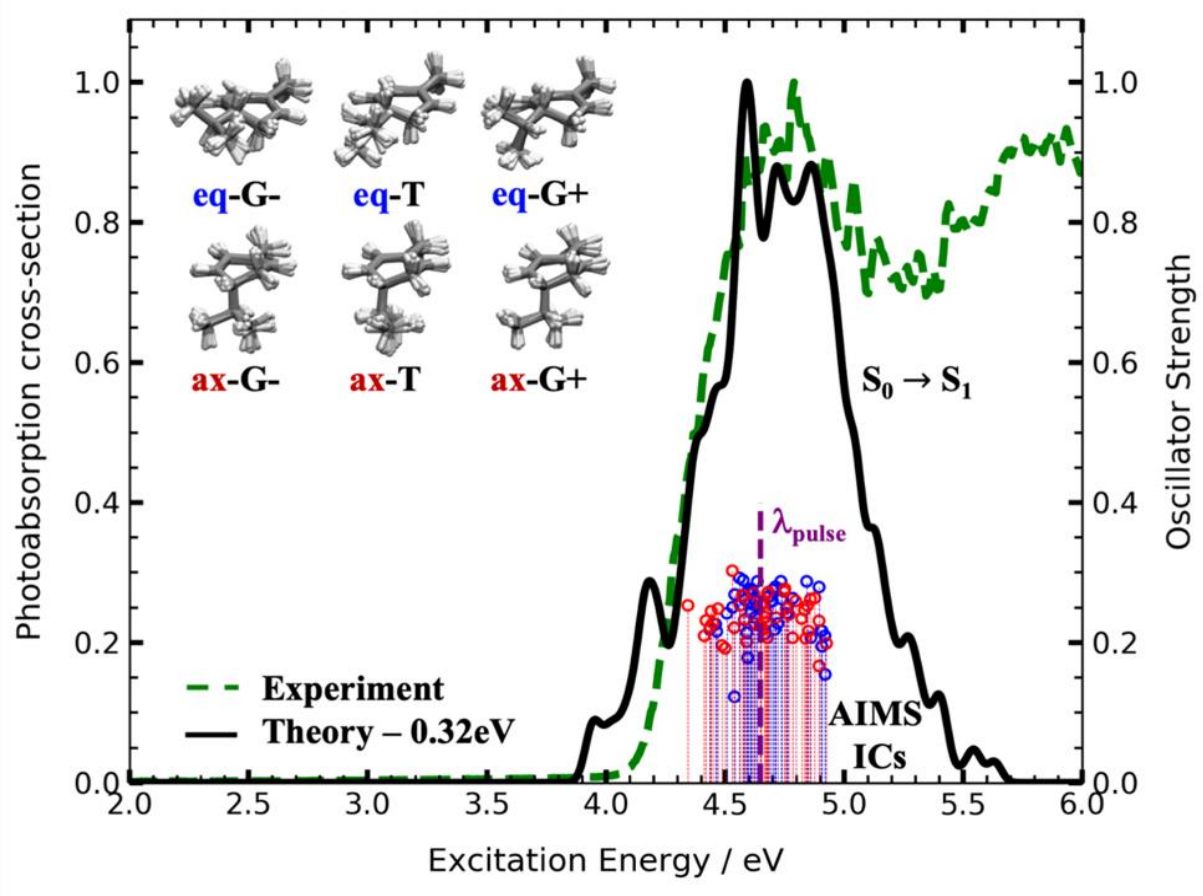


Fig. S10. UV Electronic Absorption Spectra of αPH: The UV electronic absorption spectrum was generated from 600 initial conditions sampled from a ground-state harmonic Wigner distribution. The AIMS dynamics simulations used 15 initial conditions for each conformer. The energy and oscillator strength for each of the initial conditions (randomly sampled with the restriction that they were within 0.3eV of the pump pulse energy used in the UED experiment) are shown with red/blue vertical lines for the axial/equatorial initial conditions respectively. The inset shows the starting geometries for each conformer.

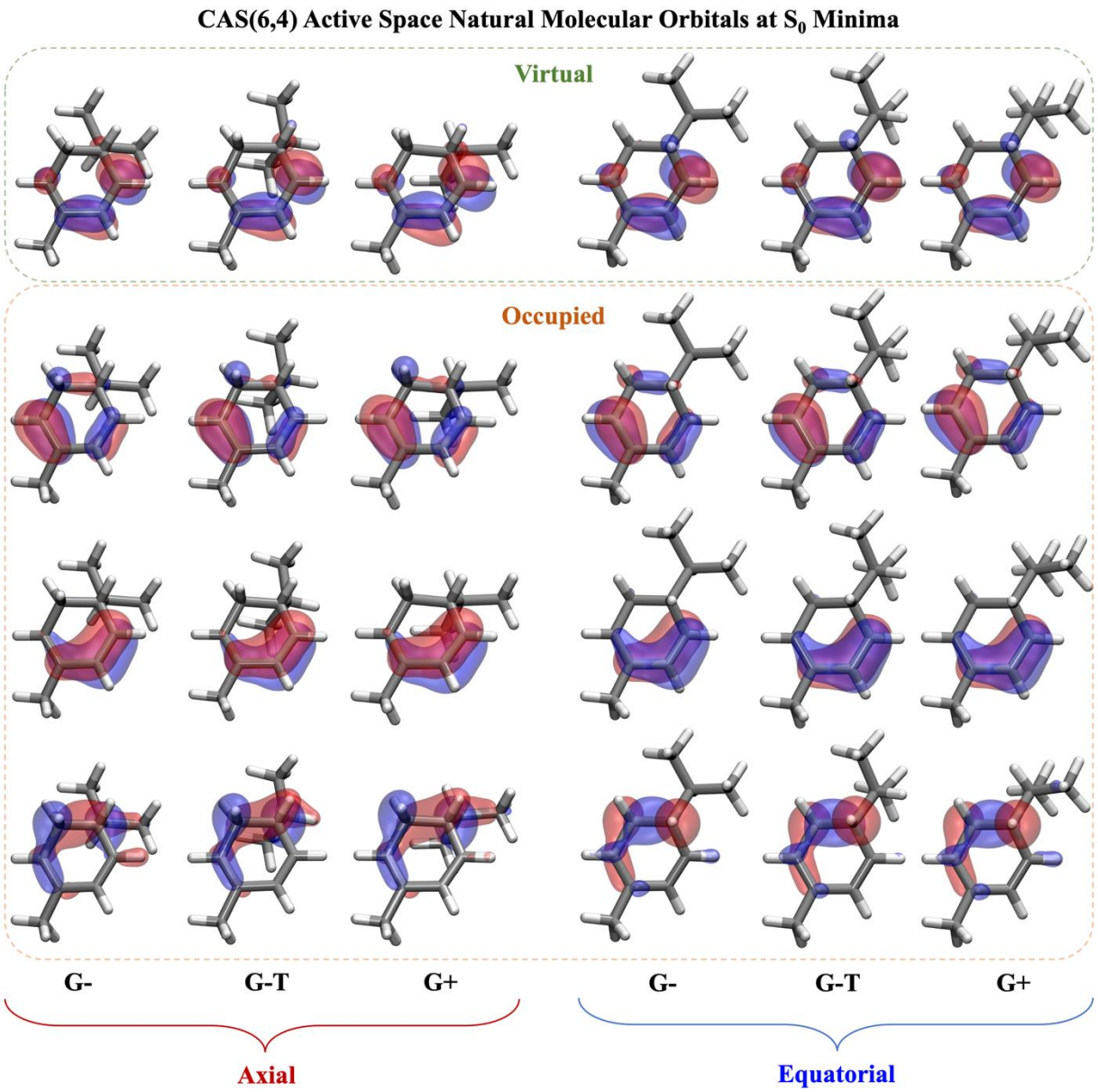
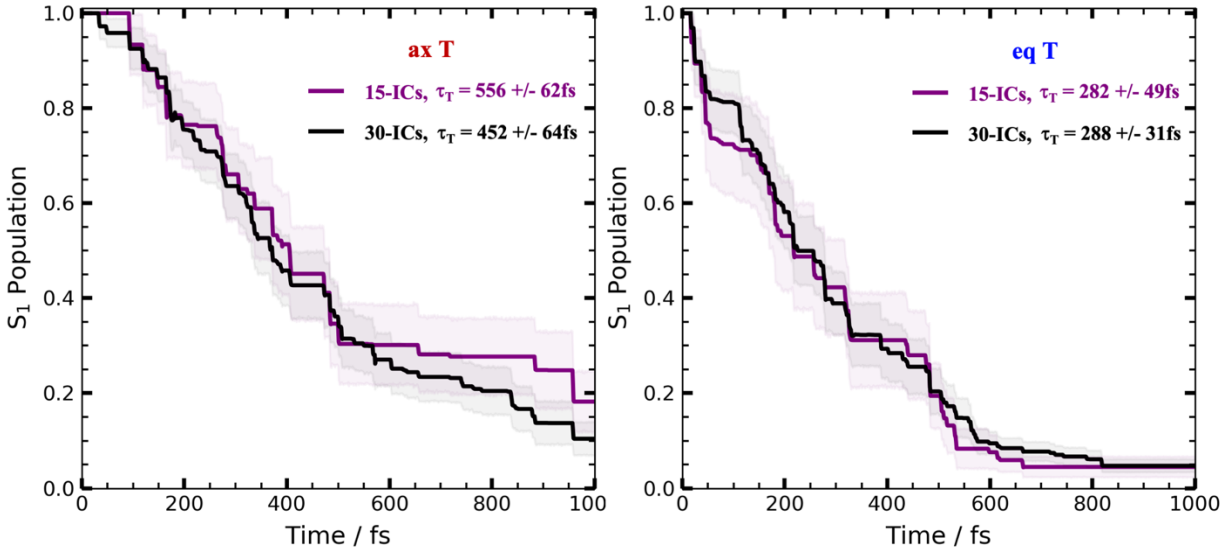
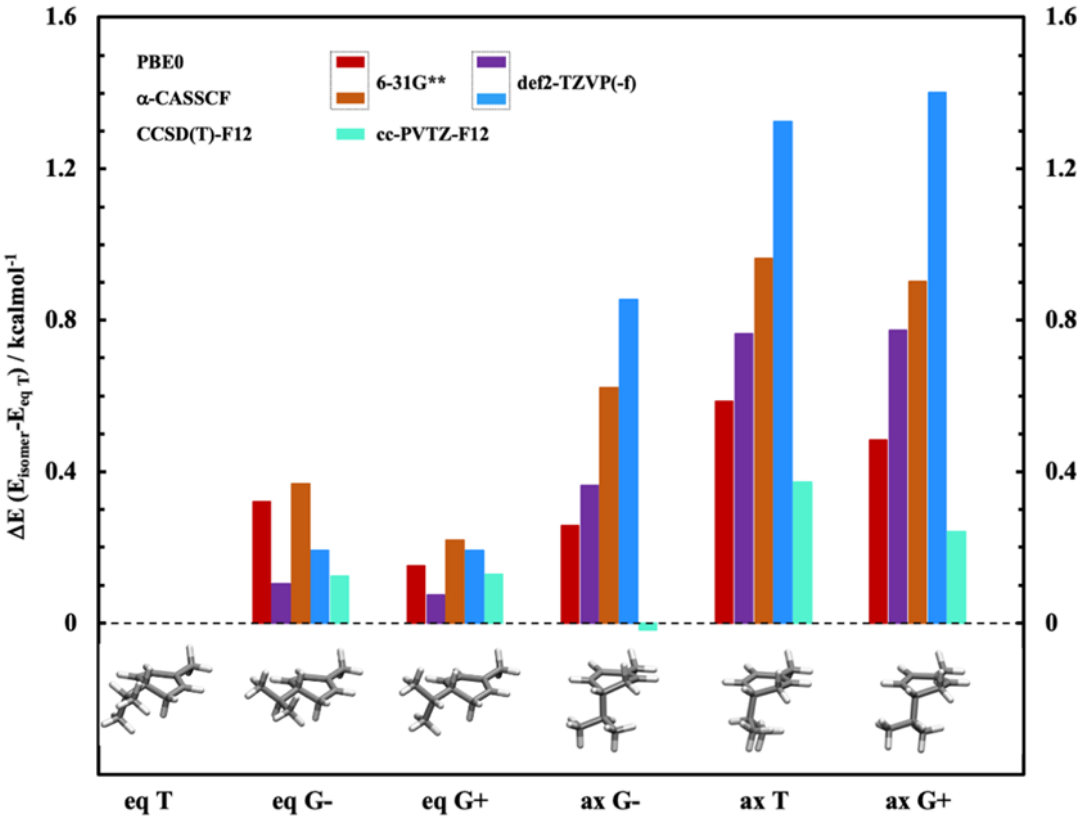


Fig. S11. SA-CASSCF Natural MOs at the S_0 Minima for all six αPH Isomers. The α(0.82)-SA2-CAS(6,4)SCF natural orbitals for the critical points along the α, β, and γ Z/E photoisomerization pathways. Blue and red correspond to 0.05 and -0.05 e-/Å^3 isovalues, respectively.



	15 ICs						30 ICs					
	CI-1 (%)		CI-2 (%)		CI-3 (%)		CI-1 (%)		CI-2 (%)		CI-3 (%)	
	αPH	ZZ/ZE-DOT	αPH	ZZ/ZE DOT	αPH	ZZ/ZE-DOT	αPH	ZZ/ZE-DOT	αPH	ZZ/ZE DOT	αPH	ZZ/ZE-DOT
ax T	12 +/- 6	0	71 +/- 8	0	3 +/- 1	14 +/- 6	9 +/- 4	0	73 +/- 7	0	8 +/- 4	10 +/- 4
eq T	6 +/- 2	0	34 +/- 8	0	30 +/- 6	30 +/- 6	4 +/- 3	0	42 +/- 9	0	26 +/- 6	28 +/- 8

Fig. S12. The S_1 excited state population dynamics for the T conformer for ax (left) and eq (right) using 15 (purple) and 30 (black) initial conditions from 67 and 130 trajectory basis functions, respectively. The decay time-constant for each trace is shown in the insets. The error bars were obtained from bootstrap analysis. The computed branching ratios between the nonradiative relaxation channels are shown below.



Method	Basis Set	ΔE (E_{isomer} – $E_{eq\ T}$) / kcalmol^{-1}					
		eq T	eq G-	eq G+	ax G-	ax T	ax G+
PBE0	6-31G**	0.00	0.32	0.15	0.26	0.59	0.48
	def2-TZVP(-f)	0.00	0.10	0.08	0.36	0.76	0.77
α-CASSCF	6-31G**	0.00	0.37	0.22	0.62	0.96	0.90
	def2-TZVP(-f)	0.00	0.19	0.19	0.86	1.32	1.40
CCSD(T)-F12	cc-pVDZ-F12	0.00	0.12	0.13	-0.02	0.37	0.24

Fig. S13. The relative energies of the S_0 minima of the six most stable αPH isomers optimized at the PBE0/6-31G** level of theory and single-point energies computed with their labeled methods. α-CASSCF corresponds to α(0.82)-SA2-CAS(6,4)SCF. The αPH conformers are shown below their computed relative energies.

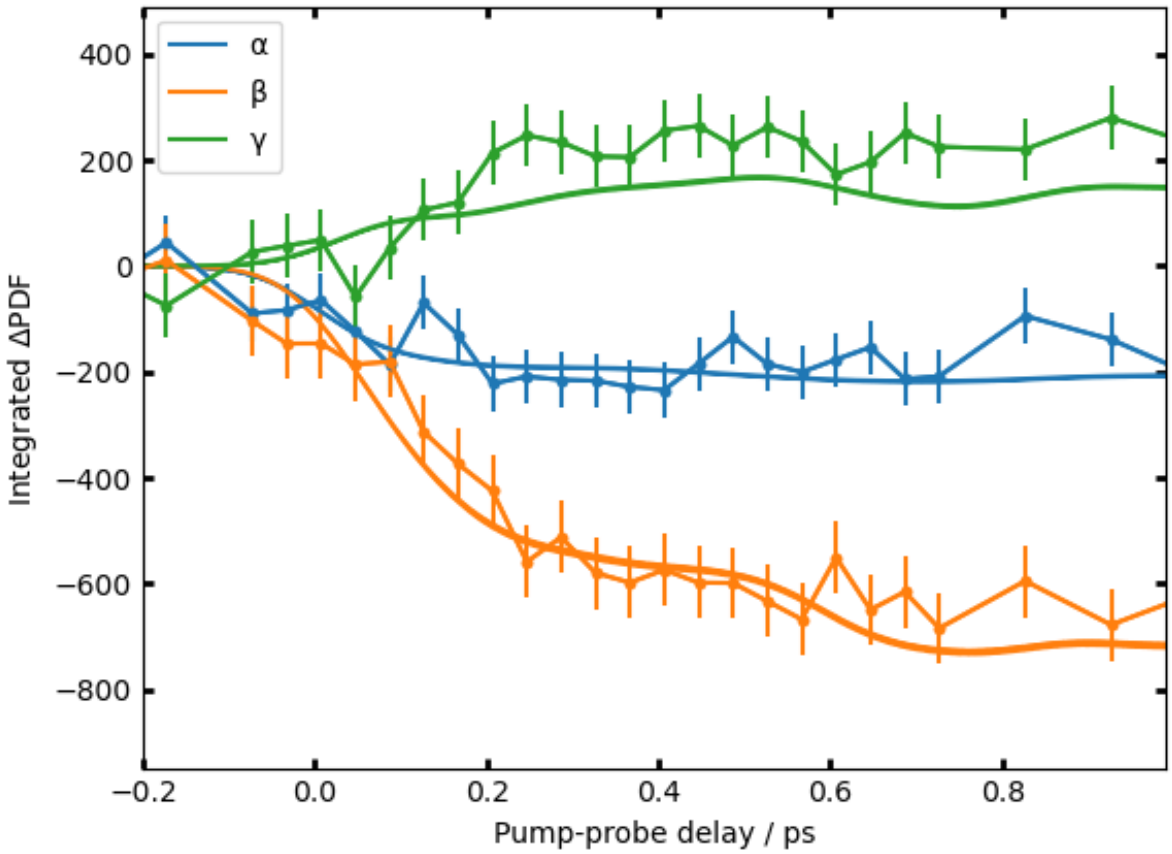


Fig. S14. Comparison of the experimental data to a linear combination of 80% eq-αPH and 20% ax-αPH, analogous to **Fig. 3d**. The intensity of the α and β features is not substantially changed by the linear combination, since both the eq-αPH and ax-αPH conformers open the ring. With a 20 % contribution from ax-αPH, the intensity of the γ-signature reduced far enough (see **Fig. S3**) that the simulation is outside the error bars (68% confidence interval) of the experiment.

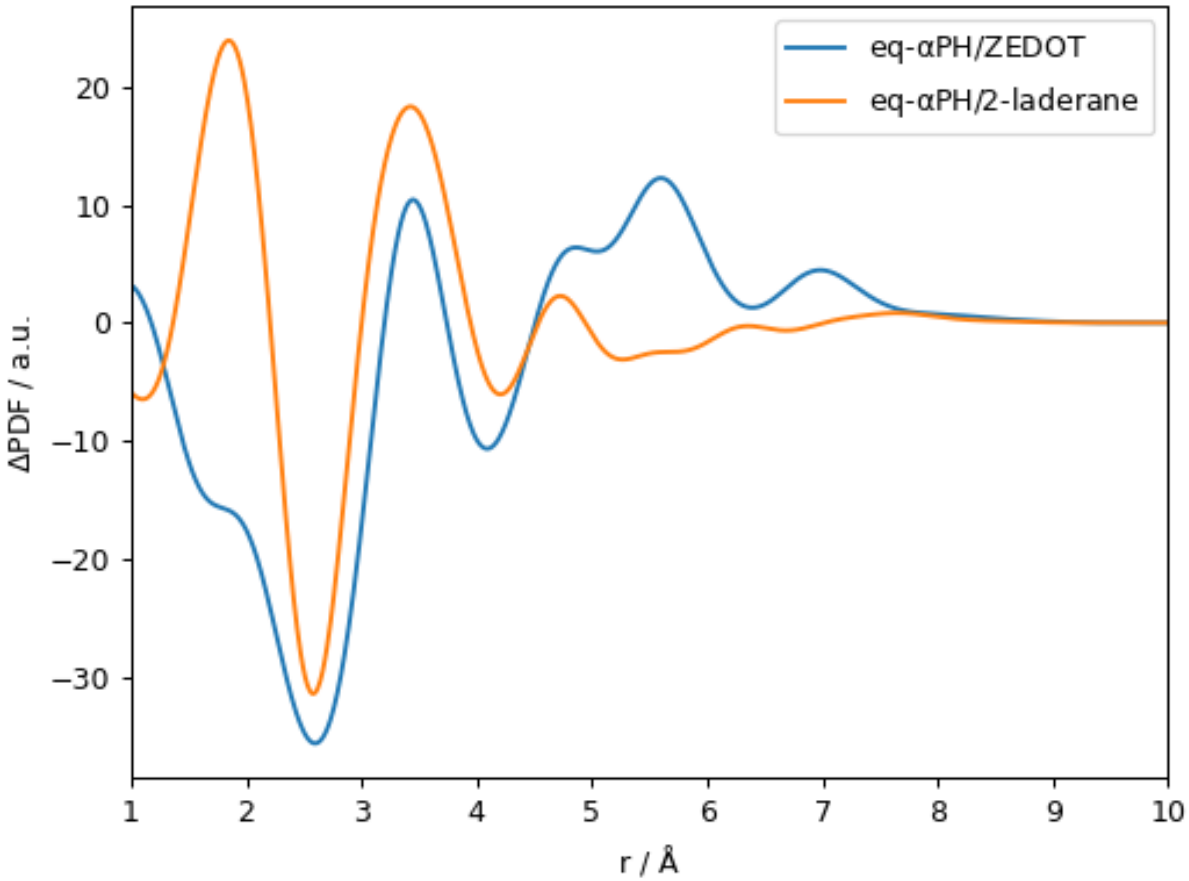
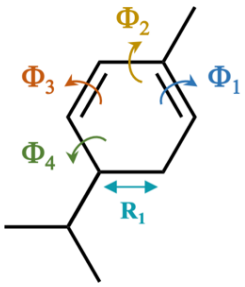


Fig. S15. Comparison of simulated ΔPDF signatures of the ZEDOT and 2-ladderane photoproducts. The ΔPDF signatures are generated analogous to **Fig. 2**.

Supplementary Tables

	CI-1 (%)		CI-2 (%)		CI-3 (%)	
Isomer	αPH	ZZ/ZE-DOT	αPH	ZZ/ZEDOT	αPH	ZZ/ZE-DOT
Axial	6 +/- 2	0	46 +/- 5	0	24 +/- 4	24 +/- 4
G-	0	0	13 +/- 6	0	50 +/- 7	37 +/- 6
T	12 +/- 6	0	71 +/- 8	0	3 +/- 1	14 +/- 6
G+	7 +/- 3	0	55 +/- 9	0	17 +/- 5	21 +/- 7
Equatorial	5 +/- 2	0	35 +/- 4	0	30 +/- 3	30 +/- 3
G-	9 +/- 4	< 1	22 +/- 6	0	38 +/- 7	31 +/- 6
T	6 +/- 2	0	34 +/- 8	0	30 +/- 6	30 +/- 6
G+	0	0	50 +/- 8	0	21 +/- 5	29 +/- 6

Table S1. Computed Quantum Yield for Eq and Ax αPH. The computed quantum yields for ax (red) and eq (blue) αPH from the AIMS simulation. Errors represent a 68% confidence interval and obtained from bootstrap analysis. The geometries associated with each CI are included in the supplementary structures.



Conformer	R_1 (Å)	$\lvert\Phi_1\rvert$ (°)	$\lvert\Phi_2\rvert$ (°)	$\lvert\Phi_3\rvert$ (°)	$\lvert\Phi_4\rvert$ (°)
αPH	≤ 1.8	≤ 80	≤ 80	≤ 80	-
cZc DOT	> 1.8	≤ 80	≤ 80	≤ 80	-
cZt/tZc DOT	> 1.8	≤ 80 or ≥ 100	≤ 80	≥ 100 or ≤ 80	-
tZt DOT	> 1.8	≥ 100	≤ 80	≥ 100	-
ZZDOT	> 1.8	≥ 100	≤ 80	≥ 100	≤ 80
ZEDOT	> 1.8	≥ 100	≤ 80	≥ 100	≥ 100

Table S2. Binning criteria for αPH conformers upon relaxation to the ground-electronic state. Each row corresponds to a specific conformer along with the structural parameters used to classify a specific geometry R(t). The carbon-carbon distance (R_1), and the absolute values of the four dihedral angles (Φ_1, Φ_2, Φ_3, and Φ_4) are shown above on the αPH structure.

Critical Point Structures

ax-G- S_0 Minimum (FC)

Cartesian coordinates / Å

26

C	0.5603236327	0.4023961588	-0.7534127770
C	0.7083580082	0.2280638902	-2.2917607550
C	-0.4806859329	1.4601042097	-0.3427323697
C	0.1905270201	-0.9037782124	-0.0835836769
C	1.1561432757	1.5217719416	-2.9836108245
C	1.6972509320	-0.8934076400	-2.6346771681
C	-1.8966775403	0.9530193094	-0.4431649948
C	-2.1892619383	-0.3262247477	-0.1896019727
C	-1.1016287345	-1.2366900564	0.1308329124
C	-3.5971279122	-0.8637417517	-0.1983626931
H	1.5295358649	0.7243728535	-0.3774203022
H	-0.2652108994	-0.0513786141	-2.6868248926
H	-0.3612853868	2.3725422211	-0.9128206563
H	-0.2910190030	1.7300974998	0.6974986094
H	0.9717223103	-1.6003674665	0.1631218703
H	2.0942398065	1.8821564697	-2.5675740747
H	1.3142229773	1.3480004559	-4.0437769645
H	0.4259905321	2.3174470212	-2.8965062503
H	2.6834867910	-0.6825871333	-2.2264033648
H	1.8034611151	-0.9919160193	-3.7107171621
H	1.3735024045	-1.8532756844	-2.2505699153
H	-2.6788309627	1.6577899201	-0.6692289336
H	-1.3468031635	-2.2011433469	0.5430824664
H	-4.3167380410	-0.0869263586	-0.4286740953
H	-3.8554407042	-1.2860978305	0.7695949806
H	-3.7080644517	-1.6572470888	-0.9328169955

S_0 energy / H: -387.96054165320811

S_0 CI eigenvector

-0.97504331747285	X36 X37 X38
0.11393573558125	X36 X37 X39
0.09694743023016	X36 X37 A38 B39
0.09694743023016	X36 X37 B38 A39
0.08914326689277	X36 X38 X39
-0.05944949541773	X36 A37 B38 X39
-0.05944949541773	X36 B37 A38 X39
-0.02940805078553	A36 X37 B38 X39
-0.02940805078553	B36 X37 A38 X39

S_1 energy / H: -387.77196192146300

S_1 CI eigenvector

0.66569875346325	X36 X37 A38 B39
0.66569875346325	X36 X37 B38 A39
0.16659600268016	X36 A37 X38 B39
0.16659600268016	X36 B37 X38 A39
0.14470360526893	X36 X37 X39
0.13321696755136	X36 X37 X38
-0.10551863283796	X36 X38 X39
0.04302315766171	X36 A37 B38 X39
0.04302315766171	X36 B37 A38 X39
-0.03902941742766	A36 X37 B38 X39
-0.03902941742766	B36 X37 A38 X39
0.02509392450520	A36 X37 X38 B39
0.02509392450520	B36 X37 X38 A39

ax-G- S_1/S_0 MECI-1 (Closed)

Cartesian coordinates / Å

26

C	0.1621130953	0.3955961655	-1.1141988442
C	0.7554693358	0.4585408063	-2.5301436349
C	-0.9982808394	1.3903029991	-0.8564786760
C	-0.5200554079	-0.8934853963	-0.7580407137
C	1.4207136966	1.8157466977	-2.7849453037
C	1.7662869611	-0.6692895249	-2.7708141217
C	-2.2081768506	0.6026907689	-0.4024733111
C	-2.1335035690	-0.4945820310	0.4651025289
C	-0.9020356518	-1.1433888871	0.6157552912
C	-3.4055396165	-1.0750878568	1.0361741662
H	0.9494501058	0.5417641763	-0.3790014621
H	-0.0620339365	0.3377675863	-3.2405277112
H	-1.2455509581	1.8841126506	-1.7897108748
H	-0.7295990292	2.1744307534	-0.1492908892
H	-0.7957838139	-1.5654818326	-1.5618515905
H	2.2390688093	1.9789179397	-2.0885236535
H	1.8288636695	1.8626898754	-3.7897525351
H	0.7259965935	2.6411199744	-2.6750474642
H	2.6222121244	-0.5717508947	-2.1085328887
H	2.1334163496	-0.6449568693	-3.7922160811
H	1.3351328597	-1.6522678531	-2.6068862224
H	-3.1783057381	1.0133707489	-0.6255953245
H	-0.8978478290	-2.1402797112	1.0182670790
H	-3.8378633989	-1.7899590253	0.3425576005
H	-4.1407189015	-0.2999167599	1.2253504958
H	-3.1938291008	-1.5950621513	1.9626938446

S_0 energy / H -387.80784501018326

S_0 CI eigenvector

0.64709438890734	X36	X37	A38	B39
0.64709438890734	X36	X37	B38	A39
0.34695217065350	X36	X37	X38	
-0.12074460502525	X36	A37	B38	X39
-0.12074460502525	X36	B37	A38	X39
0.07475597349097	X36	A37	X38	B39
0.07475597349097	X36	B37	X38	A39
-0.03931498098687	X36	X38	X39	

S_1 energy / H -387.80784494827003

S_1 CI eigenvector

0.91822500256939	X36	X37	X38	
-0.24880197931689	X36	X37	A38	B39
-0.24880197931689	X36	X37	B38	A39
-0.09515242037606	X36	X38	X39	
0.08644154315953	X36	A37	X38	B39
0.08644154315953	X36	B37	X38	A39
0.05692936396372	X36	A37	B38	X39
0.05692936396372	X36	B37	A38	X39
-0.03993705200290	X37	X38	X39	
-0.02522895954515	X36	X37	X39	

ax-G- S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å 26

C	0.2778394844	0.7402758905	-0.9436995820
C	0.6503719408	0.2715291507	-2.3871127407
C	-1.0396062394	1.5584442046	-0.8519567648
C	0.1842609901	-0.4772280282	-0.0541691708
C	0.6567092825	1.4346682168	-3.3863680272
C	2.0183001147	-0.4274011723	-2.4178296436
C	-2.3414841531	0.7087306843	-0.8612023319
C	-2.2141956516	-0.3553061164	0.0641837175
C	-0.9600545966	-1.0705232758	0.3100330113
C	-3.4061451847	-0.7973599899	0.8573050918
H	1.1179291181	1.3429610916	-0.5972064999
H	-0.0958012795	-0.4474428770	-2.7161738790
H	-1.0688533166	2.3007857938	-1.6353233566
H	-1.0285218047	2.1194928466	0.0803919283
H	1.1078654787	-0.9194881186	0.2793939825
H	1.2757531546	2.2543892213	-3.0301579862
H	1.0621302520	1.1067821862	-4.3384028664
H	-0.3369049217	1.8191988087	-3.5744596838
H	2.8050280313	0.2412133230	-2.0767374427
H	2.2643399127	-0.7320552651	-3.4299009112
H	2.0493782122	-1.3194550302	-1.8017253245
H	-1.9867231265	-0.0617963457	-1.6329539545
H	-0.9436437217	-1.9469927486	0.9350040700
H	-3.9033571669	0.0926770406	1.2255139528
H	-3.1809887850	-1.4927685603	1.6583762018
H	-4.0991488352	-1.2694627991	0.1673533469

S_0 energy / H -387.80197661779243

S_0 CI eigenvector

0.61288824429786	X36	X37	A38	B39
0.61288824429786	X36	X37	B38	A39
-0.47210234524164	X36	X37	X38	
-0.07823966371266	X36	A37	B38	X39
-0.07823966371266	X36	B37	A38	X39
0.05200492398262	A36	X37	B38	X39
0.05200492398262	B36	X37	A38	X39
-0.05053978461282	X36	A37	X38	B39
-0.05053978461282	X36	B37	X38	A39
0.03900987873768	X36	X38	X39	
0.03798693530241	X37	X38	X39	

S_1 energy / H -387.80197656569987

S_1 CI eigenvector

-0.86047987680726	X36	X37	X38	
-0.33611040007945	X36	X37	A38	B39
-0.33611040007945	X36	X37	B38	A39
-0.09283438295822	X36	A37	X38	B39
-0.09283438295822	X36	B37	X38	A39
0.07457338036087	X36	X38	X39	
0.05910489653625	X37	X38	X39	
0.03898805618125	X36	A37	B38	X39
0.03898805618125	X36	B37	A38	X39
-0.03054638312189	A36	X37	B38	X39
-0.03054638312189	B36	X37	A38	X39
0.03000672656738	A36	X37	X38	B

ax-G- S_1/S_0 MECI-3 (Open)

Cartesian coordinates / Å

26

C	0.8417220268	0.3094150283	-0.7527754442
C	0.6684700878	0.2214409531	-2.2643079427
C	-0.6958979840	1.6461909802	-0.1426474445
C	0.2844862496	-0.6297399299	0.1341828001
C	0.9992342452	1.5374316838	-2.9762029416
C	1.5616871132	-0.9016635253	-2.8201445510
C	-1.8763693304	1.0561312980	-0.6336239893
C	-2.1094764742	-0.3083304716	-0.3426723474
C	-1.0710316514	-1.1015591199	0.1157619641
C	-3.5023331242	-0.8672701793	-0.4822571987
H	1.8136285935	0.6807553281	-0.4577909945
H	-0.3608848334	-0.0334349404	-2.4824666315
H	-0.3559649374	2.5761288705	-0.5647945372
H	-0.4631322682	1.5528539700	0.9031165436
H	0.8851773650	-0.9178316287	0.9866735061
H	2.0128804599	1.8602113593	-2.7513681460
H	0.9263962167	1.4154061612	-4.0529847435
H	0.3226519642	2.3354558845	-2.6941835457
H	2.6122420179	-0.6942201329	-2.6317535898
H	1.4349543141	-1.0013416331	-3.8953038697
H	1.3229835357	-1.8563926264	-2.3635138377
H	-2.4347179111	1.5415274257	-1.4141879774
H	-1.2872180516	-2.0506155676	0.5759124282
H	-4.0695445146	-0.6663727822	0.4229638103
H	-3.4986832287	-1.9374193803	-0.6527548730
H	-4.0278662559	-0.3845268228	-1.2992176941

S_0 energy / H -387.81621596389630

S_0 CI eigenvector

-0.68422866365199	X36	X37	A38	B39
-0.68422866365199	X36	X37	B38	A39
-0.20802236504258	X36	X37	X38	
0.06916271094306	X36	A37	B38	X39
0.06916271094306	X36	B37	A38	X39
0.06569307897616	A36	X37	B38	X39
0.06569307897616	B36	X37	A38	X39
0.03658466309883	X36	X38	X39	

S_1 energy / H -387.81621591282703

S_1 CI eigenvector

0.95912177525701	X36	X37	X38	
-0.14830333425409	X36	X37	A38	B39
-0.14830333425409	X36	X37	B38	A39
-0.12097924030911	X37	X38	X39	
-0.10079638786795	X36	X38	X39	
0.06150863043967	X36	X37	X39	
0.04052344337378	X36	A37	X38	B39
0.04052344337378	X36	B37	X38	A39
0.03600610810151	A36	X37	X38	B39
0.03600610810151	B36	X37	X38	A39
-0.02612209225221	A36	B37	X38	X39
-0.02612209225221	B36	A37	X38	X39

ax-G- cZc-ZDOT Minimum

Cartesian coordinates / Å

26

C	1.3090863484	-0.5878350482	-0.7434429896
C	1.0465692236	-0.7793383837	-2.2162131453
C	-1.1432254930	2.0674572329	-0.3657589622
C	0.4441091090	-0.6690636364	0.2553290459
C	1.4842781081	0.4594064191	-3.0084413775
C	1.7748265009	-2.0329293034	-2.7220502343
C	-1.9719833495	1.0816773488	-0.7649518194
C	-2.0283354018	-0.2931430453	-0.2757166191
C	-0.9959479244	-1.0165419993	0.1787065913
C	-3.4109996727	-0.9102520116	-0.3126350699
H	2.3385346354	-0.3788405082	-0.4902012134
H	-0.0175593621	-0.9206312376	-2.3640545539
H	-1.2235225903	3.0521754435	-0.7893540989
H	-0.3877864618	1.9206509692	0.3811859555
H	0.8284274383	-0.5527355098	1.2586502807
H	2.5488757139	0.6441614973	-2.8867486787
H	1.2924245572	0.3254287432	-4.0691429647
H	0.9497915720	1.3424698104	-2.6778513910
H	2.8491079144	-1.9447799775	-2.5808029759
H	1.5920944455	-2.1841464761	-3.7820969853
H	1.4415587258	-2.9196534359	-2.1927677671
H	-2.7421950526	1.3400666511	-1.4754598184
H	-1.2265331534	-1.9934948160	0.5762032124
H	-4.1086180137	-0.3348258987	0.2898151122
H	-3.4070753781	-1.9303711735	0.0509286506
H	-3.7990724391	-0.9180916543	-1.3282781840

S_0 energy / H -387.92413487437199

S_0 CI eigenvector

0.97532175301649	X36 X37 X38
-0.09516964682509	X36 X37 X39
-0.09126436593515	X36 X37 A38 B39
-0.09126436593515	X36 X37 B38 A39
-0.08061804676734	X36 X38 X39
-0.06963203413384	X36 A37 B38 X39
-0.06963203413384	X36 B37 A38 X39
-0.03808325004110	A36 B37 X38 X39
-0.03808325004110	B36 A37 X38 X39
-0.03659396191285	X37 X38 X39
-0.03100542062448	X36 A37 X38 B39
-0.03100542062448	X36 B37 X38 A39

S_1 energy / H -387.73029552375090

S_1 CI eigenvector

-0.65810289146586	X36 X37 A38 B39
-0.65810289146586	X36 X37 B38 A39
0.16560945436037	X36 A37 X38 B39
0.16560945436037	X36 B37 X38 A39
-0.15734002442813	X36 X37 X39
-0.11706601371077	X36 X37 X38
0.09710454236041	A36 X37 X38 B39
0.09710454236041	B36 X37 X38 A39
0.08284563231944	X36 X38 X39
0.06809940224884	A36 B37 X38 X39
0.06809940224884	B36 A37 X38 X39
0.04489481348085	A36 X37 B38 X39
0.04489481348085	B36 X37 A38 X39
0.03636524577451	X37 X38 X39

ax-T S_0 Minimum (FC)

Cartesian coordinates / Å

26

C	0.4502477944	0.3858873308	-0.8255864458
C	0.7687565070	0.2731381052	-2.3441796670
C	-0.6076555934	1.4488225252	-0.4521150388
C	0.0835415899	-0.9600552283	-0.2479503836
C	-0.4571367087	0.0115373802	-3.2238624198
C	1.5524508023	1.4890979255	-2.8518281417
C	-2.0159393139	0.9246941880	-0.3377482764
C	-2.2834354747	-0.3509479971	-0.0496991026
C	-1.1812343315	-1.2891203307	0.0888161116
C	-3.6866917326	-0.8672761375	0.1401144469
H	1.3846777604	0.6900663308	-0.3597431961
H	1.4270606391	-0.5888336735	-2.4443582508
H	-0.5798836275	2.2771280132	-1.1520149567
H	-0.3371222547	1.8755561345	0.5141255427
H	0.8700396515	-1.6902880218	-0.1592491233
H	-1.1291658999	0.8640272239	-3.2373739503
H	-0.1484863682	-0.1761081315	-4.2485112680
H	-1.0169182525	-0.8506241934	-2.8821676018
H	0.9691971504	2.4031313701	-2.7936670330
H	1.8353579867	1.3532959175	-3.8915355551
H	2.4633077411	1.6393811055	-2.2794116158
H	-2.8180551472	1.6365199122	-0.4391137378
H	-1.3973619549	-2.2787426053	0.4547282112
H	-4.4198229728	-0.0783248549	0.0201542592
H	-3.8116191834	-1.2949876466	1.1318446691
H	-3.9146688072	-1.6518346421	-0.5769474763

S_0 energy / H

-387.96001187924026

S_0 CI eigenvector

-0.97523499511617	X36 X37 X38
0.11531564588785	X36 X37 X39
-0.09651088379450	X36 X37 A38 B39
-0.09651088379450	X36 X37 B38 A39
0.08816290464405	X36 X38 X39
-0.05822351679776	X36 A37 B38 X39
-0.05822351679776	X36 B37 A38 X39
0.02938383656857	A36 X37 B38 X39
0.02938383656857	B36 X37 A38 X39

S_1 energy / H

-387.77070837961162

S_1 CI eigenvector

-0.66679503700194	X36 X37 A38 B39
-0.66679503700194	X36 X37 B38 A39
-0.16389647648165	X36 A37 X38 B39
-0.16389647648165	X36 B37 X38 A39
0.14315474846456	X36 X37 X39
0.13311887925859	X36 X37 X38
-0.10301841399781	X36 X38 X39
0.04697596455500	X36 A37 B38 X39
0.04697596455500	X36 B37 A38 X39
0.03705590102833	A36 X37 B38 X39
0.03705590102833	B36 X37 A38 X39

ax-T S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å

26

C	0.1808644782	0.4500345681	-1.0668957398
C	0.7306901804	0.4416699246	-2.5058899281
C	-0.9829282960	1.4208801042	-0.7826467665
C	-0.4381036175	-0.8472752336	-0.6259978323
C	-0.3326682595	0.2274610726	-3.5901252213
C	1.5327951603	1.7166074448	-2.7840262730
C	-2.2117374626	0.5646794218	-0.5562637724
C	-2.1891123592	-0.4507695297	0.4309142767
C	-0.9494181186	-1.0030989701	0.7224953486
C	-3.4824466097	-1.0271946217	0.9467804728
H	1.0117094401	0.6391196786	-0.3859767902
H	1.4268204076	-0.3954272541	-2.5637397676
H	-1.1399214090	2.0923670604	-1.6169514010
H	-0.7745655244	2.0424358630	0.0881733393
H	-0.4454872489	-1.6854188197	-1.3093100023
H	-1.0214143992	1.0636226718	-3.6468541643
H	0.1434552956	0.1320520463	-4.5613210902
H	-0.9210161497	-0.6665709663	-3.4189634304
H	0.9088260499	2.6009700121	-2.6971309000
H	1.9423490954	1.7041018794	-3.7893597243
H	2.3596023127	1.8232361887	-2.0882471015
H	-3.1628201341	0.8978374660	-0.9351446585
H	-0.8841031802	-1.9433254484	1.2378430318
H	-3.8865408308	-1.7343607638	0.2286516487
H	-4.2189872313	-0.2438387243	1.0937466728
H	-3.3235911130	-1.5493832365	1.8823656843

S_0 energy / H

-387.80647282293432

S_0 CI eigenvector

-0.59113790085849	X36	X37	A38	B39
-0.59113790085849	X36	X37	B38	A39
0.51556069399260	X36	X37	X38	
0.11745014710862	X36	A37	B38	X39
0.11745014710862	X36	B37	A38	X39
-0.06060959378354	X36	X38	X39	
0.04043277310390	X36	A37	X38	B39
0.04043277310390	X36	B37	X38	A39
-0.02238637587029	X37	X38	X39	

S_1 energy / H

-387.80647265599879

S_1 CI eigenvector

-0.83395067122596	X36	X37	X38	
-0.36275405473977	X36	X37	A38	B39
-0.36275405473977	X36	X37	B38	A39
-0.10455299633048	X36	A37	X38	B39
-0.10455299633048	X36	B37	X38	A39
0.09196027125666	X36	X38	X39	
0.06801797704185	X36	A37	B38	X39
0.06801797704185	X36	B37	A38	X39

ax-T S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å

26

C	0.3825027852	0.4227521758	-0.8695869794
C	0.9825591475	0.2774215461	-2.3001824496
C	-0.7345064912	1.5038137890	-0.7247397624
C	-0.0544360883	-0.9383149088	-0.3781330739
C	-0.0509064085	-0.0303514342	-3.3894865337
C	1.8159616934	1.5067801491	-2.6777693529
C	-2.1972186461	0.9933194355	-0.6416488270
C	-2.3018615671	-0.2183401653	0.0768021812
C	-1.2881109985	-1.2836106789	-0.0115475886
C	-3.5024456664	-0.5108005602	0.9254816919
H	1.2307323963	0.6974915081	-0.2424082460
H	1.6730486977	-0.5649883173	-2.2619720432
H	-0.6608633583	2.2147958570	-1.5360841287
H	-0.5458803302	2.0752356565	0.1791964595
H	0.7183790077	-1.6902556425	-0.3373438151
H	-0.7414920618	0.7943437359	-3.5271475416
H	0.4476300772	-0.1992868816	-4.3395103268
H	-0.6301688817	-0.9200618565	-3.1623629051
H	1.2018960046	2.3943282812	-2.7865742496
H	2.3252935260	1.3432384308	-3.6226938174
H	2.5720026887	1.7144821443	-1.9266758971
H	-2.1563431827	0.2968832386	-1.5502115119
H	-1.4993820997	-2.2772528326	0.3455303013
H	-3.8512944056	0.4119493517	1.3690249772
H	-3.3176394320	-1.2741130684	1.6746594239
H	-4.2915500355	-0.8716910782	0.2701318010

S_0 energy / H

-387.80219477126423

S_0 CI eigenvector

-0.96804494677227	X36 X37 X38
-0.11184870321220	X36 X37 A38 B39
-0.11184870321220	X36 X37 B38 A39
0.11058939461755	X36 A37 X38 B39
0.11058939461755	X36 B37 X38 A39
0.10190087810522	X36 X38 X39
0.04912619277670	X37 X38 X39

S_1 energy / H

-387.80219451298774

S_1 CI eigenvector

-0.68943496768376	X36 X37 A38 B39
-0.68943496768376	X36 X37 B38 A39
0.15743063927787	X36 X37 X38
-0.10730489050749	X36 A37 B38 X39
-0.10730489050749	X36 B37 A38 X39

ax-T S_1/S_0 MECI-3 (Open)

Cartesian coordinates / Å

26

C	0.7600752822	0.2619303598	-0.7345672864
C	0.7830153508	0.2579166972	-2.2720168789
C	-0.7406620023	1.6333500825	-0.0491431933
C	0.1707195023	-0.6765232557	0.1320007060
C	-0.5335351606	0.1770755693	-3.0511408672
C	1.6153410954	1.4461789347	-2.7729738947
C	-1.9938387835	1.0912451088	-0.3986140253
C	-2.2399739581	-0.2727143345	-0.1342096149
C	-1.1891844003	-1.1166813565	0.1876445025
C	-3.6503216637	-0.8011281549	-0.1663487214
H	1.7277392808	0.5751582644	-0.3681904871
H	1.3441360304	-0.6391027403	-2.5394867067
H	-0.4100673102	2.5368989040	-0.5340874852
H	-0.3972326430	1.5559885046	0.9663687377
H	0.7908265143	-0.9891812069	0.9634273798
H	-1.0920788936	1.1032617880	-3.0062249426
H	-0.3070967046	-0.0179020666	-4.0960193106
H	-1.1696708477	-0.6224615044	-2.6958546887
H	1.1271822984	2.3925419434	-2.5577374951
H	1.7612025856	1.3863941928	-3.8472707733
H	2.5974036994	1.4661655867	-2.3099577936
H	-2.6080253153	1.6098152557	-1.1132925299
H	-1.3922595925	-2.0588048690	0.6667396840
H	-4.2051156166	-0.4289940506	0.6899114153
H	-3.6767037322	-1.8840670622	-0.1553257954
H	-4.1651577275	-0.4533539167	-1.0567843432

S_0 energy / H

-387.80336467764687

S_0 CI eigenvector

-0.64757822452749	X36 X37 X38
-0.52600073201432	X36 X37 A38 B39
-0.52600073201432	X36 X37 B38 A39
0.08175196382723	X36 X38 X39
0.06172453643308	X37 X38 X39
0.05633790510091	A36 X37 B38 X39
0.05633790510091	B36 X37 A38 X39
-0.05592383401504	X36 A37 B38 X39
-0.05592383401504	X36 B37 A38 X39
-0.03692629107170	X36 X37 X39
0.03170782386289	X36 A37 X38 B39
0.03170782386289	X36 B37 X38 A39

S_1 energy / H

-387.80336462500168

S_1 CI eigenvector

0.73768411723328	X36 X37 X38
-0.46159502663600	X36 X37 A38 B39
-0.46159502663600	X36 X37 B38 A39
-0.10233865251497	X37 X38 X39
-0.07053653834627	X36 X38 X39
0.04845815828915	X36 X37 X39
-0.04455288932464	X36 A37 B38 X39
-0.04455288932464	X36 B37 A38 X39
0.03739804278241	A36 X37 X38 B39
0.03739804278241	B36 X37 X38 A39
0.03634317401199	A36 X37 B38 X39
0.03634317401199	B36 X37 A38 X39
-0.02898498174395	X36 A37 X38 B39
-0.02898498174395	X36 B37 X38 A39

ax-T cZc-ZDOT Minimum

Cartesian coordinates / Å

26

C	1.2262137283	-0.4709174959	-0.7964103447
C	1.1585813768	-0.7202937895	-2.2886809088
C	-1.3126608512	2.1604922434	-0.0579900102
C	0.3182307415	-0.5479889060	0.1640824436
C	-0.0561263468	-1.4957423448	-2.8020005830
C	1.3132248648	0.6118619887	-3.0400384177
C	-2.2381946639	1.2201001551	-0.3434485250
C	-2.1974653729	-0.2160018617	-0.1001160044
C	-1.1056778271	-0.9664229034	0.1054498748
C	-3.5571628023	-0.8844251902	-0.1200457241
H	2.2107758561	-0.1605178311	-0.4785110005
H	2.0379107697	-1.3203721912	-2.5212465027
H	-1.5015201345	3.1909582647	-0.2985648791
H	-0.3728095438	1.9375343054	0.4052460106
H	0.6675242169	-0.3292544311	1.1641820086
H	-0.9680672438	-0.9183182247	-2.7200228327
H	0.0896235342	-1.7428833134	-3.8498663030
H	-0.1950702827	-2.4248326024	-2.2598014966
H	0.4596576928	1.2555880077	-2.8552361808
H	1.3879977913	0.4428947374	-4.1104168857
H	2.2073075204	1.1424309579	-2.7260763152
H	-3.1635580624	1.5697249496	-0.7744022235
H	-1.2690474142	-2.0115665824	0.3179631918
H	-4.2270671192	-0.4266243520	0.6026110694
H	-3.4893275819	-1.9419200206	0.1032179585
H	-4.0217628459	-0.7781535695	-1.0974874198

S_0 energy / H

-387.91742606262198

S_0 CI eigenvector

-0.97045088079365	X36 X37 X38
0.11630963210912	X36 X37 X39
-0.11088909562897	X36 X37 A38 B39
-0.11088909562897	X36 X37 B38 A39
0.09408824985995	X36 X38 X39
-0.06885883475258	X36 A37 B38 X39
-0.06885883475258	X36 B37 A38 X39

S_1 energy / H

-387.71958766363451

S_1 CI eigenvector

-0.64052538503022	X36 X37 A38 B39
-0.64052538503022	X36 X37 B38 A39
-0.21759427849506	X36 A37 X38 B39
-0.21759427849506	X36 B37 X38 A39
0.18894574911363	X36 X37 X39
0.14280142485137	X36 X37 X38
-0.14148612199564	X36 X38 X39
-0.03989177177915	A36 X37 X38 B39
-0.03989177177915	B36 X37 X38 A39
0.03369976424435	A36 X37 B38 X39
0.03369976424435	B36 X37 A38 X39
-0.03126773855448	A36 B37 X38 X39
-0.03126773855448	B36 A37 X38 X39
0.02478811920746	X36 A37 B38 X39
0.02478811920746	X36 B37 A38 X39

ax-G+ - S_0 Minimum (FC)

Cartesian coordinates / Å

26

C	0.2417848542	0.5701366501	-1.0365749936
C	0.8546216929	0.5714765869	-2.4499952311
C	-1.0090832397	1.4537513061	-0.8627792298
C	-0.2920112659	-0.7461200204	-0.5398810184
C	2.1808000036	-0.1977077169	-2.4771258328
C	-0.0826431040	0.0677752757	-3.5552569029
C	-2.1781085746	0.5188223250	-0.6346404501
C	-2.1199382797	-0.4347732054	0.4079666100
C	-0.8532907428	-0.8537565164	0.7953521084
C	-3.3812709159	-1.1001204819	0.8962881300
H	1.0153605740	0.8752799282	-0.3319253066
H	1.0813164136	1.6136136112	-2.6683074401
H	-1.1714313208	2.0607451758	-1.7457945641
H	-0.8916230957	2.1390167356	-0.0229087410
H	-0.2254846849	-1.6212861413	-1.1698089689
H	2.0374899805	-1.2525863255	-2.2564921360
H	2.6464459493	-0.1333569981	-3.4557466112
H	2.8820119421	0.1992920618	-1.7493746399
H	-0.2891439292	-0.9936089832	-3.4589723916
H	0.3777200529	0.2202927156	-4.5269592696
H	-1.0338969041	0.5871290276	-3.5552808382
H	-3.1318636476	0.7526938900	-1.0752606424
H	-0.7413589069	-1.7518304230	1.3744045335
H	-3.6474338275	-1.9240059857	0.2409085387
H	-4.2099822650	-0.3998897440	0.9083994734
H	-3.2353313542	-1.4981302333	1.8930299388

S_0 energy / H -387.80663156815126

S_0 CI eigenvector

-0.58318663210468	X36 X37 A38 B39
-0.58318663210468	X36 X37 B38 A39
0.53343576501733	X36 X37 X38
0.11705072203375	X36 A37 B38 X39
0.11705072203375	X36 B37 A38 X39
-0.06118923433112	X36 X38 X39
0.04007527920139	X36 A37 X38 B39
0.04007527920139	X36 B37 X38 A39
-0.02315067218226	X37 X38 X39

S_1 energy / H -387.80663149768958

S_1 CI eigenvector

-0.82259159908024	X36 X37 X38
-0.37505867221203	X36 X37 A38 B39
-0.37505867221203	X36 X37 B38 A39
-0.10593731455118	X36 A37 X38 B39
-0.10593731455118	X36 B37 X38 A39
0.09019604216599	X36 X38 X39
0.06967442377067	X36 A37 B38 X39
0.06967442377067	X36 B37 A38 X39
0.03529369718816	X37 X38 X39

Ax-G+ - S_1/S_0 MECI-1 (Closed)

Cartesian coordinates / Å 26

C	0.1979337252	0.7696784185	-1.1184560652
C	0.8099382383	0.4867837568	-2.5228037267
C	-1.2188185788	1.4210002335	-1.1895952109
C	0.2273857230	-0.4638820890	-0.2442485828
C	2.2944929198	0.1069655953	-2.4482692050
C	0.0329359314	-0.5417071924	-3.3524142698
C	-2.4336022205	0.5062040787	-0.8860299446
C	-2.1499743709	-0.4242483781	0.1376037291
C	-0.8353938360	-1.0739851565	0.2811295533
C	-3.2108939813	-0.8400664046	1.1122189883
H	0.8883631806	1.4749939816	-0.6557015851
H	0.7561913661	1.4380405851	-3.0464531356
H	-1.3497493330	1.8761058939	-2.1639416020
H	-1.2580989772	2.2400051051	-0.4773086444
H	1.1998972685	-0.8773652419	-0.0332719152
H	2.4459171497	-0.8829197728	-2.0272304194
H	2.7316716465	0.1016806575	-3.4419085203
H	2.8562318881	0.8158005489	-1.8464054960
H	-0.0056265028	-1.5070761617	-2.8549374287
H	0.5168976240	-0.6914094896	-4.3130089066
H	-0.9835836627	-0.2211635455	-3.5469311405
H	-2.1353904445	-0.3620779845	-1.5719062675
H	-0.7155419682	-1.9346002339	0.9172099065
H	-3.8297808318	0.0191453440	1.3348112218
H	-2.8106144869	-1.2922825550	2.0139165426
H	-3.8476339188	-1.5721954203	0.6218562600

S_0 energy / H -387.80181805115842

S_0 CI eigenvector

-0.64799097481248	X36	X37	A38	B39
-0.64799097481248	X36	X37	B38	A39
0.36632801375322	X36	X37	X38	
-0.10099624051597	X36	A37	B38	X39
-0.10099624051597	X36	B37	A38	X39
-0.03812499714040	X36	A37	X38	B39
-0.03812499714040	X36	B37	X38	A39
-0.03558014074478	X36	X38	X39	
-0.02337175802583	X37	X38	X39	

S_1 energy / H -387.80181795300194

S_1 CI eigenvector

0.90973354915533	X36	X37	X38	
0.26066575682312	X36	X37	A38	B39
0.26066575682312	X36	X37	B38	A39
-0.10502402148164	X36	A37	X38	B39
-0.10502402148164	X36	B37	X38	A39
-0.09587225581004	X36	X38	X39	
-0.04583590102241	X37	X38	X39	
0.03757149430946	X36	A37	B38	X39
0.03757149430946	X36	B37	A38	X39

Ax-G+ - S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å

26

C	0.1979337252	0.7696784185	-1.1184560652
C	0.8099382383	0.4867837568	-2.5228037267
C	-1.2188185788	1.4210002335	-1.1895952109
C	0.2273857230	-0.4638820890	-0.2442485828
C	2.2944929198	0.1069655953	-2.4482692050
C	0.0329359314	-0.5417071924	-3.3524142698
C	-2.4336022205	0.5062040787	-0.8860299446
C	-2.1499743709	-0.4242483781	0.1376037291
C	-0.8353938360	-1.0739851565	0.2811295533
C	-3.2108939813	-0.8400664046	1.1122189883
H	0.8883631806	1.4749939816	-0.6557015851
H	0.7561913661	1.4380405851	-3.0464531356
H	-1.3497493330	1.8761058939	-2.1639416020
H	-1.2580989772	2.2400051051	-0.4773086444
H	1.1998972685	-0.8773652419	-0.0332719152
H	2.4459171497	-0.8829197728	-2.0272304194
H	2.7316716465	0.1016806575	-3.4419085203
H	2.8562318881	0.8158005489	-1.8464054960
H	-0.0056265028	-1.5070761617	-2.8549374287
H	0.5168976240	-0.6914094896	-4.3130089066
H	-0.9835836627	-0.2211635455	-3.5469311405
H	-2.1353904445	-0.3620779845	-1.5719062675
H	-0.7155419682	-1.9346002339	0.9172099065
H	-3.8297808318	0.0191453440	1.3348112218
H	-2.8106144869	-1.2922825550	2.0139165426
H	-3.8476339188	-1.5721954203	0.6218562600

S_0 energy / H -387.80181805115842

S_0 CI eigenvector

-0.64799097481248	X36	X37	A38	B39
-0.64799097481248	X36	X37	B38	A39
0.36632801375322	X36	X37	X38	
-0.10099624051597	X36	A37	B38	X39
-0.10099624051597	X36	B37	A38	X39
-0.03812499714040	X36	A37	X38	B39
-0.03812499714040	X36	B37	X38	A39
-0.03558014074478	X36	X38	X39	
-0.02337175802583	X37	X38	X39	

S_1 energy / H -387.80181795300194

S_1 CI eigenvector

0.90973354915533	X36	X37	X38	
0.26066575682312	X36	X37	A38	B39
0.26066575682312	X36	X37	B38	A39
-0.10502402148164	X36	A37	X38	B39
-0.10502402148164	X36	B37	X38	A39
-0.09587225581004	X36	X38	X39	
-0.04583590102241	X37	X38	X39	
0.03757149430946	X36	A37	B38	X39
0.03757149430946	X36	B37	A38	X3

Ax-G+ - S_1/S_0 MECI-3 (Open)

Cartesian coordinates / Å

26			
C	0.7287161387	0.2030187308	-0.8467286336
C	0.6470982265	0.2015435846	-2.3786516980
C	-0.6802286569	1.5984392577	-0.0854244165
C	0.1821062931	-0.7173309423	0.0597495139
C	1.7227340677	-0.7705250334	-2.8997429549
C	-0.6822165347	-0.1306513745	-3.0620960643
C	-1.9711535468	1.0945290671	-0.3590505622
C	-2.2255840353	-0.2713006541	-0.1132311535
C	-1.1823834620	-1.1409658490	0.1586514114
C	-3.6416280126	-0.7829545171	-0.1295145312
H	1.7133214126	0.5342864678	-0.5464606234
H	0.9366131510	1.2003190121	-2.7016356517
H	-0.3452279821	2.4832470546	-0.6035924735
H	-0.2859495416	1.5302793727	0.9130282360
H	0.8322570126	-1.0169782959	0.8729685086
H	1.4641387215	-1.7927249911	-2.6375792745
H	1.8026831650	-0.7110449861	-3.9818652319
H	2.7006528636	-0.5566226713	-2.4802207014
H	-1.0652241982	-1.0945575777	-2.7496025960
H	-0.5194412703	-0.1702249153	-4.1356342580
H	-1.4398831915	0.6138642010	-2.8720042665
H	-2.6104205837	1.6355815820	-1.0341993391
H	-1.3860072978	-2.0946448203	0.6136039693
H	-4.1764615510	-0.4397433846	0.7508253112
H	-3.6751287676	-1.8651913987	-0.1608918579
H	-4.1693448474	-0.3969120278	-0.9961449871

S_0 energy / H -387.80483862897137

S_0 CI eigenvector

-0.95975759923633	X36	X37	X38	
-0.14781598943905	X36	X37	A38	B39
-0.14781598943905	X36	X37	B38	A39
0.11114463245535	X37	X38	X39	
0.10508230583397	X36	X38	X39	
-0.05190930957953	X36	X37	X39	
0.04650013862945	X36	A37	X38	B39
0.04650013862945	X36	B37	X38	A39
-0.02803180795458	A36	B37	X38	X39
-0.02803180795458	B36	A37	X38	X39
-0.02531857949088	A36	X37	X38	B39
-0.02531857949088	B36	X37	X38	A39
0.02438265916908	A36	X37	B38	X39
0.02438265916908	B36	X37	A38	X39

S_1 energy / H -387.80483844324084

S_1 CI eigenvector

-0.68375200325077	X36	X37	A38	B39
-0.68375200325077	X36	X37	B38	A39
0.20754459505639	X36	X37	X38	
-0.07332504654601	X36	A37	B38	X39
-0.07332504654601	X36	B37	A38	X39
0.06002297019828	A36	X37	B38	X39
0.06002297019828	B36	X37	A38	X39
-0.04455957191723	X37	X38	X39	
0.02801839030162	A36	X37	X38	B39
0.02801839030162	B36	X37	X38	A3

Ax-G+ cZc-ZDOT Minimum

Cartesian coordinates / Å

26

C	1.2167540946	-0.4263481655	-0.8569819289
C	1.1402182129	-0.6871393715	-2.3472869257
C	-1.3497894335	2.1558913897	-0.0846773421
C	0.3260912437	-0.5193955953	0.1185604699
C	2.3580028781	-1.5247600642	-2.7688914272
C	-0.1492815735	-1.3292490863	-2.8614041022
C	-2.2875347749	1.2022024154	-0.2677975836
C	-2.2046778391	-0.2343365681	-0.0422410692
C	-1.0901570403	-0.9671671327	0.0976530589
C	-3.5501090893	-0.9300777802	0.0010500629
H	2.2000225813	-0.1019978867	-0.5497176457
H	1.2362961754	0.2857772751	-2.8299142516
H	-1.5838347448	3.1837912708	-0.2947945179
H	-0.3609873960	1.9491448650	0.2707039006
H	0.6874805475	-0.2778796620	1.1091982699
H	2.3282822282	-2.5077366650	-2.3071481271
H	2.3786983156	-1.6607554925	-3.8456788845
H	3.2893071565	-1.0485454934	-2.4773758954
H	-0.3328087981	-2.2867461875	-2.3840971873
H	-0.0679507446	-1.5036173543	-3.9304102188
H	-1.0101961004	-0.6975264821	-2.6904588913
H	-3.2579232981	1.5403941351	-0.5961475093
H	-1.2230583946	-2.0206418042	0.2881621825
H	-4.1769896962	-0.5126956589	0.7845108326
H	-3.4486583050	-1.9931495903	0.1804553947
H	-4.0825162054	-0.7973653108	-0.9376006641

S_0 energy / H

-387.91686946030802

S_0 CI eigenvector

-0.96934101487212	X36 X37 X38
0.11972552996098	X36 X37 X39
-0.11476083098522	X36 X37 A38 B39
-0.11476083098522	X36 X37 B38 A39
0.09461400324175	X36 X38 X39
0.06827796568446	X36 A37 B38 X39
0.06827796568446	X36 B37 A38 X39

S_1 energy / H

-387.7188817407411

S_1 CI eigenvector

0.63712461440479	X36 X37 A38 B39
0.63712461440479	X36 X37 B38 A39
-0.22171951676535	X36 A37 X38 B39
-0.22171951676535	X36 B37 X38 A39
-0.19783083056383	X36 X37 X39
-0.14841740420460	X36 X37 X38
0.14788885665153	X36 X38 X39
0.03408096242917	A36 X37 X38 B39
0.03408096242917	B36 X37 X38 A39
-0.02928668817313	A36 X37 B38 X39
-0.02928668817313	B36 X37 A38 X39
-0.02661533151651	A36 B37 X38 X39
-0.02661533151651	B36 A37 X38 X39
0.02579770266313	X36 A37 B38 X39
0.02579770266313	X36 B37 A38 X39

eq-G- S_0 Minimum (FC)

Cartesian coordinates / Å

26

C	0.7215842185	-0.0176476731	0.1956837804
C	2.1871475914	-0.0476244843	-0.2973649979
C	-0.0231118548	1.2737258499	-0.1832592245
C	-0.0785385643	-1.2088974162	-0.2865091147
C	2.9437810903	1.2482435975	0.0212230012
C	2.9593750992	-1.2324084311	0.2987129588
C	-1.5046217313	1.1881932906	0.0822919164
C	-2.1705195596	0.0346739532	-0.0151504071
C	-1.4270730878	-1.1696272090	-0.3448711194
C	-3.6615937916	-0.0703838162	0.1758983077
H	0.7459488470	-0.0627673021	1.2883797787
H	2.1685409125	-0.1643166350	-1.3802441370
H	0.1314014948	1.4797909357	-1.2453625462
H	0.3920133693	2.1165617483	0.3563176005
H	0.4328696946	-2.1208024234	-0.5332548962
H	2.9163864131	1.4643798018	1.0867630772
H	3.9864562843	1.1578140542	-0.2675142581
H	2.5366999143	2.1042667572	-0.5037653823
H	3.0311326718	-1.1384796418	1.3793814673
H	3.9700914053	-1.2659107955	-0.0963739498
H	2.4969600581	-2.1882085833	0.0825018220
H	-2.0292503802	2.1024847742	0.3029085326
H	-1.9777469460	-2.0500451328	-0.6305709975
H	-4.1021050295	0.8942966314	0.3986780990
H	-3.9038770024	-0.7495828821	0.9891074074
H	-4.1393511169	-0.4605289679	-0.719406718

S_0 energy / H

-387.96100444601700

S_0 CI eigenvector

-0.97519068229222	X36 X37 X38
0.11632710709177	X36 X37 X39
0.09633384418636	X36 X37 A38 B39
0.09633384418636	X36 X37 B38 A39
0.08682545112113	X36 X38 X39
-0.05806737301177	X36 A37 B38 X39
-0.05806737301177	X36 B37 A38 X39
0.03061420004001	A36 X37 B38 X39
0.03061420004001	B36 X37 A38 X39

S_1 energy / H

-387.77243518781489

S_1 CI eigenvector

-0.66680452344343	X36 X37 A38 B39
-0.66680452344343	X36 X37 B38 A39
-0.16384811375325	X36 A37 X38 B39
-0.16384811375325	X36 B37 X38 A39
-0.14076336339304	X36 X37 X39
-0.13290784952594	X36 X37 X38
0.09926063151556	X36 X38 X39
-0.04867673559357	X36 A37 B38 X39
-0.04867673559357	X36 B37 A38 X39
-0.03474854513125	A36 X37 B38 X39
-0.03474854513125	B36 X37 A38 X39
0.03145485319226	A36 X37 X38 B39
0.03145485319226	B36 X37 X38 A39

eq-G- S_1/S_0 MECI-1 (Closed)

Cartesian coordinates / Å

26

C	0.8205846739	0.2056237093	0.5701030249
C	2.0239412939	0.0476758007	-0.3772567085
C	-0.0491291391	1.4578870690	0.3775027571
C	-0.2250101521	-0.8674528447	0.3842313533
C	3.0040730779	1.2122506109	-0.2100399871
C	2.7322354646	-1.2939719954	-0.1578851361
C	-1.4760188018	1.0100455143	0.6203765233
C	-2.0257626551	0.0051221609	-0.2086215388
C	-1.1090933929	-0.8737839235	-0.7721684666
C	-3.5166093311	-0.2054856091	-0.2836208056
H	1.1706646381	0.1724767687	1.5994590956
H	1.6364802501	0.0646366178	-1.3919447569
H	0.0476778765	1.8443099289	-0.6371753129
H	0.2377228012	2.2495221910	1.0592224010
H	-0.2962895087	-1.6526282735	1.1242266122
H	3.4024449218	1.2467612720	0.8011088545
H	3.8430192727	1.1104875417	-0.8919962212
H	2.5316097121	2.1673471756	-0.4132297416
H	3.0949339780	-1.3856679017	0.8633568841
H	3.5861915268	-1.3958827963	-0.8205842000
H	2.0701805684	-2.1329565228	-0.3525684046
H	-2.1230498577	1.5944887338	1.2504867304
H	-1.4321210927	-1.7893763946	-1.2317389901
H	-4.0564177275	0.7185871082	-0.1070306019
H	-3.8322956727	-0.9320161742	0.4593472024
H	-3.7848547101	-0.5927407573	-1.2599603127

S_0 energy / H

-387.80956229542915

S_0 CI eigenvector

0.58512611242490	X36 X37 X38
-0.55711001454199	X36 X37 A38 B39
-0.55711001454199	X36 X37 B38 A39
0.11460965090409	X36 A37 B38 X39
0.11460965090409	X36 B37 A38 X39
-0.06988733178561	X36 X38 X39
0.04865608199524	X36 A37 X38 B39
0.04865608199524	X36 B37 X38 A39
-0.02509910410607	X37 X38 X39

S_1 energy / H

-387.80956226639279

S_1 CI eigenvector

-0.78540814846225	X36 X37 X38
-0.41198449833168	X36 X37 A38 B39
-0.41198449833168	X36 X37 B38 A39
-0.10461145972005	X36 A37 X38 B39
-0.10461145972005	X36 B37 X38 A39
0.08889472040544	X36 X38 X39
0.07822105820126	X36 A37 B38 X39
0.07822105820126	X36 B37 A38 X39
0.03351048927819	X37 X38 X39

eq-G- S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å

26

C	0.7724558188	0.0881489672	0.2575458415
C	2.1641725098	-0.0301612690	-0.4149372244
C	-0.0953169535	1.2859829156	-0.2199619392
C	0.0013187188	-1.2022528236	0.1664981594
C	2.8643924751	1.3301594762	-0.5178322918
C	3.0899203241	-1.0125060859	0.3162115250
C	-1.5893856116	1.2244938718	0.2010323763
C	-2.1032783329	-0.0733967160	-0.0479152003
C	-1.3347114484	-1.2994743567	0.1253622107
C	-3.5198039553	-0.2291249812	-0.5082117168
H	0.9334500337	0.2393880853	1.3310635797
H	2.0086792564	-0.3982033194	-1.4288842151
H	-0.0528859469	1.3526859865	-1.3066551869
H	0.3385638732	2.2015648128	0.1573238533
H	0.5648228322	-2.1195474218	0.1592786458
H	2.3133401099	2.0305406558	-1.1321480463
H	2.9925329792	1.7761990325	0.4652017450
H	3.8500695782	1.2125511006	-0.9572133342
H	3.2938458834	-0.6673817568	1.3264566539
H	4.0407637876	-1.0957321960	-0.2006340527
H	2.6799381386	-2.0142489723	0.3880038954
H	-1.4044340302	0.8469200358	1.2705441974
H	-1.8086803251	-2.2636121218	0.0569376242
H	-4.1630174545	0.0337230138	0.3259636754
H	-3.7733680767	-1.2266639856	-0.8496290174
H	-3.6979371855	0.5169857453	-1.2733276221

S_0 energy / H

-387.80592223014224

S_0 CI eigenvector

0.69616470434947	X36 X37 A38 B39
0.69616470434947	X36 X37 B38 A39
0.09227620068639	X36 X37 X38
-0.08860596014356	A36 X37 B38 X39
-0.08860596014356	B36 X37 A38 X39
-0.05353036383453	X36 A37 B38 X39
-0.05353036383453	X36 B37 A38 X39

S_1 energy / H

-387.80592209503504

S_1 CI eigenvector

-0.97776450793694	X36 X37 X38
0.08651795125359	X37 X38 X39
-0.08511072749567	X36 A37 X38 B39
-0.08511072749567	X36 B37 X38 A39
0.06703208733617	X36 X38 X39
0.06576866316932	X36 X37 A38 B39
0.06576866316932	X36 X37 B38 A39
-0.06375019652245	A36 X37 X38 B39
-0.06375019652245	B36 X37 X38 A39

eq-G- S_1/S_0 MECI-3 (Open)

Cartesian coordinates / Å

26

C	0.8645538360	-0.0952671421	0.0089172085
C	2.3611565855	-0.2204773165	-0.2170248598
C	-0.4798137648	1.6344741216	-0.6225996939
C	-0.0263071444	-0.9367252573	-0.6613854982
C	3.0818100555	1.0908440900	0.1151330204
C	2.9729992878	-1.3780238197	0.5920812997
C	-1.6489315323	1.3311922368	0.1035809977
C	-2.1940256412	0.0547380452	-0.0246396753
C	-1.4364637360	-0.9692238870	-0.6222635145
C	-3.5818141064	-0.2367650660	0.4785190911
H	0.5757732206	0.2918034307	0.9704747946
H	2.5348859884	-0.4326971590	-1.2710366892
H	-0.4065519467	1.3349330604	-1.6502217991
H	0.1155975129	2.4877297847	-0.3504589850
H	0.4226522944	-1.6489164584	-1.3425565291
H	2.8964228245	1.3804213742	1.1467215403
H	4.1564963508	0.9939998763	-0.0104347429
H	2.7429862726	1.9010520633	-0.5229560802
H	2.8173893362	-1.2293701922	1.6572890695
H	4.0439384611	-1.4575138773	0.4188288234
H	2.5205059167	-2.3274785958	0.3227543418
H	-2.0049691761	2.0113206899	0.8566727426
H	-1.9360179036	-1.8325148995	-1.0244789700
H	-4.0772366140	0.6582876061	0.8338679088
H	-3.5503935388	-0.9690005425	1.2793224344
H	-4.1784777464	-0.6631974590	-0.3227357354

S_0 energy / H

-387.82385202031855

S_0 CI eigenvector

-0.69350859306081	X36 X37 A38 B39
-0.69350859306081	X36 X37 B38 A39
0.13019679049011	X36 X37 X38
-0.09760916431948	X36 A37 B38 X39
-0.09760916431948	X36 B37 A38 X39
-0.03104039399901	X36 X38 X39
0.02315939544216	X36 X37 X3

S_1 energy / H

-387.82385189660880

S_1 CI eigenvector

0.97107198284765	X36 X37 X38
-0.14405395540441	X36 X38 X39
0.09587170452449	X36 X37 A38 B39
0.09587170452449	X36 X37 B38 A39
-0.08012434328866	X37 X38 X39
0.06549146721486	X36 X37 X39
-0.05782472008042	X36 A37 X38 B39
-0.05782472008042	X36 B37 X38 A39

eq-G- cZc-EDOT Minimum

Cartesian coordinates / Å

26

C	1.1304329602	-0.6808460378	0.1531111476
C	2.6108857186	-0.8726431806	-0.0582562878
C	-0.8397391593	2.1781603942	-0.3330961895
C	0.1826872384	-1.1238807229	-0.6662253754
C	3.3168251808	0.4797027822	-0.2296180574
C	3.2280019423	-1.6642512586	1.1027154228
C	-1.5180011267	1.3362282260	0.4263986706
C	-2.0141919731	0.0035058644	0.0151788084
C	-1.2671213438	-0.9977242344	-0.5134790172
C	-3.5047389718	-0.1731498095	0.2036390696
H	0.8513437450	-0.1391939872	1.0426050131
H	2.7529239070	-1.4449278437	-0.9718693548
H	-0.5348543828	1.9197469593	-1.3310549044
H	-0.5581763229	3.1524309024	0.0257170257
H	0.4921310612	-1.7089542178	-1.5203398084
H	3.1929135743	1.0984489536	0.6553718593
H	4.3822420307	0.3430806567	-0.3911941615
H	2.9144137370	1.0254576344	-1.0767109078
H	3.1046789773	-1.1340957527	2.0435838755
H	4.2918904388	-1.8178571709	0.9460700741
H	2.7577650806	-2.6366969437	1.2048889576
H	-1.8250750906	1.6676335611	1.4084721413
H	-1.8128539633	-1.8591925958	-0.8652825050
H	-3.7805972017	-0.0713139520	1.2518827207
H	-3.8350880037	-1.1493028144	-0.1308188385
H	-4.0639280527	0.5824345881	-0.3433293788

S_0 energy / H

-387.92638919143826

S_0 CI eigenvector

0.98729585419654	X36 X37 X38
-0.09333196538926	X36 X37 X39
-0.07379587045791	X37 X38 X39
-0.05689852958353	A36 X37 B38 X39
-0.05689852958353	B36 X37 A38 X39
0.03806106086014	X36 X37 A38 B39
0.03806106086014	X36 X37 B38 A39
-0.03748386015648	X36 X38 X39

S_1 energy / H

-387.73789017951913

S_1 CI eigenvector

0.68854109167997	X36 X37 A38 B39
0.68854109167997	X36 X37 B38 A39
-0.11757409596283	A36 X37 X38 B39
-0.11757409596283	B36 X37 X38 A39
-0.09020469298112	X36 A37 B38 X39
-0.09020469298112	X36 B37 A38 X39
-0.05276435889037	X36 X37 X38
-0.05123689289574	X36 X37 X39
0.03517039062917	X37 X38 X39
0.02328033685207	X36 A37 X38 B39
0.02328033685207	X36 B37 X38 A39

eq-T S_0 Minimum (FC)	
Cartesian coordinates / Å	26
	C 0.7057597469 0.0237544854 0.1411151022
	C 2.1723001798 -0.0213651958 -0.3431453567
	C -0.1260218952 1.1862578378 -0.4248841664
	C -0.0132019614 -1.2857727150 -0.0859510646
	C 2.3222236753 -0.2396929353 -1.8536175369
	C 2.9686119337 1.2090630395 0.1040870397
	C -1.5944317799 1.0447811606 -0.1112177847
	C -2.1788127838 -0.1508849697 0.0088839364
	C -1.3617565860 -1.3479548047 -0.1079293012
	C -3.6580792044 -0.3159238124 0.2468169455
	H 0.7446689661 0.1675857197 1.2242459065
	H 2.6172269885 -0.8844624529 0.1506684005
	H -0.0140835236 1.2329888968 -1.5085834025
	H 0.2422429672 2.1306146352 -0.0390170489
	H 0.5697536686 -2.1895358151 -0.1363372372
	H 1.9850938788 0.6221323403 -2.4208210383
	H 3.3653477121 -0.4044559118 -2.1072800077
	H 1.7583117501 -1.1011605270 -2.1955237782
	H 2.6314201107 2.1106839297 -0.3982812198
	H 4.0228904957 1.0862604543 -0.1254590171
	H 2.8800568115 1.3709888251 1.1745859597
	H -2.1823613767 1.9447068789 -0.0466656314
	H -1.8567961662 -2.3008172372 -0.1900486800
	H -4.1601928511 0.6425655125 0.3052079878
	H -3.8468681307 -0.8537281379 1.1723299508
	H -4.1173026260 -0.8886292005 -0.5551789576
S_0 energy / H	-387.96159429897074
S_0 CI eigenvector	-0.97493281468196 X36 X37 X38
	0.11662336390680 X36 X37 X39
	-0.09735180221812 X36 X37 A38 B39
	-0.09735180221812 X36 X37 B38 A39
	0.08655202046549 X36 X38 X39
	-0.05799785652372 X36 A37 B38 X39
	-0.05799785652372 X36 B37 A38 X39
	0.03116916936685 A36 X37 B38 X39
	0.03116916936685 B36 X37 A38 X39
S_1 energy / H	-387.77315039506851
S_1 CI eigenvector	-0.66640928234247 X36 X37 A38 B39
	-0.66640928234247 X36 X37 B38 A39
	-0.16438042434047 X36 A37 X38 B39
	-0.16438042434047 X36 B37 X38 A39
	0.14207072500754 X36 X37 X39
	0.13453150546971 X36 X37 X38
	-0.09879323528164 X36 X38 X39
	0.04850522885015 X36 A37 B38 X39
	0.04850522885015 X36 B37 A38 X39
	0.03455292093703 A36 X37 B38 X39
	0.03455292093703 B36 X37 A38 X39
	0.03128328492401 A36 X37 X38 B39
	0.03128328492401 B36 X37 X38 A39

eq-T S_1/S_0 MECI-1 (Closed)

Cartesian coordinates / Å

26

C	0.7607767557	0.2409503832	0.4054968458
C	2.0450281606	0.0504225558	-0.4355621621
C	-0.1295918459	1.4669736053	0.1750342942
C	-0.2731490417	-0.8573214356	0.2861859717
C	1.8248738289	-0.1023877659	-1.9450035070
C	3.0280385578	1.1923050715	-0.1487110497
C	-1.5103882391	1.0098828195	0.5972806452
C	-2.1354034838	-0.0274553305	-0.1450278911
C	-1.2713280193	-0.9073077576	-0.7732287345
C	-3.6219740359	-0.2476692916	-0.0459023764
H	1.0697267814	0.2605708474	1.4475878802
H	2.5075801987	-0.8706427150	-0.0804400936
H	-0.1415200431	1.7610378429	-0.8734459666
H	0.2026411342	2.3188512508	0.7556178151
H	-0.2311649265	-1.6637149295	1.0069039108
H	1.4002192874	0.7941514475	-2.3834803788
H	2.7769793192	-0.2892192569	-2.4347360761
H	1.1585288062	-0.9224551794	-2.1769922009
H	2.6359064585	2.1441293527	-0.4952392475
H	3.9721958077	1.0227971808	-0.6575899357
H	3.2359829075	1.2846150026	0.9134345938
H	-2.0917254058	1.5943327642	1.2881794798
H	-1.6186748439	-1.8383577149	-1.1799877587
H	-4.1467999680	0.6964766869	0.0560510525
H	-3.8486061015	-0.8545250142	0.8257667908
H	-3.9883817482	-0.7698450793	-0.9217480950

S_0 energy / H

-387.80500974883802

S_0 CI eigenvector

0.97192763752711	X36 X37 X38
-0.11745472841741	X36 X38 X39
0.11160470710375	X36 A37 X38 B39
0.11160470710375	X36 B37 X38 A39
-0.08250169116511	X36 X37 A38 B39
-0.08250169116511	X36 X37 B38 A39
-0.04076355267413	X37 X38 X39
-0.02371222048129	X36 X37 X39

S_1 energy / H

-387.80500962784629

S_1 CI eigenvector

0.68762268207827	X36 X37 A38 B39
0.68762268207827	X36 X37 B38 A39
-0.13985120101163	X36 A37 B38 X39
-0.13985120101163	X36 B37 A38 X39
0.11400361728325	X36 X37 X38
0.02961637043922	X36 A37 X38 B39
0.02961637043922	X36 B37 X38 A39

eq-T S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å

26			
C	0.7687321046	0.1112457476	0.2414067123
C	2.1687557267	-0.0107788136	-0.4069880475
C	-0.1656619577	1.2190177012	-0.3188610698
C	0.0825120003	-1.2247692879	0.3026601893
C	2.1141315226	-0.4418339439	-1.8783183976
C	2.9729331498	1.2830718783	-0.2526130910
C	-1.6540457600	1.0944556487	0.1131239454
C	-2.0843954276	-0.2534453343	0.0020587929
C	-1.2441465497	-1.4075437311	0.2982265965
C	-3.4898173244	-0.5468893562	-0.4238838795
H	0.9296824607	0.3662585649	1.2947943040
H	2.7022737959	-0.7884113381	0.1406966856
H	-0.1334649623	1.2237338250	-1.4053593580
H	0.2128612604	2.1813995400	-0.0011049598
H	0.7176552703	-2.0920771836	0.3975985709
H	1.5724124368	-1.3745768407	-2.0098686396
H	1.6313701980	0.3074606847	-2.4959843021
H	3.1163741752	-0.5900020278	-2.2686048355
H	2.5428846835	2.0901155110	-0.8358716046
H	3.9942066581	1.1414730802	-0.5925145718
H	3.0107000051	1.6047814284	0.7840649706
H	-1.4455860259	0.8419909603	1.2144988436
H	-1.6622656444	-2.3977957067	0.3508660194
H	-4.1465833977	-0.2225633692	0.3767652152
H	-3.6833151334	-1.5921435157	-0.6391440536
H	-3.7124993752	0.0873558888	-1.2737004909

S_0 energy / H -387.80720210961749

S_0 CI eigenvector

-0.63870299452758	X36	X37	A38	B39
-0.63870299452758	X36	X37	B38	A39
0.39972856902206	X36	X37	X38	
0.07399792765471	A36	X37	B38	X39
0.07399792765471	B36	X37	A38	X39
-0.06172236205932	X36	A37	B38	X39
-0.06172236205932	X36	B37	A38	X39
-0.04076503536987	X36	A37	X38	B39
-0.04076503536987	X36	B37	X38	A39
-0.03600000405787	X37	X38	X39	
-0.02968698031213	X36	X38	X3	

S_1 energy / H -387.80720201363135

S_1 CI eigenvector

-0.89703060374286	X36	X37	X38	
-0.28448203187155	X36	X37	A38	B39
-0.28448203187155	X36	X37	B38	A39
0.08348704968869	X36	A37	X38	B39
0.08348704968869	X36	B37	X38	A39
0.07374053821242	X37	X38	X39	
0.06548869326992	X36	X38	X39	
-0.05383556111760	A36	X37	X38	B39
-0.05383556111760	B36	X37	X38	A39
0.03341790728550	A36	X37	B38	X39
0.03341790728550	B36	X37	A38	X39
-0.02359527063297	X36	A37	B38	X39

eq-T S_1/S_0 MECI-3 (Open)

Cartesian coordinates / Å 26

C	0.9095339727	-0.0484331258	-0.0145314402
C	2.4043536677	-0.0444539669	-0.3004398358
C	-0.6140307484	1.2605330511	-1.0733290568
C	0.1142566625	-1.1501561702	-0.3416282763
C	2.7170111627	-0.1369487777	-1.8004323764
C	3.0597019168	1.2034339509	0.2990071460
C	-1.7322649527	1.0753231098	-0.2360560362
C	-2.1417125342	-0.2268026002	0.0502701397
C	-1.2831609853	-1.3065251392	-0.2228198041
C	-3.5149561917	-0.4695766576	0.6178650859
H	0.5862682481	0.5806494983	0.7942841497
H	2.8691181041	-0.9107573943	0.1781022715
H	-0.5162613603	0.6694718828	-1.9631322573
H	-0.1166549753	2.2136853439	-1.1021302435
H	0.6281030632	-1.9970853961	-0.7783569712
H	2.3174378144	0.7237250566	-2.3298834921
H	3.7889243003	-0.1693223792	-1.9758097948
H	2.2879820292	-1.0284835047	-2.2474674697
H	2.6433039812	2.1096171065	-0.1342353788
H	4.1298929343	1.2109819630	0.1157456207
H	2.9071979689	1.2498611373	1.3730552513
H	-2.1539588949	1.9137546092	0.2885955467
H	-1.6910535089	-2.2986023907	-0.3061337975
H	-4.2145320376	-0.6366491780	-0.1976406605
H	-3.8650939060	0.3925009507	1.1739962064
H	-3.5360107075	-1.3399039953	1.2622727925

S_0 energy / H -387.82229947872599

S_0 CI eigenvector

0.58775178793951	X36 X37 A38 B39
0.58775178793951	X36 X37 B38 A39
0.53104751369019	X36 X37 X38
-0.09031680732821	X36 X38 X39
-0.07797737688523	X36 A37 B38 X39
-0.07797737688523	X36 B37 A38 X39
0.05596380898023	X36 X37 X39
-0.04928821467268	X37 X38 X39
0.02206405608562	X36 A37 X38 B39
0.02206405608562	X36 B37 X38 A39

S_1 energy / H -387.82229908597662

S_1 CI eigenvector

-0.82271966075544	X36 X37 X38
0.38303160573690	X36 X37 A38 B39
0.38303160573690	X36 X37 B38 A39
0.11641835123835	X36 X38 X39
0.07026407790796	X37 X38 X39
-0.06080567079592	X36 X37 X39
-0.04515824235417	X36 A37 X38 B39
-0.04515824235417	X36 B37 X38 A39
-0.03874787926089	X36 A37 B38 X39
-0.03874787926089	X36 B37 A38 X3

eq-T cZc-EDOT Minimum

Cartesian coordinates / Å

26

C	1.0962937617	-0.7437084803	0.1187906338
C	2.5784273855	-0.9430739121	-0.1005682561
C	-0.8491385437	2.0587091358	-0.7375281197
C	0.0999406563	-1.2777773747	-0.5793084452
C	2.9316018990	-1.9482684154	-1.1973467000
C	3.2538553380	0.4118305896	-0.3650625402
C	-1.4801362514	1.3720170901	0.1984734119
C	-2.0269544013	0.0042657496	0.0506468334
C	-1.3343727055	-1.0914261003	-0.3493704851
C	-3.5024156684	-0.0977276454	0.3684862025
H	0.8541511774	-0.0843802515	0.9359452259
H	2.9846312340	-1.3238424698	0.8368144877
H	-0.6298542426	1.6325425825	-1.6998220723
H	-0.5221819891	3.0691135703	-0.5659913635
H	0.3339182122	-1.9804019920	-1.3627237568
H	2.5764377184	-1.6159904974	-2.1683545036
H	4.0086103012	-2.0668852925	-1.2634683732
H	2.5030384298	-2.9246786351	-0.9971472383
H	2.9066016755	0.8382236794	-1.3016790344
H	4.3326280947	0.3018702704	-0.4238711746
H	3.0349166896	1.1233115206	0.4253637654
H	-1.7000717027	1.8659234599	1.1346346124
H	-1.9162051507	-1.9856578828	-0.5103255262
H	-3.7008369536	0.1864134829	1.4005579276
H	-3.8705728381	-1.1070557719	0.2280202815
H	-4.0883221262	0.5691235901	-0.2598557930

S_0 energy / H

-387.92443007312096

S_0 CI eigenvector

0.98724719543351	X36 X37 X38
-0.09231252203294	X36 X37 X39
-0.07473813237284	X37 X38 X39
-0.05810477880187	A36 X37 B38 X39
-0.05810477880187	B36 X37 A38 X39
0.03731851511057	X36 X37 A38 B39
0.03731851511057	X36 X37 B38 A39
-0.03662211345440	X36 X38 X39

S_1 energy / H

-387.73435296924430

S_1 CI eigenvector

-0.68776779599788	X36 X37 A38 B39
-0.68776779599788	X36 X37 B38 A39
0.12157726426136	A36 X37 X38 B39
0.12157726426136	B36 X37 X38 A39
0.09033090811472	X36 A37 B38 X39
0.09033090811472	X36 B37 A38 X39
0.05115726381170	X36 X37 X38
0.04896846654400	X36 X37 X39
-0.03442345199243	X37 X38 X39
-0.02903790866638	X36 A37 X38 B39
-0.02903790866638	X36 B37 X38 A39

eq-G+ S_0 Minimum (FC)			
Cartesian coordinates / Å	26		
	C	0.6960482445	-0.0870689034	0.1032427960
	C	2.1626863025	-0.0576844258	-0.3832934109
	C	-0.0884986580	1.1743503570	-0.2878428753
	C	-0.0793547894	-1.3184258211	-0.3060929493
	C	3.0166369418	-1.1085996037	0.3367219916
	C	2.3167036572	-0.1977258456	-1.9026816995
	C	-1.5530235132	1.0607302408	0.0506945782
	C	-2.1888588477	-0.1141951421	0.0128325073
	C	-1.4302457422	-1.3135032371	-0.3048362342
	C	-3.6681042849	-0.2510727812	0.2682471986
	H	0.7336829485	-0.0940102295	1.1955738903
	H	2.5576055164	0.9177123264	-0.1028197183
	H	0.0016911040	1.3541740970	-1.3593550705
	H	0.3463757605	2.0390329813	0.2046486454
	H	0.4495607089	-2.2299324216	-0.5185427318
	H	2.7126398569	-2.1199528478	0.0833499680
	H	4.0620250710	-1.0068359534	0.0609856035
	H	2.9468010749	-1.0026704737	1.4151857457
	H	1.9456648592	-1.1559234419	-2.2535025973
	H	3.3639117843	-0.1292760459	-2.1822904325
	H	1.7855179837	0.5777640602	-2.4427714802
	H	-2.0947893591	1.9657719398	0.2677627609
	H	-1.9718511037	-2.2187961190	-0.5217577433
	H	-4.1243692097	0.7083293507	0.4818543027
	H	-3.8594285947	-0.9124520087	1.1092605924
	H	-4.1710277119	-0.6787400518	-0.5955736373
S_0 energy / H	-387.96128271615066		
S_0 CI eigenvector	-0.97490610199104	X36 X37 X38	
	0.11644922646756	X36 X37 X39	
	-0.09740199834209	X36 X37 A38 B39	
	-0.09740199834209	X36 X37 B38 A39	
	0.08649470651096	X36 X38 X39	
	-0.05806762497663	X36 A37 B38 X39	
	-0.05806762497663	X36 B37 A38 X39	
	-0.03149315218857	A36 X37 B38 X39	
	-0.03149315218857	B36 X37 A38 X39	
S_1 energy / H	-387.77296474415903		
S_1 CI eigenvector	-0.66612638392567	X36 X37 A38 B39	
	-0.66612638392567	X36 X37 B38 A39	
	-0.16489117153764	X36 A37 X38 B39	
	-0.16489117153764	X36 B37 X38 A39	
	0.14235848364915	X36 X37 X39	
	0.13452794941286	X36 X37 X38	
	-0.09922599578473	X36 X38 X39	
	0.04801419686799	X36 A37 B38 X39	
	0.04801419686799	X36 B37 A38 X39	
	-0.03528431505315	A36 X37 B38 X39	
	-0.03528431505315	B36 X37 A38 X39	
	-0.03316164040981	A36 X37 X38 B39	
	-0.03316164040981	B36 X37 X38 A39	

eq-G+ S_1/S_0 MECI-1 (Closed)

Cartesian coordinates / Å 26

C	0.7583159085	-0.1006263508	0.4949642215
C	1.9487010256	-0.1456607667	-0.4810838568
C	0.0362621951	1.2489130232	0.6182955523
C	-0.4000957131	-0.9817307749	0.0920694465
C	3.0843608934	0.7459294013	0.0315582008
C	2.4451455340	-1.5766496329	-0.7138307309
C	-1.4294795874	0.9137438898	0.7936023980
C	-2.0935997272	0.1953150222	-0.2301624815
C	-1.2901988639	-0.6302770664	-1.0040252554
C	-3.5988551832	0.1826037232	-0.2949452518
H	1.0962516366	-0.4122297405	1.4806115447
H	1.6004122949	0.2458075544	-1.4326058947
H	0.1762541409	1.8403927503	-0.2865916253
H	0.4127924833	1.8305480182	1.4510988390
H	-0.5440764187	-1.9126056505	0.6231471687
H	3.4748676744	0.3721392274	0.9752809843
H	3.9062817777	0.7730530190	-0.6774150585
H	2.7549207141	1.7675084191	0.1912428782
H	2.7521409499	-2.0476113045	0.2173166375
H	3.3003600918	-1.5836978018	-1.3825883053
H	1.6777242467	-2.1967451010	-1.1682206727
H	-2.0081858679	1.4131702389	1.5502220112
H	-1.7213068391	-1.3786644420	-1.6428089561
H	-4.0031026839	1.1574858604	-0.0419692561
H	-3.9948556205	-0.5392439088	0.4136463770
H	-3.9349812458	-0.1001352588	-1.2851147592

S_0 energy / H -387.80940292764240

S_0 CI eigenvector

-0.57871978062015	X36	X37	A38	B39
-0.57871978062015	X36	X37	B38	A39
-0.53617385164606	X36	X37	X38	
0.11386776958470	X36	A37	B38	X39
0.11386776958470	X36	B37	A38	X39
-0.07835583232262	X36	A37	X38	B39
-0.07835583232262	X36	B37	X38	A39
0.05916993786748	X36	X38	X39	
0.02260994333456	X37	X38	X39	

S_1 energy / H -387.80940272617028

S_1 CI eigenvector

0.81952993002138	X36	X37	X38	
-0.38119570043481	X36	X37	A38	B39
-0.38119570043481	X36	X37	B38	A39
-0.09724002381702	X36	X38	X39	
0.08382713005827	X36	A37	X38	B39
0.08382713005827	X36	B37	X38	A39
0.07935555110863	X36	A37	B38	X39
0.07935555110863	X36	B37	A38	X39
-0.03504285474656	X37	X38	X39	

eq-G+ S_1/S_0 MECI-2 (Closed)

Cartesian coordinates / Å 26

C	0.8315692947	0.1936518889	0.2965853420
C	2.2488748655	0.0342300278	-0.3042589839
C	-0.0646043360	1.2102494815	-0.4584503758
C	0.1274751178	-1.1172893598	0.5143741097
C	3.2624147346	-0.4860102298	0.7208815773
C	2.2727783115	-0.8253841500	-1.5744887382
C	-1.5667438866	1.1714418026	-0.0693820186
C	-2.0160138756	-0.1735338215	-0.0062272574
C	-1.2016932727	-1.2840778700	0.4753470157
C	-3.4129099395	-0.5031336533	-0.4366770891
H	0.9513282988	0.6005013115	1.3063549915
H	2.5607728611	1.0380565790	-0.5840049119
H	0.0094683597	1.0448079098	-1.5309233253
H	0.3310577267	2.2032964669	-0.2803775304
H	0.7345817273	-1.9740067991	0.7566192562
H	3.3340578954	0.1809041148	1.5743766335
H	2.9940964084	-1.4710820752	1.0945018293
H	4.2516965260	-0.5674029528	0.2809951803
H	2.0585066510	-1.8682404251	-1.3550400536
H	3.2539034249	-0.7913808219	-2.0374618744
H	1.5512536083	-0.4870484672	-2.3095571029
H	-1.3983297640	1.0683958322	1.0628601462
H	-1.6362366087	-2.2542421784	0.6455213089
H	-4.0928127451	-0.0525943141	0.2794246599
H	-3.6239923538	-1.5647047145	-0.5067538660
H	-3.5893352794	0.0039729897	-1.3780759565

S_0 energy / H -387.80693665837327

S_0 CI eigenvector

-0.67990519954931	X36 X37 A38 B39
-0.67990519954931	X36 X37 B38 A39
-0.22899503431839	X36 X37 X38
-0.08242271308404	A36 X37 B38 X39
-0.08242271308404	B36 X37 A38 X39
0.06073958417323	X36 A37 B38 X39
0.06073958417323	X36 B37 A38 X39
-0.02504941402394	X36 A37 X38 B39
-0.02504941402394	X36 B37 X38 A39
0.02176228949323	X37 X38 X39

S_1 energy / H -387.80693659693350

S_1 CI eigenvector

0.95481877791196	X36 X37 X38
-0.16296049640291	X36 X37 A38 B39
-0.16296049640291	X36 X37 B38 A39
0.08705774046205	X36 A37 X38 B39
0.08705774046205	X36 B37 X38 A39
-0.08112785137459	X37 X38 X39
-0.06804658048944	X36 X38 X39
-0.05979856312741	A36 X37 X38 B39
-0.05979856312741	B36 X37 X38 A39
-0.02002049944278	A36 X37 B38 X39
-0.02002049944278	B36 X37 A38 X39

eq-G+ S_1/S_0 MECI-3 (Open)

Cartesian coordinates / Å

26

C	0.8393340240	-0.1842733329	0.0702667985
C	2.3413296884	-0.1757239922	-0.1744777564
C	-0.5134496424	1.2430574449	-0.9860143405
C	-0.0193656647	-1.2093660117	-0.3304106005
C	3.1105786672	-0.1531246947	1.1549305307
C	2.8517825385	-1.3127529898	-1.0644544973
C	-1.6916604615	1.1418784961	-0.2118601578
C	-2.2114439674	-0.1278473010	0.0337061001
C	-1.4289487822	-1.2635637487	-0.2356345117
C	-3.6172771574	-0.2808463004	0.5510067190
H	0.5242766161	0.4342377115	0.8904969234
H	2.5902854585	0.7546639658	-0.6886958454
H	-0.4382334611	0.6920281665	-1.9045899679
H	0.0781506110	2.1413529522	-0.9482154056
H	0.4299577159	-2.0620520236	-0.8159763421
H	2.9413193639	-1.0671242670	1.7168988304
H	4.1797277991	-0.0522195241	0.9870992124
H	2.7947026510	0.6807948467	1.7749008549
H	2.7103178607	-2.2822464684	-0.5947365760
H	3.9141255320	-1.1935633428	-1.2520552820
H	2.3489934244	-1.3288369831	-2.0268865176
H	-2.0564048330	2.0022742172	0.3195550163
H	-1.9062515518	-2.2198941063	-0.3581808740
H	-4.2872514452	-0.4717969091	-0.2839040172
H	-3.9576001172	0.6240130942	1.0403949788
H	-3.7000937252	-1.1123041585	1.2408739903

S_0 energy / H -387.82076950452392

S_0 CI eigenvector

-0.68673998548323	X36 X37 A38 B39
-0.68673998548323	X36 X37 B38 A39
0.19740638436937	X36 X37 X38
-0.08824148116916	X36 A37 B38 X39
-0.08824148116916	X36 B37 A38 X39

S_1 energy / H -387.82076928014169

S_1 CI eigenvector

0.95997457664482	X36 X37 X38
-0.14086373112353	X36 X38 X39
0.13894945635338	X36 X37 A38 B39
0.13894945635338	X36 X37 B38 A39
-0.08507873053137	X37 X38 X39
0.07221049275525	X36 X37 X39
-0.05062706457381	X36 A37 X38 B39
-0.05062706457381	X36 B37 X38 A39
0.02550730321154	X36 A37 B38 X39
0.02550730321154	X36 B37 A38 X39

eq-G+ cZc-EDOT Minimum				
Cartesian coordinates / Å	26			
	C	1.1069891144	-0.7071434348	0.1435385351
	C	2.5967442049	-0.8780873330	-0.0446227292
	C	-0.8185241000	2.1256866707	-0.5383397457
	C	0.1373462659	-1.1905767785	-0.6249294365
	C	3.2136466248	-1.5081232905	1.2136645063
	C	2.9961560918	-1.6619931778	-1.2953199812
	C	-1.4972466021	1.3737901447	0.3107580425
	C	-2.0211864692	0.0157608187	0.0450907957
	C	-1.3049009896	-1.0389914637	-0.4182374975
	C	-3.5030402028	-0.1267083574	0.3145846343
	H	0.8335645302	-0.1257240997	1.0085965066
	H	3.0151856688	0.1248179686	-0.1377011611
	H	-0.5372310951	1.7670350185	-1.5118288134
	H	-0.5130731037	3.1242137821	-0.2797404200
	H	0.4008133456	-1.8205237740	-1.4592070886
	H	2.8462630536	-2.5202705978	1.3556113861
	H	4.2961272098	-1.5491988451	1.1367846848
	H	2.9652700445	-0.9374212340	2.1033944019
	H	2.6298581219	-2.6836014882	-1.2549705960
	H	4.0774024363	-1.7034303514	-1.3817157185
	H	2.6087423078	-1.2007468222	-2.1976855500
	H	-1.7781139413	1.8046241389	1.2615862602
	H	-1.8710859596	-1.9242776642	-0.6627375201
	H	-3.7320318991	0.0763063957	1.3593564204
	H	-3.8538589751	-1.1266271484	0.0886782979
	H	-4.0815956827	0.5785109230	-0.2776982141
S_0 energy / H	-387.92458684230434			
S_0 CI eigenvector	0.98734756732215	X36 X37 X38		
	-0.09243563086125	X36 X37 X39		
	-0.07448575785208	X37 X38 X39		
	0.05767436211655	A36 X37 B38 X39		
	0.05767436211655	B36 X37 A38 X39		
	-0.03797202759569	X36 X38 X39		
	0.03607817069294	X36 X37 A38 B39		
	0.03607817069294	X36 X37 B38 A39		
S_1 energy / H	-387.73530515519013			
S_1 CI eigenvector	-0.68823877641986	X36 X37 A38 B39		
	-0.68823877641986	X36 X37 B38 A39		
	-0.11913239829799	A36 X37 X38 B39		
	-0.11913239829799	B36 X37 X38 A39		
	0.09078221553536	X36 A37 B38 X39		
	0.09078221553536	X36 B37 A38 X39		
	0.04950738469998	X36 X37 X38		
	0.04666626926509	X36 X37 X39		
	-0.03212382714577	X37 X38 X39		
	-0.03169745228226	X36 A37 X38 B39		
	-0.03169745228226	X36 B37 X38 A39		

Table S3.

Coordinates, Energies and CI Eigenvectors for S_0 And S_1 at Critical Points Along the Ring-Closed and Ring-Open Pathways of αPH. For the CI eigenvectors, XYY indicates that the YYth molecular orbital is doubly occupied, and AYY/BYY indicate that the YYth molecular orbital is singly occupied with alpha or beta spin, respectively.

References and Notes

1. Y.-P. Chang, K. Długołęcki, J. Küpper, D. Rösch, D. Wild, S. Willitsch, Specific chemical reactivities of spatially separated 3-aminophenol conformers with cold Ca^+ ions. *Science* **342**, 98–101 (2013).

2. K. A. Dill, J. L. MacCallum, The protein-folding problem, 50 years on. *Science* **338**, 1042–1046 (2012).

3. R. B. Woodward, R. Hoffmann, The Conservation of Orbital Symmetry. *Angew. Chem. Int. Ed.* **8**, 781–853 (1969).

4. T. Bach, J. P. Hehn, Photochemical reactions as key steps in natural product synthesis. *Angew. Chem. Int. Ed.* **50**, 1000–1045 (2011).

5. E. Havinga, J. L. M. A. Schlatmann, Remarks on the specificities of the photochemical and thermal transformations in the vitamin D field. *Tetrahedron* **16**, 146–152 (1961).

6. J. E. Baldwin, S. M. Krueger, Stereoselective photochemical electrocyclic valence isomerizations of α-phellandrene conformational isomers. *J. Am. Chem. Soc.* **91**, 6444–6447 (1969).

7. M. M. de Christo Scherer, F. M. Marques, M. M. Figueira, M. C. O. Peisino, E. F. P. Schmitt, T. P. Kondratyuk, D. C. Endringer, R. Scherer, M. Fronza, Wound healing activity of terpinolene and α-phellandrene by attenuating inflammation and oxidative stress in vitro. *J. Tissue Viability* **28**, 94–99 (2019).

8. W. G. Dauben, J. Rabinowitz, N. D. Vietmeyer, P. H. Wendschuh, Photoequilibriums between 1,3-cyclohexadienes and 1,3,5-hexatrienes. Photochemistry of 3-alkyl-6,6,9,9-tetramethyl-Δ3,5(10)-hexalins. *J. Am. Chem. Soc.* **94**, 4285–4292 (1972).

9. C. W. Spangler, R. P. Hennis, The influence of ground state conformation on the photochemical ring-opening of 5-alkylcyclohexa-1,3-dienes. *Chem. Commun.* **1972**, 24–25 (1972).

10. M. K. Lawless, S. D. Wickham, R. A. Mathies, Resonance Raman View of Pericyclic Photochemical Ring-Opening Reactions: Beyond the Woodward-Hoffmann Rules. *Acc. Chem. Res.* **28**, 493–502 (1995).

11. P. J. Reid, S. J. Doig, R. A. Mathies, Picosecond time-resolved UV resonance Raman spectroscopy of the photochemical ring opening of 1,3,5-cyclooctatriene and α-phellandrene. *J. Phys. Chem.* **94**, 8396–8399 (1990).

12. M. Garavelli, C. S. Page, P. Celani, M. Olivucci, W. E. Schmid, S. A. Trushin, W. Fuss, Reaction Path of a sub-200 fs Photochemical Electrocyclic Reaction. *J. Phys. Chem. A* **105**, 4458–4469 (2001).

13. B. C. Arruda, B. Smith, K. G. Spears, R. J. Sension, Ultrafast ring-opening reactions: A comparison of α-terpinene, α-phellandrene, and 7-dehydrocholesterol with 1,3-cyclohexadiene. *Faraday Discuss.* **163**, 159–171 (2013).

14. O. Njoya, S. Matsika, T. Weinacht, Angle-resolved strong-field ionization of polyatomic molecules: More than the orbitals matters. *ChemPhysChem* **14**, 1451–1455 (2013).

15. B. C. Arruda, R. J. Sension, Ultrafast polyene dynamics: The ring opening of 1,3-cyclohexadiene derivatives. *Phys. Chem. Chem. Phys.* **16**, 4439–4455 (2014).

16. M. Ben-Nun, T. J. Martínez, Ab initio quantum molecular dynamics. *Adv. Chem. Phys.* **121**, 439–512 (2002).

17. M. Ben-Nun, T. J. Martínez, Nonadiabatic molecular dynamics: Validation of the multiple spawning method for a multidimensional problem. *J. Chem. Phys.* **108**, 7244–7257 (1998).

18. M. Ben-Nun, J. Quenneville, T. J. Martínez, Ab Initio Multiple Spawning: Photochemistry from First Principles Quantum Molecular Dynamics. *J. Phys. Chem. A* **104**, 5161–5175 (2000).

19. S. Matsika, P. Krause, Nonadiabatic events and conical intersections. *Annu. Rev. Phys. Chem.* **62**, 621–643 (2011).

20. A. Hofmann, R. de Vivie-Riedle, Adiabatic approach for ultrafast quantum dynamics mediated by simultaneously active conical intersections. *Chem. Phys. Lett.* **346**, 299–304 (2001).

21. K. M. Marzec, I. Reva, R. Fausto, L. M. Proniewicz, Comparative matrix isolation infrared spectroscopy study of 1,3- and 1,4-diene monoterpenes (α-phellandrene and γ-terpinene). *J. Phys. Chem. A* **115**, 4342–4353 (2011).

22. J. W. Snyder Jr., R. M. Parrish, T. J. Martínez, α-CASSCF: An Efficient, Empirical Correction for SA-CASSCF To Closely Approximate MS-CASPT2 Potential Energy Surfaces. *J. Phys. Chem. Lett.* **8**, 2432–2437 (2017).

23. T. J. A. Wolf, D. M. Sanchez, J. Yang, R. M. Parrish, J. P. F. Nunes, M. Centurion, R. Coffee, J. P. Cryan, M. Gühr, K. Hegazy, A. Kirrander, R. K. Li, J. Ruddock, X. Shen, T. Vecchione, S. P. Weathersby, P. M. Weber, K. Wilkin, H. Yong, Q. Zheng, X. J. Wang, M. P. Minitti, T. J. Martínez, The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction. *Nat. Chem.* **11**, 504–509 (2019).

24. M. H. Kim, L. Shen, H. Tao, T. J. Martinez, A. G. Suits, Conformationally controlled chemistry: Excited-state dynamics dictate ground-state reaction. *Science* **315**, 1561–1565 (2007).

25. S. T. Park, S. K. Kim, M. S. Kim, Observation of conformation-specific pathways in the photodissociation of 1-iodopropane ions. *Nature* **415**, 306–308 (2002).

26. K.-W. Choi, D.-S. Ahn, J.-H. Lee, S. K. Kim, A highly conformationally specific α- and β-Ala^+ decarboxylation pathway. *Chem. Commun.* **2007**, 1041–1043 (2007).

27. F. Filsinger, G. Meijer, H. Stapelfeldt, H. N. Chapman, J. Küpper, State- and conformer-selected beams of aligned and oriented molecules for ultrafast diffraction studies. *Phys. Chem. Chem. Phys.* **13**, 2076–2087 (2011).

28. Y.-P. Chang, D. A. Horke, S. Trippel, J. Küpper, Spatially-controlled complex molecules and their applications. *Int. Rev. Phys. Chem.* **34**, 557–590 (2015).

29. T. Endo, S. P. Neville, V. Wanie, S. Beaulieu, C. Qu, J. Deschamps, P. Lassonde, B. E. Schmidt, H. Fujise, M. Fushitani, A. Hishikawa, P. L. Houston, J. M. Bowman, M. S. Schuurman, F. Légaré, H. Ibrahim, Capturing roaming molecular fragments in real time. *Science* **370**, 1072–1077 (2020).

30. T. J. A. Wolf, Figures for “Conformer-specific photochemistry imaged in real space and time”. DOI:10.5281/zenodo.5214798.

31. X. Shen, J. P. F. Nunes, J. Yang, R. K. Jobe, R. K. Li, M.-F. Lin, B. Moore, M. Niebuhr, S. P. Weathersby, T. J. A. Wolf, C. Yoneda, M. Guehr, M. Centurion, X. J. Wang, Femtosecond gas-phase mega-electron-volt ultrafast electron diffraction. *Struct. Dyn.* **6**, 054305 (2019).

32. S. P. Weathersby, G. Brown, M. Centurion, T. F. Chase, R. Coffee, J. Corbett, J. P. Eichner, J. C. Frisch, A. R. Fry, M. Gühr, N. Hartmann, C. Hast, R. Hettel, R. K. Jobe, E. N. Jongewaard, J. R. Lewandowski, R. K. Li, A. M. Lindenberg, I. Makasyuk, J. E. May, D. McCormick, M. N. Nguyen, A. H. Reid, X. Shen, K. Sokolowski-Tinten, T. Vecchione, S. L. Vetter, J. Wu, J. Yang, H. A. Dürr, X. J. Wang, Mega-electron-volt ultrafast electron diffraction at SLAC National Accelerator Laboratory. *Rev. Sci. Instrum.* **86**, 073702 (2015).

33. J. W. Snyder Jr., B. S. Fales, E. G. Hohenstein, B. G. Levine, T. J. Martínez, A direct-compatible formulation of the coupled perturbed complete active space self-consistent field equations on graphical processing units. *J. Chem. Phys.* **146**, 174113 (2017).

34. J. W. Snyder Jr., B. F. Curchod, T. J. Martínez, GPU-accelerated state-averaged complete active space self-consistent field interfaced with ab initio multiple spawning unravels the photodynamics of provitamin D3. *J. Phys. Chem. Lett.* **7**, 2444–2449 (2016).

35. J. W. Snyder Jr., E. G. Hohenstein, N. Luehr, T. J. Martínez, An atomic orbital-based formulation of analytical gradients and nonadiabatic coupling vector elements for the state-averaged complete active space self-consistent field method on graphical processing units. *J. Chem. Phys.* **143**, 154107 (2015).

36. I. S. Ufimtsev, T. J. Martínez, Quantum chemistry on graphical processing units. 1. Strategies for two-electron integral evaluation. *J. Chem. Theory Comput.* **4**, 222–231 (2008).

37. I. S. Ufimtsev, T. J. Martinez, Quantum chemistry on graphical processing units. 2. Direct self-consistent-field implementation. *J. Chem. Theory Comput.* **5**, 1004–1015 (2009).

38. I. S. Ufimtsev, T. J. Martinez, Quantum chemistry on graphical processing units. 3. Analytical energy gradients, geometry optimization, and first principles molecular dynamics. *J. Chem. Theory Comput.* **5**, 2619–2628 (2009).

39. J. P. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **77**, 3865–3868 (1996).

40. T. J. A. Wolf, https://github.com/ThomasJAWolf/Diffraction_simulation.

41. F. Salvat, A. Jablonski, C. J. Powell, ELSEPA—Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules. *Comput. Phys. Commun.* **165**, 157–190 (2005).