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Supporting Information

Nanosecond Laser Flash Photolysis of a 6-Nitroindolinospiropyran in Solution and in Nanocrystalline Suspension Under Single Excitation Conditions

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General Information. All commercially obtained reagents/solvents were used as received without further purification. UV-Vis absorption and transmission spectra were recorded on an Ocean Optics spectrometer (DT-MINI-2-GS UV-VIS-NIR LightSource and USB2000+ using SpectraSuite software package). Dynamic Light Scattering (DLS) data were recorded using a Beckman-Coulter N4 Plus particle analyzer with a 10 mW helium-neon laser at 632.8 nm. The particle size was determined using the 62.6° detection angle and was calculated using the size distribution processor (SDP) analysis package provided by the manufacturer. Powder X-ray diffraction measurements were performed on a flat stage using a PANalytical.Inc X'Pert Pro Cu K-α = 1.5406 Å radiation source at power settings of 45 kV and 40 mA and a slit width of 0.5°. Data were collected at room temperature in the range of 2θ = 4–45°. Nanosecond transient absorption experiments were performed using a laser flash photolysis (LFP) instrument from Edinburgh Instruments in conjunction with a Q-switched Nd:YAG laser (Brilliant b, Quantel®) with a 355 nm output

wavelength, 5–8 ns pulse width, 1 Hz repetition rate, and 36–40 mJ pulse energy. The optical detection is based on a pulsed Xenon arc lamp (450 W), a monochromator (TMS300, Czerny-Turner), a photomultiplier detector (Hamamatsu R928), and a digital oscilloscope (TDS3012C, 100 MHz and 1.25 GS/s from Tektronix). Transient absorption data was processed using the L900 software package provided by Edinburgh Instruments. Laser flash photolysis experiments were performed with a 1 cm quartz flow cell mounted on a home-built sample holder that is placed at the cross-section of the laser incident beam and the probe flashlamp. Samples were flowed through a Masterflex L/S peristaltic pump at a rate of 15 mL/min for acetonitrile solutions and at a rate of 1.9 mL/min for nanocrystalline suspension samples.

Synthesis of 1',3',3'-Trimethyl-6-nitrospiro[chromene-2,2'-indoline] (SP1): compound was prepared as previously reported.[1]

General preparation of solutions for LFP experiments
730 μL of a stock solution (17.2 mM) of **SP1** in acetonitrile was diluted to 500 mL to give a final sample concentration of 0.025 mM with an optical density of ca. 0.25 at 355 nm.

General preparation of nanocrystalline suspensions for LFP experiments
15 μL of a stock solution (~50 mM) of **SP1** in acetonitrile was injected via a micropipette into a graduated cylinder containing a vigorously stirring solution of 16 mL of Millipore water and 4 mL of a CTAB (cetyltrimethylammonium bromide) solution (0.193 mM). The vigorous stirring was continued for 30 seconds after injection. The newly created suspension was gently poured into a large culture tube and sonicated for 2 minutes. The suspension was then immediately used for LFP studies and new suspensions were made as needed. Nanocrystalline suspensions had an optical density of ca. 0.365 at 355 nm.

Laser flash photolysis of SP1 in solution (argon degassed and air saturated)
Degassed acetonitrile solutions of **SP1** were purged with argon for 3 hours prior to conducting laser flash photolysis experiments, and a continuous flow of argon was maintained for the duration of data collection. Air saturated acetonitrile solutions of **SP1** were allowed to equilibrate overnight under normal atmospheric conditions prior to conducting laser flash photolysis experiments.

Time-resolved transient absorption maps were then recorded from 325–685 nm in 20 nm steps while continuously flowing the sample solutions through the quartz cell at 15 mL/min. Absorption bands with λ_{max} values of 370, 440, 550, and 590 nm were observed, and the kinetics at 440, 550, and 590 nm were then measured with a 1.5 nm bandwidth and 20–30 scans averaged together. Flashlamp settings were set where the frequency was 10 Hz, width at 40 μs, and delay at 4000 μs. Q-switch settings were set where the frequency was at 1.0 Hz, width at 20 μs, and delay at 280 μs. All transient data was reproduced in triplicate.

Laser flash photolysis of SP1 in nanocrystalline suspension
Suspensions were prepared immediately prior to performing kinetic measurements as described above. Time-resolved transient absorption maps were then recorded from 325–685 nm in 20 nm steps while continuously flowing the sample suspensions through a quartz cell at 1.9 mL/min. Kinetic measurements were made at the same wavelengths, same bandwidth, and same number of averaged scans as in solution due to no real absorption bands being observed in nanocrystalline suspension. Flashlamp settings were set where the frequency was 10 Hz, width at 40 μs, and delay at 4000 μs. Q-switch settings were set where the frequency was at 1.0 Hz, width at 20 μs, and delay at 300 μs. All transient data was reproduced in triplicate.

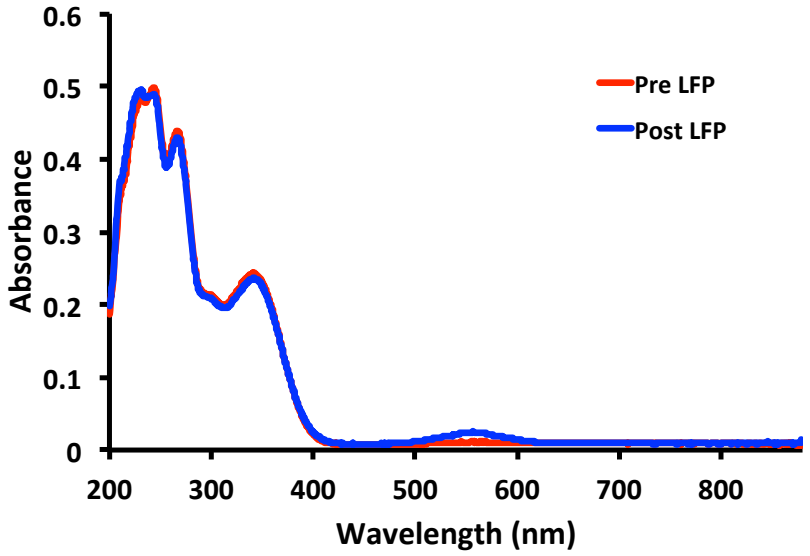

Figure S1. UV-vis absorption spectra of **SP1** in acetonitrile pre-laser flash photolysis (LFP) irradiation (red) and post-LFP irradiation.

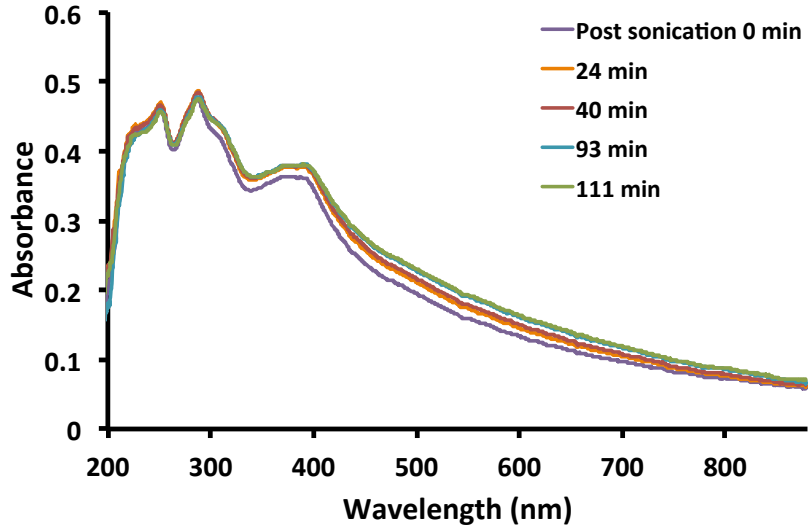

Figure S2. UV-vis absorption spectra of **SP1** in nanocrystalline suspension over time.

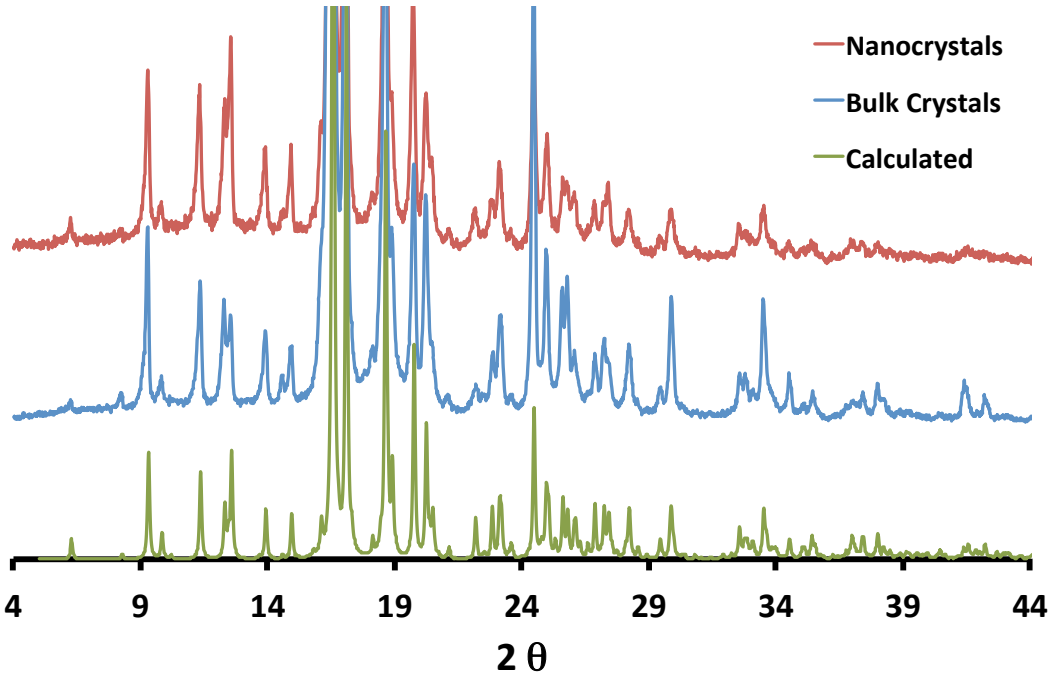

Figure S3. PXRD comparison of experimentally obtained nanocrystals (top) and bulk crystals (middle) to the calculated (bottom) diffractogram from the CSD for **SP1**.

Unimodal Results Summary

Rept#.	Mean (nm)	Std.Dev (nm)	Baseline Error	P.I.	Counts/s	Diff.Coef (m^2/s)	Overflow
Rept.1	365.8	178.9	-0.00%	-2.763	1.15e+05	1.24e-12	0
Rept.2	234.8	114.2	0.00%	2.170	1.15e+05	1.93e-12	0
Rept.3	206.0	100.4	0.00%	2.343	1.15e+05	2.20e-12	1
Average	268.9	131.16		0.583			

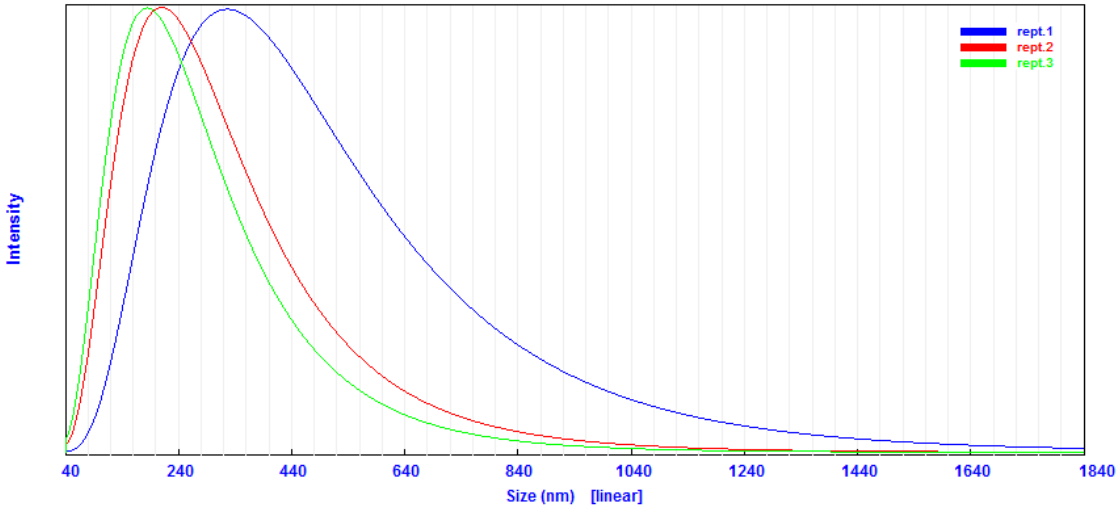

Figure S4. Dynamic light scattering (DLS) results for the nanocrystalline suspensions of SP1 showing the average particle size to be 269 nm.

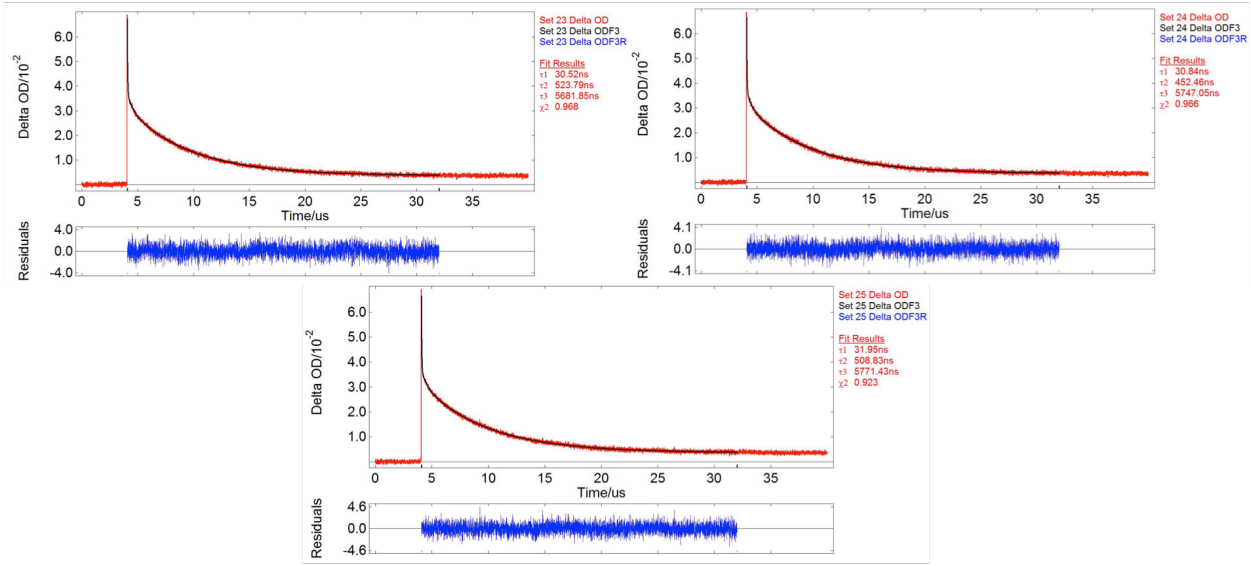

Figure S5. Laser flash photolysis transient kinetic decay plots at 440 nm in argon degassed acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetimes shown.

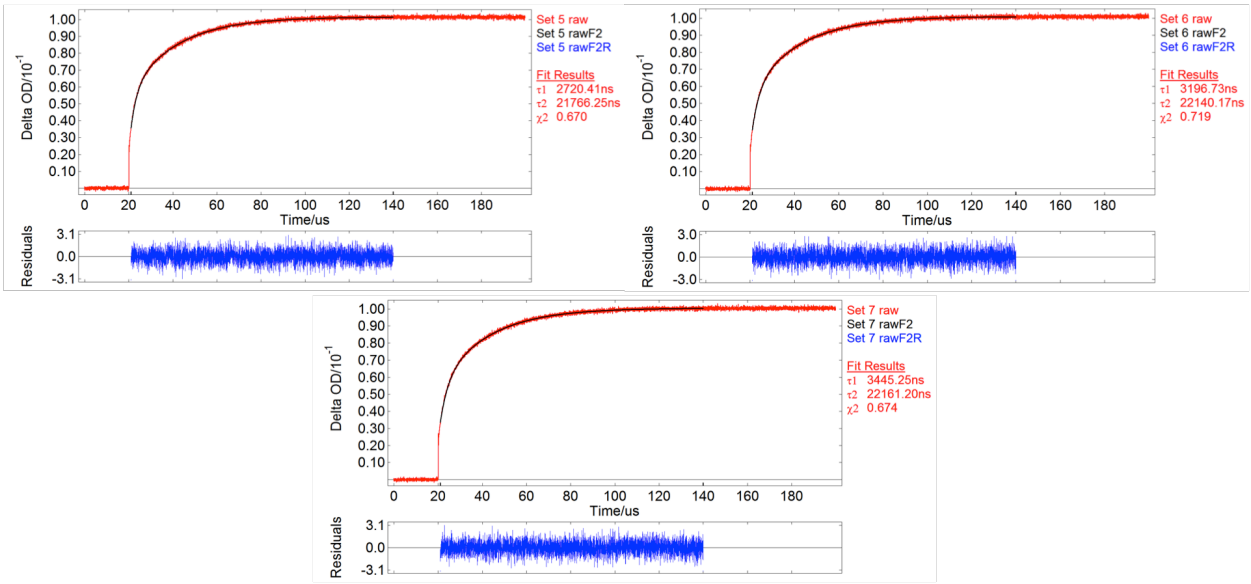

Figure S6. Laser flash photolysis transient kinetic growth plots at 550 nm in argon degassed acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetimes shown.

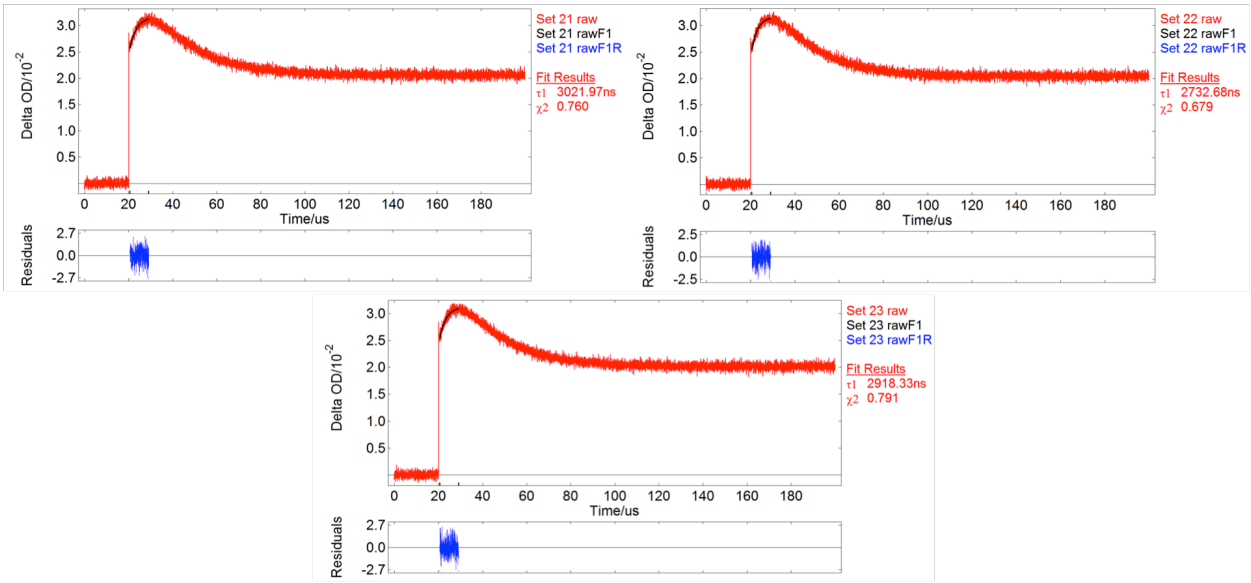

Figure S7. Laser flash photolysis transient kinetic growth plots at 590 nm in argon degassed acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetime shown.

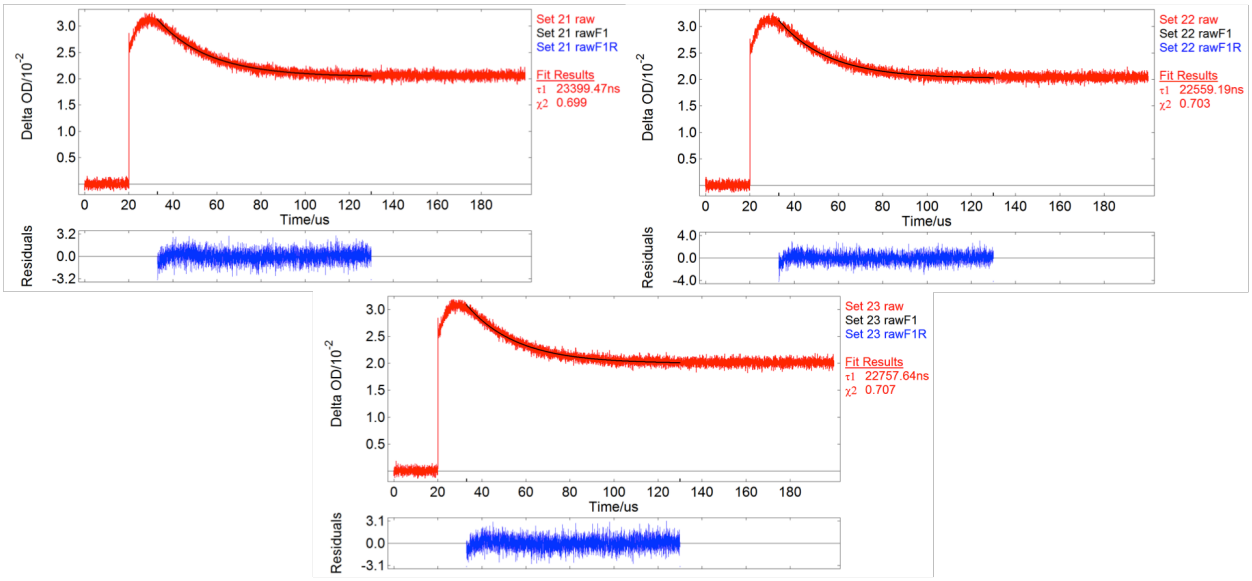

Figure S8. Laser flash photolysis transient kinetic decay plots at 590 nm in argon degassed acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetime shown.

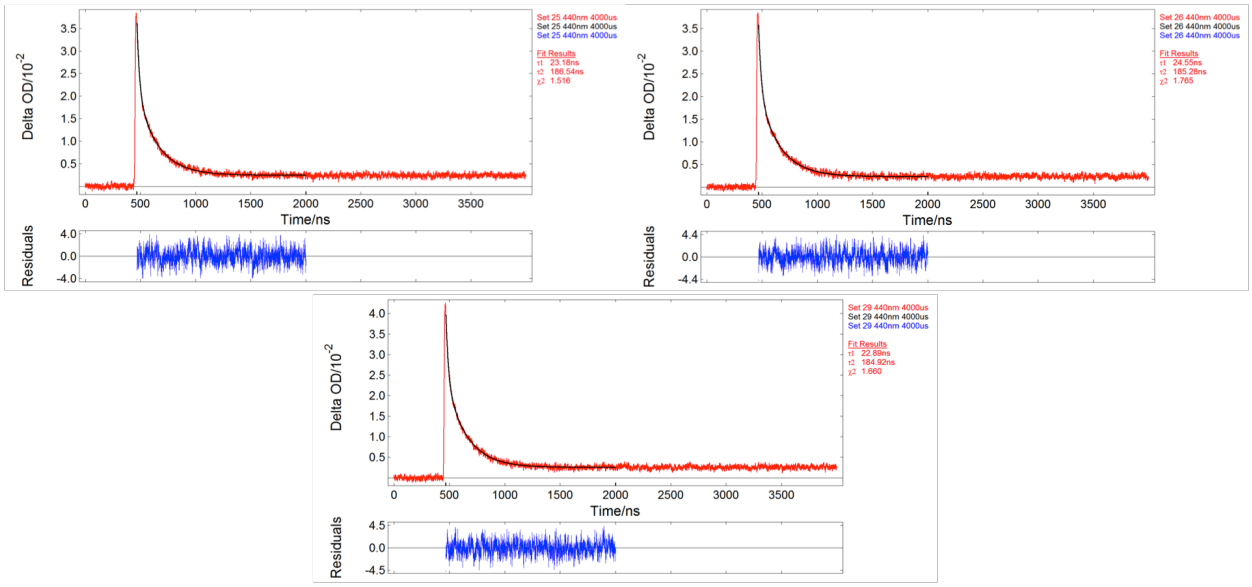

Figure S9. Laser flash photolysis transient kinetic decay plots at 440 nm in air saturated acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetimes shown.

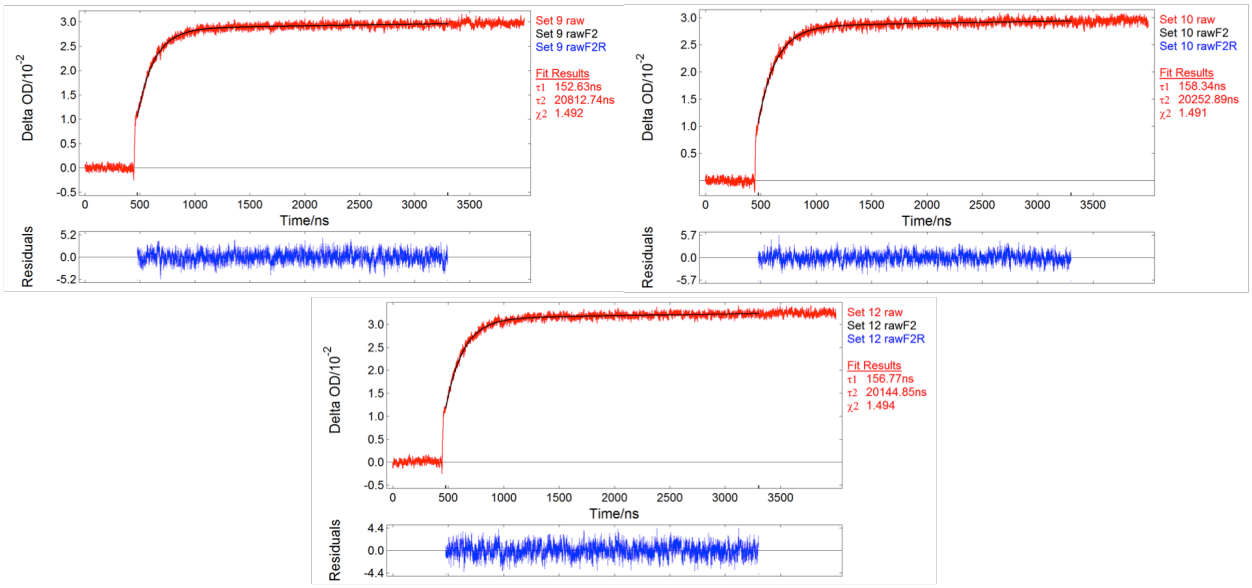

Figure S10. Laser flash photolysis transient kinetic growth plots at 550 nm in air saturated acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetimes shown.

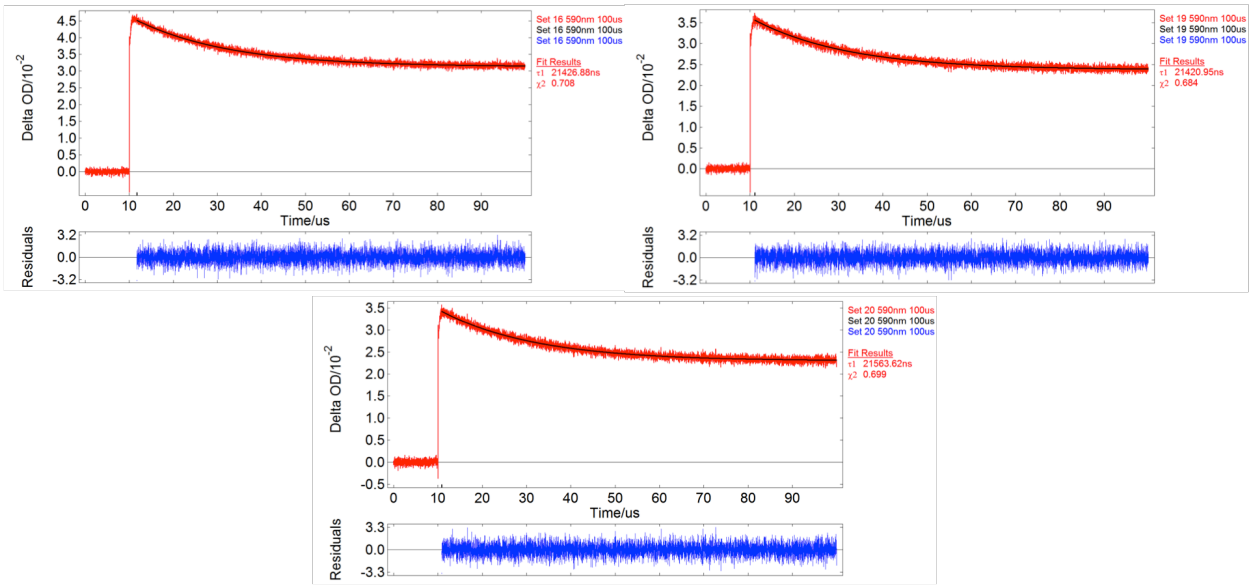

Figure S11. Laser flash photolysis transient kinetic decay plots at 590 nm in air saturated acetonitrile with the kinetic trace (red), fit line (black), residual (blue), and lifetime shown.

Computational methods

We used density functional theory (DFT) and TD-DFT calculations to explain the blue shift we observed from 590 to 550 nm in our transient absorption spectra (main text Figures 2a and 3a). To understand the origin of this shift and the molar absorptivity difference between the bands at 550 and 590 nm we performed a conformational search to identify the lowest energy conformer for the spiropyran (**SP1**), *Z*-merocyanine (*Z*-MC), and *E*-merocyanine (*E*-MC) on the ground state (S_0) and first excited singlet state (S_1) potential energy surfaces (PESs). The conformational search on **SP1** and *E*- and *Z*-MC isomers was performed with the MMFF94[2] force field using Maestro/Macromodel[3,4] in the Schrödinger Suite of Programs (energy cutoff and other information). Each of the resulting conformers were optimized to their ground state geometries (S_0) and excited state geometries (S_1) using the TD-CAM-B3LYP[5] density functional at the 6-311++G(d,p) level of theory utilizing the IEFPCM-(CH_3CN) continuum solvent method[6,7] and D3 empirical dispersion with Becke-Johnson damping[8] within Gaussian16 Revision A[9]. Upon vibrational analysis, each optimized structure only had positive frequencies, indicating a local minimum. A transition state between **MCZ-a$_0$** and **MCE-c$_0$** was also optimized and confirmed to be a transition state with one imaginary frequency along the calculated intrinsic reaction coordinate (IRC). Single point energies, corrections to thermal free energies, and free energies are provided for each stationary point.

We computed a full torsional potential about the central C=C π bond ($C_2C_3C_4C_5$–highlighted in green in Figure S12) to explore relatively high-energy structures and their absorbance properties. We obtained the torsional potentials with the IEFPCM-(CH_3CN) solvation model instead of with multiscale (QM/MM) modeling to maintain reasonable computational cost. The key stationary points **MCZ-a$_0$**, **TS(MCZ$_0$→MCE$_0$)**, and **MCE-c$_0$** are shown in Figure S12.

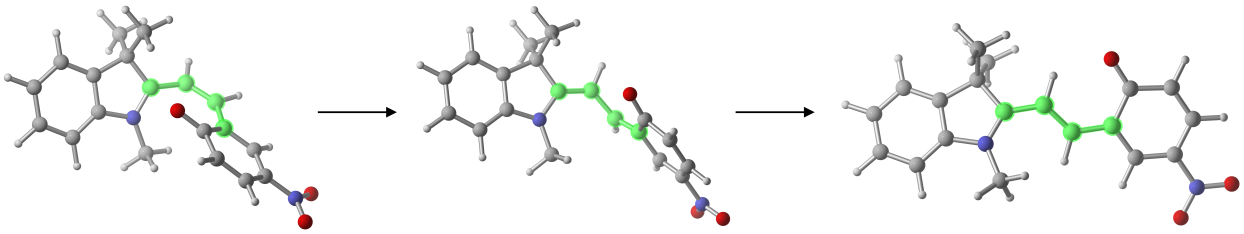

Figure S12. Key stationary points from the torsional potential of the *E*- and *Z*-MCs: **MCZ-a$_0$**, **TS(MCZ$_0$→MCE$_0$)**, and **MCE-c$_0$**. Computed with CAM-B3LYP-(D3BJ)/6-31+G(d,p)/IEFPCM-(CH_3CN) level of theory.

In aiming to understand how the absorption profile varies as a function of structure, we performed single-point calculations on each structure along the torsional potential shown in Fig. 6 of the main text using the TD-CAM-B3LYP method and 6-311++G(d,p) basis set. From this we obtained vertical excitations in order to generate predicted UV-vis absorbance spectra, as shown below in Figure S13. The spectra show that the *E*-like MC structures have a higher absorptivity compared to the *Z*-like MCs, which is in agreement with our solution experimental results shown in Figures 2a and 3a of the main text.

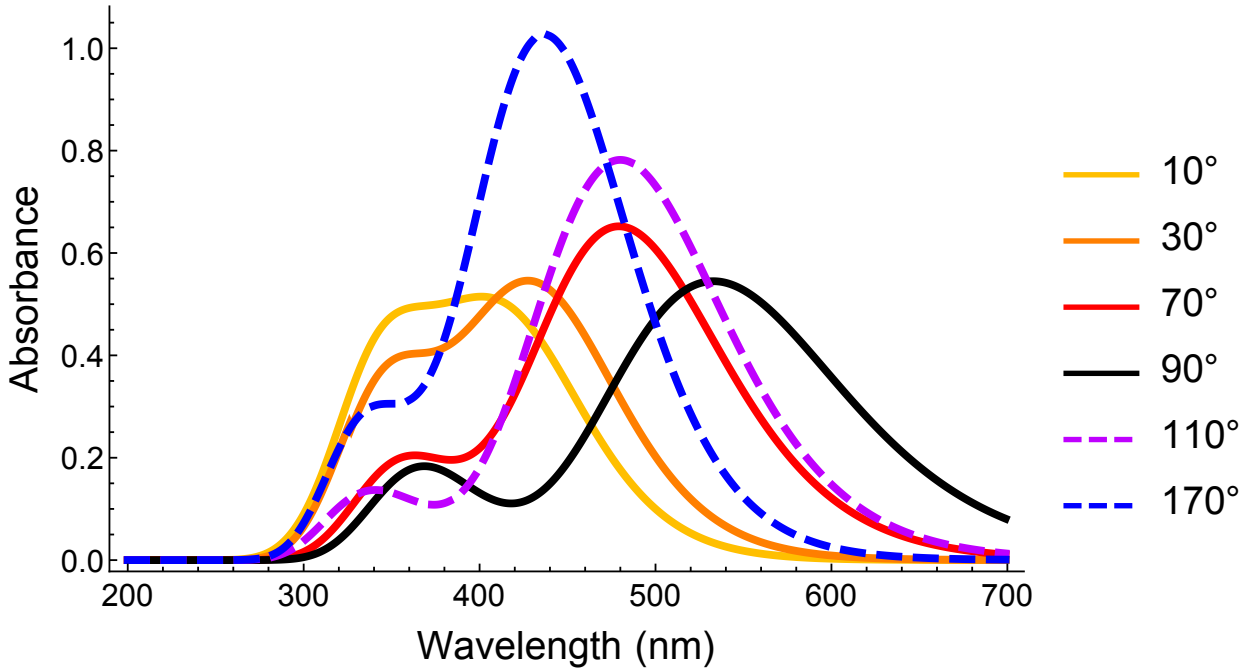

Figure S13. Calculated UV-vis spectra for MC geometries along the relaxed scan about the central π-bond (highlighted in green in Figure S12). MC geometries were computed at the CAM-B3LYP-(D3BJ)/6-31+G(d,p) IEFPCM-(CH_3CN) level of theory. Absorbance spectra were predicted with the 6-311++G(d,p) basis set. The thick black line indicates the structure closest to the transition state between *Z*- and *E*-MC. The yellow, orange, and red solid lines correlate to *Z*-like MCs, and the purple and blue dashed lines correlate to *E*-like MCs.

MCZ-a_0
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.73029003
Sum of electronic and zero-point Energies (Eh)	-1069.393029
Sum of electronic and thermal Energies (Eh)	-1069.372308
Sum of electronic and enthalpy Energies (Eh)	-1069.371364
Sum of electronic and thermal Free Energies (Eh)	-1069.442609
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

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__Frequencies__ (Top 10 out of 120)

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2. 33.0515 cm-1 (Symmetry: A)
3. 44.9047 cm-1 (Symmetry: A)
4. 68.1971 cm-1 (Symmetry: A)
5. 97.4352 cm-1 (Symmetry: A)
6. 108.2468 cm-1 (Symmetry: A)
7. 118.1617 cm-1 (Symmetry: A)
8. 142.7425 cm-1 (Symmetry: A)
9. 159.7737 cm-1 (Symmetry: A)
10. 170.0243 cm-1 (Symmetry: A)
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MCZ-b_0
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Datum	Value
Charge	0
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Number of Basis Functions	654
Electronic Energy (Eh)	-1069.72748733
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Sum of electronic and thermal Energies (Eh)	-1069.369411
Sum of electronic and enthalpy Energies (Eh)	-1069.368466
Sum of electronic and thermal Free Energies (Eh)	-1069.44039
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

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__Frequencies__ (Top 10 out of 120)

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Sum of electronic and thermal Energies (Eh)	-1069.285577
Sum of electronic and enthalpy Energies (Eh)	-1069.284632
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Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

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H       -1.426570     -3.262571     -0.575432
H       -0.875924      1.008574     -1.454798
H        0.374493      0.820506     -2.701593
H       -0.581450     -0.580204     -2.182822
H       -1.126943      1.481548      2.294031
H       -3.354537      2.060535      1.343934
H       -3.403665     -1.593074     -0.895511
```

__Frequencies__ (Top 10 out of 120)

```
 1.     22.2076 cm-1 (Symmetry: A)
 2.     35.7714 cm-1 (Symmetry: A)
 3.     39.8258 cm-1 (Symmetry: A)
 4.     55.1850 cm-1 (Symmetry: A)
 5.     81.9393 cm-1 (Symmetry: A)
 6.    109.7023 cm-1 (Symmetry: A)
 7.    116.8738 cm-1 (Symmetry: A)
 8.    147.9268 cm-1 (Symmetry: A)
 9.    158.5456 cm-1 (Symmetry: A)
10.    167.7947 cm-1 (Symmetry: A)
```

MCZ-b_1
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.71891541
Sum of electronic and zero-point Energies (Eh)	-1069.308911
Sum of electronic and thermal Energies (Eh)	-1069.287869
Sum of electronic and enthalpy Energies (Eh)	-1069.286924
Sum of electronic and thermal Free Energies (Eh)	-1069.359141
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -4.364804      1.817698      0.218242
C       -3.466224      2.331608      1.152175
C       -2.281944      1.670714      1.448730
C       -2.032678      0.485105      0.769268
C       -2.926066     -0.047642     -0.159975
C       -4.100377      0.618366     -0.442429
```

```
N       -0.925716    -0.355057     0.889092
C       -1.029099    -1.410165     0.030327
C       -2.380655    -1.358012    -0.672045
C       -3.264139    -2.536900    -0.217838
C       -2.230005    -1.362878    -2.199642
C       -0.070267    -2.387235    -0.220001
C        1.318231    -2.347070    -0.043141
C        2.143159    -1.201984    -0.058996
C       -0.036868    -0.237551     2.037429
C        3.554084    -1.378281     0.372831
C        4.387172    -0.195777     0.428059
C        3.921745     1.020658     0.049928
C        2.590451     1.143591    -0.421697
C        1.728589     0.064798    -0.498914
O        3.982204    -2.495810     0.685307
N        2.121870     2.431883    -0.839508
O        0.954049     2.538858    -1.213769
O        2.900037     3.386131    -0.811596
H       -5.280539     2.355369     0.006854
H       -3.692496     3.263997     1.654109
H       -1.582149     2.074782     2.167813
H       -4.809984     0.220767    -1.158180
H       -2.833028    -3.486752    -0.538197
H       -4.254684    -2.443683    -0.666544
H       -3.374894    -2.550273     0.867065
H       -1.604837    -0.534678    -2.535755
H       -1.779498    -2.297135    -2.537926
H       -3.210598    -1.267651    -2.669311
H       -0.470833    -3.310079    -0.629955
H        1.839439    -3.294677     0.017988
H        0.601363    -1.111780     2.095718
H       -0.645379    -0.171751     2.941338
H        0.582904     0.655565     1.956234
H        5.403189    -0.325567     0.777922
H        4.545564     1.901887     0.093276
H        0.741223     0.216185    -0.902942
```

__Frequencies__ (Top 10 out of 120)

```
 1.     27.8221 cm-1 (Symmetry: A)
 2.     31.9058 cm-1 (Symmetry: A)
 3.     39.7660 cm-1 (Symmetry: A)
 4.     59.3789 cm-1 (Symmetry: A)
 5.     71.0199 cm-1 (Symmetry: A)
 6.     93.6238 cm-1 (Symmetry: A)
 7.    105.2528 cm-1 (Symmetry: A)
 8.    140.2641 cm-1 (Symmetry: A)
 9.    150.5079 cm-1 (Symmetry: A)
10.    184.3533 cm-1 (Symmetry: A)
```

```

**MCE-$a_0$**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.73666717 |
| Sum of electronic and zero-point Energies (Eh) | -1069.399809 |
| Sum of electronic and thermal Energies (Eh) | -1069.378484 |
| Sum of electronic and enthalpy Energies (Eh) | -1069.37754 |
| Sum of electronic and thermal Free Energies (Eh) | -1069.452254 |
| Number of Imaginary Frequencies | 0 |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -5.946764    -1.262551    -0.000325
C       -6.190592     0.106685    -0.000377
C       -5.144217     1.024622    -0.000239
C       -3.860436     0.512280    -0.000043
C       -3.598533    -0.848841    -0.000010
C       -4.642201    -1.752079    -0.000142
N       -2.623716     1.204278     0.000120
C       -1.591565     0.366929     0.000179
C       -2.103395    -1.071539     0.000213
C       -1.678901    -1.823769     1.273436
C       -1.678528    -1.823981    -1.272752
C       -0.269255     0.847151     0.000137
C        0.836054     0.040258     0.000093
C        2.199682     0.440369     0.000030
C       -2.507642     2.656586     0.000110
C        2.626401     1.841430     0.000042
C        4.058379     2.067788    -0.000060
C        4.958246     1.055477    -0.000132
C        4.506629    -0.288870    -0.000125
C        3.161006    -0.576132    -0.000042
O        1.825737     2.796462     0.000052
N        5.456772    -1.355300    -0.000207
O        6.653780    -1.075608    -0.000095
O        5.053531    -2.516775    -0.000012
H       -6.779279    -1.954654    -0.000432
H       -7.210431     0.470063    -0.000533
H       -5.347057     2.086511    -0.000302
H       -4.457586    -2.819589    -0.000102
H       -0.604867    -1.999587     1.301984
H       -2.181098    -2.791521     1.298142
H       -1.962470    -1.268196     2.168051
```
```

H -2.180740 -2.791726 -1.297452
H -1.961806 -1.268551 -2.167548
H -0.604488 -1.999836 -1.300934
H -0.107739 1.913471 0.000077
H 0.692796 -1.033045 0.000090
H -1.974955 2.987970 -0.890488
H -3.500175 3.093063 0.000673
H -1.974035 2.987882 0.890182
H 4.386360 3.099890 -0.000074
H 6.021302 1.252618 -0.000201
H 2.844292 -1.611119 -0.000041
```

__Frequencies__ (Top 10 out of 120)

```
 1.    13.1754 cm-1 (Symmetry: A)
 2.    22.5362 cm-1 (Symmetry: A)
 3.    45.0096 cm-1 (Symmetry: A)
 4.    46.5029 cm-1 (Symmetry: A)
 5.    64.5998 cm-1 (Symmetry: A)
 6.    81.4031 cm-1 (Symmetry: A)
 7.    96.6464 cm-1 (Symmetry: A)
 8.   109.9929 cm-1 (Symmetry: A)
 9.   137.0822 cm-1 (Symmetry: A)
10.   150.7862 cm-1 (Symmetry: A)
```

MCE-b_0
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.73517504
Sum of electronic and zero-point Energies (Eh)	-1069.398353
Sum of electronic and thermal Energies (Eh)	-1069.377057
Sum of electronic and enthalpy Energies (Eh)	-1069.376113
Sum of electronic and thermal Free Energies (Eh)	-1069.449944
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C 6.081304 0.196500 0.046953
C 5.961564 -1.188623 0.018936
C 4.712940 -1.803119 -0.012134
C 3.605939 -0.975310 -0.014289
C 3.705997 0.406855 0.016394
```
```

```
C        4.948324      1.007630      0.046357
N        2.232873     -1.323416     -0.044043
C        1.452577     -0.245995     -0.026008
C        2.320074      1.010780      0.012140
C        2.088953      1.815704      1.302979
C        2.122682      1.878257     -1.243413
C        0.052402     -0.351814     -0.032198
C       -0.794092      0.723197     -0.025081
C       -2.211243      0.711779     -0.018527
C        1.748292     -2.696785     -0.080648
C       -2.884801      2.014291     -0.026973
C       -4.334460      1.980236     -0.015928
C       -5.028106      0.817729      0.001902
C       -4.335719     -0.422486      0.010487
C       -2.961627     -0.465993      0.000310
O       -2.256227      3.088379     -0.043390
N       -5.078826     -1.643838      0.032545
O       -6.306354     -1.583651      0.042435
O       -4.472881     -2.713442      0.040739
H        7.064659      0.648704      0.070549
H        6.852012     -1.804448      0.021686
H        4.633781     -2.881142     -0.030947
H        5.047723      2.086125      0.069618
H        2.214729      1.184784      2.183922
H        1.093827      2.256405      1.332792
H        2.819309      2.623984      1.354536
H        1.135115      2.335836     -1.270626
H        2.256385      1.287851     -2.150812
H        2.865097      2.677212     -1.243366
H       -0.360108     -1.351195     -0.039375
H       -0.383217      1.723829     -0.025653
H        1.101888     -2.841094     -0.945122
H        1.199843     -2.926543      0.832641
H        2.594124     -3.370181     -0.163151
H       -4.849735      2.932614     -0.022360
H       -6.109223      0.813200      0.010303
H       -2.476846     -1.432443      0.010021
```

__Frequencies__ (Top 10 out of 120)

```
1.    18.8757 cm-1 (Symmetry: A)
2.    34.8338 cm-1 (Symmetry: A)
3.    42.7373 cm-1 (Symmetry: A)
4.    54.1121 cm-1 (Symmetry: A)
5.    71.6471 cm-1 (Symmetry: A)
6.    86.4490 cm-1 (Symmetry: A)
7.    93.4419 cm-1 (Symmetry: A)
8.   119.9013 cm-1 (Symmetry: A)
9.   121.9486 cm-1 (Symmetry: A)
```

10. 143.2805 cm-1 (Symmetry: A)
```

**MCE-$c_0$**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.73399849 |
| Sum of electronic and zero-point Energies (Eh) | -1069.396541 |
| Sum of electronic and thermal Energies (Eh) | -1069.375673 |
| Sum of electronic and enthalpy Energies (Eh) | -1069.374729 |
| Sum of electronic and thermal Free Energies (Eh) | -1069.447133 |
| Number of Imaginary Frequencies | 0 |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       6.128493    -0.563103     0.374109
C       5.681352    -1.839265     0.049443
C       4.336483    -2.084844    -0.214747
C       3.478418    -1.004923    -0.139967
C       3.902901     0.272478     0.190163
C       5.238612     0.507020     0.447672
N       2.074205    -0.976012    -0.366535
C       1.581465     0.235189    -0.149605
C       2.712125     1.196123     0.190715
C       2.478775     1.835759     1.567152
C       2.835691     2.274250    -0.899564
C       0.242902     0.674143    -0.212411
C      -0.873015    -0.107980    -0.104080
C      -2.231704     0.320802    -0.104947
C       1.354873    -2.143197    -0.853719
C      -2.634524     1.715703    -0.289701
C      -4.059797     1.974360    -0.249919
C      -4.976076     0.993718    -0.062899
C      -4.547718    -0.346423     0.106830
C      -3.206910    -0.661507     0.085921
O      -1.818492     2.641169    -0.471019
N      -5.512975    -1.379175     0.302801
O      -6.704726    -1.075838     0.317069
O      -5.129261    -2.538429     0.451096
H       7.179692    -0.400328     0.575756
H       6.386620    -2.659326     0.003073
H       3.994499    -3.081638    -0.456989
H       5.592905     1.498059     0.703970
H       2.376259     1.075508     2.342664
H       1.577767     2.449936     1.558655
```
```

```
H        3.327137      2.473540      1.818698
H        2.976240      1.826176     -1.884056
H        3.698508      2.904661     -0.681358
H        1.948282      2.907324     -0.924259
H        0.097781      1.742983     -0.261987
H       -0.751174     -1.172635      0.052418
H        0.945662     -2.723175     -0.026280
H        2.045131     -2.763884     -1.418550
H        0.553872     -1.821177     -1.514684
H       -4.370105      3.003612     -0.381086
H       -6.034214      1.214536     -0.040202
H       -2.907729     -1.692894      0.220518
```

__Frequencies__ (Top 10 out of 120)

```
 1.     20.8483 cm-1 (Symmetry: A)
 2.     32.8935 cm-1 (Symmetry: A)
 3.     42.2406 cm-1 (Symmetry: A)
 4.     59.6128 cm-1 (Symmetry: A)
 5.     83.1470 cm-1 (Symmetry: A)
 6.     97.4296 cm-1 (Symmetry: A)
 7.    109.8800 cm-1 (Symmetry: A)
 8.    130.0148 cm-1 (Symmetry: A)
 9.    154.1232 cm-1 (Symmetry: A)
10.    160.3054 cm-1 (Symmetry: A)
```

MCE-d_0
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.73263546
Sum of electronic and zero-point Energies (Eh)	-1069.395432
Sum of electronic and thermal Energies (Eh)	-1069.374422
Sum of electronic and enthalpy Energies (Eh)	-1069.373478
Sum of electronic and thermal Free Energies (Eh)	-1069.446661
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C        6.081675     -0.559876      0.163301
C        5.979380      0.808876     -0.059621
C        4.739088      1.422704     -0.213239
C        3.624710      0.609633     -0.135787
```

```
C         3.706278     -0.754568      0.094766
C         4.940050     -1.355236      0.243289
N         2.254915      0.971357     -0.264521
C         1.465308     -0.080286     -0.083989
C         2.312972     -1.327097      0.135442
C         2.086343     -2.337570     -1.001413
C         1.996357     -1.958560      1.499575
C         0.059932     -0.143727     -0.084230
C        -0.816835      0.899376      0.033958
C        -2.235212      0.831978      0.067642
C         1.847604      2.322599     -0.615566
C        -2.952788      2.096981      0.248921
C        -4.399344      2.008468      0.279700
C        -5.052954      0.829972      0.145657
C        -4.318858     -0.372208     -0.031892
C        -2.943432     -0.362332     -0.068986
O        -2.361656      3.186526      0.368195
N        -5.017901     -1.610334     -0.174668
O        -6.246631     -1.598818     -0.138909
O        -4.374981     -2.647128     -0.328319
H         7.058777     -1.011364      0.279781
H         6.876537      1.412489     -0.112736
H         4.669877      2.489195     -0.376922
H         5.025094     -2.420586      0.420409
H         2.765404     -3.180806     -0.869590
H         2.281394     -1.887095     -1.975380
H         1.065242     -2.720126     -0.989121
H         2.660013     -2.807704      1.666818
H         2.142305     -1.241828      2.308694
H         0.967205     -2.317638      1.532524
H        -0.329941     -1.152881     -0.115167
H        -0.446389      1.907624      0.156579
H         2.678539      2.819694     -1.107018
H         1.009694      2.279665     -1.308103
H         1.566930      2.888216      0.273346
H        -4.946315      2.933227      0.414936
H        -6.132902      0.784792      0.170532
H        -2.426046     -1.301440     -0.208154
```

__Frequencies__ (Top 10 out of 120)

```
1.    15.6085 cm-1 (Symmetry: A)
2.    29.9872 cm-1 (Symmetry: A)
3.    42.1366 cm-1 (Symmetry: A)
4.    55.1428 cm-1 (Symmetry: A)
5.    77.1501 cm-1 (Symmetry: A)
6.    90.4973 cm-1 (Symmetry: A)
7.   110.6823 cm-1 (Symmetry: A)
8.   132.0327 cm-1 (Symmetry: A)
```

9. 141.1834 cm-1 (Symmetry: A)
10. 155.3242 cm-1 (Symmetry: A)

```

**MCE-$a_1$**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.73291353 |
| Sum of electronic and zero-point Energies (Eh) | -1069.310421 |
| Sum of electronic and thermal Energies (Eh) | -1069.288724 |
| Sum of electronic and enthalpy Energies (Eh) | -1069.28778 |
| Sum of electronic and thermal Free Energies (Eh) | -1069.363542 |
| Number of Imaginary Frequencies | 0 |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C 5.991425 -1.208044 0.008142
C 6.212272 0.169045 -0.022263
C 5.157478 1.069112 -0.037953
C 3.866652 0.543589 -0.021974
C 3.633236 -0.836155 0.009145
C 4.693068 -1.716864 0.023951
N 2.651840 1.205776 -0.031937
C 1.600402 0.326856 -0.006360
C 2.144418 -1.094012 0.020348
C 1.733317 -1.893590 -1.231145
C 1.741675 -1.841604 1.305901
C 0.285491 0.775700 -0.004987
C -0.850434 -0.035196 0.016016
C -2.203702 0.380694 0.018577
C 2.504202 2.647700 -0.067716
C -2.632227 1.806331 0.042426
C -4.057987 2.074799 0.022366
C -4.984248 1.084780 -0.000092
C -4.548794 -0.261530 -0.009237
C -3.206142 -0.601842 -0.000993
O -1.818293 2.737219 0.080398
N -5.534651 -1.302435 -0.029287
O -6.727166 -0.992844 -0.042379
O -5.152299 -2.472754 -0.032705
H 6.835559 -1.885876 0.019821
H 7.227226 0.546470 -0.033824
H 5.345987 2.133436 -0.061213
H 4.526568 -2.787343 0.047735
H 0.659946 -2.077032 -1.255328
```
```

```
H        2.241981     -2.859028     -1.227359
H        2.013174     -1.361135     -2.140949
H        2.244963     -2.809371      1.334997
H        2.033372     -1.275497      2.191367
H        0.667479     -2.016893      1.347378
H        0.117940      1.842202     -0.021908
H       -0.718126     -1.108871      0.020593
H        1.968736      2.995444      0.817158
H        3.484842      3.110969     -0.088048
H        1.954119      2.948614     -0.960806
H       -4.349843      3.117200      0.033964
H       -6.043167      1.298301     -0.009624
H       -2.929626     -1.646545     -0.012804
```

__Frequencies__ (Top 10 out of 120)

```
 1.      9.8530 cm-1 (Symmetry: A)
 2.     21.8081 cm-1 (Symmetry: A)
 3.     40.3088 cm-1 (Symmetry: A)
 4.     46.4103 cm-1 (Symmetry: A)
 5.     71.4801 cm-1 (Symmetry: A)
 6.     76.8825 cm-1 (Symmetry: A)
 7.     92.5265 cm-1 (Symmetry: A)
 8.    114.2938 cm-1 (Symmetry: A)
 9.    128.9918 cm-1 (Symmetry: A)
10.    150.5827 cm-1 (Symmetry: A)
```

MCE-b_1
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.73075115
Sum of electronic and zero-point Energies (Eh)	-1069.315096
Sum of electronic and thermal Energies (Eh)	-1069.294061
Sum of electronic and enthalpy Energies (Eh)	-1069.293117
Sum of electronic and thermal Free Energies (Eh)	-1069.364736
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -6.103763      0.112435      0.015368
C       -5.940233     -1.275383      0.006827
C       -4.675389     -1.854857     -0.003086
```

```
C       -3.578493    -0.994064    -0.004428
C       -3.728233     0.397911     0.005180
C       -4.991104     0.958441     0.014900
N       -2.221605    -1.301059    -0.013958
C       -1.454430    -0.171436    -0.007698
C       -2.364299     1.050282     0.003474
C       -2.182230     1.913011    -1.261967
C       -2.171108     1.896446     1.278331
C       -0.063323    -0.230425    -0.008786
C        0.808988     0.863963    -0.007425
C        2.218585     0.751104    -0.004795
C       -1.686824    -2.649208    -0.027266
C        2.988993     2.023865    -0.008405
C        4.434568     1.942948    -0.005129
C        5.080042     0.744221     0.001382
C        4.320682    -0.453548     0.004561
C        2.929830    -0.460319     0.001344
O        2.396081     3.117893    -0.014443
N        5.019020    -1.701415     0.010110
O        6.258631    -1.698806     0.018176
O        4.357316    -2.748846     0.006896
H       -7.102278     0.535527     0.022983
H       -6.814474    -1.917432     0.008348
H       -4.565847    -2.932283    -0.007942
H       -5.122773     2.035710     0.022278
H       -2.318548     1.313339    -2.164874
H       -1.192486     2.370036    -1.296460
H       -2.926452     2.713210    -1.264425
H       -1.181757     2.354553     1.308624
H       -2.297185     1.284706     2.174682
H       -2.916524     2.695195     1.298815
H        0.373516    -1.222202    -0.010512
H        0.429804     1.875166    -0.008995
H       -1.093274    -2.831053     0.872643
H       -1.059581    -2.797518    -0.909886
H       -2.505101    -3.362756    -0.057355
H        4.981654     2.878775    -0.008124
H        6.160308     0.682815     0.003659
H        2.419317    -1.412706     0.004153
```

__Frequencies__ (Top 10 out of 120)

```
 1.     30.7604 cm-1 (Symmetry: A)
 2.     48.8058 cm-1 (Symmetry: A)
 3.     52.4879 cm-1 (Symmetry: A)
 4.     78.0951 cm-1 (Symmetry: A)
 5.     93.5588 cm-1 (Symmetry: A)
 6.    106.6723 cm-1 (Symmetry: A)
 7.    119.6570 cm-1 (Symmetry: A)
```

8. 123.5237 cm-1 (Symmetry: A)
9. 137.5522 cm-1 (Symmetry: A)
10. 154.3294 cm-1 (Symmetry: A)

```

**MCE-$c_1$**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.72890487 |
| Sum of electronic and zero-point Energies (Eh) | -1069.30694 |
| Sum of electronic and thermal Energies (Eh) | -1069.285562 |
| Sum of electronic and enthalpy Energies (Eh) | -1069.284618 |
| Sum of electronic and thermal Free Energies (Eh) | -1069.358619 |
| Number of Imaginary Frequencies | 0 |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C 6.168532 -0.488948 0.328032
C 5.745670 -1.779433 0.012019
C 4.407384 -2.063168 -0.220923
C 3.504718 -1.007216 -0.126177
C 3.915727 0.289972 0.195328
C 5.249205 0.555855 0.421122
N 2.128583 -1.021499 -0.317231
C 1.588838 0.213881 -0.082623
C 2.712285 1.197328 0.214162
C 2.531126 1.869820 1.584155
C 2.805703 2.264244 -0.893565
C 0.250506 0.584851 -0.070487
C -0.893214 -0.217576 -0.102502
C -2.236389 0.229973 -0.128133
C 1.424258 -2.191946 -0.808987
C -2.621493 1.648633 -0.356181
C -4.029319 1.981450 -0.258412
C -4.983707 1.040075 -0.050932
C -4.593672 -0.311262 0.100301
C -3.265712 -0.704204 0.063780
O -1.786241 2.516927 -0.639295
N -5.610975 -1.300143 0.309886
O -6.789126 -0.942345 0.351205
O -5.268868 -2.475425 0.441516
H 7.219563 -0.298038 0.504474
H 6.473043 -2.579275 -0.050471
H 4.091526 -3.070725 -0.453971
H 5.582964 1.557076 0.666482
```
```

```
H        2.454222      1.126211      2.378441
H        1.630101      2.484830      1.595362
H        3.385636      2.515252      1.795503
H        2.933581      1.801001     -1.872789
H        3.659959      2.916946     -0.704068
H        1.903526      2.877627     -0.912883
H        0.085623      1.649085      0.020038
H       -0.785173     -1.290708     -0.029998
H        0.966162     -2.752283      0.008984
H        2.130979     -2.837552     -1.323564
H        0.659498     -1.886857     -1.518946
H       -4.288472      3.023110     -0.398453
H       -6.032061      1.296453     -0.003839
H       -3.022738     -1.747882      0.203843
```

__Frequencies__ (Top 10 out of 120)

```
 1.    21.2691 cm-1 (Symmetry: A)
 2.    27.8696 cm-1 (Symmetry: A)
 3.    33.6638 cm-1 (Symmetry: A)
 4.    51.6944 cm-1 (Symmetry: A)
 5.    73.4394 cm-1 (Symmetry: A)
 6.    80.3798 cm-1 (Symmetry: A)
 7.   109.9831 cm-1 (Symmetry: A)
 8.   127.3913 cm-1 (Symmetry: A)
 9.   148.0966 cm-1 (Symmetry: A)
10.   156.9242 cm-1 (Symmetry: A)
```

MCE-d_1
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.72873385
Sum of electronic and zero-point Energies (Eh)	-1069.311851
Sum of electronic and thermal Energies (Eh)	-1069.290519
Sum of electronic and enthalpy Energies (Eh)	-1069.289574
Sum of electronic and thermal Free Energies (Eh)	-1069.363493
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C        6.069297     -0.609664      0.135161
C        5.993191      0.763238     -0.091236
```

```
C        4.769405      1.404608     -0.229600
C        3.625120      0.620497     -0.133188
C        3.687242     -0.754794      0.098442
C        4.909550     -1.378251      0.231726
N        2.290681      1.010769     -0.238777
C        1.456231     -0.046315     -0.040428
C        2.286543     -1.309721      0.145771
C        2.042419     -2.295800     -1.012075
C        1.990443     -1.986660      1.493299
C        0.068420     -0.047945      0.013554
C       -0.827429      1.022179      0.080350
C       -2.231638      0.866287      0.078534
C        1.902902      2.361055     -0.608498
C       -3.038482      2.103849      0.246661
C       -4.478363      1.973391      0.263134
C       -5.084351      0.765950      0.124264
C       -4.290867     -0.393119     -0.043388
C       -2.904425     -0.353348     -0.073716
O       -2.481551      3.202353      0.369106
N       -4.952459     -1.657453     -0.193414
O       -6.183804     -1.691562     -0.184562
O       -4.261302     -2.667548     -0.326822
H        7.037805     -1.082332      0.239114
H        6.903980      1.345147     -0.157972
H        4.723881      2.472305     -0.394224
H        4.973866     -2.445318      0.408388
H        2.702138     -3.158451     -0.902559
H        2.243177     -1.826371     -1.975868
H        1.011174     -2.652107     -1.005106
H        2.649997     -2.845998      1.625954
H        2.149914     -1.296453      2.322616
H        0.959383     -2.341452      1.529337
H       -0.351272     -1.046171      0.058790
H       -0.483105      2.038861      0.175100
H        2.734000      2.836908     -1.121706
H        1.055527      2.324511     -1.288129
H        1.644944      2.952360      0.272249
H       -5.053792      2.881377      0.389383
H       -6.160181      0.668612      0.136845
H       -2.366976     -1.277199     -0.221245
```

__Frequencies__ (Top 10 out of 120)

```
1.  17.9158 cm-1 (Symmetry: A)
2.  29.2594 cm-1 (Symmetry: A)
3.  38.7421 cm-1 (Symmetry: A)
4.  50.6717 cm-1 (Symmetry: A)
5.  69.9383 cm-1 (Symmetry: A)
6.  90.9733 cm-1 (Symmetry: A)
```

7. 109.7162 cm-1 (Symmetry: A)
8. 123.3627 cm-1 (Symmetry: A)
9. 138.5261 cm-1 (Symmetry: A)
10. 152.0655 cm-1 (Symmetry: A)

```

**TS($MCZ_0 \rightarrow MCE_0$)**
Run with Gaussian 16revision A.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.69279642 |
| Sum of electronic and zero-point Energies (Eh) | -1069.358298 |
| Sum of electronic and thermal Energies (Eh) | -1069.33723 |
| Sum of electronic and enthalpy Energies (Eh) | -1069.336286 |
| Sum of electronic and thermal Free Energies (Eh) | -1069.410158 |
| Number of Imaginary Frequencies | 1 |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -3.487043     2.313168    -0.285248
C       -2.939265     1.082305     0.043768
C       -3.709205    -0.081091     0.023485
C       -5.043797    -0.027740    -0.312550
C       -5.616719     1.204787    -0.639611
C       -4.839743     2.354616    -0.625154
C       -2.843926    -1.260810     0.412682
C       -1.474859    -0.590357     0.598924
N       -1.634168     0.779862     0.429081
O        0.944329    -1.438590    -1.720688
C        1.925125    -0.914294    -1.214025
C        2.024163    -0.616880     0.247010
C        1.000019    -0.769541     1.121270
C       -0.355261    -1.267662     0.870529
C        3.091223    -0.553857    -2.024448
C        4.210805    -0.049442    -1.484345
C        4.292503     0.169081    -0.062098
C        3.267956    -0.098968     0.764684
C       -3.322765    -1.882863     1.731334
C       -2.810163    -2.317918    -0.695478
C       -0.574650     1.758618     0.504125
N        5.529186     0.705222     0.490307
O        6.440891     0.940698    -0.285850
O        5.599683     0.893942     1.693065
H       -2.896763     3.219752    -0.288674
H       -5.646026    -0.929392    -0.327029
H       -6.664106     1.261092    -0.908351
```
```

```
H       -5.286091     3.307005    -0.885767
H        1.241379    -0.535256     2.158483
H       -0.445289    -2.346673     0.963641
H        3.012313    -0.733129    -3.088809
H        5.067513     0.198717    -2.094913
H        3.360130     0.087140     1.826352
H       -2.660460    -2.696662     2.033618
H       -3.341251    -1.139064     2.529802
H       -4.330669    -2.286491     1.613359
H       -2.139034    -3.137044    -0.430497
H       -3.808708    -2.733230    -0.847043
H       -2.470241    -1.886284    -1.637809
H       -1.007586     2.748170     0.633800
H        0.058129     1.567504     1.369507
H        0.046024     1.762953    -0.396727
```

__Frequencies__ (Top 10 out of 120)

```
 1.   -278.7828 cm-1 (Symmetry: A)  *
 2.     16.2316 cm-1 (Symmetry: A)
 3.     27.2383 cm-1 (Symmetry: A)
 4.     38.6509 cm-1 (Symmetry: A)
 5.     47.6830 cm-1 (Symmetry: A)
 6.     56.8206 cm-1 (Symmetry: A)
 7.     82.3079 cm-1 (Symmetry: A)
 8.    105.6593 cm-1 (Symmetry: A)
 9.    125.9377 cm-1 (Symmetry: A)
10.    135.5584 cm-1 (Symmetry: A)
```

Scans:

MCZ 30.0°
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.72782629
Sum of electronic and zero-point Energies (Eh)	N/A
Sum of electronic and thermal Energies (Eh)	N/A
Sum of electronic and enthalpy Energies (Eh)	N/A
Sum of electronic and thermal Free Energies (Eh)	N/A
Number of Imaginary Frequencies	N/A
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -5.136607     -1.633338      0.257180
C       -4.322514     -2.506184     -0.464261
C       -3.055697     -2.115257     -0.900664
C       -2.656028     -0.829550     -0.580853
C       -3.447648      0.053505      0.142528
C       -4.704397     -0.341025      0.566178
N       -1.431872     -0.181912     -0.904701
C       -1.380378      1.023991     -0.374383
C       -2.699928      1.353711      0.306173
C       -3.413714      2.504231     -0.430442
C       -2.465276      1.718288      1.780348
C       -0.311538      1.957951     -0.493155
C        1.031845      1.735021     -0.573578
C        1.847610      0.684612     -0.025667
C       -0.427442     -0.814501     -1.739797
C        1.353945     -0.275157      0.959967
C        2.330243     -1.200914      1.497165
C        3.631934     -1.206435      1.101784
C        4.076525     -0.255421      0.149672
C        3.198097      0.674261     -0.380962
O        0.158511     -0.302790      1.342408
N        5.440264     -0.243484     -0.253589
O        5.819093      0.592152     -1.084568
O        6.214388     -1.073770      0.239474
H       -6.116186     -1.963523      0.585362
H       -4.674293     -3.507012     -0.689356
H       -2.422298     -2.798615     -1.453136
H       -5.342322      0.332365      1.129316
H       -4.397954      2.656897      0.017827
H       -3.549184      2.276682     -1.490412
H       -2.851712      3.436136     -0.336724
H       -3.427938      1.877912      2.271725
H       -1.923910      0.922724      2.293548
H       -1.881749      2.639215      1.854119
H       -0.645953      2.975992     -0.674130
H        1.605991      2.579432     -0.950909
H        0.217859     -1.455932     -1.137076
H       -0.932255     -1.408183     -2.500497
H        0.173128     -0.045114     -2.219582
H        1.970661     -1.915043      2.230170
H        4.337762     -1.920552      1.507150
H        3.571467      1.402933     -1.091280
```

MCZ 50.0°
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0

Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.72154366
Sum of electronic and zero-point Energies (Eh)	N/A
Sum of electronic and thermal Energies (Eh)	N/A
Sum of electronic and enthalpy Energies (Eh)	N/A
Sum of electronic and thermal Free Energies (Eh)	N/A
Number of Imaginary Frequencies	N/A
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -5.320059    -1.487346     0.200745
C       -4.517144    -2.425783    -0.446431
C       -3.210755    -2.116155    -0.828606
C       -2.757804    -0.841370    -0.534132
C       -3.538530     0.104765     0.119128
C       -4.834273    -0.209100     0.488712
N       -1.488030    -0.270527    -0.817098
C       -1.402685     0.960968    -0.333102
C       -2.732133     1.368802     0.288098
C       -3.364966     2.545461    -0.476585
C       -2.526611     1.731886     1.767890
C       -0.295716     1.832153    -0.416545
C        1.027954     1.554976    -0.677657
C        1.899872     0.591518    -0.084257
C       -0.490118    -0.966488    -1.606446
C        1.467753    -0.302265     0.991119
C        2.503336    -1.107853     1.609622
C        3.794321    -1.089240     1.185670
C        4.171088    -0.226411     0.122338
C        3.243540     0.597812    -0.482094
O        0.277636    -0.367545     1.376491
N        5.528094    -0.196460    -0.314418
O        5.848516     0.557923    -1.240235
O        6.348070    -0.930893     0.248311
H       -6.331307    -1.754319     0.487789
H       -4.908816    -3.415265    -0.655533
H       -2.588166    -2.852744    -1.321688
H       -5.462772     0.516370     0.995154
H       -4.354696     2.751248    -0.062517
H       -3.476465     2.315707    -1.538812
H       -2.761091     3.449733    -0.371895
H       -3.494157     1.943574     2.229136
H       -2.045945     0.913235     2.306174
H       -1.897907     2.621176     1.856376
H       -0.593788     2.864980    -0.584342
H        1.561601     2.362433    -1.177867
H        0.176848    -1.545314    -0.966039
H       -0.998590    -1.627634    -2.306085
```

H 0.093286 -0.235415 -2.164100
H 2.194495 -1.758114 2.420957
H 4.545441 -1.717529 1.647651
H 3.565386 1.262931 -1.275070
```

**MCZ 70.0°**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.71152376 |
| Sum of electronic and zero-point Energies (Eh) | N/A |
| Sum of electronic and thermal Energies (Eh) | N/A |
| Sum of electronic and enthalpy Energies (Eh) | N/A |
| Sum of electronic and thermal Free Energies (Eh) | N/A |
| Number of Imaginary Frequencies | N/A |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C -5.543255 -1.291335 0.104761
C -4.764612 -2.311792 -0.438365
C -3.415205 -2.110488 -0.735683
C -2.891251 -0.856357 -0.468033
C -3.650448 0.171083 0.082318
C -4.987545 -0.036129 0.369006
N -1.568914 -0.391577 -0.677822
C -1.432139 0.868233 -0.251054
C -2.775533 1.389814 0.251979
C -3.276987 2.559034 -0.614095
C -2.658885 1.817037 1.723468
C -0.276692 1.649215 -0.271808
C 1.018060 1.334926 -0.691251
C 1.970963 0.477051 -0.095035
C -0.574375 -1.171394 -1.387967
C 1.633670 -0.364046 1.057781
C 2.745258 -1.035546 1.708489
C 4.012477 -0.970035 1.227276
C 4.290655 -0.185527 0.071317
C 3.297483 0.520777 -0.564045
O 0.461561 -0.487720 1.470466
N 5.630792 -0.115180 -0.424650
O 5.867584 0.570246 -1.423880
O 6.511325 -0.747355 0.166187
H -6.588529 -1.474370 0.328770
H -5.208897 -3.282278 -0.631271
H -2.814501 -2.912901 -1.146299
```
```

H -5.596792 0.754960 0.794543
H -4.279497 2.847045 -0.289116
H -3.323910 2.278817 -1.669088
H -2.625398 3.429904 -0.510517
H -3.639122 2.124914 2.095583
H -2.292763 0.995302 2.342396
H -1.970788 2.659988 1.823122
H -0.522563 2.702025 -0.410433
H 1.474357 2.103693 -1.315861
H 0.082798 -1.698917 -0.696432
H -1.083284 -1.884270 -2.034327
H 0.023080 -0.499820 -2.005782
H 2.512651 -1.630864 2.584635
H 4.823291 -1.502492 1.708228
H 3.543126 1.128065 -1.427395
```

**MCZ 90.0°**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.69913102 |
| Sum of electronic and zero-point Energies (Eh) | N/A |
| Sum of electronic and thermal Energies (Eh) | N/A |
| Sum of electronic and enthalpy Energies (Eh) | N/A |
| Sum of electronic and thermal Free Energies (Eh) | N/A |
| Number of Imaginary Frequencies | N/A |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C -5.773380 -1.038596 0.002469
C -5.055823 -2.147485 -0.440088
C -3.676605 -2.079919 -0.652899
C -3.054114 -0.865301 -0.409135
C -3.756126 0.250730 0.041485
C -5.121000 0.174538 0.246592
N -1.690588 -0.531720 -0.546691
C -1.467135 0.751503 -0.178631
C -2.793719 1.403667 0.214714
C -3.145690 2.563870 -0.731196
C -2.739184 1.893021 1.669672
C -0.262019 1.412433 -0.141598
C 1.007288 1.054869 -0.678476
C 2.042674 0.335667 -0.084035
C -0.708581 -1.419654 -1.133837
C 1.829491 -0.418913 1.162022
```
```

```
C       3.027250    -0.911897     1.826968
C       4.254480    -0.801051     1.265530
C       4.408143    -0.138876     0.006583
C       3.342001     0.411134    -0.646683
O       0.693066    -0.616343     1.625154
N       5.719792    -0.030858    -0.571970
O       5.850864     0.544445    -1.653527
O       6.669600    -0.522750     0.039535
H      -6.843126    -1.117320     0.163008
H      -5.571632    -3.084813    -0.619930
H      -3.127993    -2.953172    -0.984778
H      -5.680856     1.037444     0.593838
H      -4.139185     2.947742    -0.486493
H      -3.150035     2.236337    -1.773685
H      -2.430497     3.383597    -0.625468
H      -3.711534     2.298801     1.960584
H      -2.486524     1.075911     2.349282
H      -1.989920     2.680795     1.781262
H      -0.422653     2.488173    -0.242010
H       1.354721     1.736908    -1.457008
H      -0.080793    -1.881270    -0.371278
H      -1.220837    -2.189195    -1.708756
H      -0.075228    -0.845724    -1.814616
H       2.890487    -1.419917     2.775112
H       5.132567    -1.206101     1.752386
H       3.492666     0.928604    -1.586868
```

MCZ 110.0°
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.70748315
Sum of electronic and zero-point Energies (Eh)	N/A
Sum of electronic and thermal Energies (Eh)	N/A
Sum of electronic and enthalpy Energies (Eh)	N/A
Sum of electronic and thermal Free Energies (Eh)	N/A
Number of Imaginary Frequencies	N/A
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       5.516807    -0.701217    -1.348719
C       5.070299    -1.990423    -1.064787
C       3.866933    -2.206755    -0.389991
C       3.143368    -1.086514    -0.015456
C       3.569725     0.207789    -0.296629
```

```
C        4.762648      0.411826     -0.966059
N        1.912151     -1.020409      0.682032
C        1.501646      0.248535      0.821441
C        2.542528      1.189268      0.216274
C        3.114987      2.118432      1.298747
C        1.936736      2.007146     -0.937633
C        0.317548      0.729617      1.381251
C       -0.923741      0.080073      1.361933
C       -2.080365      0.449100      0.644842
C        1.243072     -2.179236      1.241485
C       -2.236744      1.747354     -0.026665
C       -3.405511      1.889789     -0.879546
C       -4.350553      0.922953     -0.983219
C       -4.200675     -0.295158     -0.257620
C       -3.103527     -0.515974      0.536940
O       -1.422817      2.682651      0.112946
N       -5.204223     -1.308684     -0.367834
O       -5.063469     -2.364759      0.255745
O       -6.184046     -1.090483     -1.086084
H        6.455375     -0.560528     -1.873603
H        5.663175     -2.844867     -1.372890
H        3.526391     -3.213765     -0.181627
H        5.110458      1.414735     -1.192423
H        3.900678      2.741049      0.863938
H        3.544307      1.546671      2.124787
H        2.337812      2.776709      1.694080
H        2.716715      2.621176     -1.394373
H        1.521600      1.350286     -1.706171
H        1.139233      2.659221     -0.576010
H        0.234770      1.800836      1.240795
H       -0.955021     -0.958732      1.684038
H        0.376640     -2.458231      0.635441
H        1.937662     -3.015473      1.270172
H        0.927722     -1.961301      2.262805
H       -3.506737      2.827566     -1.414662
H       -5.223828      1.057207     -1.609050
H       -3.010879     -1.457803      1.064988
```

MCZ 130.0°
Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.72027101
Sum of electronic and zero-point Energies (Eh)	N/A
Sum of electronic and thermal Energies (Eh)	N/A
Sum of electronic and enthalpy Energies (Eh)	N/A
Sum of electronic and thermal Free Energies (Eh)	N/A

| Number of Imaginary Frequencies | N/A |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       5.683183    -0.596738    -1.253937
C       5.351153    -1.869347    -0.791724
C       4.155919    -2.099903    -0.107859
C       3.326776    -1.008858     0.087607
C       3.635993     0.266483    -0.370904
C       4.822882     0.485065    -1.046993
N       2.072097    -0.961974     0.752062
C       1.542900     0.257086     0.692523
C       2.511723     1.205691    -0.005634
C       2.971243     2.302357     0.971479
C       1.862419     1.826281    -1.254209
C       0.283718     0.698461     1.144976
C      -0.875926    -0.049484     1.082868
C      -2.140914     0.356457     0.571937
C       1.515388    -2.103476     1.458093
C      -2.463475     1.746802     0.236882
C      -3.742836     1.966822    -0.411279
C      -4.627806     0.961534    -0.638406
C      -4.301283    -0.366756    -0.251637
C      -3.088837    -0.650761     0.342351
O      -1.692501     2.701281     0.486018
N      -5.231059    -1.419738    -0.489259
O      -4.936455    -2.573267    -0.154484
O      -6.311438    -1.146790    -1.024996
H       6.617754    -0.445429    -1.782937
H       6.028170    -2.698337    -0.966651
H       3.899500    -3.093094     0.240568
H       5.084491     1.472869    -1.412293
H       3.711358     2.936346     0.477826
H       3.427221     1.870801     1.865386
H       2.130582     2.931331     1.272754
H       2.600644     2.436335    -1.779889
H       1.504946     1.052677    -1.937967
H       1.019772     2.462531    -0.975761
H       0.141787     1.767007     1.045514
H      -0.793129    -1.129050     1.179864
H       0.865955    -2.688173     0.802003
H       2.331914    -2.733362     1.806912
H       0.954636    -1.752167     2.323494
H      -3.977411     2.987729    -0.692453
H      -5.583249     1.152801    -1.110655
H      -2.862388    -1.674925     0.615559
```

MCZ 150.0°

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C19H18N2O3
Number of Basis Functions	654
Electronic Energy (Eh)	-1069.72927072
Sum of electronic and zero-point Energies (Eh)	N/A
Sum of electronic and thermal Energies (Eh)	N/A
Sum of electronic and enthalpy Energies (Eh)	N/A
Sum of electronic and thermal Free Energies (Eh)	N/A
Number of Imaginary Frequencies	N/A
Mean of alpha and beta Electrons	85

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -5.931552     -0.561296      0.925404
C       -5.570151     -1.827787      0.467789
C       -4.305341     -2.065802     -0.072764
C       -3.438657     -0.988080     -0.130942
C       -3.776215      0.280127      0.325807
C       -5.033030      0.506719      0.858051
N       -2.109898     -0.951358     -0.637282
C       -1.571013      0.251141     -0.477660
C       -2.599041      1.202308      0.122398
C       -2.921584      2.328081     -0.877770
C       -2.088487      1.784818      1.450896
C       -0.256976      0.678231     -0.776380
C        0.864715     -0.107716     -0.684703
C        2.196731      0.316618     -0.394301
C       -1.507014     -2.092117     -1.309093
C        2.592766      1.724687     -0.314818
C        3.964428      1.980323      0.080787
C        4.853738      0.981698      0.324277
C        4.442246     -0.372125      0.204849
C        3.143195     -0.684452     -0.148822
O        1.807840      2.668127     -0.570198
N        5.372828     -1.418145      0.457366
O        5.003450     -2.594863      0.355107
O        6.531274     -1.119766      0.772982
H       -6.920750     -0.404224      1.341281
H       -6.279316     -2.645606      0.533446
H       -4.027243     -3.053962     -0.418716
H       -5.319894      1.489460      1.217807
H       -3.714623      2.955973     -0.465275
H       -3.263015      1.924164     -1.833622
H       -2.045295      2.955944     -1.052781
H       -2.867645      2.407249      1.896494
H       -1.833486      0.991712      2.157662
H       -1.204393      2.404279      1.286364
```

H -0.099467 1.748232 -0.743481
H 0.741421 -1.185905 -0.647521
H -0.984499 -2.732522 -0.594966
H -2.294205 -2.665539 -1.795611
H -0.813358 -1.735802 -2.069159
H 4.261651 3.020218 0.162556
H 5.875630 1.199223 0.608858
H 2.854913 -1.726617 -0.225101
```

**MCZ 170.0°**
Run with Gaussian 16revisionA.03.

| Datum | Value |
|---|---|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C19H18N2O3 |
| Number of Basis Functions | 654 |
| Electronic Energy (Eh) | -1069.73337853 |
| Sum of electronic and zero-point Energies (Eh) | N/A |
| Sum of electronic and thermal Energies (Eh) | N/A |
| Sum of electronic and enthalpy Energies (Eh) | N/A |
| Sum of electronic and thermal Free Energies (Eh) | N/A |
| Number of Imaginary Frequencies | N/A |
| Mean of alpha and beta Electrons | 85 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C -6.104801 -0.563882 0.518058
C -5.677219 -1.836407 0.141114
C -4.345832 -2.078261 -0.200911
C -3.481580 -0.997971 -0.148338
C -3.885450 0.275719 0.232207
C -5.207940 0.506200 0.567226
N -2.090914 -0.965009 -0.450071
C -1.584634 0.242879 -0.232900
C -2.692877 1.198213 0.190844
C -2.868309 2.307591 -0.863406
C -2.384604 1.805535 1.569639
C -0.244269 0.675978 -0.358191
C 0.869136 -0.114244 -0.246671
C 2.230029 0.314650 -0.178682
C -1.400174 -2.118561 -1.007501
C 2.641025 1.713942 -0.315652
C 4.062158 1.976432 -0.193208
C 4.973488 0.990666 0.019993
C 4.539006 -0.355912 0.136200
C 3.196926 -0.672895 0.037847
O 1.829075 2.645700 -0.527431
N 5.490924 -1.389015 0.358122
O 5.101841 -2.559814 0.457225
```
```

```
O       6.687550    -1.086491    0.445998
H      -7.145052    -0.404127    0.779753
H      -6.386772    -2.656072    0.114899
H      -4.018610    -3.071633   -0.482611
H      -5.546097     1.493474    0.864280
H      -3.716717     2.935636   -0.582562
H      -3.062044     1.888078   -1.853215
H      -1.979070     2.939377   -0.915674
H      -3.220476     2.435423    1.882666
H      -2.238750     1.026289    2.321219
H      -1.485012     2.423174    1.526287
H      -0.091210     1.746215   -0.392458
H       0.741005    -1.182842   -0.109725
H      -0.966492    -2.733929   -0.216533
H      -2.116650    -2.712605   -1.571672
H      -0.619324    -1.776369   -1.684912
H       4.375703     3.010641   -0.285938
H       6.029923     1.213342    0.103374
H       2.893373    -1.709088    0.134141
```

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