Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Modulation of the carboxamidine redox potential through photoinduced spiropyran or fulgimide isomerization.

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Supplementary Information

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S1 Experimental Details

S1.1 General Methods

Compounds **6**[1], **9**[2], **10**[3], **12**[4], **16**[5] and **17**[6] (see Schemes S1 and S2)were synthesized according to reported literature. All other materials were either purchased from commercial sources without further purification. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a JEOL ECS-400 unless otherwise noted. A Rayonet Photochemical Chamber Reactor RPR-200 with a cooling fan and 253.7 nm Hg bulbs was used for the UV-irradiation of all samples. ATR-IR spectra were collected on a Thermo Scientific Nicolet iS5 spectrometer with a Specac Di Quest ATR accessory.

S1.2 UV-vis spectroscopy

Absorption spectra were recorded using a Super Range TEC Spectrometer equipped with VIS-NIR (SL1 Tungsten Halogen Lamp) and UV sources (SL3 Deuterium Lamp). The spectrometer was connected to a thermostated temperature control system having cuvette holders, a stirrer, and flow cells. Unless stated otherwise, UV-vis spectra were recorded at 298 K with stirring. Photoconversion of **1**(o) (to give **1**(c)) and **2**(c) (to give **2**(o)) was obtained by using a RPR-200 Photochemical Reactor (intense source of UV light approximately 1.65x 10 photons/sec/cm^3 at 253.7 nm and 350 nm). Some photoconversions were done in situ in the sample-holder using a pen light LED source (378 nm). Photoconversion of **1**(c) to give **1**(o) and **2**(o) to give **2**(c) was obtained by using a green (530 nm) LED source while keeping out of ambient light. Stirring was used in all photoconversions unless otherwise stated.

S1.3 Cyclic Voltammetry

All CV measurements were done under strictly anaerobic conditions. Experiments were performed at 298 K, using Pine Research instruments, WaveDriver 10 Potentiostat/Galvanostat

System. The cell contained a glassy carbon working electrode, a Pt wire auxiliary electrode, and a 0.5 mm diameter Ag wire, as reference electrode.

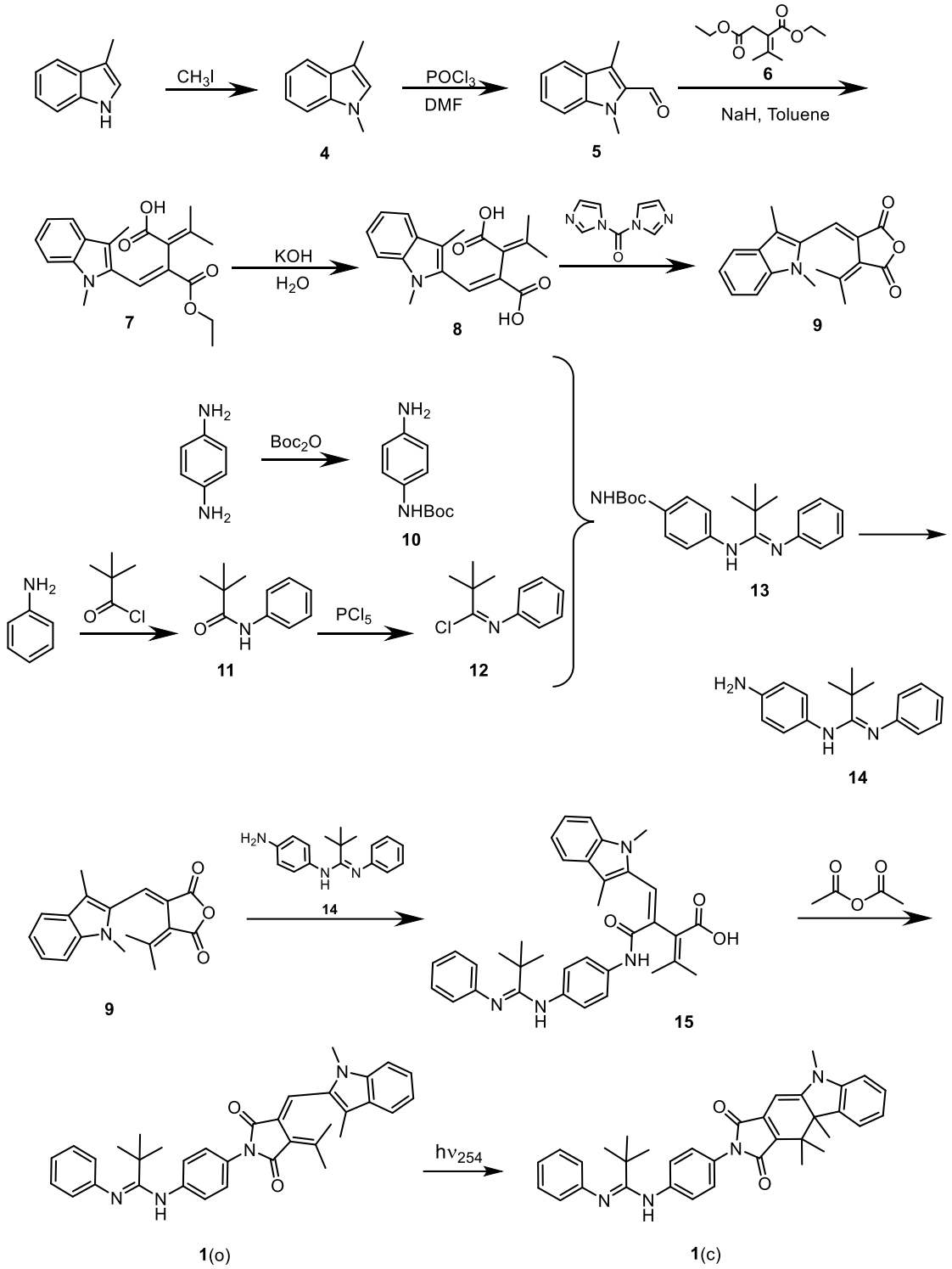
S1.4 Photoelectrochemistry

Photoelectrochemical cyclic voltammetric (CV) measurements were done upon irradiation with 254 nm light at regular intervals of 30 minutes (i.e., 0, 30 minutes, 60 minutes, 90 minutes, and 120 minutes).

S1.5 Spectroelectrochemistry

Spectroelectrochemical measurements were performed using a Honeycomb Spectroelectrochemical cell (cuvette with cap, Pt honeycomb electrode, and reference electrode) from Pine Research. Experiments were performed in CH_3CN (0.1 M Bu_4NPF_6) at 298 K, and the spectra were recorded from 235 – 800 nm.

S1.6 Synthesis



Scheme S1. Synthesis of compound 1(o) and 1(c).

Synthesis of tert-butyl (4-(N'-phenylpivalimidamido)phenyl)carbamate (13)

N-phenylpivalimidoyl chloride (**12**, 3.10 g, 15.8 mmol) in 5 mL toluene was added dropwise to a solution of tert-butyl(4-aminophenyl)carbamate (**10**, 3.30 g, 15.8 mmol) and triethylamine (3.20 g, 31.7 mmol). The mixture was refluxed for 24 hours. The solvent was removed in vacuo, and water (50 mL) was added. The product was extracted using 50 mL dichloromethane. The solution was dried and the solvent removed in vacuo, yielding 5.60 g crude product (96% yield) which was used in subsequent steps without further purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.96 (s, 4H), 6.70 (m, 5H), 6.15 (m, 2H), 1.46 (s, 9H), 1.34 (s, 2 H).

Synthesis of N-(4-aminophenyl)-N'-phenylpivalimidamide (14)

Tert-butyl(4-(N'-phenylpivalimidamido)phenyl)carbamate (0.500 g, 1.36 mmol) was added into a solution of trifluoroacetic acid in dichloromethane (1:1, 10 mL). The reaction was stirred at room temperature overnight. The solvent was removed in vacuo. The residual solid was washed with diethyl ether yielding a brown product (quantitative yield) that was used without further purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.39 (d, 2H, J = 2.0 Hz), 7.02 (m, 3H), 6.68 (d, 2H, J = 7.2 Hz), 6.56 (d, 2H, J = 8.4 Hz), 6.24 (d, 2H, J = 8.4 Hz), 1.48 (s, 9H).

Synthesis of (*E*)-2-((1,3-dimethyl-1H-indol-2-yl)methylene)-4-methyl-3-((4-(N'-phenylpivalimidamido)phenyl)carbamoyl)pent-3-enoic acid (15)

N-(4-aminophenyl)-N'-phenylpivalimidamide (**14**, 0.490 g, 1.86 mmol) and (E)-3-((1,3-dimethyl-1H-indol-2-yl)methylene)-4-(propan-2-ylidene)dihydrofuran-2,5-dione (**9**, 0.500 g, 1.69 mmol) were dissolved in 5 mL toluene. The mixture was stirred overnight. The solvent was removed in vacuo. The product was obtained by column chromatography (ethyl acetate:methanol = 20:1) 57% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.66 (s, 1H), 7.51 (d, 1H, J = 7.2 Hz), 7.20

(d, 2H, J = 3.2 Hz), 7.07 (m, 3H), 6.94 (m, 2H), 6.82 (m, 1H), 6.70 (m, 4H), 3.61(s, 3H), 2.18(s, 3H), 2.09(s, 3H), 1.49(s, 3H), 1.45(s, 9H).

Synthesis of N'-(4-((*E*)-3-((1,3-dimethyl-1H-indol-2-yl)methylene)-2,5-dioxo-4-(propan-2-ylidene)pyrrolidin-1-yl)phenyl)-N-phenylpivalimidamide (1(o))

(*E*)-2-((1,3-dimethyl-1H-indol-2-yl)methylene)-4-methyl-3-((4-(N'-phenylpivalimidamido)phenyl)carbamoyl)pent-3-enoic acid (**15**, 7.00 mg, 12.4 mmol) was dissolved into 50 mL toluene. Acetic anhydride (50 mL) was added, and the mixture was stirred at room temperature for 3 hours. After 3 hours, the solution was poured onto 500 mL water. The mixture was neutralized with a concentrated solution of aqueous $NaHCO_3$. The crude product was purified by column chromatography (ethyl acetate:hexanes = 4:1) to give 5.71 g (84% yield) of light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.66 (s, 1H), 7.57 (d, 1H, J = 8.0 Hz), 7.29 (d, 2H, J = 4.0 Hz), 7.07 (m, 5H), 6.88 (m, 2H), 6.72 (d, 2H, J = 8.0 Hz), 6.3 (s, 1H), 3.74 (s, 3H), 2.47 (s, 3H), 1.97 (s, 3H), 1.38 (s, 9H), 1.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 168.46, 167.76, 153.62, 138.54, 133.02, 128.47, 127.74, 127.20, 126.43, 123.56, 122.29, 121.39, 121.35, 119.60, 115.21, 109.18, 39.37, 30.92, 29.69, 29.13, 27.10, 22.77, 10.78. MS (EI): m/z = 545.67 $[M+H]^+$.

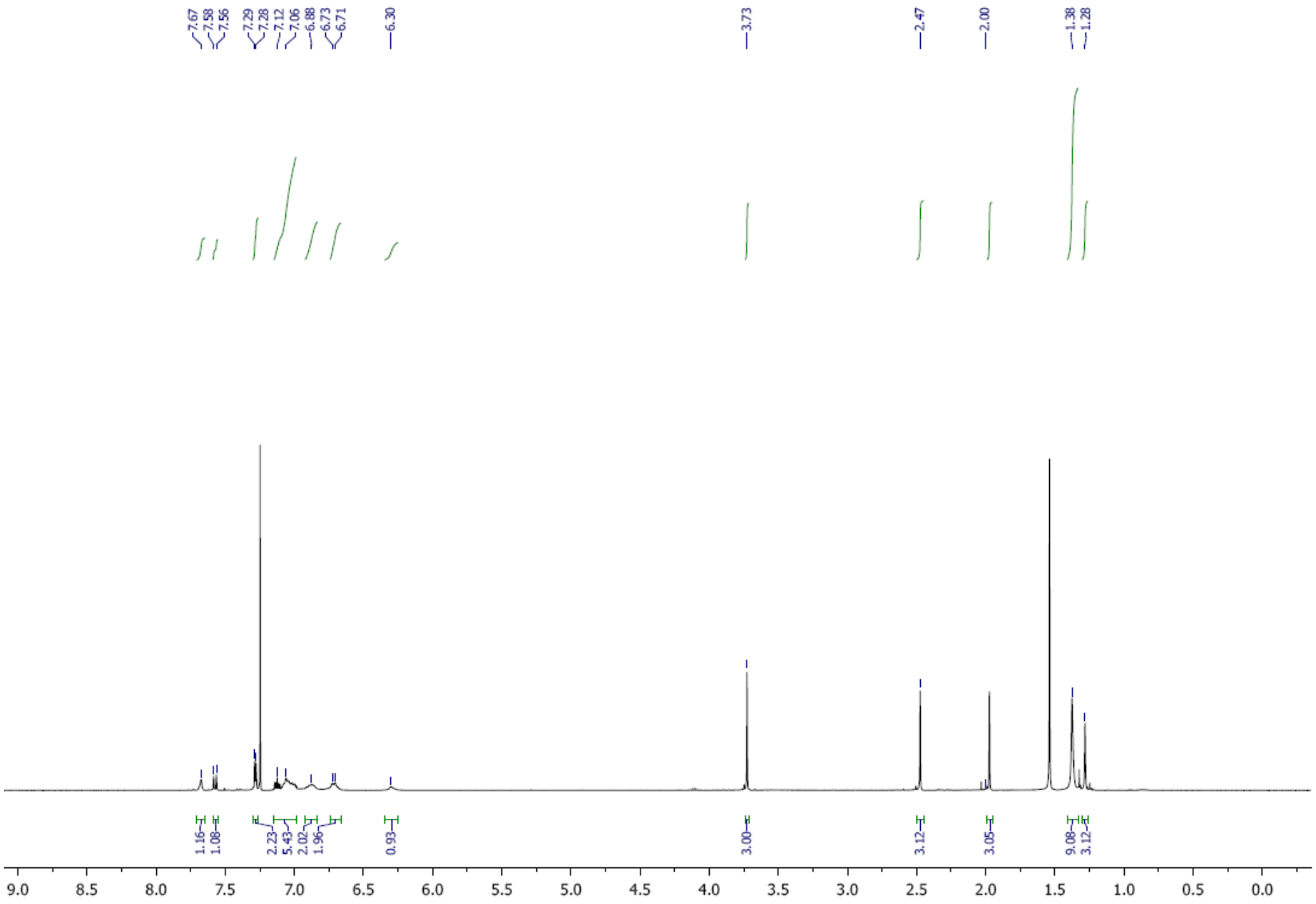


Figure S1. ^{1}H NMR of **1**(o) in $CDCl_3$.

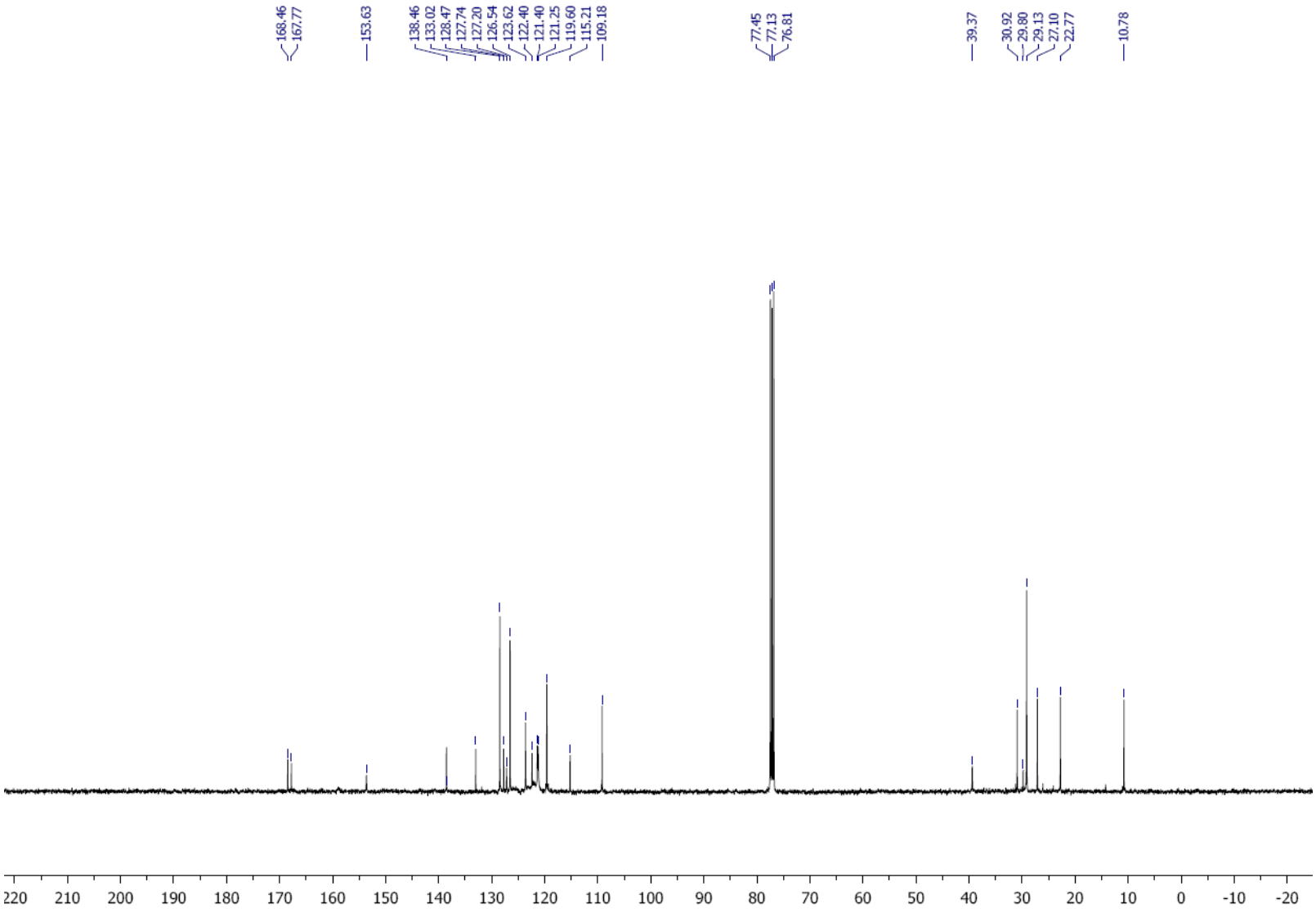


Figure S2. ^{13}C NMR of **1**(o) in $CDCl_3$.

Isolation of 1(c)

Compound **1**(o) (8.9 mg, 0.017 mmol) was dissolved in 0.500 mL of dichloromethane in a large quartz test tube (15.5 cm x 2.5 cm) with a stir bar. The test tube was placed in a photoreactor and stirred for 30 minutes while irradiating with 350 nm light. After 30 minutes, the solvent was removed under vacuum while continuing to irradiate. After the solvent was removed, the dry, red solid was recovered quantitatively. The ^{1}H NMR shows that the resulting solid is a mixture of **1**(o) (6%) and **1**(c) (94%).

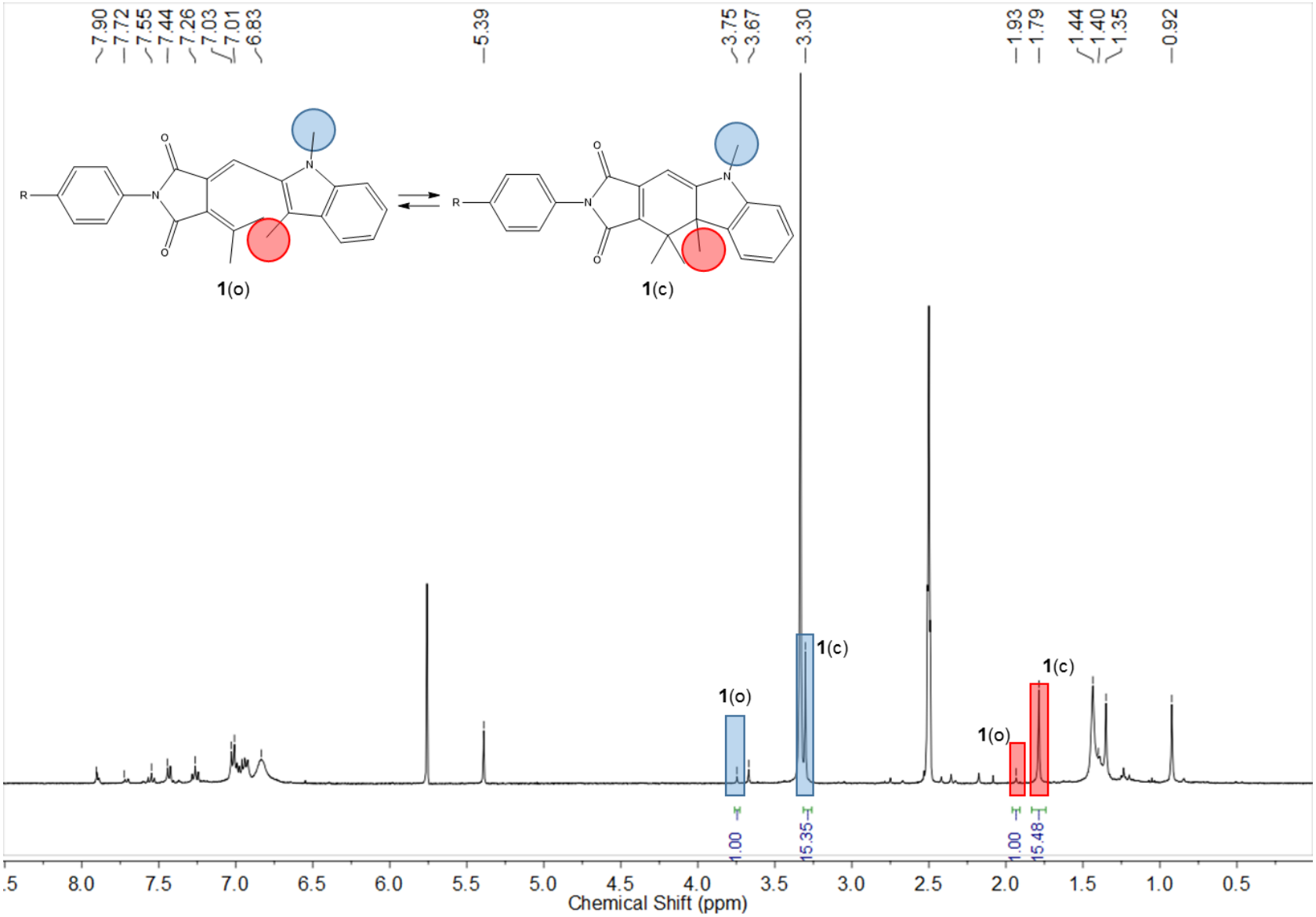
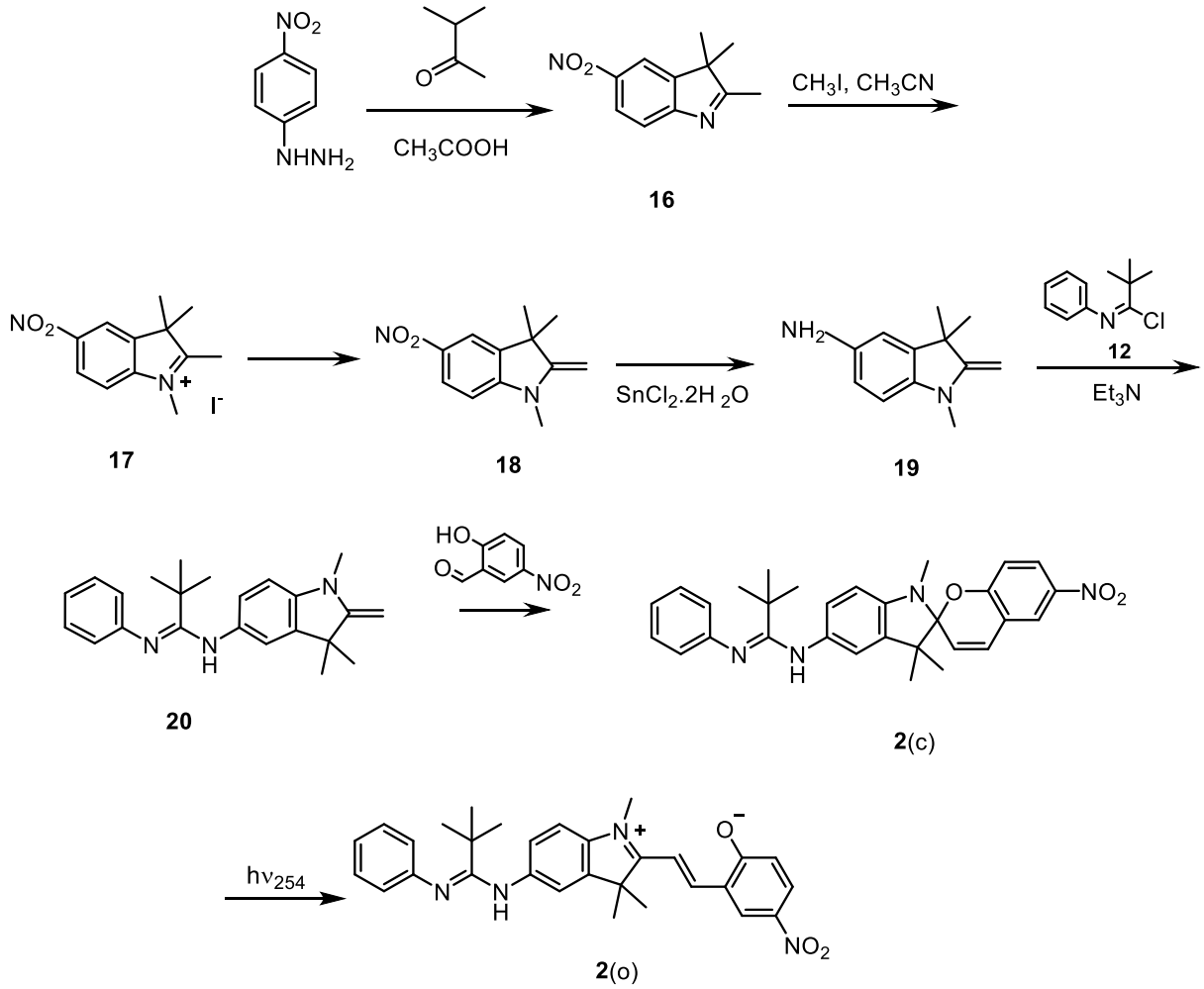


Figure S3. [1]H NMR spectrum of isolated **1**(c) in d_6-DMSO.



Scheme S2. Synthesis of compound **2**(c) and **2**(o).

Synthesis of 1,3,3-trimethyl-2-methylene-5-nitroindoline (18)

NaOH (3.47 g, 86.7 mmol) was dissolved into 100 mL water, followed by the addition of 1,2,3,3-tetramethyl-5-nitro-3H-indolium iodide (10.0 g, 28.9 mmol). The mixture was stirred over 2 hours at 50 °C. The red solid was obtained by filtering and used without purification (quantitative yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.13 (quartet, 8H, J_{12} = 2.4 Hz, J_{13} = 8.4 Hz), 7.93 (d, 1H, J = 2.4 Hz), 6.51 (d, 1H, J = 8.8 Hz), 4.09 (s, 2H), 3.12 (s, 3H), 1.53 (s, 6H).

Synthesis of 1,3,3-trimethyl-2-methyleneindolin-5-amine (19)

$SnCl_2 \cdot 2H_2O$ (49.6 g, 122 mmol) and 1,3,3-trimethyl-2-methylene-5-nitroindoline (**18**, 8.00 g, 36.5 mmol) were added to concentrated HCl (200 mL). The mixture was refluxed overnight under N_2. After cooling, the solution was neutralized with an aqueous NaOH solution. The product was extracted with ethyl acetate (500 mL). The solution was dried, and the solvent was removed to get the crude product (92 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.54 (d, 1H, J = 2.4 Hz), 6.50 (quartet, 1H, J_{12} = 2.4 Hz, J_{13} = 8.4 Hz), 6.33 (d, 1H, J = 8.0 Hz), 3.73 (d, 2H, J = 5.2 Hz), 3.34 (s, 2H), 2.96 (s, 3H), 1.30 (s, 6H).

Synthesis of N'-phenyl-N-(1,3,3-trimethyl-2-methyleneindolin-5-yl)pivalimidamide (20)

1,3,3-trimethyl-2-methyleneindolin-5-amine (**19**, 6.30 g, 33.5 mmol) and triethyl amine (6.77 g, 66.9 mmol) were dissolved in 70 mL tetrahydrofuran. To this solution, a solution of (*E*)-N-(tert-butyl)benzimidoyl chloride (**12**, 7.86g, 40.2 mmol) in 10 mL tetrahydrofuran was added. The mixture was allowed to stir overnight. The solvent was removed in vacuo, and the crude product was purified by column chromatography (hexanes:ethyl acetate= 1:6) (75% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.88 (t, 2H, J = 7.2 Hz), 6.57 (d, 4H, J = 7.2 Hz), 6.54 (s, 1H), 6.14 (d, 1H, J = 8.4 Hz), 3.72 (s, 2H), 2.89 (s, 3H), 1.37 (s, 9H), 1.15 (s, 6H).

Synthesis of N-phenyl-N'-(1',3',3'-trimethyl-6-nitrospiro[chromene-2,2'-indolin]-5'-yl)pivalimidamide (2(c))

N'-phenyl-N-(1,3,3-trimethyl-2-methyleneindolin-5-yl)pivalimidamide (**20**, 8.50 g, 24.5 mmol) and 2-hydroxy-5-nitrobenzaldehyde (4.09 mg, 24.5 mmol) were added to 85 mL ethanol. The mixture was refluxed overnight. After cooling, the product was obtained by filteration (91% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01 (quartet, 1H, J_{12} = 2.8 Hz, J_{13} = 8.8 Hz), 7.95 (d, 1H, J = 2.8 Hz), 6.91 (m, 3H), 6.65 (m, 5H), 6.44 (s, 1H), 6.17 (d, 1H, J = 8.0 Hz), 5.73 (d, 1H, J = 10.4

Hz), 2.57 (s, 3H), 1.37 (s, 9H), 1.11 (s, 3H), 0.96 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 135.82, 128.09, 125.92, 122.74, 118.76, 115.35, 51.64, 28.60, 25.15, 19.93 MS (EI): m/z = 497.45 $[M+H]^+$.

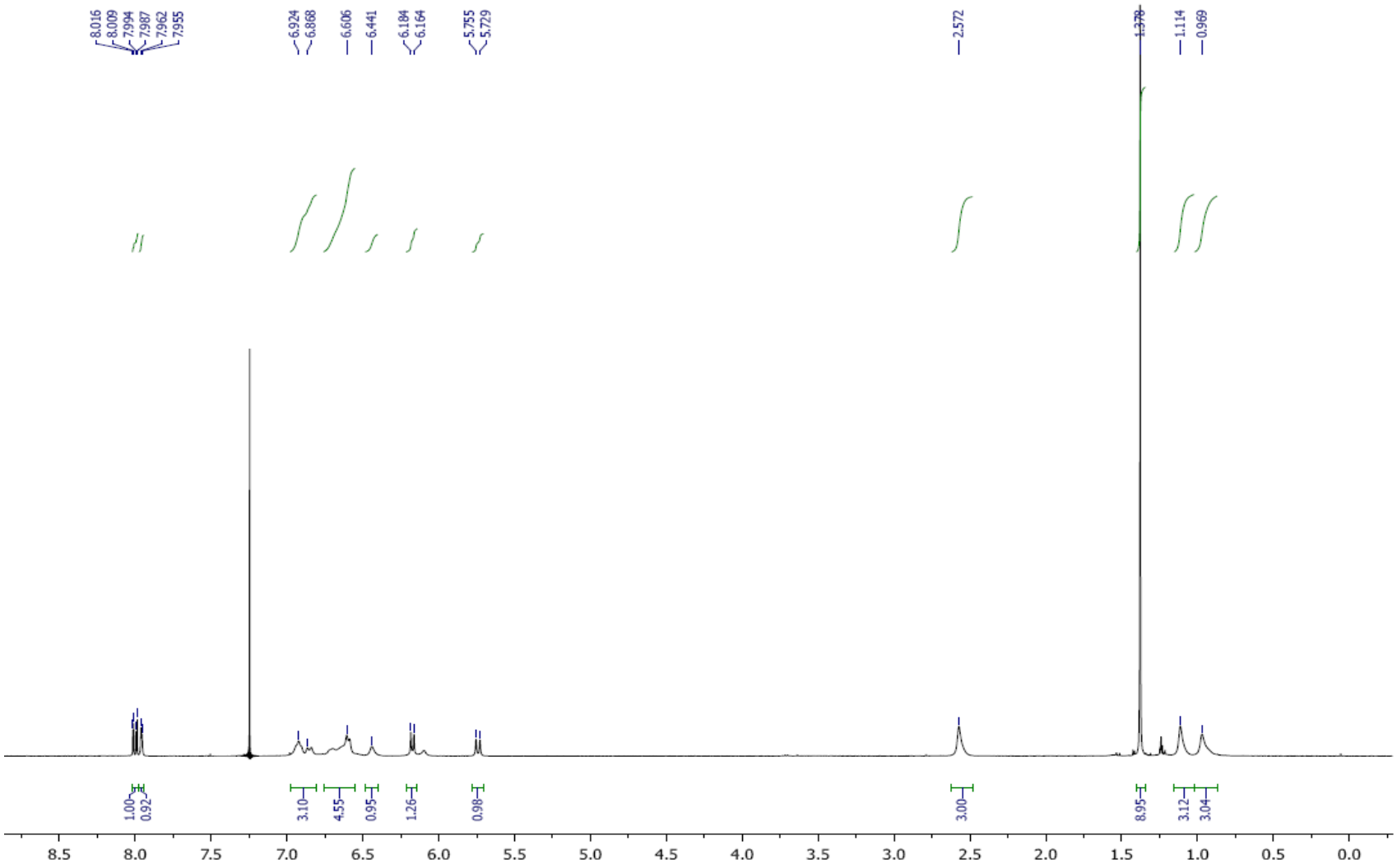


Figure S4. ^{1}H NMR of **2**(c) in $CDCl_3$.

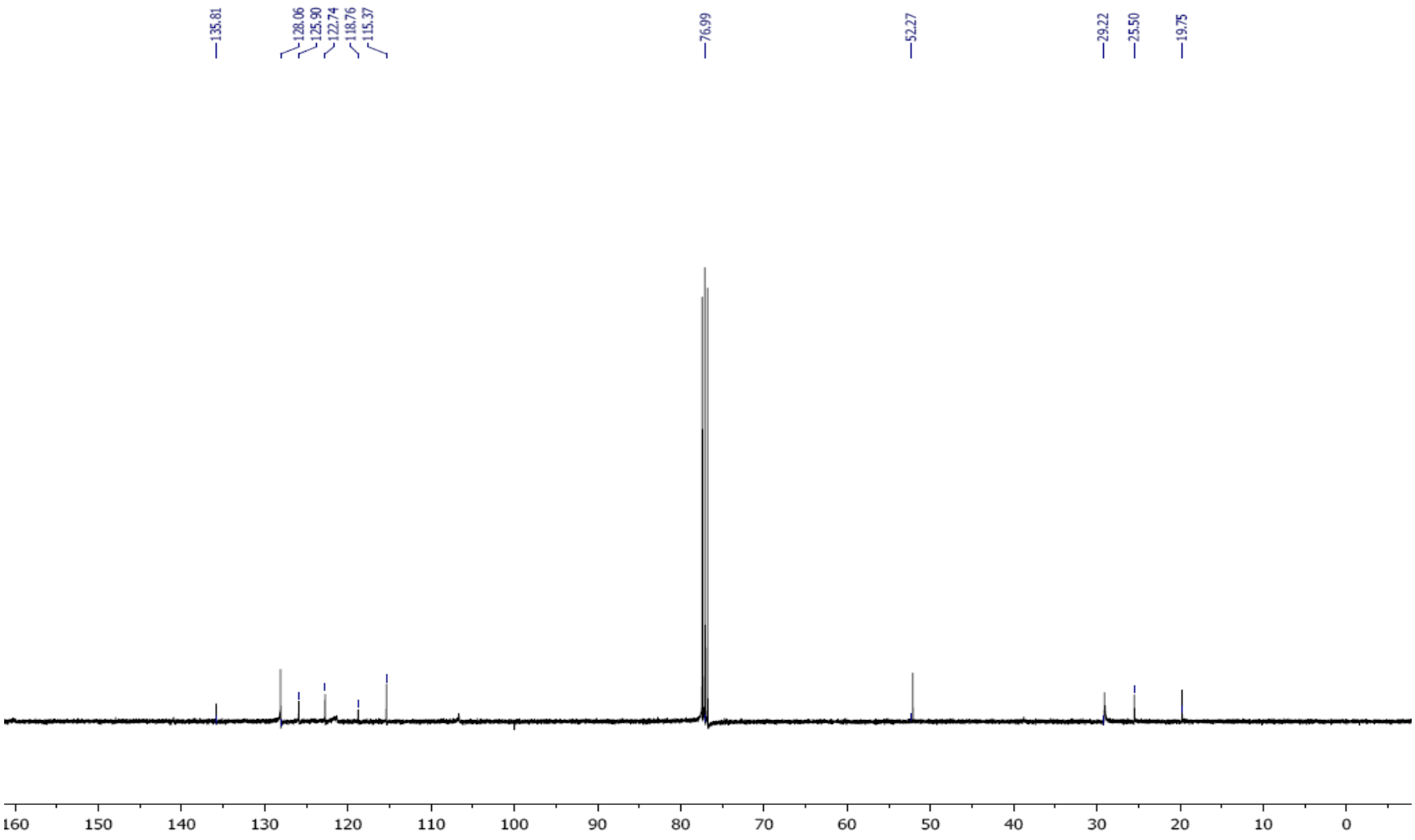


Figure S5. ^{13}C NMR of **2**(c) in $CDCl_3$.

Isolation of 2(o)

Compound **2**(c) (8.0 mg, 0.016 mmol) was dissolved in a small amount of dichloromethane in a large quartz test tube (15.5 cm x 2.5 cm) with a stir bar. The test tube was placed in a photoreactor and stirred for 15 minutes while irradiating with 350 nm light. After 15 minutes, the solvent was removed using a Schlenk line while continuing to irradiate. After the solvent was removed, the dry, blue-purple solid was recovered quantitatively. The ^{1}H NMR spectrum shows only one species, **2**(o).

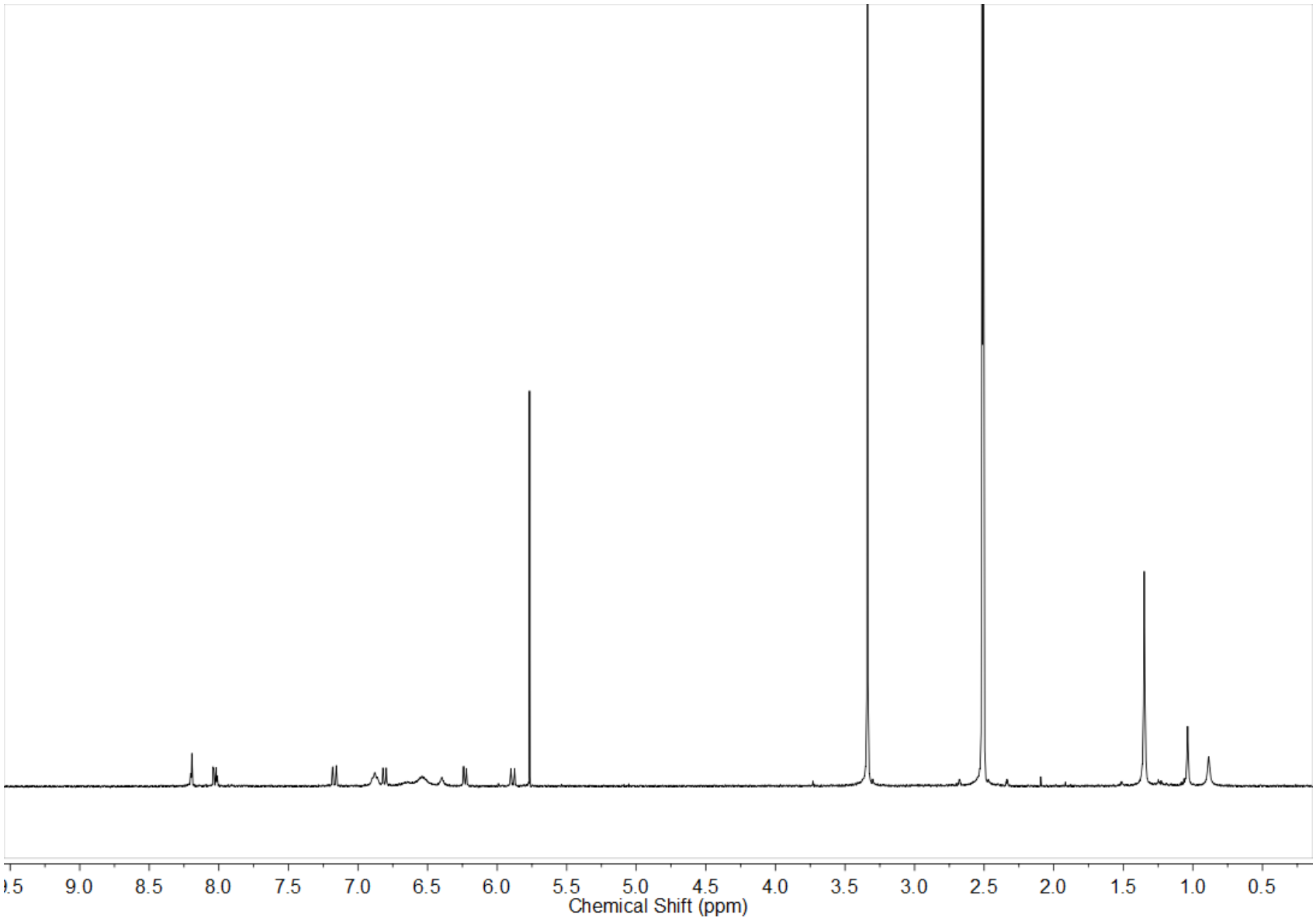


Figure S6. ^{1}H NMR spectrum of isolated **2**(o) in d_6-DMSO.

S1.7 Photostationary state composition of 1

To determine the relative concentrations of **1**(o) and **1**(c) upon photoswitching, a 2.00 mM solution of **1**(o) in d_6-DMSO was irradiated with 350 nm in a quartz flask with stirring for 10 minutes. An aliquot was removed and a ^{1}H NMR spectrum was taken. The ^{1}H NMR showed 100% conversion to **1**(c) in DMSO and 100% conversion to **1**(o) upon irradiation with 530 nm light in DMSO. The same procedure was repeated in CD_3OD.

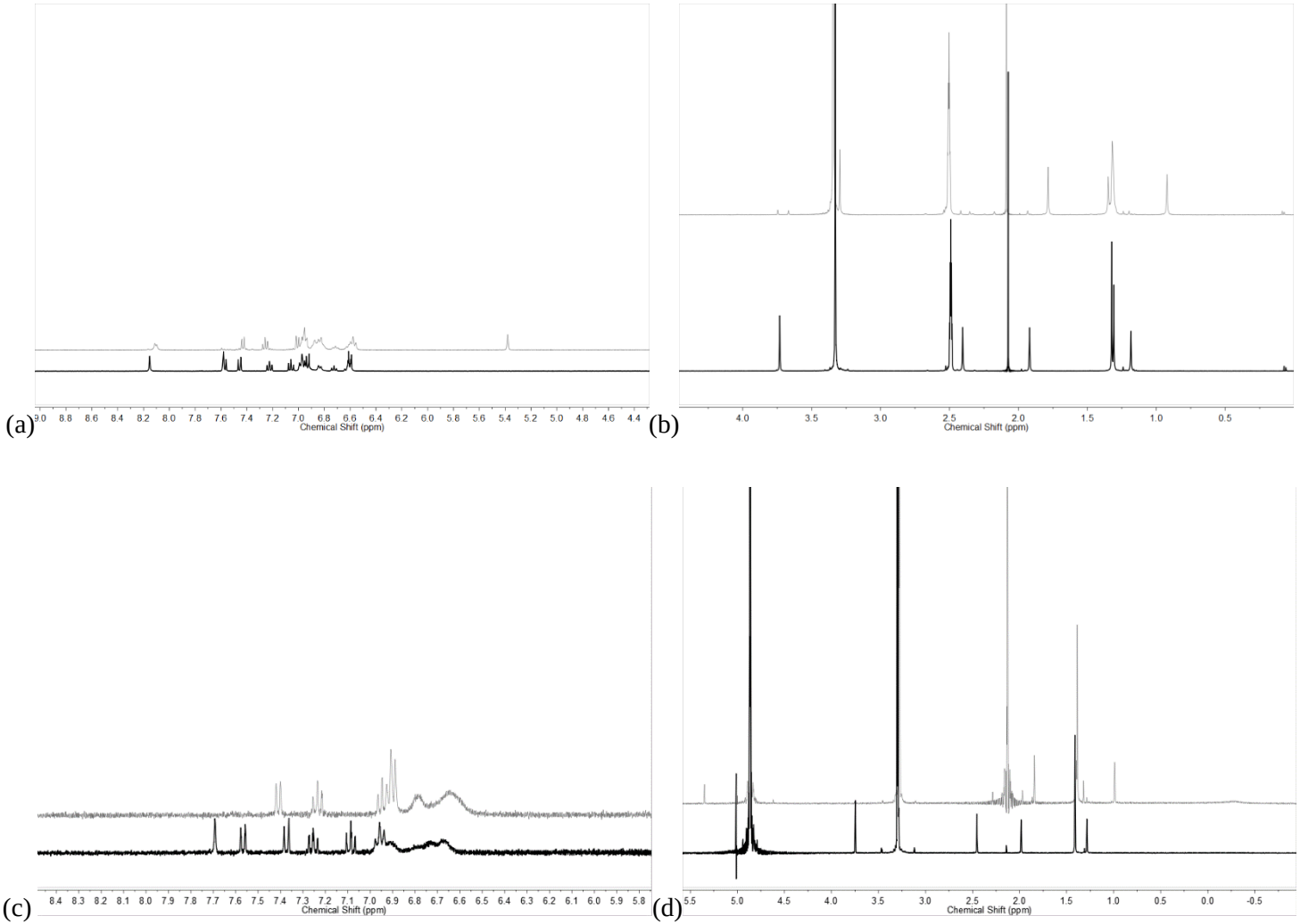


Figure S7. ^{1}H NMR spectra of **1**(o) in d_6-DMSO before (black) and after (grey) 10 minutes UV irradiation (350 nm) to give **1**(c). (a) aromatic region (b) aliphatic region. ^{1}H NMR spectra of **1**(o) in CD_3OD before (black) and after (grey) 10 minutes UV irradiation (350 nm) to give **1**(c). (c) aromatic region (d) aliphatic region.

S1.8 Thermal equilibrium composition of 2

To determine the relative concentrations of **2**(c) and **2**(o) upon thermal switching, a 4.27 mM solution of **2**(c) in CD_3OD was heated with stirring at 323 K. After 1 hour, an aliquot was removed and placed in an NMR tube. The NMR spectra were taken in triplicate at 323 K, and the *t*-butyl peaks and the peaks associated with the methyl group on the nitrogen of the indoline moiety were used to determine relative concentrations. MestReNova was used to fit the peaks. The average of the relative concentrations of the thermal equilibrium state was determined to be 24.05% **2**(o) and 75.95% **2**(c).

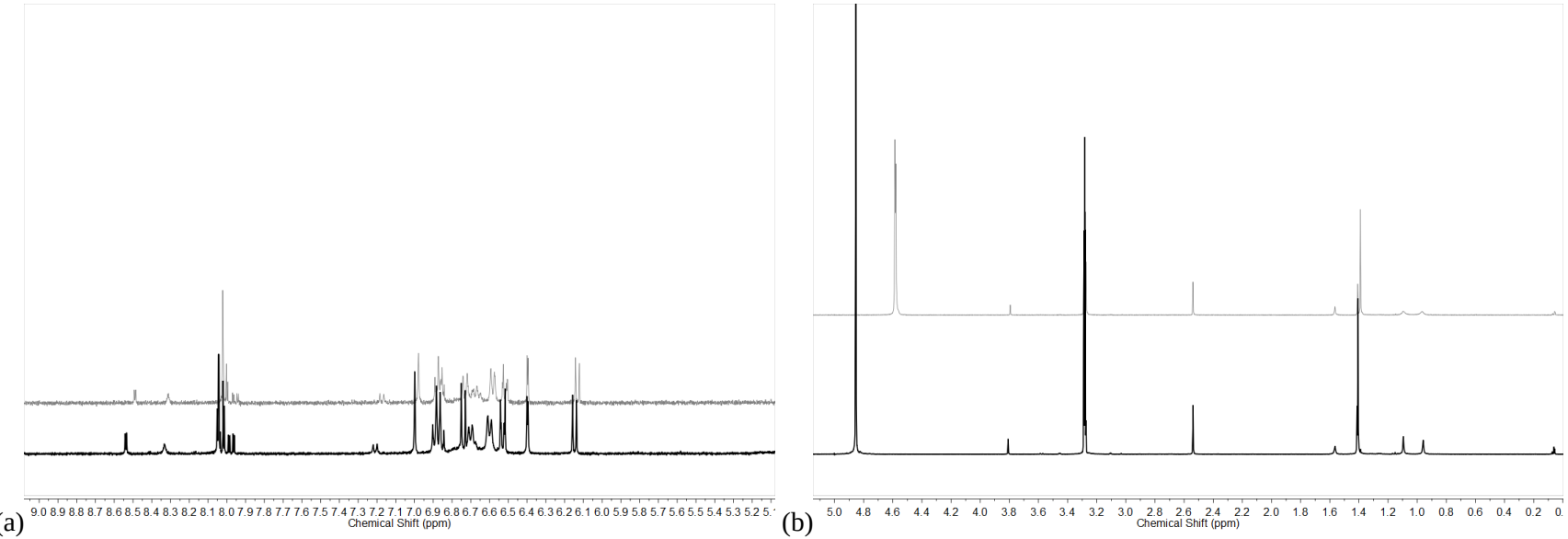


Figure S8. ^{1}H NMR spectra of **2**(c) in CD_3OD before (black) and after (grey) heating at 323 K to give **2**(o). (a) aromatic region (b) aliphatic region.

S1.9 Molar extinction coefficients

Molar extinction coefficients (ε) were determined by irradiating 50 μM solutions of **1** in DMSO and **2** in CH_3OH. UV-vis spectra were taken in triplicate at 298 K with stirring.

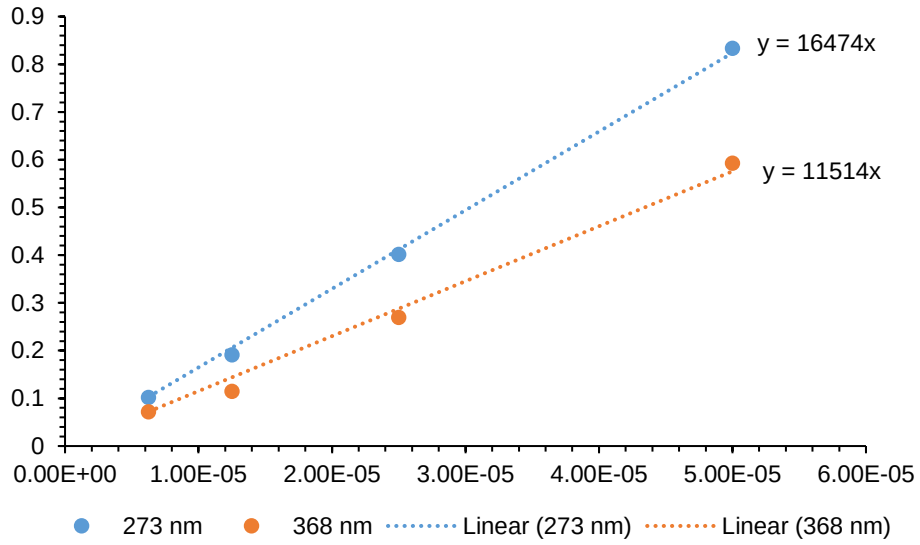


Figure S9. Absorbance of bands vs. concentration for **1**(o) in DMSO.

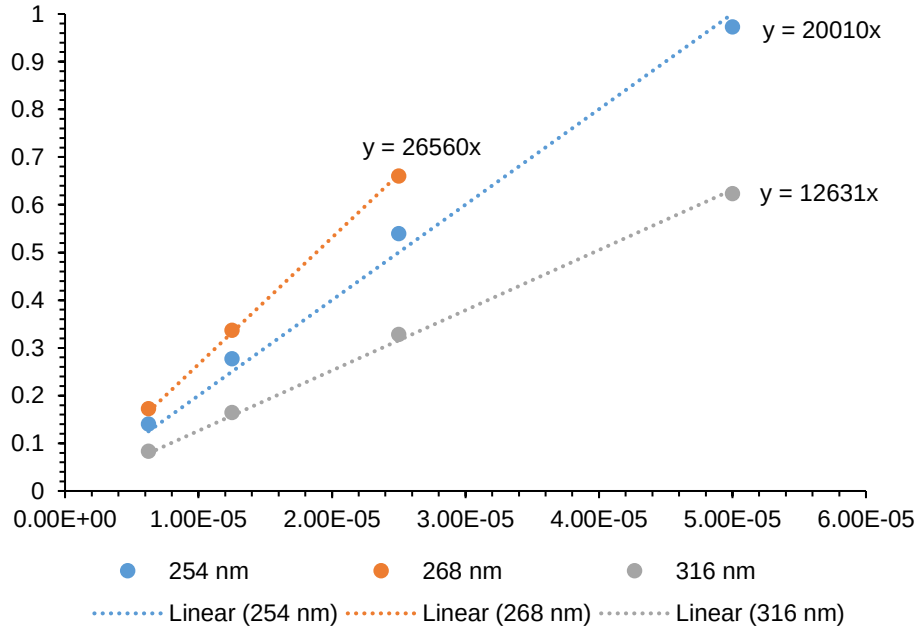


Figure S10. Absorbance of bands vs. concentration for **2**(c) in methanol.

For **1**(o) in DMSO, average absorbances at 273 nm and 368 nm were graphed as a function of concentration. For **2**(c) in methanol, average absorbances at 254 nm, 268 nm, and 316 nm were graphed as a function of concentration. Beer's law ($A = \varepsilon lc$) was then used to determine ε in M^{-1} cm^{-1}. Because the path length is 1 cm, the slope of each line is equal to ε. The solutions of **1**(o) were then irradiated in situ in the sample-holder with 378 nm light for 5 minutes with stirring to ensure full photoconversion. UV-vis spectra were taken in intervals of about 20 seconds. This procedure was repeated with 25 μM and 12.5 μM solutions of **1** in DMSO. For **1**(c), average absorbances at 279 nm and 535 nm were graphed as a function of concentration.

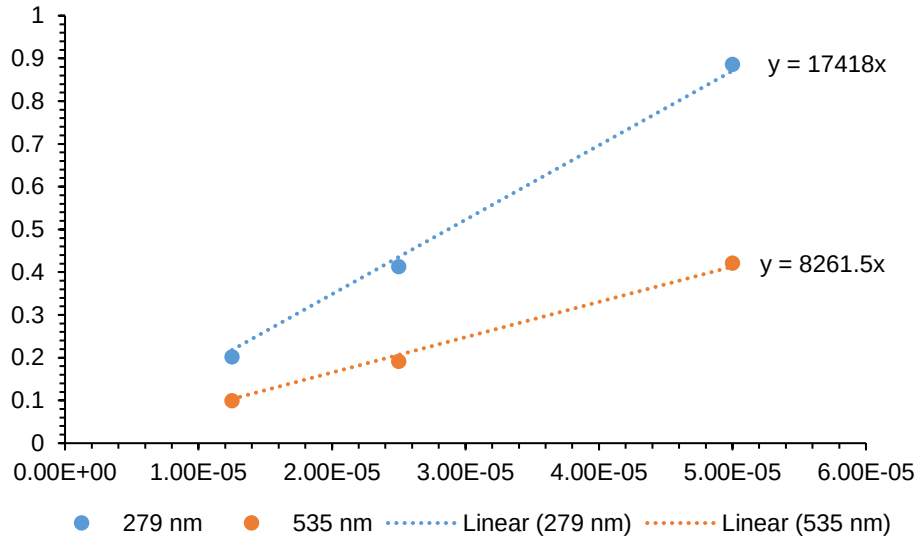


Figure S11. Absorbance of bands vs. concentration for **1**(c) in DMSO.

The molar absorptivity of **2**(c) was determined by measuring samples following irradiation at 530 nm. Attempts to determine the molar absorptivity for **2**(o) were confounded by the incomplete photochemical conversion and the competing thermal isomerization process (vide infra). To obtain an accurate value for **2**(o), the relative concentrations of **2**(c) and **2**(o) were determined after achieving thermal equilibrium by heating a 4.27 mM solution of **2** in CD_3OD at 323 K in the dark. The ^1H NMR spectrum was then taken at 323 K to ensure that the sample was at thermal equilibrium. The peaks associated with the *t*-butyl group and the methyl group on the indoline nitrogen could be used to determine the relative concentrations of **2**(c)

and **2**(o) at thermal equilibrium (1:3 **2**(o):**2**(c) – see 8). This method prevented the competing photoisomerisation, and the ε could then be used with absorption spectra to calculate the relative concentration of **2**(o) following irradiation in situ. Because there are competing thermal and photochemical reactions taking place simultaneously, a true photostationary state cannot be achieved, rather an equilibrium state under irradiation conditions.

A procedure similar to the one used for **1** was used for the thermal switching of **2** after determining the percent photoconversion (vide supra). A 50 μM stock solution of **2** in methanol was heated at 323 K for one hour. A UV-vis spectrum was taken while stirring and maintaining the sample holder at 323 K. Spectra were recorded every 5 minutes until no change was observed in the peak at 537 nm. This procedure was repeated at 25 and 12.5 μM concentrations, using the 50 μM solution for dilutions. The glassware used for this experiment were heated to 323 K in an oven until needed in order to minimize heat loss during dilutions. Utilizing the composition of the thermal equilibrium state determined by ^{1}H NMR, corrections were made to the concentrations, and Beer's law was applied. For **2**(o), average absorbances at 267 nm, 315 nm, and 537 nm were graphed as a function of concentration. It should be noted that for the peaks at 267 and 315 nm, contributions from **2**(c) had to be accounted for as well (the relative ratio of **2**(o):**2**(c) was determined by ^{1}H NMR).

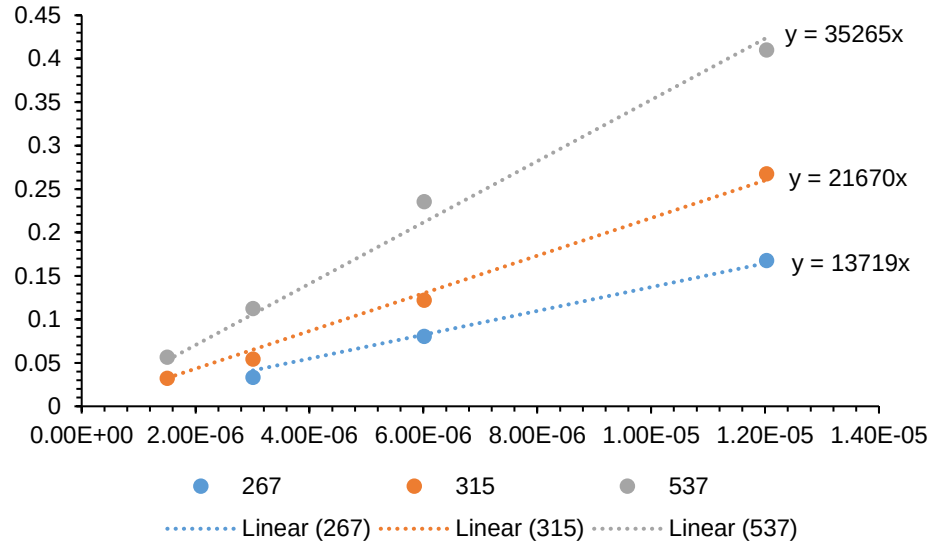


Figure S12. Absorbance of bands vs. Concentration for thermally switched **2**(o) in methanol.

Table S1. TDDFT calculated transitions that contribute more than 10% and experimental absorptions for fulgimide **1**(o) and **1**(c). Transitions that contribute more than 50% shown in bold.

1(o)			
Band	Calc λ (nm) (*f*)	Expt λ (nm) (ε* ($L \cdot mol^{-1} \cdot cm^{-1}$))	Transition (contribution)
1	426.4 (0.49)	368 (1.15×10^4)	**H→L (74%)**
			H-1→L (24%)
	401.3 (0.17)		**H-1→L (68%)**
			H→L (18%)
	360.1 (0.11)		**H-3→L (64%)**
			H→L+1 (19%)
			H-2→L (10%)
	349.7 (0.22)		**H→L+1 (67%)**
			H-3→L (17%)
	337.5 (0.30)		**H-1→L+1 (86%)**
2	305.5 (0.10)	273 (1.65×10^4)	H→L+2 (44%)
			H-1→L+2 (34%)
	222.9 (0.50)		H-11→L (30%)
			H-2→L+4 (12%)
1(c)			
Band	Calc λ (nm) (*f*)	Expt λ (ε* ($L \cdot mol^{-1} \cdot cm^{-1}$))	Transition (contribution)
1	542.0 (0.05)	535 (8.26×10^3)	**H→L (93%)**
	431.5 (0.28)		**H-1→L (92%)**
2	321.2 (0.37)	279 (1.74×10^4)	**H→L+2 (86%)**
	296.0 (0.14)		**H→L+3 (75%)**
	253.3 (0.22)		H→L+6 (23%)
			H-9→L (15%)
			H→L+5 (13%)
			H-2→L+3 (11%)
	224.8 (0.12)		H-5→L+2 (32%)
			H-2→L+8 (13%)

*ε determined in DMSO at concentrations of 50.0, 25.0, and 12.5 μM. Irradiation to obtain **1**(c) was done using a 378 nm light source with stirring.

Table S2. TDDFT calculated transitions that contribute more than 10% and experimental absorptions for spiropyran **2**(c) and **2**(o). Transitions that contribute more than 50% shown in bold.

2(c)			
Band	Calc λ (nm) (*f*)	Expt λ (nm) (ε* ($L \cdot mol^{-1} \cdot cm^{-1}$))	Transition (contribution)
	526.4 (0.02)	not observed	**H→L (99%)**
1	339.4 (0.27)	316 (1.26×10^4)	**H→L+2 (76%)**
			H-2→L (17%)
2	274.8 (0.13)	268 (2.66×10^4)	**H-6→L (55%)**
			H-2→L+1 (14%)
			H-1→L+2 (13%)
	271.1 (0.18)		**H-1→L+2 (58%)**
			H→L+6 (15%)
	263.0 (0.12)		H-1→L+3 (39%)
			H→L+6 (38%)
	257.4 (0.16)		H-1→L+3 (35%)
			H→L+6 (28%)
			H-1→L+2 (12%)
	250.6 (0.10)		**H-4→L+1 (70%)**
			H-6→L+1 (17%)
3	234.7 (0.24)	254 (2.00×10^4)	H-6→L+1 (37%)
			H-2→L+4 (28%)
	216.1 (0.23)		H-2→L+4 (27%)
			H-6→L+1 (14%)
2(o)			
Band	Calc λ (nm) (*f*)	Expt λ (nm) (ε* ($L \cdot mol^{-1} \cdot cm^{-1}$))	Transition (contribution)
1	500 (1.27)	537 (3.53×10^4)	**H→L (92%)**
2	351.4 (0.12)	315 (2.17×10^4)	**H→L+1 (72%)**
			H→L+2 (17%)
	339.7 (0.11)		**H→L+2 (69%)**
			H→L+1 (16%)
	327.1 (0.32)		**H-4→L (57%)**
			H→L+3 (21%)
3	305.4 (0.12)	267 (1.37×10^4)	**H-1→L+1 (73%)**
	282.9 (0.15)		**H→L+5 (83%)**
	229.2 (0.13)		H-1→L+6 (29%)
			H→L+10 (18%)
			H-12→L (11%)

*ε determined in methanol at concentrations of 50.0, 25.0, and 12.5 μM. Solutions of **2**(o) were obtained by heating each solution until no change was observed in the absorbance at 537 nm and determining the amount of **2**(o) by ^{1}H NMR.

S1.10 Activation energies

For the determination of activation energy, a solution (0.100 mM) of **2**(c) in CH_3OH was placed in the thermostated sample holder with stirring. The thermal conversion of **2**(c) to **2**(o) was monitored by UV-vis absorption spectroscopy. Episodic data capture was used to ensure that

spectra were taken at regular intervals. Measurements were collected at intervals of approximately 30 seconds over 2 hours at 323 K, intervals of approximately 1 minute over 4 hours at 313 K, and intervals of approximately 3 minutes over 12 hours at 303 K.

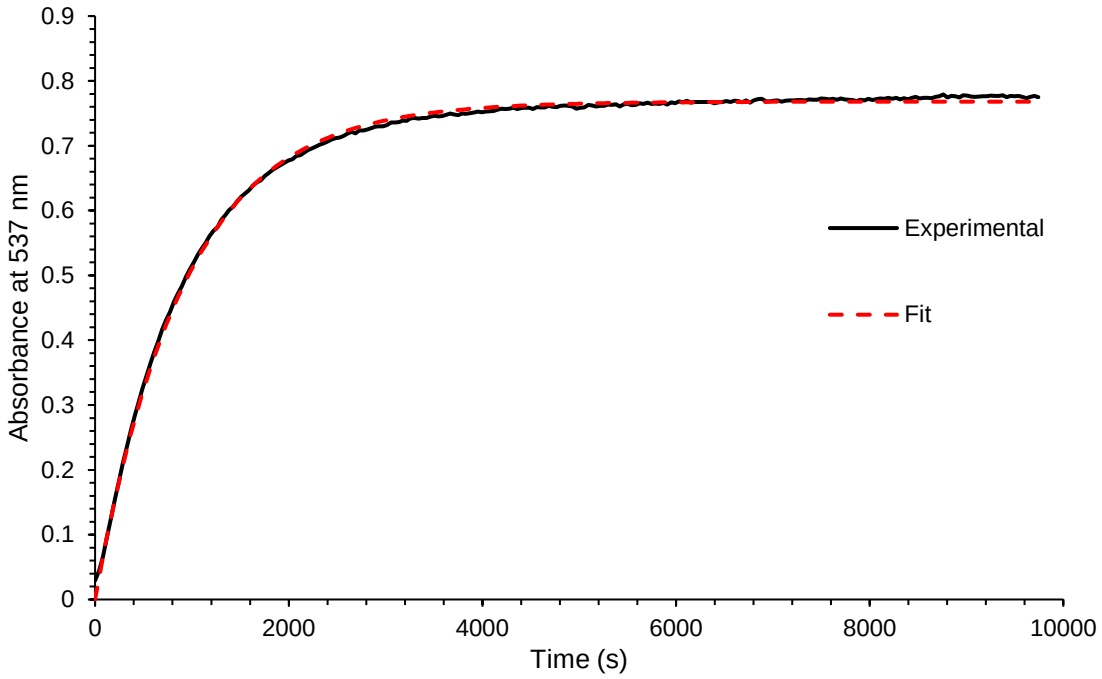


Figure S13. Absorbance of a 0.100 mM solution of **2** in methanol at 537 nm as a function of time at 323 K.

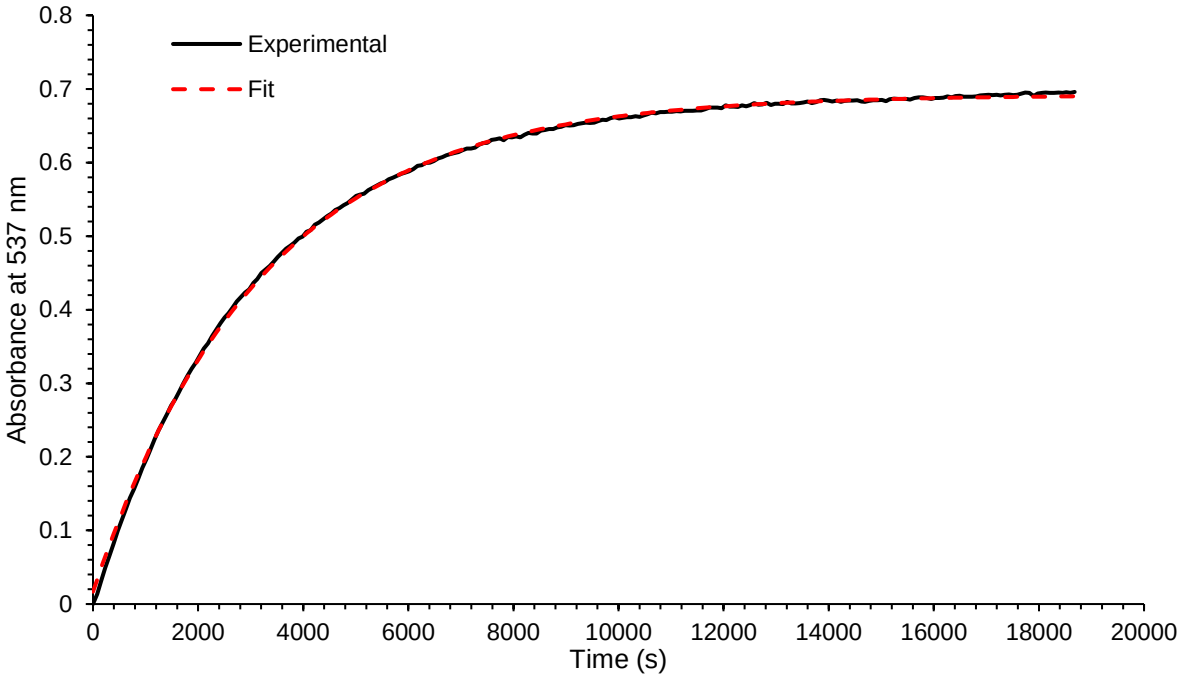


Figure S14. Absorbance of a 0.100 mM solution of **2** in methanol at 537 nm as a function of time at 313 K.

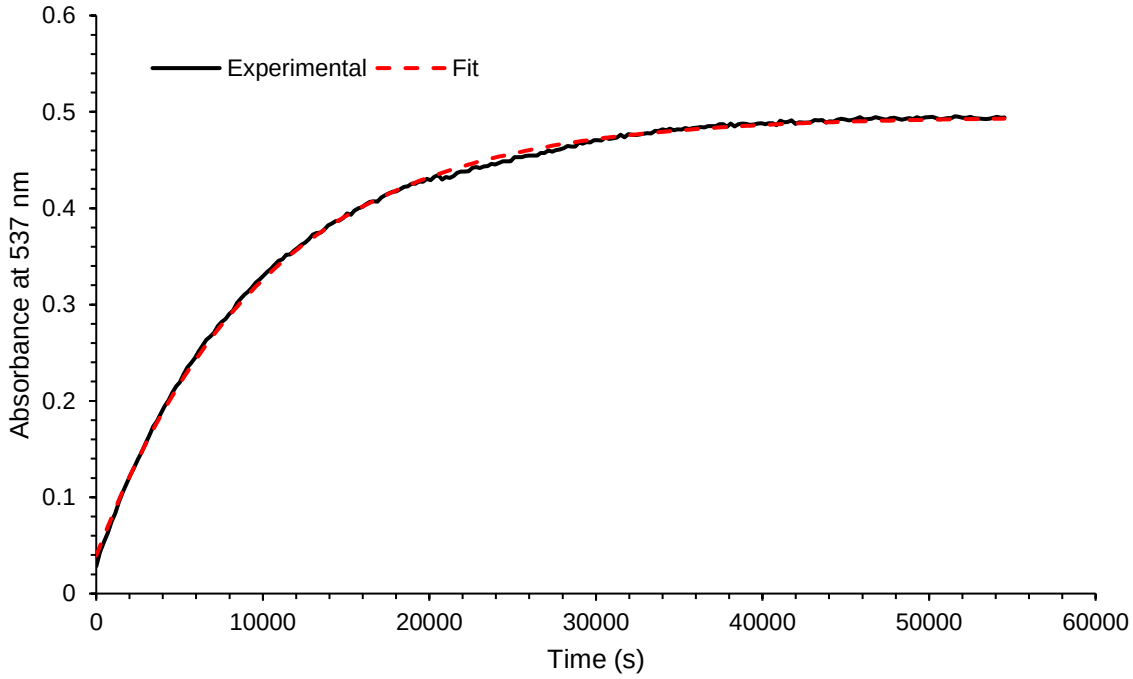


Figure S15. Absorbance of a 0.100 mM solution of **2** in methanol at 537 nm as a function of time at 303 K.

In each case a generic reaction $A \leftrightarrow B$, where A is **2**(c) and B is **2**(o), the forward reaction rate as written is represented by k_1 and the reverse reaction rate by k_2, was used to fit the data. The following form of rate law equations for first-order reversible reactions were used:

$$[A] = \frac{k_2[A]_0}{k_1 + k_2}\left[1 + \frac{k_1}{k_2}e^{-(k_1+k_2)t}\right]$$

$$[B] = \frac{k_1[A]_0}{k_1 + k_2}\left[1 - e^{-(k_1+k_2)t}\right]$$

In order to use the absorbance data as obtained, the concentrations were then multiplied by the molar extinction coefficients that were determined as described above and the path length. The solver function of Microsoft Excel was then used to minimize the sum of the squares of differences between the fitted and experimental data by varying the K_{eq} (which is equal to $\frac{k_1}{k_2}$) and k_1 at each temperature. These values were then used to calculate k_2 at each temperature. The Eyring-Polanyi plot (Figure S16) was used to determine the $\Delta H^{‡}$ and $\Delta S^{‡}$ for the forward and for the reverse reactions per the linear Eyring-Polayi equation:

$$\ln\frac{k}{T} = -\frac{\Delta H^{‡}}{R}\left(\frac{1}{T}\right) + \ln\frac{k_B}{h} + \frac{\Delta S^{‡}}{R}$$

where k is the rate constant in s^{-1}, T is the temperature in K, R is the ideal gas constant in $J•mol^{-1}•K^{-1}$, k_B is Boltzmann's constant in $J•K^{-1}$, and h is Planck's constant in J•s.

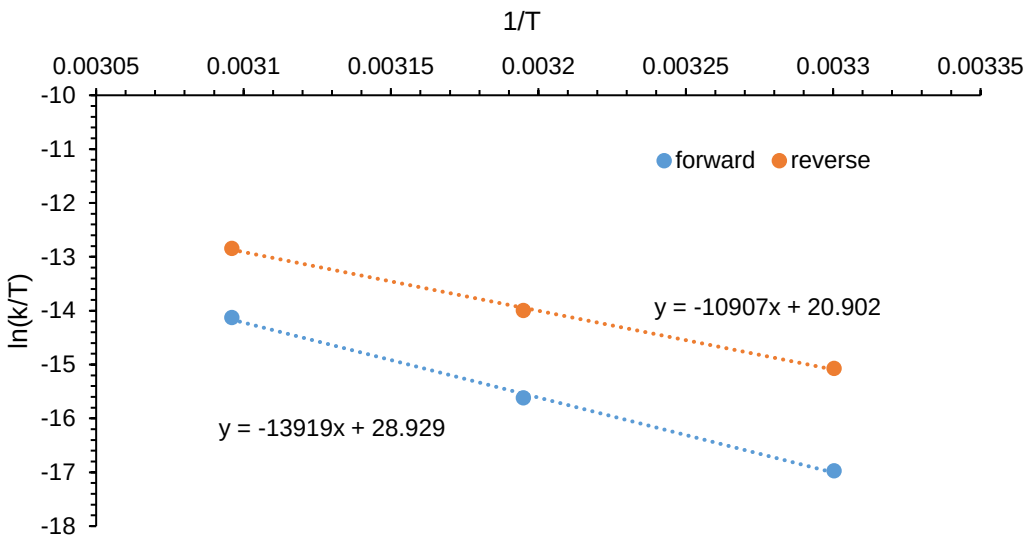


Figure S16. Eyring-Polanyi plot for both forward and reverse thermal reactions of **2** in methanol.

S1.11 Crystallography

Data was collected on a Bruker PLATFORM three circle diffractometer equipped with an APEX II CCD detector and operated at 1500 W (50 kV, 30 mA) to generate graphite monochromated Mo K_α radiation (λ = 0.71073 Å). Crystals were transferred from the vial and placed on a glass slide in polyisobutylene. A Zeiss Stemi 305 microscope was used to identify a suitable specimen for X-ray diffraction from a representative sample of the material. The crystal and a small amount of the oil were collected on a MiTiGen cryoloop and transferred to the instrument where it was placed under a cold nitrogen stream (Oxford) maintained at 100 K throughout the duration of the experiment. The sample was optically centered with the aid of a video camera to insure that no translations were observed as the crystal was rotated through all positions.

A unit cell collection was then carried out. After it was determined that the unit cell was not present in the CCDC database a sphere of data was collected. Omega scans were carried out with a 120 sec/frame exposure time and a rotation of 0.50° per frame. After data collection, the crystal was measured for size, morphology, and color. These values are reported in Table S3.

After data collection, the unit cell was re-determined using a subset of the full data collection. At this point, it was determined that the data consisted of a 2-component non-merohedral twin as determined by CELL_NOW.[7] Intensity data were corrected for Lorentz, polarization, and background effects using the Bruker program APEX 3. A semi-empirical correction for adsorption was applied using the program *TWINABS*[8]. The *SHELXL-2014*[9], series of programs was used for the solution and refinement of the crystal structure. Hydrogen atoms bound to carbon atoms were located in the difference Fourier map and were geometrically constrained using the appropriate AFIX commands.

Table S3. Crystal data and structure refinement for **1**(o).

Identification code	**coz14_03**
Crystal Color	orange
Crystal Habit	plate
Empirical formula	C35 H35 N4 O2
Formula weight	543.67
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 19.675(11) Å alpha = 90 °
	b = 16.984(10) Å beta = 95.450(9) °
	c = 8.859(5) Å gamma = 90 °
Volume	2947(3) $Å^3$
Z	4
Calculated density	1.225 Mg/m^3
Absorption coefficient	0.077 mm^{-1}
F(000)	1156

Crystal size	0.400 x 0.200 x 0.050 mm
Theta range for data collection	1.587 to 23.243 °
Limiting indices	?<=h<=?, ?<=k<=?, ?<=l<=?
Reflections collected / unique	4169 / 4169 [R(int) = 0.1150]
Completeness to theta = 25.242°	98.90%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4169 / 336 / 377
Goodness-of-fit on F^2	0.973
Final R indices [I>2sigma(I)]	R1 = 0.1172, wR2 = 0.2797
R indices (all data)	R1 = 0.2281, wR2 = 0.3399
Largest diff. peak and hole	0.524 and -0.443 $e.A^{-3}$

Table S4. Bond lengths for **1**(o).

Atoms	Distance (Å)
O(1)-C(21)	1.224(8)
O(2)-C(18)	1.208(10)
N(1)-C(1)	1.264(9)
N(1)-C(12)	1.447(10)
N(2)-C(1)	1.378(10)
N(2)-C(6)	1.419(10)
N(3)-C(21)	1.355(9)
N(3)-C(18)	1.428(10)
N(3)-C(15)	1.449(9)
N(4)-C(29)	1.403(10)
N(4)-C(26)	1.407(10)
N(4)-C(35)	1.458(10)
C(1)-C(2)	1.543(11)
C(2)-C(3)	1.506(12)
C(2)-C(5)	1.518(12)
C(2)-C(4)	1.530(11)
C(3)-H(3A)	0.98
C(3)-H(3B)	0.98
C(3)-H(3C)	0.98
C(4)-H(4A)	0.98
C(4)-H(4B)	0.98
C(4)-H(4C)	0.98
C(5)-H(5A)	0.98
C(5)-H(5B)	0.98
C(5)-H(5C)	0.98
C(6)-C(7)	1.348(12)
C(6)-C(11)	1.410(12)
C(7)-C(8)	1.370(13)
C(7)-H(7)	0.95
C(8)-C(9)	1.395(15)
C(8)-H(8)	0.95
C(9)-C(10)	1.331(14)
C(9)-H(9)	0.95
C(10)-C(11)	1.417(13)
C(10)-H(10)	0.95
C(11)-H(11)	0.95
C(12)-C(13)	1.385(11)
C(12)-C(17)	1.404(11)
C(13)-C(14)	1.394(10)
C(13)-H(13)	0.95
C(14)-C(15)	1.429(10)
C(14)-H(14)	0.95
C(15)-C(16)	1.319(10)
C(16)-C(17)	1.388(11)
C(16)-H(16)	0.95
C(17)-H(17)	0.95
C(18)-C(19)	1.495(11)

C(19)-C(22)	1.380(11)	C(28)-C(29)	1.378(10)
C(19)-C(20)	1.454(11)	C(28)-C(33)	1.382(10)
C(20)-C(25)	1.323(10)	C(29)-C(30)	1.446(10)
C(20)-C(21)	1.490(10)	C(30)-C(31)	1.352(11)
C(22)-C(24)	1.487(12)	C(30)-H(30)	0.95
C(22)-C(23)	1.511(12)	C(31)-C(32)	1.388(11)
C(23)-H(23A)	0.98	C(31)-H(31)	0.95
C(23)-H(23B)	0.98	C(32)-C(33)	1.413(10)
C(23)-H(23C)	0.98	C(32)-H(32)	0.95
C(24)-H(24A)	0.98	C(33)-H(33)	0.95
C(24)-H(24B)	0.98	C(34)-H(34A)	0.98
C(24)-H(24C)	0.98	C(34)-H(34B)	0.98
C(25)-C(26)	1.471(10)	C(34)-H(34C)	0.98
C(25)-H(25)	0.95	C(35)-H(35A)	0.98
C(26)-C(27)	1.370(10)	C(35)-H(35B)	0.98
C(27)-C(28)	1.387(9)	C(35)-H(35C)	0.98
C(27)-C(34)	1.461(9)		

Table S5. Bond angles for **1**(o).

Atoms	**Angle (°)**		
C(1)-N(1)-C(12)	122.4(7)	C(29)-N(4)-C(35)	129.0(7)
C(1)-N(2)-C(6)	127.8(7)	C(26)-N(4)-C(35)	127.2(7)
C(21)-N(3)-C(18)	112.9(6)	N(1)-C(1)-N(2)	128.5(7)
C(21)-N(3)-C(15)	123.9(6)	N(1)-C(1)-C(2)	116.9(7)
C(18)-N(3)-C(15)	123.1(6)	N(2)-C(1)-C(2)	114.5(7)
C(29)-N(4)-C(26)	103.6(7)	C(3)-C(2)-C(5)	110.7(8)
		C(3)-C(2)-C(4)	110.2(7)

C(5)-C(2)-C(4)	106.9(8)
C(3)-C(2)-C(1)	111.2(7)
C(5)-C(2)-C(1)	105.8(7)
C(4)-C(2)-C(1)	111.9(7)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(11)	121.2(8)
C(7)-C(6)-N(2)	120.7(8)
C(11)-C(6)-N(2)	118.0(8)

C(6)-C(7)-C(8)	120.3(10)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	119.8(10)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	120.2(10)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	121.4(11)
C(9)-C(10)-H(10)	119.3
C(11)-C(10)-H(10)	119.3
C(6)-C(11)-C(10)	116.7(10)
C(6)-C(11)-H(11)	121.6
C(10)-C(11)-H(11)	121.6
C(13)-C(12)-C(17)	120.1(8)
C(13)-C(12)-N(1)	121.5(7)
C(17)-C(12)-N(1)	118.2(8)
C(12)-C(13)-C(14)	119.8(7)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(13)-C(14)-C(15)	118.6(8)
C(13)-C(14)-H(14)	120.7
C(15)-C(14)-H(14)	120.7
C(16)-C(15)-C(14)	120.6(7)

C(16)-C(15)-N(3)	122.4(6)
C(14)-C(15)-N(3)	117.0(7)
C(15)-C(16)-C(17)	122.1(7)
C(15)-C(16)-H(16)	119
C(17)-C(16)-H(16)	119
C(16)-C(17)-C(12)	118.8(8)
C(16)-C(17)-H(17)	120.6
C(12)-C(17)-H(17)	120.6
O(2)-C(18)-N(3)	123.5(8)
O(2)-C(18)-C(19)	131.9(8)
N(3)-C(18)-C(19)	104.6(7)
C(22)-C(19)-C(20)	128.4(8)
C(22)-C(19)-C(18)	122.7(8)
C(20)-C(19)-C(18)	107.0(6)
C(25)-C(20)-C(19)	136.3(7)
C(25)-C(20)-C(21)	118.1(7)
C(19)-C(20)-C(21)	105.5(7)
O(1)-C(21)-N(3)	125.4(7)
O(1)-C(21)-C(20)	126.7(7)
N(3)-C(21)-C(20)	107.8(6)
C(19)-C(22)-C(24)	123.9(8)
C(19)-C(22)-C(23)	121.9(8)
C(24)-C(22)-C(23)	114.2(7)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(20)-C(25)-C(26)	130.7(7)
C(20)-C(25)-H(25)	114.6
C(26)-C(25)-H(25)	114.6
C(27)-C(26)-N(4)	110.4(7)
C(27)-C(26)-C(25)	120.1(6)
N(4)-C(26)-C(25)	128.8(7)
C(26)-C(27)-C(28)	108.2(6)
C(26)-C(27)-C(34)	125.7(6)
C(28)-C(27)-C(34)	126.0(7)
C(29)-C(28)-C(33)	125.3(7)
C(29)-C(28)-C(27)	106.6(7)
C(33)-C(28)-C(27)	128.0(7)
C(28)-C(29)-N(4)	111.1(6)
C(28)-C(29)-C(30)	117.7(7)
N(4)-C(29)-C(30)	131.1(8)

C(31)-C(30)-C(29)	117.7(8)
C(31)-C(30)-H(30)	121.2
C(29)-C(30)-H(30)	121.2
C(30)-C(31)-C(32)	123.1(7)
C(30)-C(31)-H(31)	118.5
C(32)-C(31)-H(31)	118.5
C(31)-C(32)-C(33)	121.0(8)
C(31)-C(32)-H(32)	119.5
C(33)-C(32)-H(32)	119.5
C(28)-C(33)-C(32)	115.1(7)
C(28)-C(33)-H(33)	122.4
C(32)-C(33)-H(33)	122.4

C(27)-C(34)-H(34A)	109.5
C(27)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(27)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
N(4)-C(35)-H(35A)	109.5
N(4)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
N(4)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5

S2 Spectroscopic Data

S2.1 IR spectra

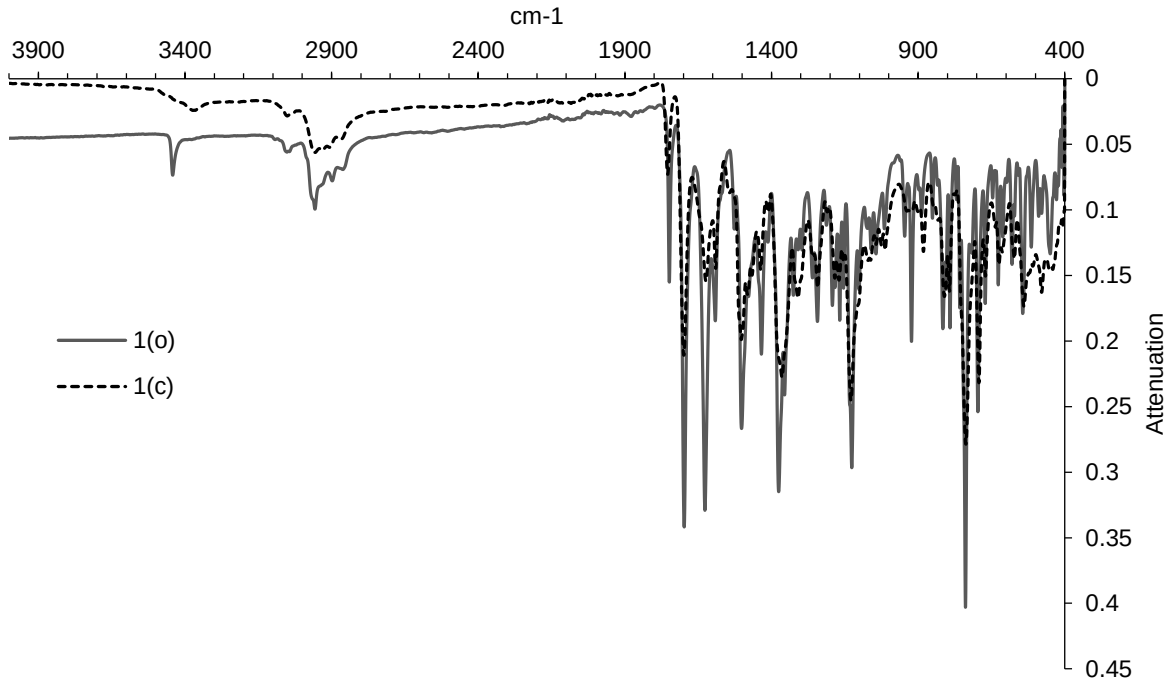


Figure S17. Di-ATR FT-IR spectra of **1**(o) and **1**(c).

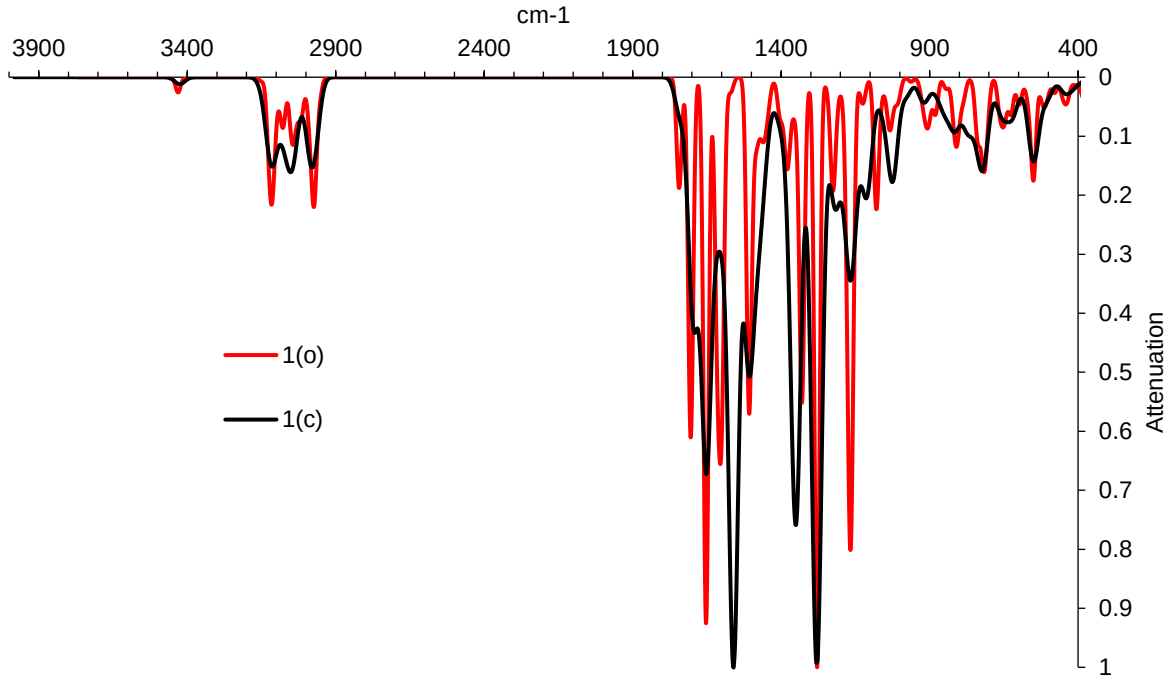


Figure S18. Calculated (PW91, TZP(d)) IR spectra of **1**(o) and **1**(c).

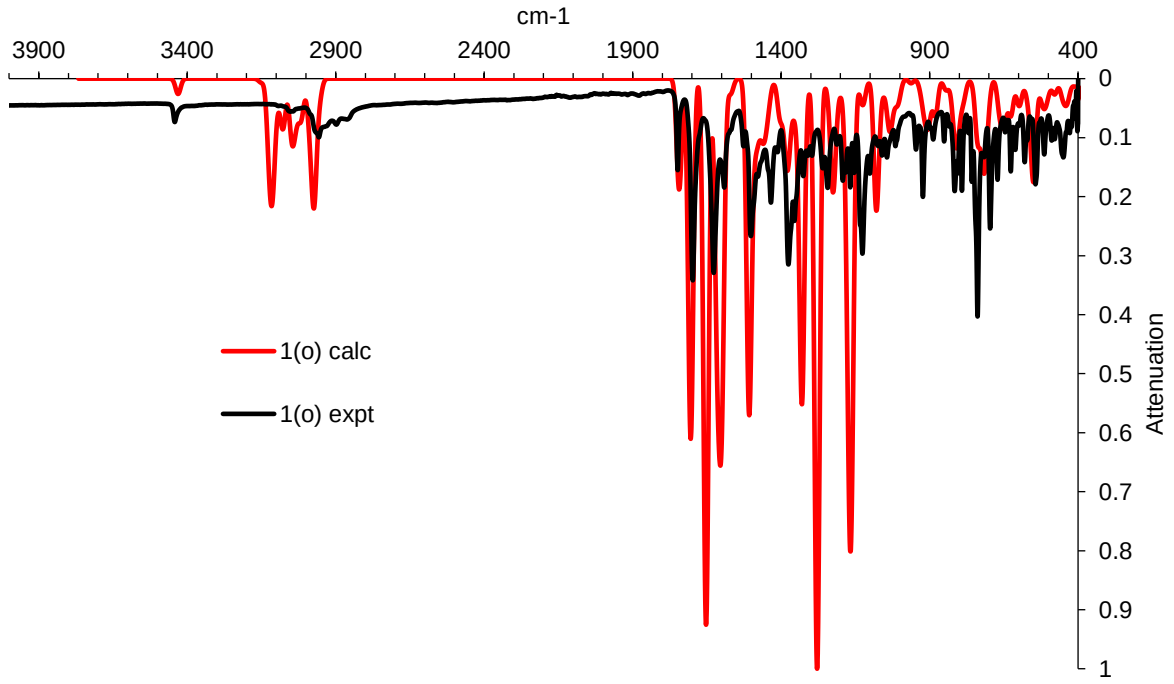


Figure S19. Calculated (PW91, TZP(d)) and experimental IR spectra of **1**(o).

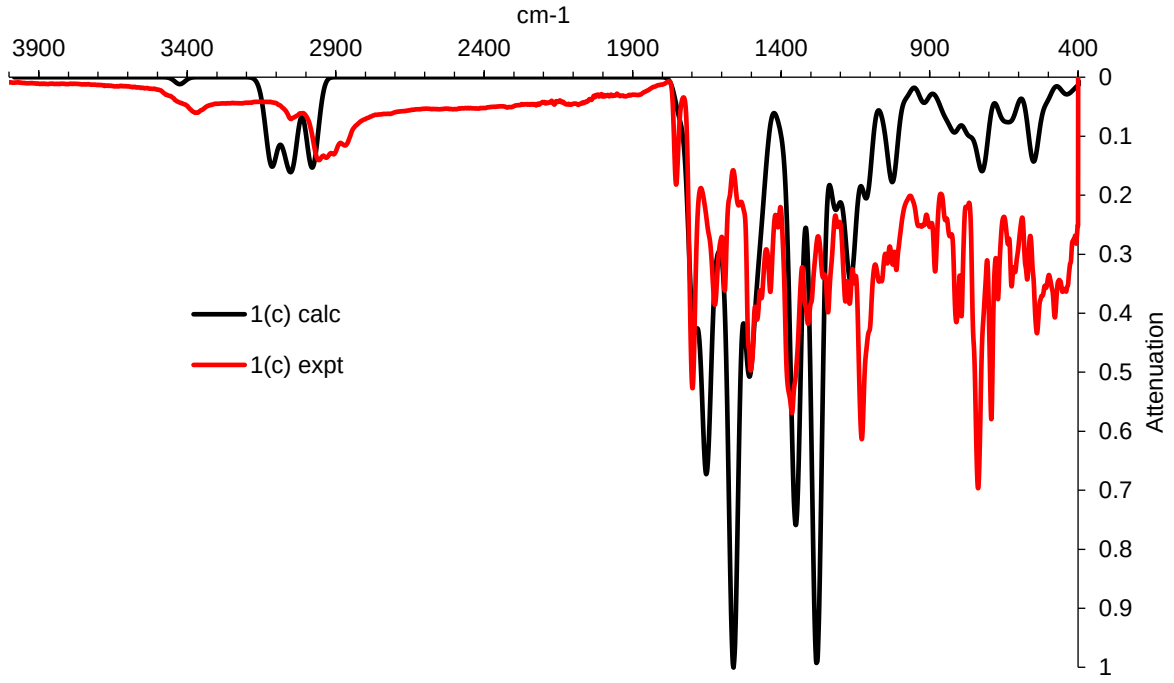


Figure S20. Calculated (PW91, TZP(d)) and experimental IR spectra for **1**(c).

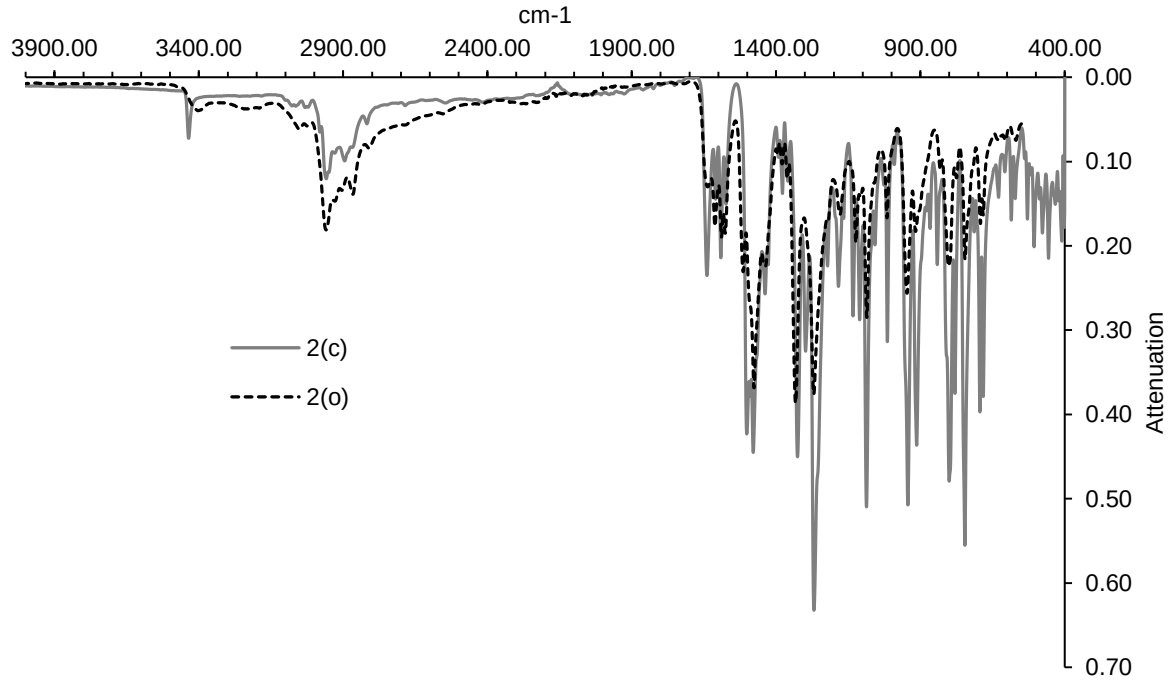


Figure S21. Di-ATR FT-IR spectra of **2**(c) and **2**(o).

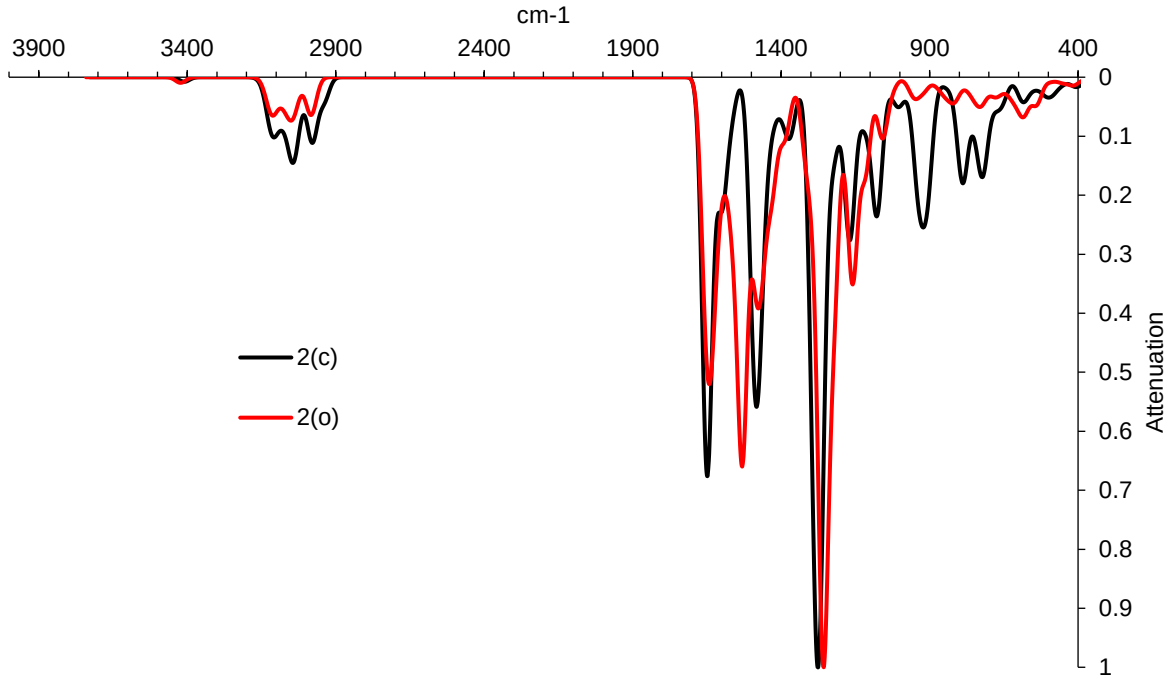


Figure S22. Calculated (PW91, TZP(d)) IR spectra of **2**(c) and **2**(o).

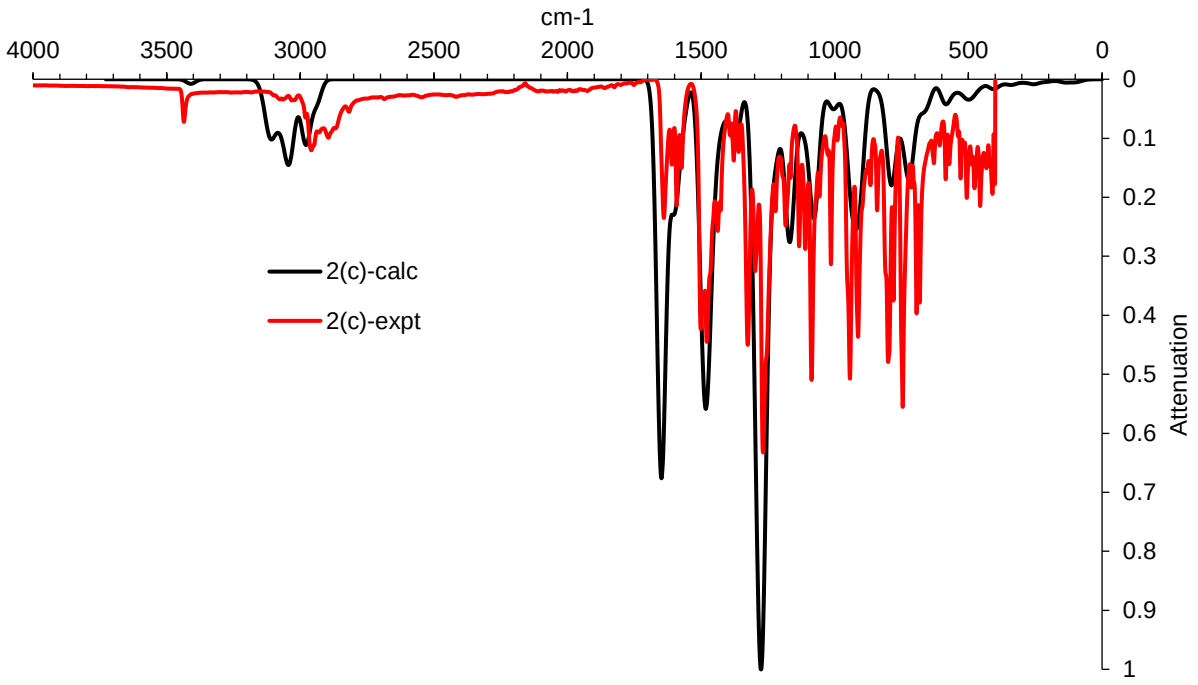


Figure S23. Calculated (PW91, TZP(d)) and experimental IR spectra for **2**(c).

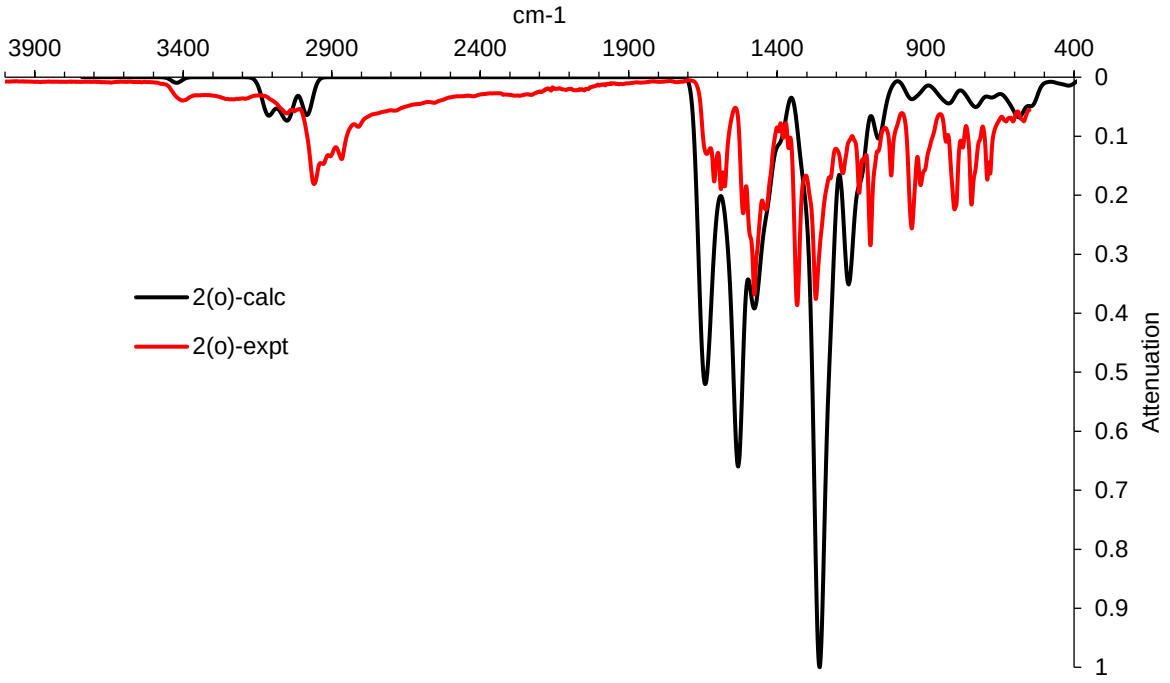


Figure S24. Calculated (PW91, TZP(d)) and experimental IR spectra for **2**(o).

S2.2 UV-vis spectroscopy

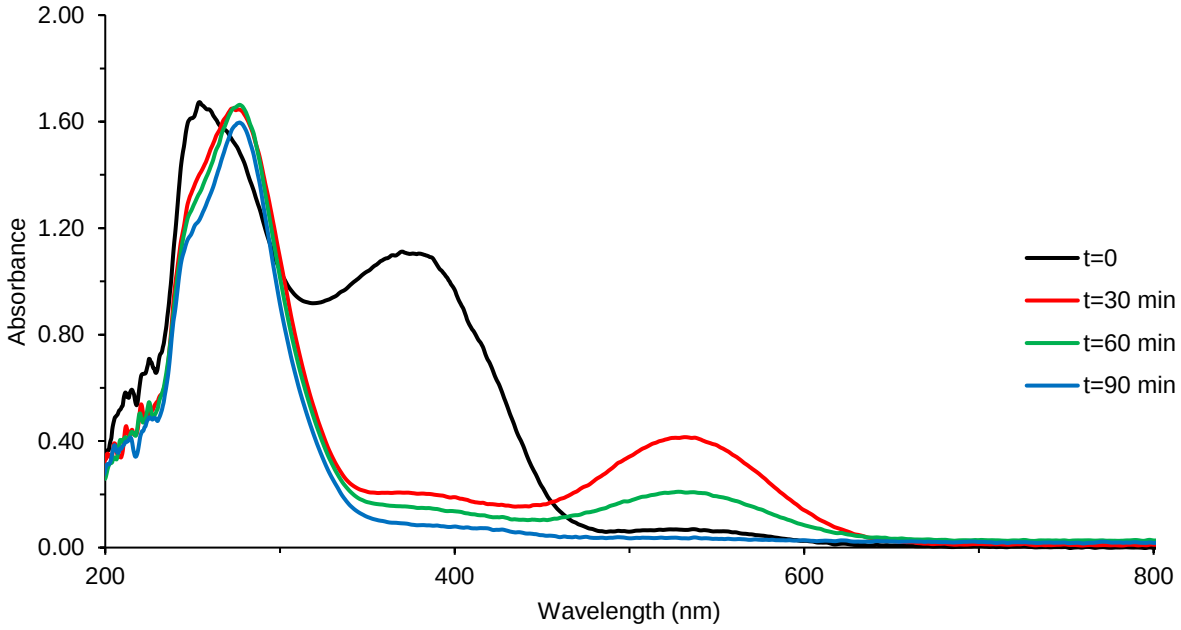


Figure S25. Experimental UV-vis of **1**(o) (0.1 mM in methanol) upon 254 nm irradiation to give **1**(c). Times indicated are the amount of time of UV-irradiation.

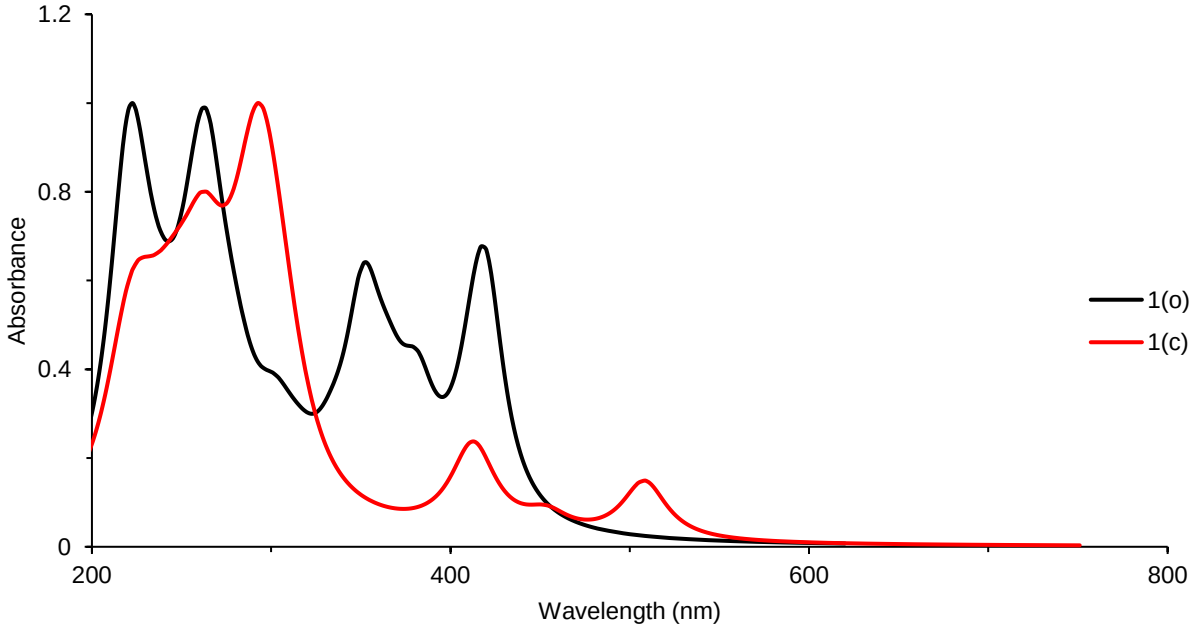


Figure S26. Calculated (B3LYP, TZV(2d)) electronic transitions for **1**(o) and **1**(c).

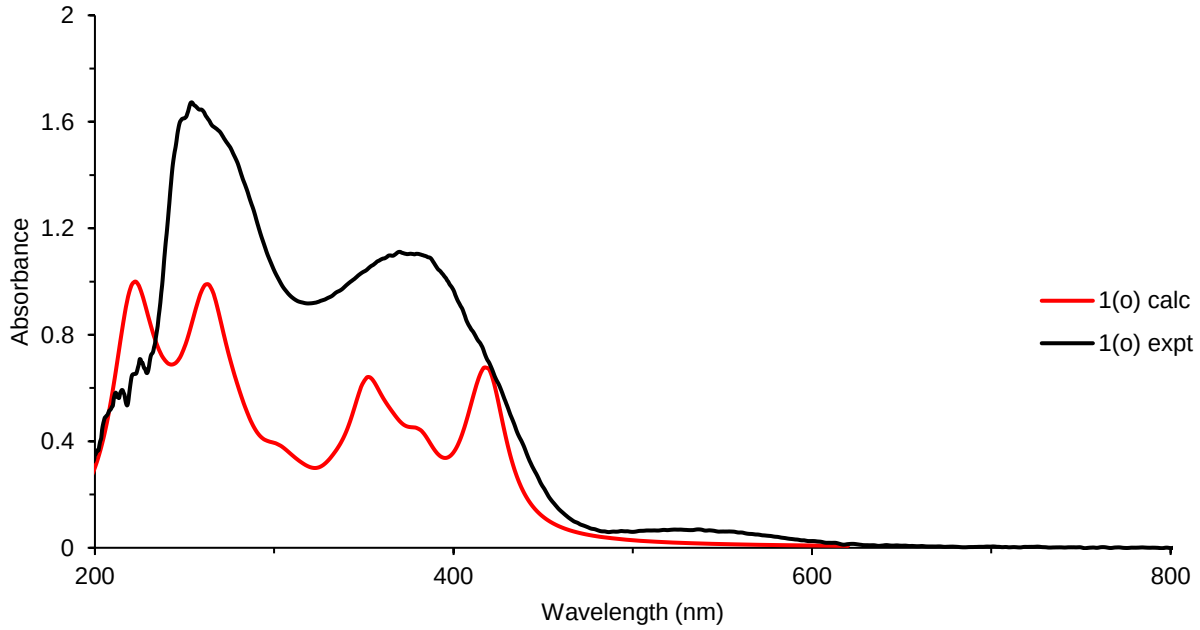


Figure S27. Experimental UV-vis spectrum of **1**(o) and the calculated (B3LYP, TZV(2d)) electronic transitions of **1**(o).

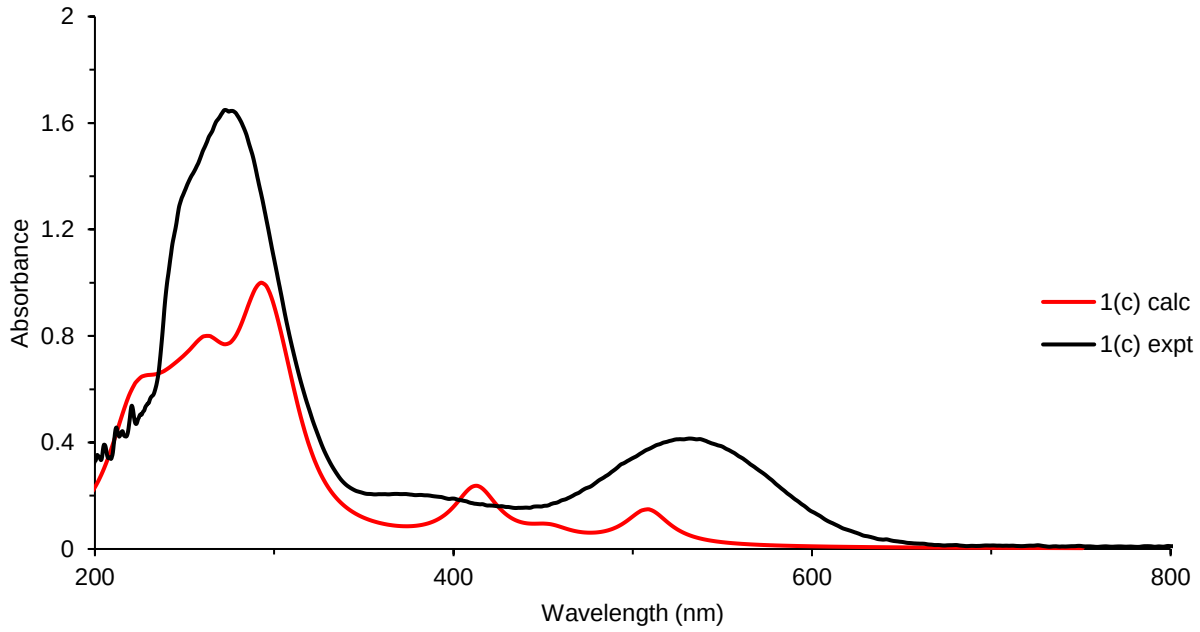


Figure S28. Experimental UV-vis spectrum of **1**(c) and calculated (B3LYP, TZV(2d)) electronic transitions of **1**(c).

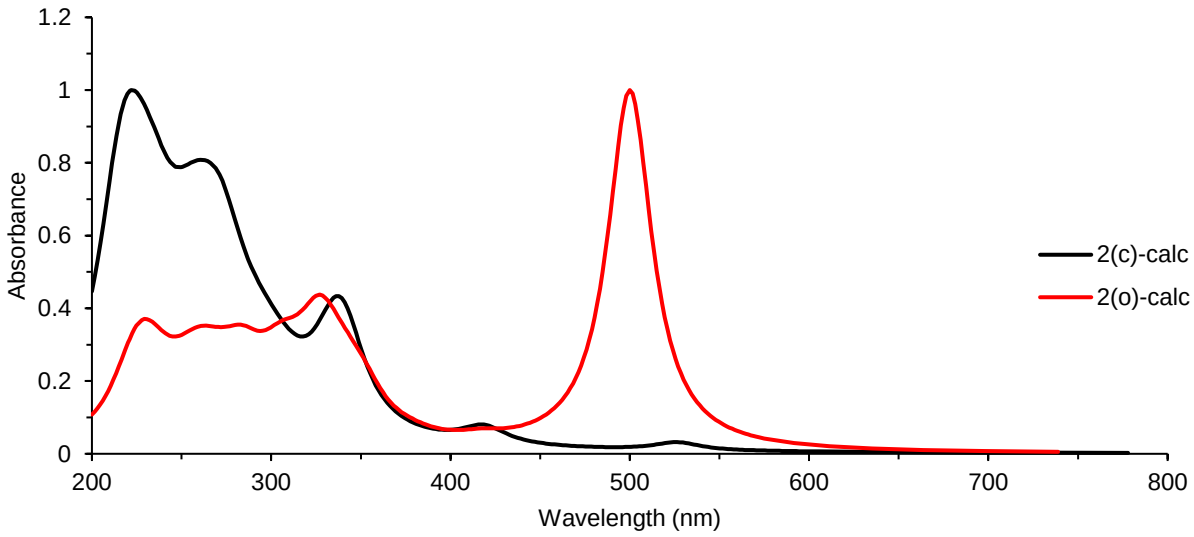


Figure S29. Calculated (B3LYP, TZV(2d)) electronic transitions for **2**(c) and **2**(o).

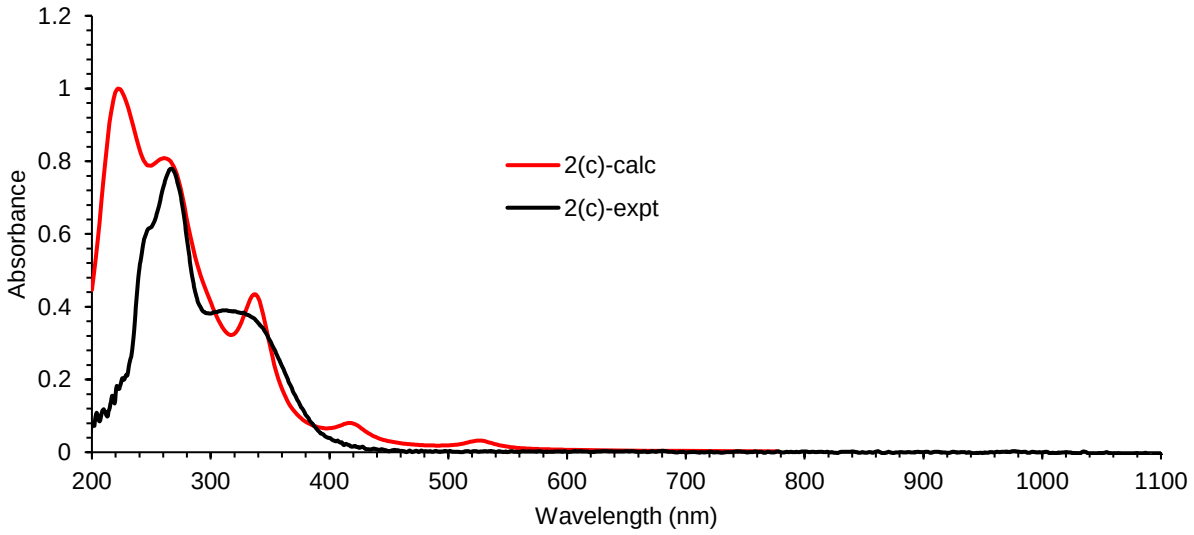


Figure S30. Experimental UV-vis spectrum of **2**(c) and the calculated (B3LYP, TZV(2d)) electronic transitions of **2**(c).

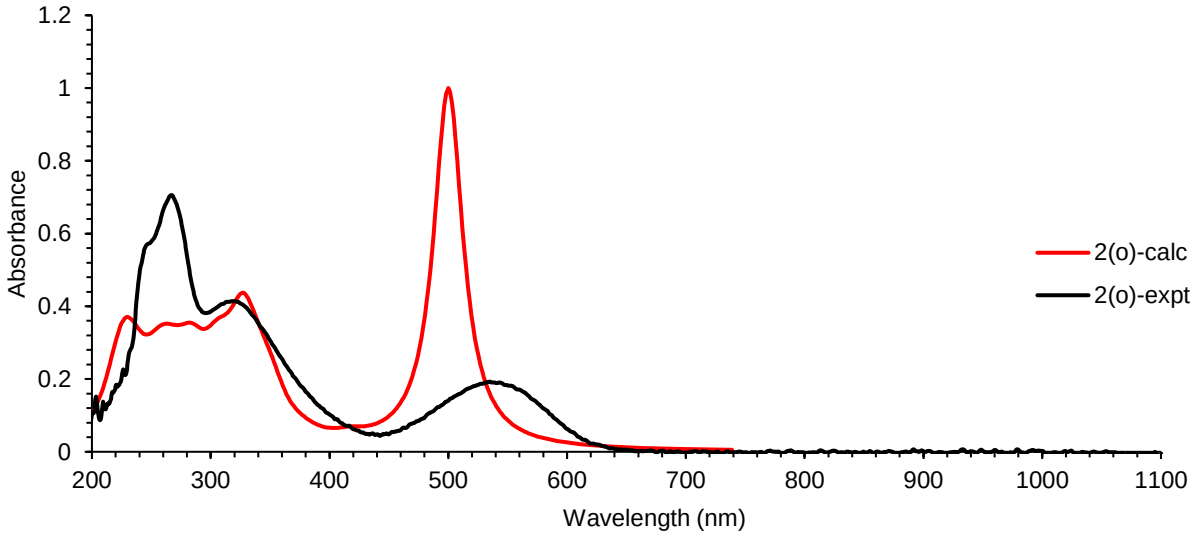


Figure S31. Experimental UV-vis spectrum of **2**(o) and the calculated (B3LYP, TZV(2d)) electronic transitions of **2**(o).

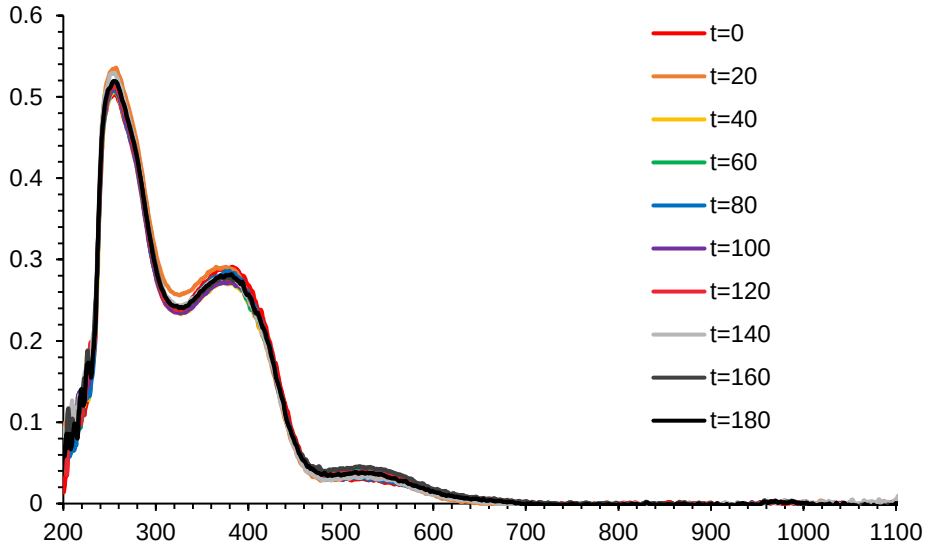


Figure S32. Experimental UV-vis spectra of **1**(o). Time intervals indicated are in minutes irradiation. Irradiation was done in 10 minute intervals, alternating with 350 nm and then 535 nm light. The spectra shown here are only of the solution before any irradiation (t=0) and after the 535 nm irradiation.

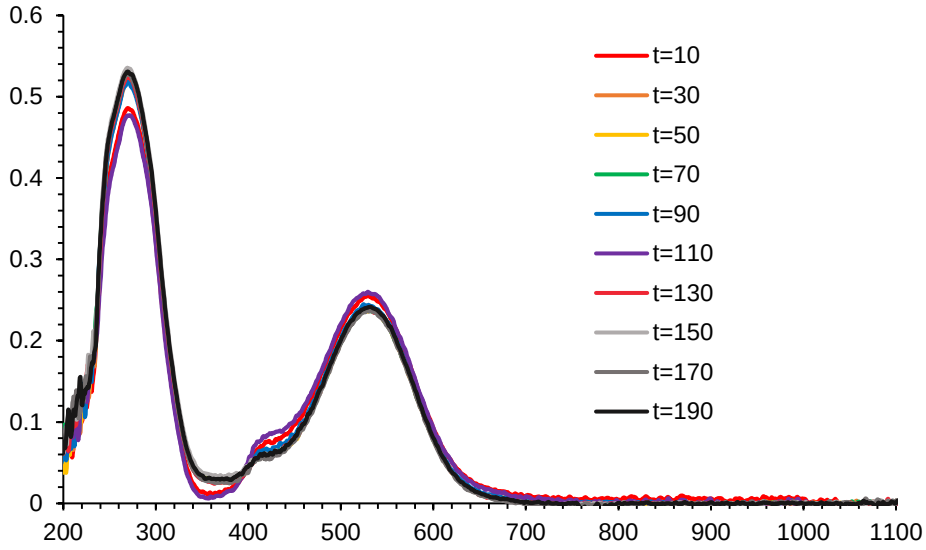


Figure S33. Experimental UV-vis spectra of **1**(c). Time intervals indicated are in minutes irradiation. Irradiation was done in 10 minute intervals, alternating with 350 nm and then 535 nm light. The spectra shown here are only of the solution after the 350 nm irradiation.

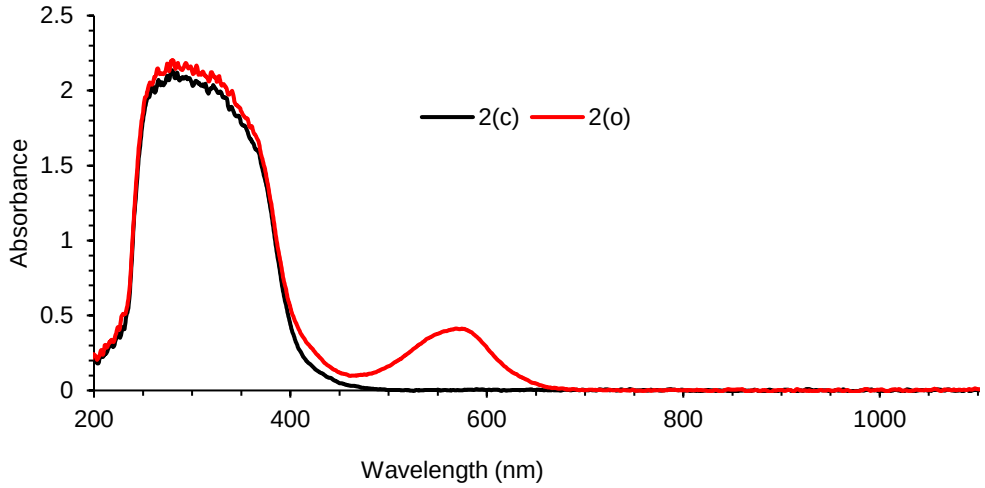


Figure S34. Experimental UV-vis of **2** (0.1 mM in CH_3CN) upon 254 nm irradiation to give **2**(o).

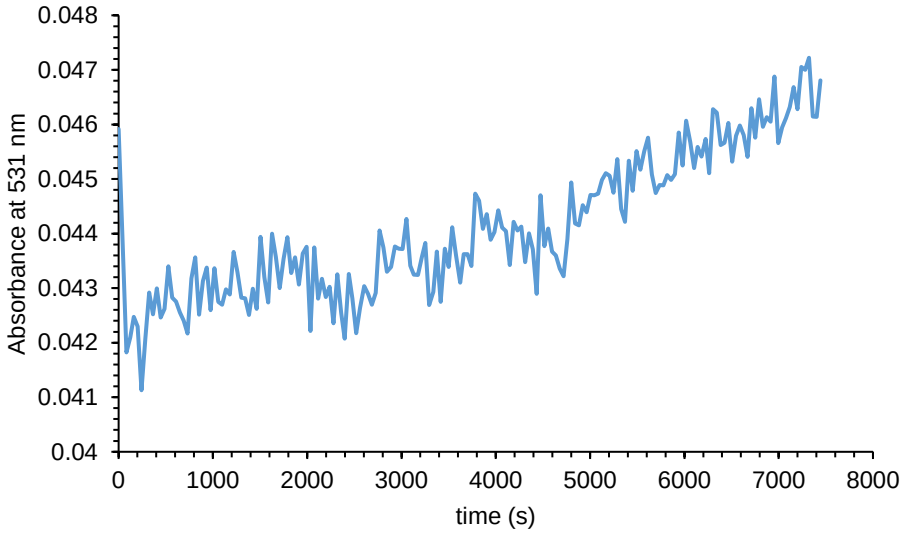


Figure S35. Absorbance of **1**(o) at 531 nm as a function of time at 323 K to demonstrate a lack of thermal isomerization.

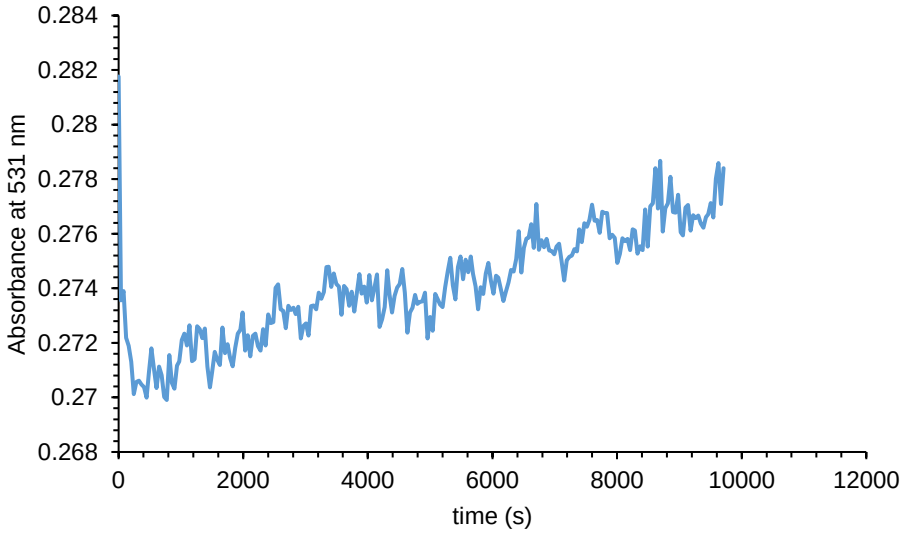


Figure S36. Absorbance of **1**(c) at 531 nm as a function of time at 323 K to demonstrate a lack of thermal isomerization.

S3 Cyclic Voltammetry

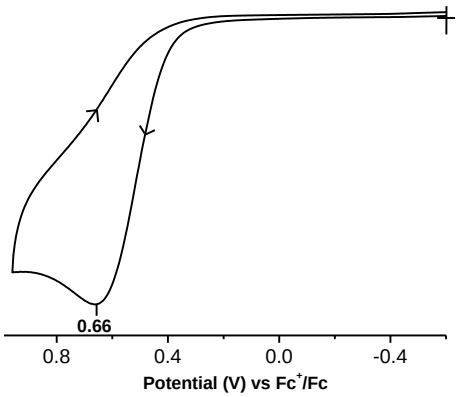


Figure S37. CV (100 mV/s) of a 1.0 mM solution of **3** in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode. Indicated peak potentials are in V vs. Fc^+/Fc.

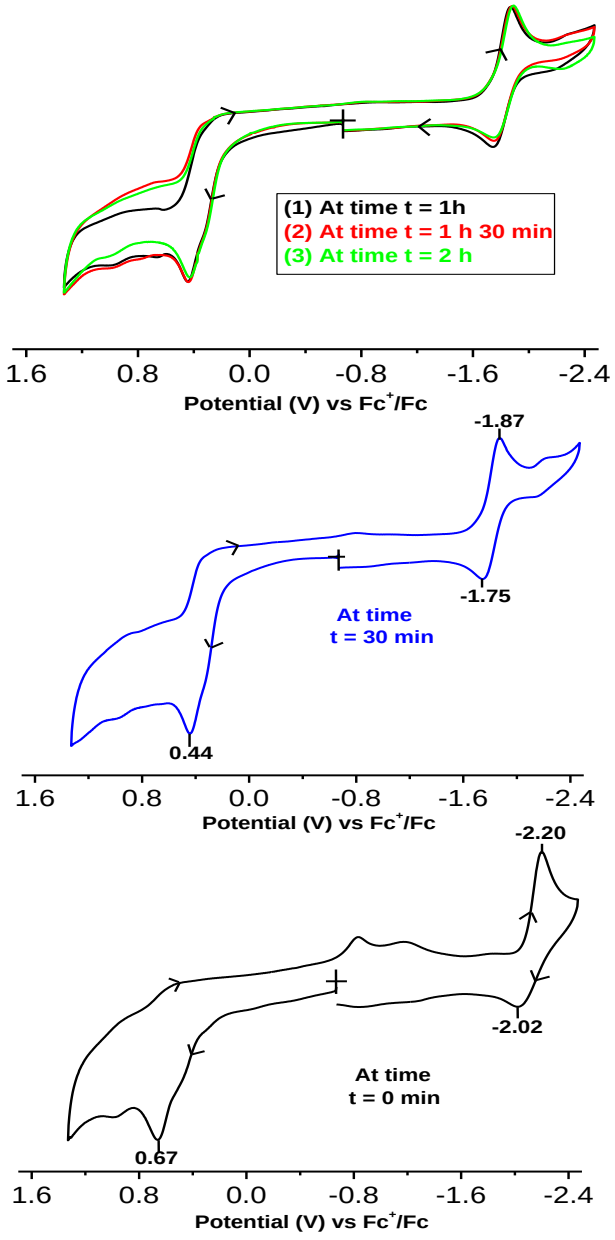


Figure S38. Photoelectrochemistry (100 mV/s) of a 1.0 mM solution of **1**(o) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode upon irradiation of 254 nm light to give **1**(c). Indicated peak potentials are in V vs. Fc^+/Fc.

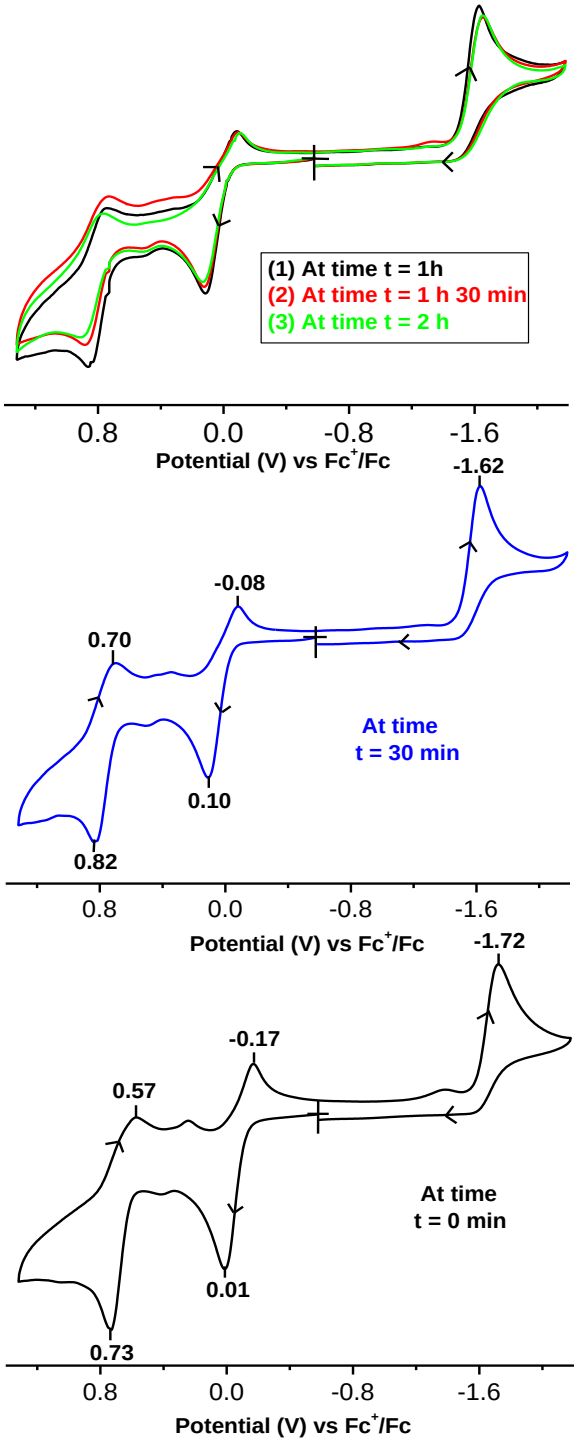


Figure S39. Time dependent CV (100 mV/s) of a 1.0 mM solution of **2**(c) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode upon irradiation of 254 nm light to give **2**(o). Indicated peak potentials are in V vs. Fc^+/Fc.

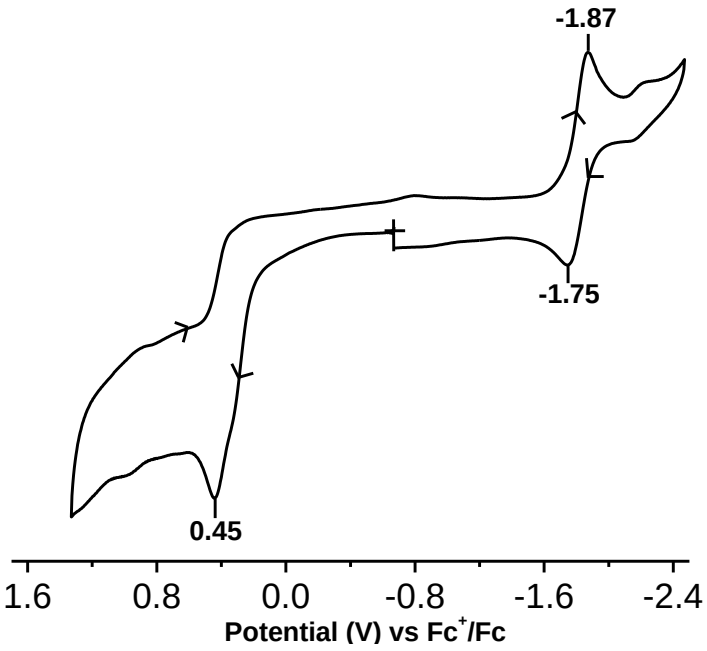


Figure S40. CV (100 mV/s) of a 1.0 mM solution of **1**(c) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode. Indicated peak potentials are in V vs. Fc^+/Fc.

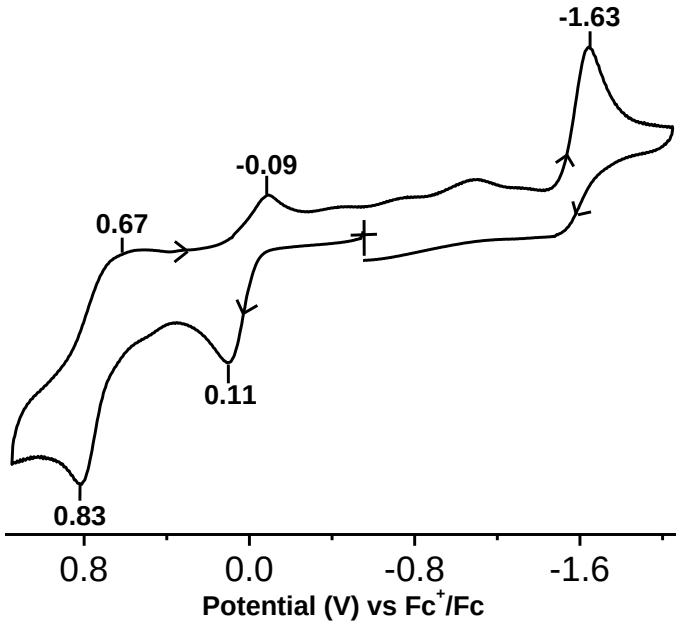


Figure S41. CV (100 mV/s) of a 1.0 mM solution of **2**(o) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode. Indicated peak potentials are in V vs. Fc^+/Fc.

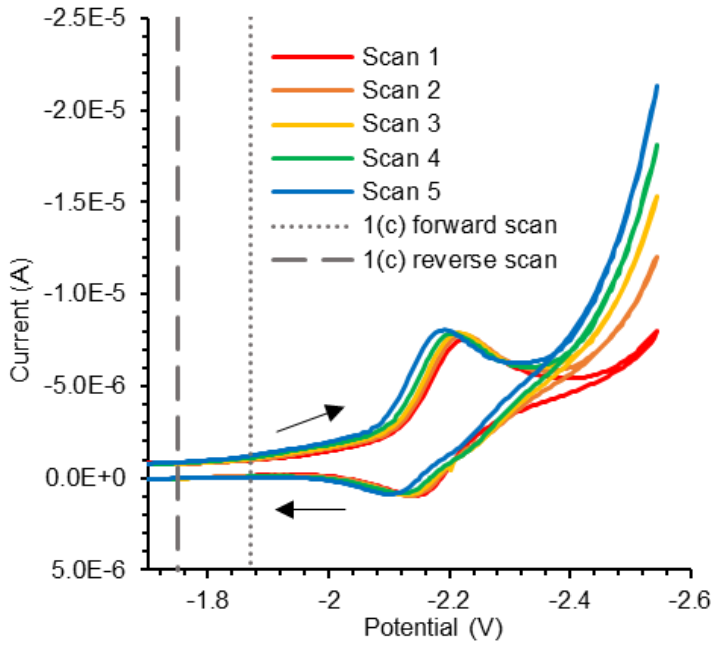


Figure S42. Multiple CV scans of 1.0 mM solution **1**(o) in CH_3CN at 50 mV/s (0.1 M Bu_4NPF_6). Indicated peak potentials are in V vs. Fc/Fc^+. Arrows indicate direction of scans. Vertical bars represent potentials of **1**(c).

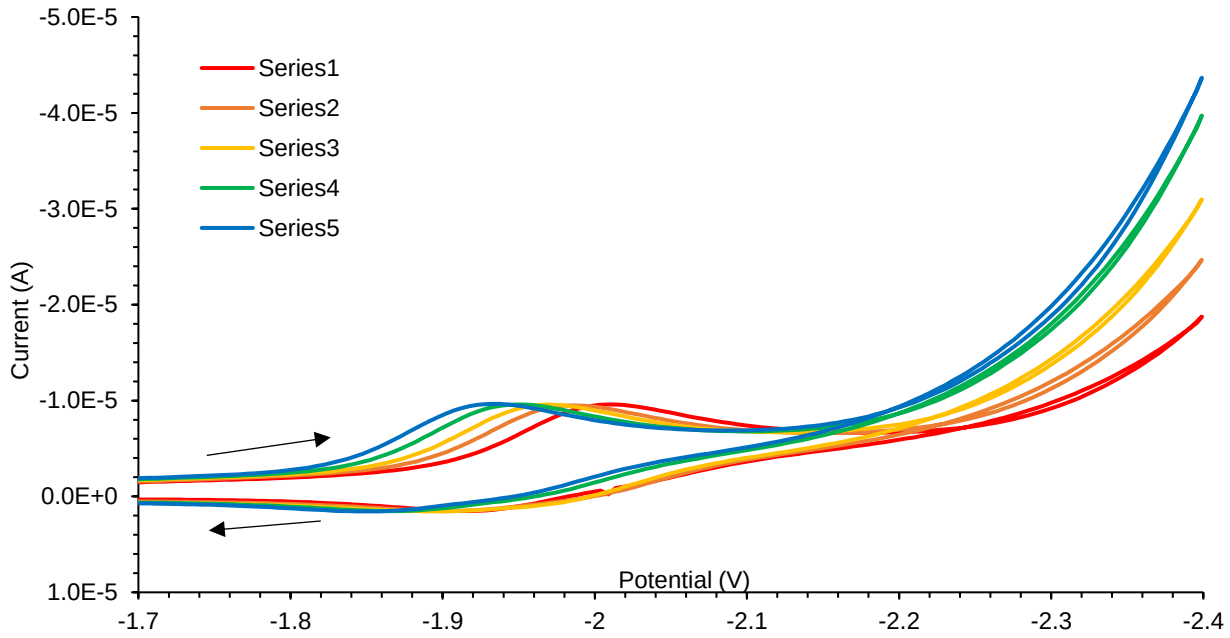


Figure S43. CV (75 mV/s) of a 1.0 mM solution of **1**(o) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode. Indicated peak potentials are in V vs. Fc^+/Fc. Arrows indicate direction of scans and colors are used to depict scan number.

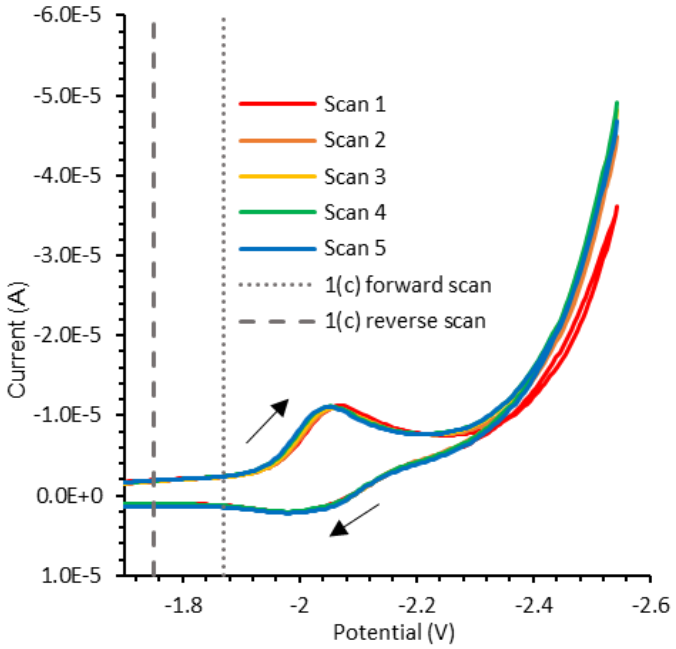


Figure S44. Multiple CV scans of 1.0 mM solution **1**(o) in CH3CN at 100 mV/s (0.1 M Bu4NPF6). Indicated peak potentials are in V vs. Fc/Fc+. Arrows indicate direction of scans. Vertical bars represent potentials of **1**(c).

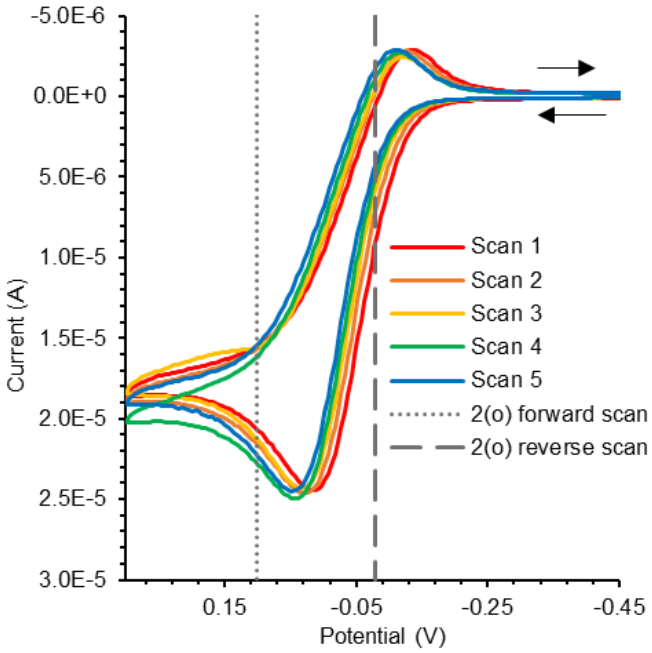


Figure S45. Multiple CV scans of 1.0 mM solution **2**(c) in CH_3CN at 50 mV/s (0.1 M Bu_4NPF_6). Indicated peak potentials are in V vs. Fc/Fc^+. Arrows indicate direction of scans. Vertical bars represent potentials of **2**(o).

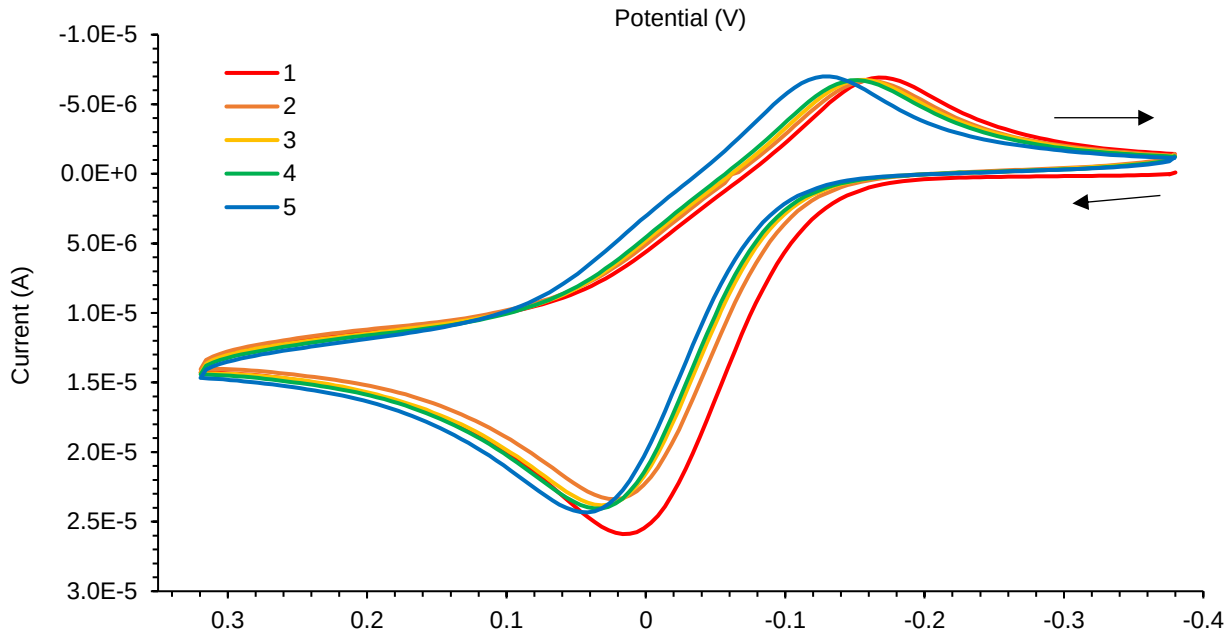


Figure S46. CV (75 mV/s) of a 1.0 mM solution of **2**(c) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode. Indicated peak potentials are in V vs. Fc^+/Fc. Arrows indicate direction of scans and colors are used to depict scan number.

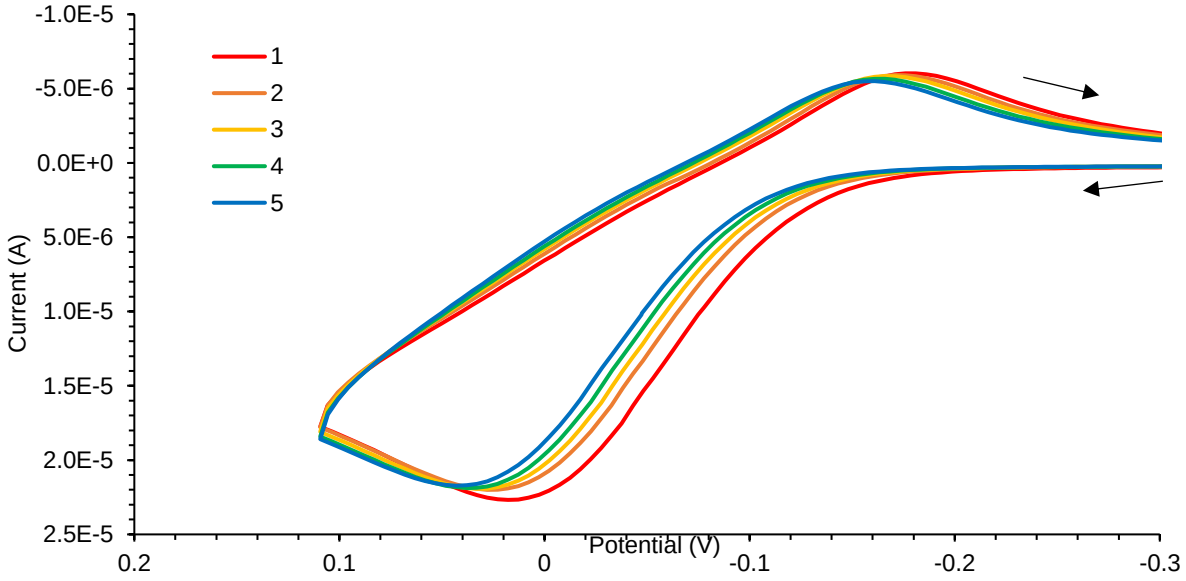


Figure S47. CV (100 mV/s) of a 1.0 mM solution of **2**(c) in CH_3CN (0.1 M in Bu_4NPF_6) at a platinum working electrode. Indicated peak potentials are in V vs. Fc^+/Fc. Arrows indicate direction of scans and colors are used to depict scan number.

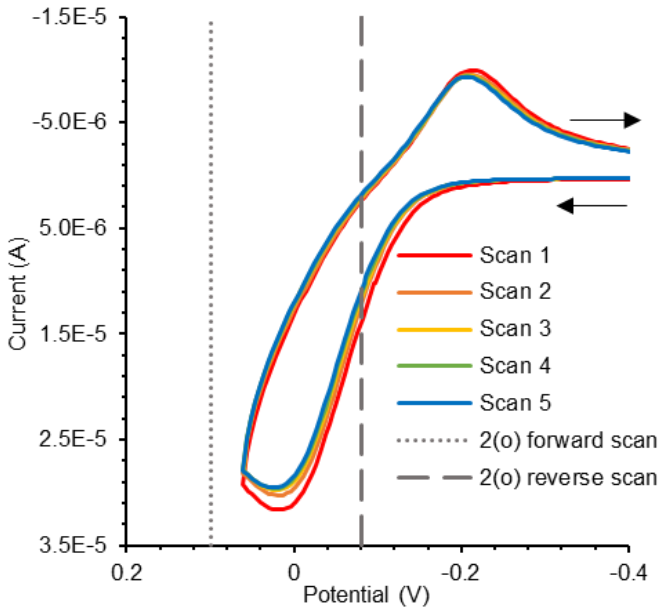


Figure S48. Multiple CV scans of 1.0 mM solution **2**(c) in CH_3CN at 200 mV/s (0.1 M Bu_4NPF_6). Indicated peak potentials are in V vs. Fc/Fc^+. Arrows indicate direction of scans. Vertical bars represent potentials of **2**(o).

S4 Computational Details

Calculations were performed using the ORCA 3.0 quantum chemistry program package from the development team at the Max Planck Institute for Bioinorganic Chemistry.[10] For geometry optimizations the LDA and GGA functionals employed were those of Perdew and Wang (PW-LDA, PW91).[11] In the case of thermodynamic calculations, the hybrid functional (30% HF)[12] of Becke (B88)[13] was used for exchange and Perdew and Wang (PW91)[11] for the correlation. The geometry optimizations employed the Ahlrichs-TZV[14] basis sets (def2-TZV[15]), designated as Default-Basis-3[14] in the Orca 3.0 program. The Ahlrichs (2d,2p) polarization functions were obtained from the TurboMole basis set library under ftp.chemie.uni-karlsruhe.de/pub/basen. Frequency calculations were performed on gas-phase optimized structures and no negative frequencies were determined. Electronic excitations were calculated with TDDFT using the B3LYP[12,16] functional and the Ahlrichs-TZV[14] basis sets (def2-TZV[15]) designated as Default-Basis-4[14] in the Orca 3.0 program. The Ahlrichs (2d2fg,3p2df) polarization functions were obtained from the TurboMole basis set library under ftp.chemie.uni-karlsruhe.de/pub/basen.

Table S6. Relative energies (kJ·mol^{-1}) of different configurations of **1** and **2** before and after isomerisation (PW91, TZP(d)).

Tautomer 1	**Z**	**Z′**	**E**	**E′**
1(o)	1.22	10.66	0*	40.10
1(c)	1.23	10.31	0.31	40.97
$\Delta E_{photoisomerisation}$	0.01	–0.35	0.31	0.87
Tautomer 2	**Z**	**E**	**Z′**	**E′**
1(o)	3.10	1.47	10.17	32.05
1(c)	1.85	–0.06	7.13	27.78
$\Delta E_{photoisomerisation}$	–1.25	–1.53	–3.04	–4.27
Tautomer 1	**Z**	**Z′**	**E**	**E′**
2(c)	0*	11.23	3.28	48.40
2(o)	9.80	23.13	12.12	52.17
$\Delta E_{photoisomerisation}$	9.80	11.90	8.84	3.77
Tautomer 2	**Z**	**E**	**Z′**	**E′**
2(c)	6.87	2.21	8.17	29.00
2(o)	14.87	14.79	27.08	47.19
$\Delta E_{photoisomerisation}$	8.00	12.58	18.91	18.19

*The lowest energy configuration for each photoswitch of Tautomer 1 (consistent with crystal structure of **1**(o)) was chosen as zero. The remaining values represent the energies relative to that species.

S4.1 DFT Optimized Cartesian Coordinates

Table S7. Cartesian Coordinates (in Å) of *Z*-**1**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-1.69322892698206	4.24606294047296	3.13692183283875
C	-1.86347964077352	4.68015894537969	1.82427369662526
C	-0.78491377775167	4.68629680680264	0.93825477151817
C	0.47040162401939	4.27164677071685	1.38643032250671
C	0.65527880280772	3.85234962993586	2.70236757517702
C	-0.43288806690584	3.82310904365921	3.58575440734925
N	-0.29167512989144	3.44245791206494	4.93897733808732
C	0.60757235528827	2.56603593904112	5.53240797971302
C	0.89344130934062	2.87880502589967	7.01792270715134

C	-0.42485925722756	2.96936504949640	7.81653744066216
C	1.64750949176403	4.22051222589555	7.11228416070075
C	1.75566700840817	1.77048277180817	7.63256053101699
N	1.22251521813243	1.57712364506265	4.98293258929056
H	-2.85084577399746	4.99869921181282	1.48799568259568
H	-2.54484972236278	4.21543487918969	3.81992251425775
H	-0.92261242712752	5.00838641602947	-0.09370249718935
H	1.32272815786857	4.27845587555701	0.70618554098007
H	1.64207057784114	3.54912172599767	3.04670456022940
H	-0.19795185821571	3.09822098996391	8.88339549244766
H	-1.05209038669634	3.82789285954637	7.53090279431184
H	-1.02461243018931	2.05567378477308	7.70783896900554
H	1.86398313040297	4.45800820605383	8.16332742457052
H	2.60307116527941	4.17065870235919	6.57337431437673
H	1.06667953562362	5.05313767064384	6.69254637581159
H	1.25483881090344	0.79632794595951	7.57748542740178
H	1.95381480748463	2.00321268588102	8.68844765756397
H	2.71253429462317	1.67486788903714	7.10857780490356
C	0.94745235586771	0.99394351591099	3.74847125909979
C	-0.35209966828645	0.62290952251982	3.34781206023812
C	-0.56513031494868	-0.06483623377237	2.16010063870012
C	0.51419760651750	-0.38532778592363	1.32601007884130
C	2.02382092140738	0.62910965594692	2.91712196125075
C	1.81334674290036	-0.03117448712176	1.71297601549756
N	0.28602959062136	-1.07131057109300	0.09951069403275
H	-1.57594630097228	-0.33970335203091	1.86594512420022
H	-1.20054210632173	0.86755410978625	3.98684975280916
H	3.03621438872495	0.87838148094524	3.23604722303128

H	2.65960230986359	-0.29936877921327	1.08463936390686
C	-0.73742277601885	-0.73548907684618	-0.81830205203413
C	1.06086718805632	-2.17165607588002	-0.35693041766142
C	0.40557546986326	-2.66381617070263	-1.61456413039561
C	-0.55999217547391	-1.63443677318589	-1.99777129884821
C	0.52027248342335	-3.94675052191065	-2.06890863655730
C	1.52381147646214	-4.92891737004211	-1.54083286442675
C	-0.40778586297516	-4.51198285498738	-3.10262009769227
O	-1.55426224104722	0.15839881559402	-0.66684243053610
O	2.03488791206029	-2.60513170938264	0.23726031600694
C	-1.20698084800218	-1.27636543505642	-3.14665368802598
C	-1.06005788830272	-1.67804542509044	-4.51715612929149
H	1.00555832119030	-5.77031274598066	-1.05279340470200
H	2.08145493067330	-5.37070820590313	-2.38283528234272
H	2.22938677379989	-4.49060207684242	-0.83399022671250
H	0.06905679868573	-4.55636725735958	-4.09441319410501
H	-0.66464222439780	-5.54791016433735	-2.83750237174738
H	-1.33133233185683	-3.93530066601302	-3.20910177566147
H	-1.96367889789615	-0.50042352590050	-2.98706501663610
N	0.15096784767413	-2.06322750680724	-5.12145383570027
C	-2.08472581535659	-1.73620270965864	-5.46900234056643
C	-0.10007268099731	-2.36331313125134	-6.44472640808636
C	1.48764031608762	-1.82850585047485	-4.60380006366648
C	-1.49585903285809	-2.19226819902720	-6.68699582060007
C	-2.00496831834403	-2.46163336489598	-7.97138217192831
C	-1.13031154073819	-2.86405942644615	-8.97227791518658
C	0.24975123553310	-3.00542272726356	-8.71752593925131
C	0.78395602860418	-2.75449012037473	-7.45666335765551

C	-3.53368773960856	-1.46004866226322	-5.24110836082364
H	1.99639549937335	-2.76706855005592	-4.34220930950281
H	2.08825728684522	-1.29775678380389	-5.35457759485731
H	1.42901230354526	-1.20969428590900	-3.70545449089786
H	1.85070925196002	-2.87878115226926	-7.26885795568409
H	0.91230160576173	-3.32269524477162	-9.52337299575970
H	-1.51148679100292	-3.07359834690286	-9.97215174780091
H	-3.07032326651447	-2.35189160936666	-8.17907525332045
H	-3.70056927891642	-0.83710150911564	-4.35349801539137
H	-4.11132379803444	-2.38673783383424	-5.09670084987333
H	-3.97434484248171	-0.93951781759652	-6.10277895964748
H	-0.85110179581566	3.98718044692085	5.58852250205779

Table S8. Cartesian Coordinates (in Å) of *Z*′-**1**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.61307112645106	5.50110014820558	3.69154018911386
C	0.03424508237797	6.76796354061752	3.62033260848030
C	-1.28644376343805	6.96034670582532	4.03122035881770
C	-2.03118012013342	5.87448997282395	4.49546048416578
C	-1.45910580607689	4.60323655314108	4.55464122411488
C	-0.12436174521856	4.41087540439922	4.17351301483993
N	0.46352725242528	3.10972274632366	4.15489231520161
C	0.75788910828007	2.20857101344808	5.16858145688908
C	0.96667450788514	2.68236527663193	6.62043749780023
C	-0.38448707769912	2.98129757696558	7.30512635888487
C	1.86466055222023	3.93281388861618	6.66783628609318
C	1.65704385920407	1.56086863462385	7.41518949662926

N	0.97076001069740	0.96045817257794	4.90220035664421
H	0.61921259201270	7.60866120797647	3.24581745029399
H	1.64729874340662	5.34282723694431	3.38447864587935
H	-1.73761688464971	7.95151102823725	3.97907675587912
H	-3.07041729920528	6.01227137399628	4.79618475631824
H	-2.05098679688494	3.74671227366128	4.87591716577476
H	-0.21426540082846	3.16231310040545	8.37578563611554
H	-0.87411895762801	3.87016540206831	6.89388646203355
H	-1.07040292615662	2.12772510009674	7.21547353316298
H	2.07231302070176	4.19054997763985	7.71572703888100
H	2.82715687751620	3.74687185105946	6.17161964726085
H	1.39948683048738	4.80653305462863	6.19839570367467
H	1.05482342128265	0.64620442023504	7.43008145462189
H	1.80973863591596	1.89994422933799	8.44966376884877
H	2.63206797030555	1.30486040057233	6.98390411676907
C	0.75440420637358	0.42256005045640	3.63132790532323
C	-0.54570370730904	0.22426932619521	3.11986780741089
C	-0.74713476965168	-0.39949484474206	1.89364977857201
C	0.34871968563343	-0.82957972045084	1.13450407199999
C	1.84325290193104	-0.03009426844122	2.86091412199143
C	1.64665283454395	-0.63809851464449	1.62589826747791
N	0.13730291852202	-1.45501823972806	-0.12671640973924
H	-1.75744011620048	-0.54589917246480	1.51728909226471
H	-1.40302574280019	0.54611389162795	3.71237511057552
H	2.85200703508108	0.09884644820209	3.25344467607074
H	2.50141254194916	-0.98328658119772	1.04856126377609
C	-0.76086651698448	-0.97358564245208	-1.10811634139800
C	0.80730207937688	-2.63204430051605	-0.55768427442577

C	0.19972966167344	-3.00975402349122	-1.87722568818175
C	-0.60221997259074	-1.86096915384150	-2.29834338632557
C	0.19715907941392	-4.28571369757955	-2.36451104081698
C	1.03363304614360	-5.39378590878068	-1.79622229603059
C	-0.70550846912981	-4.71046166579114	-3.48410883904454
O	-1.46928422425711	0.01336460079664	-0.98946585792135
O	1.67190675742506	-3.19352188423596	0.09534431280990
C	-1.10891129875967	-1.39995992993944	-3.48078997391212
C	-0.90297790289162	-1.78612790955205	-4.84816254145559
H	0.38354800300460	-6.18087998274387	-1.38095635530105
H	1.60289525389088	-5.87528606187202	-2.60819276192108
H	1.72544914598109	-5.06108676637947	-1.02157836004717
H	-0.15452568735842	-4.80500798496600	-4.43322401360889
H	-1.11479941571430	-5.70762995852406	-3.26566586376359
H	-1.53462107876157	-4.01759278288177	-3.65400066614513
H	-1.77688171031627	-0.54103466197633	-3.35434055352821
N	0.29771394154629	-2.30259081813584	-5.36968919977666
C	-1.84834496167811	-1.69913355777218	-5.87685043582993
C	0.11856286232383	-2.54154030629853	-6.71681375261247
C	1.60820245308827	-2.23779334548815	-4.74630614399438
C	-1.22296953336364	-2.19739186569232	-7.05964993438003
C	-1.65671335163539	-2.37473514965008	-8.38695989407150
C	-0.75929830252182	-2.85846977169664	-9.32999269304322
C	0.56939830662065	-3.17162297533918	-8.97494486687881
C	1.02767803732711	-3.01458307623908	-7.66983044979439
C	-3.26714300221346	-1.25261665471013	-5.75468625998545
H	1.98742293669150	-3.23605177490841	-4.48571587895445
H	2.32099083576123	-1.75584282716663	-5.42887797569142

H	1.54886540683035	-1.64503931819479	-3.83078949907162
H	2.05388666956005	-3.27037697865009	-7.40494716457828
H	1.25143968286370	-3.54914780591187	-9.73736288386032
H	-1.08165426294747	-2.99814734474543	-10.36220529805400
H	-2.68122174320361	-2.13133642084188	-8.67221235592363
H	-3.44132269523184	-0.67512939196010	-4.83858032268625
H	-3.96526613158984	-2.10452530945776	-5.73588519872939
H	-3.55547899107684	-0.62274724837350	-6.60795481106205
H	0.48723149137967	2.67834099008737	3.22940405108391

Table S9. Cartesian Coordinates (in Å) of *E*-**1**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-7.26458720737628	1.19708684399878	-1.10212466143067
C	-8.23182328159712	1.09436093527746	-2.10368252273358
C	-9.56180884341093	1.44218564581486	-1.87025896879520
C	-9.92849944149543	1.90417107900918	-0.60335085469162
C	-8.97780878394769	2.01242793217503	0.40480084688621
C	-7.63287467908923	1.66127285846235	0.17218196621758
N	-6.75253933165336	1.80649464871374	1.25941108520701
C	-5.39799696144033	1.56584751394659	1.37955954224931
C	-4.80913307423570	1.87929276663877	2.78957033935256
C	-5.85911575205328	2.37244175319711	3.80438043919867
C	-3.74075772421950	2.98215171852671	2.65250369690004
C	-4.17303279732586	0.59821382569229	3.36319805987509
N	-4.75525092959615	1.11876620095533	0.36049229003647
H	-7.92902136520035	0.73156140549166	-3.08688854724033
H	-6.23155027355871	0.92469225031076	-1.28973042424552

H	-10.30522627147230	1.35587757927495	-2.66283287417268
H	-10.96262546724240	2.18251228906283	-0.39660813038151
H	-9.27741292416517	2.37491883578235	1.39198489020024
H	-5.35958820188048	2.55787665400635	4.76427872568802
H	-6.32384157218780	3.32481383676922	3.50813535813061
H	-6.64508359267603	1.62797564057767	4.00054573364935
H	-3.34138635263509	3.23262654574107	3.64572955854439
H	-2.90201775280697	2.66388202989736	2.02576335140458
H	-4.16640817690418	3.89775110600803	2.21876791281906
H	-4.91439780446002	-0.20779233476766	3.45387129368847
H	-3.77254321040914	0.80447708043230	4.36600192230822
H	-3.34846446382825	0.23686686245801	2.74110649402943
C	-3.41904723386397	0.80058316908172	0.17798326202207
C	-2.50993919918902	1.75254385803798	-0.33099158863232
C	-1.20045598682210	1.40394055045897	-0.63871008843037
C	-0.75822150152988	0.08743147138725	-0.45964226896037
C	-2.96735233487431	-0.52970798250957	0.31122237077880
C	-1.65563034839747	-0.87881737209726	0.01203338667869
N	0.59010932668008	-0.25711846892909	-0.75862530107416
H	-0.51324984716449	2.15937061345068	-1.01435549821520
H	-2.85163718139771	2.77485275252699	-0.49340274341104
H	-3.66717815027374	-1.29143936296048	0.65515349565780
H	-1.33062197247720	-1.91057406970482	0.12778495629558
C	1.70927972557948	0.50087216462731	-0.34160729993272
C	0.97752238343018	-1.40542894108340	-1.49949233923476
C	2.46484515874001	-1.31347600783195	-1.68172191819734
C	2.91967588936975	-0.25732854198625	-0.77736173652244
C	3.13356080070710	-1.90817821200667	-2.71330290405380

C	2.52370028953524	-2.94317112458002	-3.61194278760111
C	4.53433796572337	-1.52151115891825	-3.08373307906542
O	1.65666779852523	1.53905458683402	0.29822297167614
O	0.18866725251302	-2.24187489764943	-1.90932685134498
C	4.10675109947287	0.09584347522807	-0.20019776036461
C	5.38533347809860	-0.55281134881204	-0.11923506446234
H	2.47065406510119	-2.56088376982745	-4.64418779127298
H	3.18330629669890	-3.82535829726282	-3.65455994174802
H	1.52665309591860	-3.25578478502146	-3.29899555891736
H	5.26483179816494	-2.27013773755600	-2.73823763269475
H	4.62670107811761	-1.48447466399326	-4.17898546115046
H	4.83508098339857	-0.55435056371985	-2.67046287341222
H	4.05453288802627	1.04934075822008	0.33613110743546
N	5.58345872538037	-1.94504050010450	-0.07002500520404
C	6.62832860503364	0.08824405361703	-0.06327298007489
C	6.93902392492101	-2.18801547278866	0.01646313027837
C	4.57940277554409	-2.95013541870088	0.23186763247425
C	7.62178123609490	-0.93533098793955	-0.00195256368792
C	9.02801456174353	-0.92161871269322	0.05495802938848
C	9.71026645919815	-2.12770656875592	0.14981191563124
C	9.01512613590205	-3.35433642334933	0.18889418587696
C	7.62513751075693	-3.40274231015274	0.12715283500404
C	6.88411441437021	1.55672183277394	-0.13676877342733
H	4.37875940394649	-3.60072287355624	-0.63117910233796
H	4.91702516178087	-3.57128894664581	1.07210361362686
H	3.64487104855004	-2.46056045968215	0.51518852724236
H	7.09973432451698	-4.35780624997347	0.14646847951825
H	9.57782145193384	-4.28531514985204	0.26423025483450

H	10.79962325857320	-2.13120072370535	0.19686286798483
H	9.57404470463782	0.02247915161069	0.02966147859974
H	5.98015009781977	2.14424232184884	0.06476412179026
H	7.25073151392209	1.85978021386155	-1.13031681909260
H	7.64988485744725	1.85937900618284	0.59143347294674
H	-7.20135955301660	2.15684862114889	2.09741811408789

Table S10. Cartesian Coordinates (in Å) of *E'*-**1**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-7.828311478	3.887128344	1.39562883
C	-8.958756669	4.417018476	2.019022
C	-9.968275206	3.570947661	2.481916455
C	-9.844496958	2.19016566	2.313512562
C	-8.708318801	1.657290841	1.704932319
C	-7.681114766	2.500813624	1.25873812
N	-6.5659922	1.947757791	0.559575535
C	-5.259672876	1.610506857	0.907652361
C	-4.670275482	2.070601925	2.267666475
C	-5.677133096	1.886186469	3.423992608
C	-4.258853242	3.554488669	2.173652385
C	-3.426811585	1.240843385	2.637456629
N	-4.676144662	0.907009938	-0.003812643
H	-9.059276042	5.497706804	2.125563121
H	-7.059023091	4.545718182	0.99416651
H	-10.85427448	3.987000555	2.962226316
H	-10.63477727	1.523537432	2.660547655
H	-8.598404601	0.578958772	1.583344329

H	-5.155792682	2.073620255	4.372713867
H	-6.525407343	2.573619315	3.377523579
H	-6.068091394	0.860198338	3.457592581
H	-3.81354674	3.870991639	3.127790944
H	-3.510530368	3.710951331	1.386596045
H	-5.115047525	4.207879649	1.972064735
H	-3.64575168	0.165458493	2.65101254
H	-3.103195385	1.53132126	3.646346305
H	-2.583936365	1.405145229	1.960951331
C	-3.355475063	0.572151041	-0.227308174
C	-2.404569416	1.532349924	-0.636656083
C	-1.105074424	1.16486859	-0.963746583
C	-0.711889962	-0.177513925	-0.893462649
C	-2.953055756	-0.779561631	-0.207405769
C	-1.650336879	-1.148148169	-0.516162653
N	0.627740837	-0.545178995	-1.203889441
H	-0.386167776	1.924488647	-1.264110043
H	-2.705669967	2.577810355	-0.711768284
H	-3.68414561	-1.53901865	0.070137204
H	-1.361501916	-2.196378181	-0.482483804
C	1.766822699	0.141320841	-0.722290282
C	0.98624629	-1.652363793	-2.018395176
C	2.478960112	-1.60547631	-2.17146921
C	2.956256373	-0.630028379	-1.191642315
C	3.143921829	-2.157628956	-3.228840564
C	2.511406387	-3.105150692	-4.205091881
C	4.565763936	-1.804644016	-3.549546874
O	1.742748409	1.135686312	-0.014501351

O	0.175315629	-2.42809706	-2.49876606
C	4.145503749	-0.361448163	-0.574794772
C	5.39595701	-1.065102889	-0.515887247
H	2.482710943	-2.647973303	-5.207561503
H	3.142421482	-4.003371636	-4.305143408
H	1.500617848	-3.404785413	-3.925364427
H	5.260338789	-2.599023335	-3.23342257
H	4.683048419	-1.708493748	-4.638799144
H	4.893508073	-0.875016856	-3.07506185
H	4.120652055	0.556833394	0.021884681
N	5.537475719	-2.464680451	-0.549739701
C	6.662272013	-0.480357147	-0.400107681
C	6.880251876	-2.768013474	-0.457395589
C	4.487870465	-3.444229246	-0.33047616
C	7.612867064	-1.545583619	-0.386794973
C	9.017298518	-1.594037548	-0.30734849
C	9.648583747	-2.830884236	-0.277901787
C	8.90416381	-4.027875374	-0.326968553
C	7.51469843	-4.0146043	-0.412962914
C	6.975547578	0.978742153	-0.379921499
H	4.278096742	-4.029677056	-1.236918929
H	4.78349111	-4.131148055	0.473651528
H	3.568627646	-2.934901179	-0.03226447
H	6.95067531	-4.946324795	-0.462198762
H	9.427406864	-4.984211399	-0.301994175
H	10.73593088	-2.882189306	-0.214505046
H	9.601684196	-0.673747804	-0.265120489
H	6.102958599	1.5847519	-0.106129464

H	7.321839093	1.33873236	-1.361699722
H	7.775038003	1.198672864	0.34137703
H	-6.797620772	1.507597815	-0.331403418

Table S11. Cartesian Coordinates (in Å) of *Z*-**1**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-1.45747586661691	4.57155252413720	3.52523725635406
C	-1.73875462726756	5.16065275945721	2.29479837100225
C	-0.75696584193796	5.22726073865944	1.30459791379938
C	0.51422945114868	4.71410182280525	1.56809206019775
C	0.81131379779552	4.13865646137239	2.80188310690149
C	-0.18087585095354	4.05059676437754	3.78877678366513
N	0.07227382212337	3.51305420121937	5.06863209875222
C	1.01931072749521	2.57965601018671	5.47855049769904
C	1.45314577648940	2.74383607567375	6.95175022096364
C	0.22038219726582	2.70176249878715	7.88114887742716
C	2.18216586440667	4.09176405981041	7.12036257720952
C	2.39822134300369	1.60564178349691	7.35289719668514
N	1.56011215849419	1.64492667345312	4.77797706554816
H	-2.73773440916233	5.55467765788454	2.10447990969016
H	-2.23602075324598	4.49614540022516	4.28755688662532
H	-0.98200602515376	5.67181075148006	0.33529648059125
H	1.29210737992019	4.76520654269899	0.80546462243285
H	1.81098127670567	3.75855475455738	3.00154192934185
H	0.54977034517100	2.73211465654137	8.92853941560979
H	-0.45968322276849	3.55731317489038	7.74706509698919
H	-0.35885295733165	1.77997105075420	7.73616720332804

H	2.50271345915031	4.21947535369216	8.16389740930040
H	3.07651986836463	4.13479244222310	6.48446389504619
H	1.54280155014080	4.94610031875965	6.85924772027514
H	1.91676556075040	0.62690912141259	7.24020821992937
H	2.69748285276477	1.73067036808263	8.40333400880558
H	3.29873795077829	1.59815126709730	6.72944794598385
C	1.15083815679156	1.18736654316771	3.52456041267290
C	-0.19135573442706	0.89471654292974	3.21156746403788
C	-0.53362069390664	0.31869413068870	1.99385324505972
C	0.45264493401013	0.04816498656175	1.03573775460845
C	2.13376261729464	0.87007503378244	2.56875541855987
C	1.79172506473941	0.33413283925293	1.33274791594177
N	0.10149703125993	-0.51875124606636	-0.21866318269455
H	-1.57583184451283	0.09585007221640	1.77378397446897
H	-0.97104582333224	1.10416480626836	3.94411643759153
H	3.17919763324024	1.05872624772824	2.81480801361154
H	2.56852559860916	0.10499669196084	0.60606391305719
C	-1.00185731772809	-0.14950068946629	-1.00068369029716
C	0.82125395436006	-1.59078153208458	-0.86853263244044
C	0.14757934129446	-1.83176280023188	-2.15293425544474
C	-0.94721362797496	-1.01830372508535	-2.22320150994215
O	-1.83819849222124	0.70086928237707	-0.74007741512763
O	1.78049239526449	-2.16118681787886	-0.37028558646492
C	-1.93602595648051	-1.07743422489256	-3.24362805321867
C	0.40376104796665	-2.94492521775157	-3.15701372603037
C	-1.63126985588739	-1.88967181595286	-4.30092499028654
C	-0.22126231843377	-2.45856454782853	-4.52041968567318
C	1.90396789025748	-3.25663249544706	-3.28057051795560

C	-0.32724487629484	-4.20687863043686	-2.64075514019466
N	-2.44427179783991	-2.30837678821780	-5.32177991541829
C	-0.49309870671715	-3.49513385946096	-5.60449141872543
C	0.61029478324898	-1.31184605922802	-5.15886814102577
C	-1.81144924034283	-3.31855258049425	-6.06969199941564
C	0.32292532467651	-4.42525395458547	-6.23357616875677
C	-2.33756986614747	-4.06924369689073	-7.11844071628619
C	-1.50447906124408	-5.02074143994196	-7.71950056127202
C	-0.19044731176019	-5.19809495745342	-7.28755700371215
C	-3.83847299550321	-1.94231644499917	-5.45657759697748
H	-2.88815992457904	-0.56526236216566	-3.11566259619738
H	2.48765594893623	-2.38344366696284	-3.59495568950130
H	2.29180366659748	-3.56567158274968	-2.30414234176443
H	2.08194913236067	-4.07300873977627	-3.99163125574064
H	-0.18605435928369	-5.05429951003192	-3.32432355429402
H	-1.40584985641925	-4.02836436484873	-2.53275172914611
H	0.07267299906701	-4.48862737323080	-1.65883634219055
H	0.78344055533672	-0.50482379795956	-4.43639280508062
H	0.07737566030989	-0.89759920997463	-6.02390224527470
H	1.57751863303893	-1.68777163538715	-5.51170392026943
H	1.35776301022855	-4.56250854215915	-5.92260159871574
H	0.44471529453472	-5.94041100497073	-7.77072192771922
H	-1.89330984968255	-5.62691697477282	-8.53811818283432
H	-3.36237509211047	-3.93639702147794	-7.46403705785036
H	-4.13645191088214	-2.00089891419815	-6.50912190414715
H	-4.49231198183008	-2.60068064258558	-4.86346165362013
H	-3.98020203673925	-0.90953551698454	-5.12044486011239
H	-0.41461096867349	3.98705397396062	5.82359525205518

Table S12. Cartesian Coordinates (in Å) of *Z′*-**1**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.98185705692282	5.62746574901779	4.03797691739371
C	0.48063453251374	6.92733048393649	4.11559659074447
C	-0.82642848040993	7.15009059515724	4.55301499049229
C	-1.63506010160248	6.06524556130712	4.89840325276549
C	-1.13857597717462	4.76426587272665	4.81341594335948
C	0.18115754800059	4.53616227679105	4.40002485099140
N	0.68088917414556	3.20826224187642	4.22747482943830
C	1.04528311258417	2.22101074272880	5.13327001305742
C	1.39112425505865	2.56844092502383	6.59369797155409
C	0.14085382595960	3.01829534579213	7.37838186456552
C	2.46373057725132	3.67486741822938	6.63741614492951
C	1.95619272391297	1.31839147316187	7.28668038247887
N	1.19753070245744	0.99552791480265	4.74858986036170
H	1.11420842708201	7.76864391312199	3.83260711369325
H	2.00089284984546	5.44251891168335	3.69720575759637
H	-1.21804894778969	8.16586350025883	4.61443599157558
H	-2.66317578076668	6.23062631992717	5.22266950545335
H	-1.77337170503812	3.91230807694195	5.05695673157361
H	0.39903060682168	3.11732225463139	8.44218981492207
H	-0.24516178718192	3.98566713315093	7.04130646605273
H	-0.66415876106515	2.27427355244589	7.29926115055347
H	2.76458742559609	3.85095709402374	7.67973945451202
H	3.35910962046508	3.37512419562019	6.07557521151358
H	2.10270564297645	4.62599871533759	6.23049734694621

H	1.22985359094011	0.49804104275279	7.29281674321768
H	2.20940655842624	1.57231239578442	8.32601786801066
H	2.85898332660468	0.95204651488839	6.78523057382108
C	0.88606131899758	0.59203492570257	3.44416780422555
C	-0.44500748571921	0.36472786097031	3.04018996430032
C	-0.73791929979750	-0.12647786485280	1.77156998821104
C	0.29286259896648	-0.38097456164927	0.85738974255660
C	1.91136460458285	0.31431347295715	2.51996985202645
C	1.62078704678013	-0.15227434462724	1.24184865077860
N	-0.00467720906418	-0.86876674320013	-0.44312742064814
H	-1.77232425311640	-0.30200317074587	1.48289894245558
H	-1.25241136261269	0.55187215674801	3.74965372739265
H	2.94718887502479	0.46710216046574	2.82433043330121
H	2.42927932055387	-0.36096323710955	0.54413041099496
C	-1.05720108087673	-0.42813624766821	-1.25658492096999
C	0.71779901530282	-1.92781091260554	-1.11293918607929
C	0.09930741605834	-2.08587961729938	-2.43681006893818
C	-0.96957263587523	-1.23893776598515	-2.51615684505097
O	-1.87918606572239	0.43576813696987	-0.99311141699322
O	1.63667889306290	-2.54829617001323	-0.59907780153613
C	-1.91410146974468	-1.22279904086552	-3.57866269942042
C	0.37216407873243	-3.15769067355935	-3.48045801798984
C	-1.58819414019139	-1.99832290752602	-4.65728817849776
C	-0.18608457889305	-2.59762762127821	-4.84444577899056
C	1.86988691370504	-3.49584734852187	-3.55857698165617
C	-0.40419375583911	-4.42531028171415	-3.05172569116405
N	-2.36877720972360	-2.34962224756479	-5.72724403073801
C	-0.44063861073704	-3.57962576542441	-5.98239144334297

C	0.69997620943386	-1.44857534380980	-5.40068129077837
C	-1.73292448654151	-3.34490726437189	-6.49230354290051
C	0.37431457363394	-4.50637738263838	-6.61788109518308
C	-2.23624015397763	-4.03430761613891	-7.59296084949462
C	-1.40591757729055	-4.98380716637319	-8.20088591064648
C	-0.11644526202123	-5.21815505832851	-7.72432348933005
C	-3.74556263638298	-1.93897648695709	-5.90606468510065
H	-2.85615967278227	-0.68864120594124	-3.46713002934162
H	2.48262364850765	-2.62113731680621	-3.80636704768179
H	2.21090425746093	-3.86061501942072	-2.58393521845561
H	2.06134525700100	-4.28016549037271	-4.30149733974265
H	-0.25189291375376	-5.24368721501925	-3.76747516788113
H	-1.48259078391917	-4.22868033348859	-2.97861239044930
H	-0.05006066144389	-4.75965598705794	-2.06876988133960
H	0.86548966001032	-0.67709441951843	-4.63851531610252
H	0.21280078798464	-0.98397068302245	-6.26713252526710
H	1.67020857500024	-1.83647581199428	-5.73142850290074
H	1.39089090302764	-4.68834965919504	-6.27177819448762
H	0.51717168377756	-5.95809298642617	-8.21311830294257
H	-1.77712374621092	-5.54304681114544	-9.06007839648640
H	-3.24191115330385	-3.85633947434455	-7.97278488884122
H	-3.98988464265857	-1.91809066387695	-6.97397013278333
H	-4.44363708035272	-2.61935869824307	-5.39395783835891
H	-3.88120566473715	-0.92836040518360	-5.50676274303091
H	0.56868293914833	2.84137108695141	3.28041540372565

Table S13. Cartesian Coordinates (in Å) of *E*-**1**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-7.06837268910300	1.65021213235061	-0.52836405661890
C	-8.02216468225027	1.66462608859086	-1.54786750302325
C	-9.34829685439072	2.01758095144520	-1.30047779951127
C	-9.72487119192247	2.36386488860449	0.00014552431694
C	-8.78786079029282	2.35471064378123	1.02656367549534
C	-7.44648649439054	1.99846063761759	0.77972238284893
N	-6.58005367408409	2.02153255242984	1.88645215562401
C	-5.23225830949198	1.73556111176304	2.00233081752561
C	-4.66370146837923	1.89368548242243	3.44678749226632
C	-5.71519000066043	2.33346140986842	4.48434743903414
C	-3.54991880893314	2.95939105122725	3.43439846022076
C	-4.09184362285647	0.53965482279778	3.91047380552601
N	-4.58408855282546	1.37622166187004	0.95296333982889
H	-7.71173789887624	1.39151918185781	-2.55742924570490
H	-6.03807258234762	1.37464593549575	-0.72629010524098
H	-10.08089026795690	2.02381914812863	-2.10772880917641
H	-10.75628615952370	2.64328355008038	0.21903234908295
H	-9.09524614405753	2.62771592893235	2.03986078487861
H	-5.22707302475870	2.41564739832845	5.46455297425226
H	-6.14166524802484	3.32381621298830	4.26564128009359
H	-6.52943378505685	1.60306777500863	4.60305404665920
H	-3.16299907402266	3.09827416589816	4.45409177369992
H	-2.71178381415080	2.66770425703800	2.79438513624303
H	-3.93047382815153	3.92838325699855	3.08220993213103
H	-4.86685555994102	-0.23939195891187	3.91447232665746
H	-3.70354358043590	0.63638377778392	4.93465689141435
H	-3.27073180448297	0.20265777980600	3.27039311948086

C	-3.24770032162320	1.04222319806335	0.76969720162407
C	-2.30936809019155	2.01119080918202	0.35886109625299
C	-1.00274807707985	1.65912948097710	0.03824378715230
C	-0.58798803791917	0.32375686310107	0.11694988908973
C	-2.82675746755845	-0.30308253065170	0.79813771726388
C	-1.51517990090824	-0.65478648646895	0.49652748145878
N	0.75197884147018	-0.03348250337750	-0.19209125472963
H	-0.29529967034447	2.42799610509341	-0.26641129361074
H	-2.62614690202009	3.05137475144574	0.27878466139722
H	-3.54860911053450	-1.07621215113412	1.06257430916592
H	-1.21402440559491	-1.69995547557583	0.53461287640547
C	1.89414210754808	0.66683579161673	0.21761098823412
C	1.13886306824958	-1.16440026036472	-1.00429597852259
C	2.60893653603982	-1.18031732882033	-1.02952269291684
C	3.06222203630752	-0.08615671713528	-0.34889286528425
O	1.93141708002355	1.68299465382648	0.89395636814282
O	0.33875851099684	-1.90508195086625	-1.55671670022072
C	4.42164877683302	0.32737361144115	-0.29201651071137
C	3.52725292982939	-2.06584633741994	-1.85731058860116
C	5.32103353710622	-0.56100200811410	-0.81389969528742
C	4.93984773698637	-2.00866017613215	-1.15917877332987
C	2.98462133189136	-3.50071648777301	-1.95702763076598
C	3.59535663759704	-1.45846329396935	-3.27834156872656
N	6.65122009232468	-0.37431088585473	-1.08548956446416
C	6.16236587350232	-2.44731374458381	-1.95735008125048
C	4.94893542836749	-2.78578216022379	0.18670805009427
C	7.15606084592287	-1.45631255698451	-1.83020173178249
C	6.46699713559156	-3.62147840989690	-2.63242248843906

C	8.42533468495558	-1.59865580447437	-2.38581341932166
C	8.70073759110795	-2.78006190038877	-3.08509019570902
C	7.73797379546349	-3.78152040890512	-3.20749560951000
C	7.36598825333418	0.86334393083341	-0.85436441176694
H	4.67823599337852	1.32126853574256	0.07092991867308
H	2.86176115234415	-3.96996993532342	-0.97381599199797
H	1.99684875279226	-3.48406644412582	-2.42967238960672
H	3.64372340863021	-4.13108831766608	-2.56695726214862
H	4.24591151250504	-2.05377881385241	-3.93250744858562
H	3.97904893888237	-0.42920196599707	-3.25636532437255
H	2.59138095154497	-1.43916324627967	-3.71987041751549
H	4.12360119502345	-2.46015992576969	0.83138027248152
H	5.89474497301759	-2.61015887266144	0.71439147824449
H	4.86021052661288	-3.86373367872342	0.00989716329654
H	5.73361143536616	-4.42211471987867	-2.72092528414154
H	7.97181370754865	-4.69633192869701	-3.75176063326152
H	9.68418687912817	-2.91445425577365	-3.53622337358812
H	9.18405350353122	-0.82196680520519	-2.29368258624331
H	8.43130199344892	0.65360230349001	-0.70812262027556
H	7.25276484891898	1.56328828112093	-1.69698967928306
H	6.98589993891812	1.34178446552067	0.05457012549740
H	-7.03508264789836	2.29715286341228	2.74858749349192

Table S14. Cartesian Coordinates (in Å) of *E′*-**1**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-2.54022559511083	1.86396954461414	4.97480476940414
C	-3.48311368445641	2.26824991313569	4.03290572783680

C	-3.18579415334994	3.28720284192565	3.12477295099537
C	-1.93019409915332	3.89765419306377	3.17330697900651
C	-0.97280367278717	3.48245359551661	4.09577046714331
C	-1.25879370102272	2.44718564945378	5.00867217694462
N	-0.37785515607282	2.06669404842759	6.02136913212448
C	0.88411430442725	1.83548451235017	5.91388921787559
C	1.68600673479887	1.65783110182517	7.22675519871015
C	1.49660602408188	0.19328209662298	7.67379190550285
C	1.12683083477821	2.60102586900769	8.30141256581341
C	3.19134145286899	1.93758951854711	7.06262975085437
N	1.62093598466255	1.64542783443217	4.75254401806762
H	-4.46415315630655	1.79085891679494	4.01519095309615
H	-2.77551091575938	1.08684130894920	5.70326468485639
H	-3.92671957952774	3.60726326907684	2.39197189015682
H	-1.68849520166526	4.70246823861790	2.47698107751880
H	0.00470379916253	3.96508095393310	4.12579994338567
H	2.05129153536791	0.00414061681785	8.60433075768175
H	0.43525446906421	-0.01727893419826	7.85424517895496
H	1.86353257125808	-0.50914649235546	6.91216228479358
H	1.63218299009784	2.42004761885397	9.26051328052046
H	1.28257210796580	3.65341497075354	8.02603169862439
H	0.05114441821639	2.44695319029890	8.43088274654451
H	3.70236393721241	1.19021603368830	6.43661051025241
H	3.67551322472921	1.89029793193137	8.04670851626124
H	3.38602295800070	2.94117040863705	6.65624914492583
C	1.21079433433485	1.21819174163279	3.47163139577820
C	0.13150609075585	0.34562494474630	3.27824093759945
C	-0.19015603032257	-0.10458064585924	2.00226699284442

C	0.55867098749393	0.30611955784380	0.89119397962356
C	1.96158908698502	1.62121192748702	2.35765076067162
C	1.64158975430413	1.17502270260154	1.08066649322600
N	0.22977189499824	-0.15146533024713	-0.41057996798401
H	-1.03397823648686	-0.77707343439429	1.86811382606700
H	-0.45301323245550	0.00463513612499	4.12995504824862
H	2.79922855693562	2.30859954669694	2.49196960424308
H	2.23618923994837	1.49766805187834	0.22948847165135
C	-1.06896836238691	-0.32555951149181	-0.91431657321622
C	1.19614449034103	-0.54073776928039	-1.41634150298617
C	0.43212851086072	-0.90027017108211	-2.61684198320146
C	-0.89957588384949	-0.81543603491107	-2.32192655608629
O	-2.11953747197549	-0.12373847765036	-0.32781042779971
O	2.40220178680647	-0.57043579626107	-1.21781413416337
C	-1.94899182897093	-1.23911909002534	-3.18125167613151
C	0.94539320480391	-1.51369295518213	-3.91038038315558
C	-1.56010594094421	-1.57743071570280	-4.44875851360662
C	-0.16465490922639	-1.24281992788392	-4.99687604433332
C	2.30685219887442	-0.92078178054040	-4.30894222047650
C	1.11219851224312	-3.03214188605838	-3.66733870112630
N	-2.28423887037998	-2.20437459459384	-5.42749369474835
C	-0.14790007076340	-2.07546515310056	-6.27381756878367
C	-0.21493077741235	0.25491029042643	-5.40818266614749
C	-1.44666642359352	-2.57411603458045	-6.49670388193595
C	0.83257467267884	-2.30309137166496	-7.22996326574830
C	-1.77639190903648	-3.31482470420952	-7.62906876199759
C	-0.76469769389879	-3.55400686167846	-8.56700598949260
C	0.52336508357192	-3.05519273626752	-8.37464369870429

C	-3.65780987653982	-2.63791457591765	-5.27766699635788
H	-2.96134565870639	-1.35233577933686	-2.79714096683469
H	2.26667868591555	0.16794050498540	-4.43220292877852
H	3.03815703715146	-1.12750202355496	-3.52045184701582
H	2.67620651175801	-1.36525079343351	-5.24144762446677
H	1.48297719363191	-3.53914432267855	-4.56786795309579
H	0.16054346692033	-3.49846375954888	-3.37799922704885
H	1.83430820211547	-3.19971073078004	-2.85851185983728
H	-0.29614148836605	0.90107597658626	-4.52545719394231
H	-1.08173063477802	0.43782754556764	-6.05541804210995
H	0.68506845514977	0.53001647566743	-5.96988866814462
H	1.83875340519392	-1.90520345558083	-7.10533686396825
H	1.29708322230562	-3.24828934225573	-9.11756733091697
H	-0.99329225574538	-4.13728067707850	-9.45930181885040
H	-2.78024902144320	-3.70765325462832	-7.78755601032937
H	-4.14360549035974	-2.67334396620684	-6.25894279423938
H	-3.72210402171217	-3.63335825741712	-4.81150808165597
H	-4.20264413496817	-1.92090547397479	-4.65448323298514
H	2.62599520676261	1.73748924209160	4.86005961459780

Table S15. Cartesian Coordinates (in Å) of *Z*-**2**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	1.57316851508478	-0.22570594944339	0.26486948596022
C	1.04136888427456	-0.70584400230898	1.44712018410507
C	0.26551936289097	0.14517096286048	2.26890366679792
C	0.10115551026360	1.48791322220938	1.88030575135111
C	0.66337242156918	1.98661336809551	0.70118708955387

C	1.38663744881795	1.11336861935116	-0.10853601137153
C	2.46367687207602	-0.89913587912235	-0.76637383281966
C	2.31729087959054	0.11061349694542	-1.97837940751573
N	2.03088475951472	1.36746129494530	-1.33227107405062
C	2.05604633889435	-2.32652349268892	-1.13155578353226
C	3.91139729447469	-0.89904389685075	-0.23424626721166
C	1.72655837675951	2.55515578985217	-2.10652523166809
O	1.07333916487076	-0.33325039466038	-2.71182436319204
C	3.48203740328703	0.19511723635123	-2.91226663021498
C	0.94756288251230	-0.20585849666813	-4.04489001262715
C	3.35784170081820	0.17207368063769	-4.25176927284064
C	2.06570506560755	0.02473558347257	-4.88569370698412
C	-0.33689943341688	-0.35819256307091	-4.59338866885854
C	1.86882801944517	0.09424931947611	-6.26695867597238
C	-0.51763474682135	-0.28902224573259	-5.96615517242542
C	0.58905840985430	-0.06111864276076	-6.79359248555830
H	1.19560491813592	-1.73733900697678	1.76882176252643
N	-0.19170717897578	-0.36339596597093	3.48941373278621
H	-0.47749370885666	2.15668658847193	2.51728393055408
H	0.51078633350326	3.02985219445995	0.42434613107674
H	2.67005573330382	-2.71037920283541	-1.95831592068199
H	2.21428689152449	-2.98682089118688	-0.26822198006339
H	1.00328914848257	-2.38839878019779	-1.42393977216171
H	4.26809665035219	0.11777405224987	-0.02470781014275
H	4.60072244640787	-1.38124981301266	-0.94146244641417
H	3.94662740596458	-1.46339586605877	0.70584528506861
H	0.66900108769013	2.59280408175996	-2.41978332897248
H	1.94527600474061	3.45220131154661	-1.51295756289474

H	2.36272717850195	2.57973171560091	-2.99821667918937
H	4.23868661750421	0.27404191823611	-4.88888016735691
H	4.45530386219301	0.33643706887851	-2.44654443453129
H	2.70712868667808	0.26718767633782	-6.94045717662155
N	0.39720971450681	0.01384031179873	-8.24910935723084
H	-1.50200498318125	-0.40715092700070	-6.41363864952102
H	-1.17687154761228	-0.53265417370065	-3.92180096213670
O	-0.75142641059162	-0.13562423611912	-8.68896273719986
O	1.39464282300286	0.22245139372720	-8.95460748408903
C	-1.33879785124420	-0.14714116047428	4.03261279555462
C	-1.55786934548639	-0.57649428361602	5.49896061742055
N	-2.46247648341688	0.43682828815092	3.44732428020870
C	-2.02036682175702	0.63128879772073	6.34403412480374
C	-2.62815644775534	-1.68483745637721	5.55274315371897
C	-0.25019037535608	-1.10956133865782	6.09501821664858
C	-2.89452784571859	0.42167157840988	2.10659032588873
C	-2.50154025885629	-0.57306796837093	1.19860614895229
C	-2.99278362627319	-0.55779532199456	-0.10531699787840
C	-3.89151621819069	0.42635387818570	-0.52202999362174
C	-4.29921958949052	1.40542950910053	0.38645014150254
C	-3.80082463375881	1.40956174184760	1.68706989156845
H	-1.81915539342118	-1.35828789265306	1.51605301704693
H	-2.67399281849458	-1.33588885396171	-0.80024470193415
H	-4.27512982347244	0.42817876565455	-1.54239581843128
H	-5.00304086762079	2.17995048165512	0.07945385439078
H	-4.10558750328317	2.19028368203874	2.38739735800313
H	-2.08886947622814	0.33593152735215	7.39970035038733
H	-3.01683796547108	1.00587556328122	6.06336989917209

H	-1.30918226251845	1.46520213414997	6.27253666560297
H	-2.79050422060820	-2.00328653953722	6.59208285621778
H	-2.30987293940678	-2.56372022494049	4.97618727597829
H	-3.59416204901918	-1.35067304975855	5.15014116686531
H	-0.41850162495415	-1.40704762505497	7.13983726425080
H	0.11515969986583	-1.97838539274892	5.53691794241915
H	0.54041267626355	-0.35010492930887	6.06993804014049
H	-3.15931373796996	0.77437862900971	4.10487217139404

Table S16. Cartesian Coordinates (in Å) of *Z′*-**2**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	1.89069065043673	0.12189735521948	-0.07880254669247
C	1.49309806609948	-0.33588691054785	1.16454858922682
C	0.62622565150428	0.45003848137682	1.96063578666638
C	0.20461977236889	1.69888030129052	1.46311866257785
C	0.61455799548646	2.17149126917109	0.20985429539990
C	1.45851719293482	1.36912456250338	-0.55461848294856
C	2.85363205014360	-0.47873326093058	-1.08980381004568
C	2.50567852139484	0.38264632507196	-2.37336340488446
N	2.01432925080922	1.62074494229386	-1.82116406581327
C	2.68633529516640	-1.98101873266292	-1.31871152794488
C	4.29344409678474	-0.18930653082179	-0.61805442508687
C	1.49411866073083	2.67066803801677	-2.67459294247048
O	1.34711632513193	-0.33316878418875	-3.02679610672084
C	3.61884111336833	0.59154393778839	-3.34969803701222
C	1.17474092540571	-0.34050386422065	-4.36159474768799
C	3.47382587917984	0.43965056251855	-4.67846267102026

C	2.21593323391674	0.01720479473166	-5.25489084494698
C	-0.07080539444848	-0.76518090887081	-4.85323028303118
C	1.98189563601766	-0.05866520741793	-6.63014602056578
C	-0.28881966141050	-0.83775315517663	-6.22050730398633
C	0.74075311626136	-0.48048872318323	-7.09983639956801
H	1.83556957353468	-1.29426531517450	1.55829286622231
N	0.30039563081080	0.00761953949066	3.25333974551063
H	-0.44299312166471	2.32026714061772	2.08349742848493
H	0.26995270033350	3.14275053654067	-0.14543475895647
H	3.33475955199808	-2.32769232668633	-2.13542903699436
H	2.97870750646776	-2.52605323248557	-0.41109086967927
H	1.65262359092381	-2.24583734043152	-1.56072495458252
H	4.47795443752311	0.88729847703968	-0.50829337869056
H	5.03528813508981	-0.61066861477568	-1.31066527902841
H	4.44873897899459	-0.65432481499714	0.36329308092887
H	0.44093696395707	2.50062414195926	-2.95792287128299
H	1.56322576897012	3.63737080384392	-2.15907847320100
H	2.10033390191757	2.73259076074157	-3.58487938765388
H	4.30991835404738	0.64194527833329	-5.35084336534040
H	4.56109050674575	0.93744852155736	-2.92950525907897
H	2.76146713526665	0.20731622202802	-7.34269938381829
N	0.50860327522922	-0.55423793525072	-8.54993112085411
H	-1.24445833791614	-1.16555407968035	-6.62386458247044
H	-0.85089040941761	-1.03728999776410	-4.14334996594351
O	-0.60291934982671	-0.94001452637575	-8.93791848124457
O	1.43722150979208	-0.22607582179977	-9.30204937825016
C	-0.92014801715489	-0.24731697426696	3.59936598174078
C	-1.18468089313809	-0.67906499328537	5.05688518663783

N	-1.93990381744699	-0.28765064828480	2.65322148603705
C	-1.81610044049603	0.46593492343600	5.87877475843912
C	-2.09927791672965	-1.91716414789801	5.10258902178305
C	0.15681874731040	-1.04133802819215	5.71741037538553
C	-3.33897720480546	-0.04847855230660	2.77412357428918
C	-3.84016605429678	1.14773997026974	3.30705262569159
C	-5.21584659293312	1.37567561352016	3.35409059306993
C	-6.10535466296998	0.42798480686416	2.84419595235677
C	-5.60993839012862	-0.75104125673624	2.28269886959562
C	-4.23667122377624	-0.99047884662994	2.25066480604404
H	-3.14375434543857	1.90672787198536	3.66216682652595
H	-5.59317040324148	2.30914709501166	3.77368132402301
H	-7.17952386092164	0.61171959086683	2.87546255863795
H	-6.29684743210527	-1.49332190339272	1.87466155915033
H	-3.84257204282406	-1.91696530919069	1.83153834802789
H	-1.82689593883179	0.18426141581321	6.94104206085636
H	-2.84996719393246	0.67241555590965	5.58248593813704
H	-1.22975729990802	1.39043927125177	5.78448418533169
H	-2.20524011517277	-2.25299383127613	6.14349951595089
H	-1.67044789205384	-2.74641569877050	4.52363960975997
H	-3.10474640543771	-1.71511731172824	4.71603366918310
H	-0.03086190309954	-1.36431623679445	6.75127615193349
H	0.65969156095450	-1.85611324570636	5.18284492801348
H	0.84243469518086	-0.18749598831140	5.73374783334871
H	-1.58237763666240	-0.16315805085002	1.70370897252812

Table S17. Cartesian Coordinates (in Å) of *E*-**2**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.84562149478189	-0.06350253414070	-0.89160691327610
C	-0.05346007175995	0.96346272064931	-0.66397350370242
C	-1.44120157737052	0.73992840095899	-0.84250151731200
C	-1.85766751369637	-0.52191304977852	-1.30772050923274
C	-0.94987945441088	-1.56356298005801	-1.53763987719435
C	0.40387882573694	-1.32311698736894	-1.31943260470973
C	2.36453828831099	-0.07488282099280	-0.83103626604857
C	2.64269810023395	-1.63434964411264	-0.80666186576118
N	1.50277213708297	-2.18764205465236	-1.49032803062034
C	2.96405059386516	0.65583407397410	0.37047642977547
C	2.90607245476348	0.54991243302631	-2.13318306009366
C	1.31648473457209	-3.62070590286868	-1.60203051266087
O	2.55571490338190	-2.02485477282657	0.65314409878772
C	3.94127293720105	-2.08345430992613	-1.39679899848287
C	3.30194599194976	-3.01745397602376	1.17017076918356
C	4.75690852225961	-2.97076456837957	-0.79891209013860
C	4.44254456849445	-3.52683543174374	0.49910312381588
C	2.94202765035082	-3.50943442629637	2.43607428053097
C	5.20087023750034	-4.52384882947662	1.11772988131181
C	3.70484098315362	-4.49732956101119	3.03939859532331
C	4.82943703851525	-4.99954679185505	2.37270700197081
H	0.28481894978107	1.95198848290833	-0.34910888348838
N	-2.34140828956858	1.80096953847784	-0.74264749256309
H	-2.91951365633124	-0.68420900710874	-1.49427664432187
H	-1.31271500023696	-2.53411266733414	-1.87666472404189
H	4.05360364633428	0.51775129959825	0.40936211076099
H	2.77111494209843	1.73346289176738	0.27950981467078

H	2.53703404876207	0.30808275338600	1.31602830733963
H	2.55337950798137	0.00938398051897	-3.02110802982335
H	4.00473630859042	0.57327785945698	-2.14121417964539
H	2.54837795758383	1.58420152542674	-2.20962436299173
H	0.85533611885598	-4.05756800291684	-0.69912356141627
H	0.67394300054060	-3.84618984836129	-2.46306726580129
H	2.28612271218907	-4.10107447128685	-1.77273249117076
H	5.67547390567475	-3.29471815744405	-1.29245706616811
H	4.17395235139088	-1.69385012325600	-2.38586109055319
H	6.08401779080353	-4.93414438192217	0.62994448149324
N	5.63700222502371	-6.04877620454501	3.01131924926885
H	3.44671993916310	-4.89119485493806	4.02002769507202
H	2.06229226562936	-3.09710412944485	2.92869052425895
O	5.28643371933707	-6.44638245149174	4.13128127278644
O	6.62278455471428	-6.47700480072084	2.39410183615533
C	-3.05015965927150	2.20515105056919	0.25109941093798
C	-3.09867328574714	1.59384074231251	1.68729339374139
N	-3.87838056954734	3.29791954047942	0.07331835905836
C	-4.03777243710800	2.34465760345104	2.65140751644535
C	-3.59625830980977	0.13765578093162	1.59439215367666
C	-1.68424325593299	1.62744994132202	2.29846334912343
C	-4.12799923062048	4.10766557570119	-1.04865476128515
C	-5.04530807623199	5.16264994077920	-0.86725568455696
C	-5.36417704529052	6.01967473672814	-1.91377667484240
C	-4.77573358486626	5.84726148243071	-3.16974924833478
C	-3.86758263817936	4.80501592049136	-3.35225196834472
C	-3.53603626073387	3.93510534795436	-2.31163225301601
H	-5.51240782462648	5.30865075374689	0.11053378695615

H	-6.07735847850423	6.82769566769283	-1.74595317243353
H	-5.02397454632547	6.51775485965809	-3.99261978351057
H	-3.39976422773011	4.65689249661110	-4.32661944122500
H	-2.82875982120909	3.12566807158123	-2.45758278395061
H	-4.00135432038677	1.85223902692400	3.63202088768289
H	-5.08954293832551	2.31630360229758	2.32957972230359
H	-3.73294001893632	3.38886742338911	2.81566964460658
H	-3.66785529915896	-0.29229022866609	2.60389839276618
H	-2.91492478718869	-0.48699268427963	1.00861712754645
H	-4.59281019340235	0.08644126989915	1.13400475518813
H	-1.71446884863006	1.21631065715530	3.31783973264480
H	-0.97388460591003	1.03209010981682	1.71656706689722
H	-1.30159432787972	2.65576498416056	2.36051157460732
H	-4.40900925168054	3.57183110899531	0.89154096603024

Table S18. Cartesian Coordinates (in Å) of *E'*-**2**(c), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	-0.08161613836684	3.04096535117599	-4.15968552926017
C	-1.40109271732665	3.44233308731531	-3.96504722464278
C	-2.40895497109488	2.49475163232336	-3.76805608927273
C	-2.07652771997269	1.13741596786730	-3.77036871749997
C	-0.75599513847367	0.72888042431550	-3.94124910824570
C	0.26984080144409	1.67741238940752	-4.12938959652732
N	1.58609540352689	1.31946090701791	-4.41845090978903
C	2.30873424518208	0.43656064365358	-3.82211469322774
C	3.65506881408934	0.05769052633081	-4.48796172046095
C	4.66770630734158	1.15752458520079	-4.10689236976921

C	3.47927976781173	0.02422595276519	-6.01305813354952
C	4.20203720647768	-1.30513503875018	-4.02585286825092
N	2.06757605852114	-0.17962082011098	-2.60203302158467
H	-1.64770544997588	4.50526315181137	-3.98504532162195
H	0.70455772860821	3.77478595653567	-4.34202692518633
H	-3.44416419357471	2.80900319370647	-3.63210976612799
H	-2.85597008626634	0.38555144084175	-3.63398260611110
H	-0.50743936333296	-0.33303079628872	-3.94465364178338
H	5.65091830586711	0.94015548081287	-4.54867039184771
H	4.32913308043024	2.13312892226570	-4.47627173015827
H	4.79370437772351	1.22580451618748	-3.01691319528836
H	4.44868654811357	-0.15126459085394	-6.50019298564100
H	2.79434262260882	-0.78012003124470	-6.31610868825490
H	3.06446931247572	0.96971640868152	-6.37587084401283
H	4.50872899625426	-1.30974538816007	-2.96896338274949
H	5.10285900288398	-1.54669380395644	-4.60499751514211
H	3.48414579466835	-2.12108519893652	-4.19663734623109
C	1.27550241466380	0.24521222926014	-1.51215408109438
C	1.12198293403848	1.60032795445291	-1.19792784881297
C	0.36294191140852	1.97868399342634	-0.08250878541593
C	-0.21088146162217	1.01264934141721	0.72655822630472
C	0.70003720822653	-0.74957997952613	-0.69641183160044
C	-0.03971512452819	-0.34903705943184	0.41379760499338
C	-1.13699158339710	1.13156486369465	1.92414890525928
H	0.24173178636336	3.03918788034375	0.14454749942993
H	1.59841551646162	2.35651450531040	-1.81707316690207
H	0.82209955623372	-1.80245087375811	-0.95399258895706
N	-0.71299141405844	-1.14819984634376	1.33699758768726

C	-1.00861432958145	-0.32815190510832	2.52716437129136
C	-0.44038120695567	-2.56580767405446	1.46441985671723
C	-2.57181350244198	1.37788839537097	1.41361837414353
C	-0.75966036153390	2.22112499478767	2.92856740536200
O	-2.29923056476311	-0.73369980036662	3.05543051769802
C	0.09563740661526	-0.47533396076727	3.53249383034369
C	-0.04949307564583	-1.11456040311414	4.70461146330479
C	-2.43069605241999	-1.41486488797774	4.22180160754277
C	-1.34277664036964	-1.63291439273425	5.09982906359054
C	-3.71426803688474	-1.87994173242845	4.53786526716210
C	-1.57125094511007	-2.32941451579721	6.28927390460544
C	-3.92811792153688	-2.56745977332063	5.72448665417751
C	-2.85159841559578	-2.78767279054551	6.58971894098817
N	-3.07562041375681	-3.52039266617096	7.84778042100904
O	-4.22507207200605	-3.91114100415635	8.09025813051772
O	-2.10123678255382	-3.70391328122907	8.58979188998982
H	-3.28600693911118	1.44223204014546	2.24404089844290
H	-2.59269617237522	2.32569745929498	0.86063243275477
H	-2.89885867382148	0.58067958875905	0.73583087820880
H	-1.40576154748104	2.17437417968390	3.81620511599091
H	-0.89795351573123	3.21151979874754	2.47450165069032
H	0.28352595029757	2.14888196396114	3.25812651717898
H	1.06478736753426	-0.09340498899463	3.20984045071604
H	0.79837172116514	-1.25497005878499	5.37779374188627
H	-0.75730189217554	-2.51692646614619	6.98810901613783
H	-4.91475504634970	-2.93846646627056	5.99274639528461
H	-4.52969832762305	-1.69166451317664	3.84077544030415
H	0.60399049312918	-2.78940895753066	1.74489149058014

H	-1.10583812913355	-2.99693084956671	2.22019803337618
H	-0.66012593203455	-3.06622280567550	0.51219482791032
H	2.61196721881704	-1.01794340559394	-2.42638178656047

Table S19. Cartesian Coordinates (in Å) of *Z*-**2**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.32401331431094	0.51304095675445	0.34859590578399
C	0.21907005372925	1.43625561663628	-0.67518818658517
C	1.00135523207296	1.28292712143918	-1.84346442428770
C	1.91051093547197	0.20487830749877	-1.91272749000027
C	2.04068129379186	-0.71359259330992	-0.87175501754346
C	1.22683833616027	-0.55215807538082	0.24803901864537
C	-0.40607512437250	0.43136734234016	1.67984888341843
N	1.14340315317398	-1.32852321261568	1.42235102239952
C	0.22506457810918	-0.82591540287076	2.29859840729379
C	1.93844671659698	-2.51929364439167	1.66868546381227
C	-1.92112522598523	0.25116173615569	1.44289458529073
C	-0.12079916867089	1.69019070024457	2.52598906910133
C	-0.02739086507874	-1.42500006547906	3.52928177246231
C	-0.95528763398341	-0.97498723460179	4.46764884644511
C	-1.26007506903281	-1.53192124631960	5.71844088413935
C	-0.63610656699609	-2.68960228699504	6.23789996372459
C	-2.31342009387207	-0.83329258381850	6.51818262021801
C	-0.98721043216754	-3.18027467450437	7.47378141177673
C	-2.61741533853443	-1.42560050997247	7.81663650164707
C	-1.98681527465102	-2.54384292597650	8.27326180065416
O	-2.89363086629324	0.18729697944897	6.10141342981118

H	-0.45475370507347	2.29179081462618	-0.61013984515568
N	0.94113238359818	2.27980702283279	-2.81191206542943
H	2.53536095389938	0.09755867294435	-2.79881074916335
H	2.76015172097752	-1.52757813487898	-0.95836846981694
H	1.29074230981727	-3.38795025930672	1.84556665875043
H	2.59080132338392	-2.38036476676888	2.54147945144347
H	2.56271185487234	-2.72480537168708	0.79643845808083
H	-2.47465516184270	0.17167054848340	2.38484103626625
H	-2.30926851523878	1.11841335816190	0.89273224876804
H	-2.12184045983607	-0.64803163081578	0.84681938883722
H	-0.47728129556008	2.57943898962415	1.98991517837361
H	0.95508153477486	1.81053469896290	2.70374482581053
H	-0.62893945765216	1.65269807199806	3.49585307434203
H	-1.54602352777512	-0.08318450423297	4.25031065829840
H	0.55132907784944	-2.31889419872008	3.77004864209024
H	0.13346208107665	-3.22003516166679	5.67773590655328
N	-0.32392374107205	-4.37796440066457	7.98014239801169
H	-2.22263915633738	-2.97730715816362	9.24383135050277
H	-3.38237040379922	-0.92645513536119	8.41135400016014
O	0.54361397717207	-4.91961764337048	7.27122068765098
O	-0.66352434766463	-4.79769467927244	9.09969989466255
C	0.90387487581893	2.12368019907942	-4.09093510785060
N	0.65351150905369	0.95058842200325	-4.78959958775360
C	1.12371802973884	3.35609200220517	-4.99311940445689
C	1.57206577414586	4.55471205475565	-4.14909870016767
C	-0.20282160719488	3.69996686154563	-5.70048743460952
C	2.21436794225751	3.06714908271385	-6.04751245280949
H	3.15307496725255	2.74416955560011	-5.57755091020032

H	2.42163878628437	3.98234622143217	-6.61758839787848
H	1.92009894570725	2.30652103350640	-6.78686138569506
H	2.51030593346678	4.34530882192945	-3.62097123934017
H	0.82219574243509	4.81298492553644	-3.39396073646309
H	1.72698994872775	5.42492067223989	-4.80214059762760
H	-0.06802511228902	4.57809454209709	-6.34700611697491
H	-0.98605793014185	3.93700925891135	-4.96826793896465
H	-0.56529797657593	2.87448999288098	-6.32820082117746
C	-0.07622143826545	-0.19607932672793	-4.40272741984645
C	0.24781939515532	-1.42651478820060	-4.99443838771614
C	-0.48696803820366	-2.57035800652596	-4.68879904033352
C	-1.54378042511388	-2.50655192070030	-3.77855409258847
C	-1.86857173676188	-1.28140546401364	-3.19219279386963
C	-1.15111126529428	-0.12832874290690	-3.50500955332822
H	1.08720332581002	-1.48337627969410	-5.69055173598693
H	-0.22460579084864	-3.51854537915652	-5.15922717952073
H	-2.11422375585397	-3.40243068408229	-3.53385487616748
H	-2.70313153541961	-1.21542881799881	-2.49305864313392
H	-1.42936933420070	0.82717706539143	-3.06446046878785
H	0.90013437096035	0.97868326117269	-5.77472617399544

Table S20. Cartesian Coordinates (in Å) of *Z′*-**2**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.54361837836923	0.28296357979555	0.78442945753095
C	0.56204959010737	1.24614425136992	-0.20911613596368
C	1.37745158965889	1.06163294896335	-1.35116957856165
C	2.15919713278614	-0.11240383845983	-1.44157061693341
C	2.15095682253799	-1.08300244386078	-0.43760540238579
C	1.33302754606084	-0.86817129664035	0.66984911851678

C	-0.22711327587112	0.23731435205900	2.09475366876336
N	1.13611339943708	-1.66773828274803	1.81488268353004
C	0.24877318533917	-1.09960224992058	2.68384681468767
C	1.79983295258817	-2.93958995003814	2.04419047389336
C	-1.74614086792014	0.23367344935360	1.82000115636789
C	0.17346494663051	1.42961728322981	2.98979462269317
C	-0.10257862198857	-1.70989849966114	3.88372404010050
C	-1.00360347616983	-1.19601190694698	4.81604612753463
C	-1.40045770111706	-1.76205501557431	6.03605336467456
C	-0.91579453834231	-2.99762715247988	6.52487848494562
C	-2.39645998160612	-0.98538398197316	6.83739058103345
C	-1.35005720923085	-3.49226154002374	7.73211309385810
C	-2.79596608967821	-1.58834616788889	8.10475766173435
C	-2.29887181165614	-2.78272942946401	8.53225089227120
O	-2.85501100321505	0.10491950913291	6.44684166469853
H	-0.02656358015422	2.16117139556174	-0.13015755070221
N	1.47837868924726	2.07805789855376	-2.30046834833845
H	2.80570169702536	-0.24292781863003	-2.30981592817507
H	2.78020443522389	-1.96733296975410	-0.53681058592490
H	1.06503662339524	-3.74918443001024	2.14672438510576
H	2.41256440637309	-2.90047216769615	2.95481021438124
H	2.45100800888111	-3.16709332078035	1.19750523423385
H	-2.32793508239239	0.19360223742170	2.74752085294176
H	-2.02263398529697	1.15226578504447	1.28618151492728
H	-2.03268243826484	-0.62212289395445	1.19593653360456
H	-0.07295845014169	2.36942424756657	2.47881070715108
H	1.25160529308076	1.42641186898810	3.19225816804307
H	-0.35789913352887	1.41500274051189	3.94776388222830

H	-1.48994151067647	-0.23852826733840	4.61954806665020
H	0.36938984404043	-2.66953436116115	4.10421732585166
H	-0.19085250960549	-3.58565458187585	5.96264587200505
N	-0.83003365553387	-4.77140051543288	8.20729482703706
H	-2.60501686569665	-3.22343158173494	9.47963165456282
H	-3.52020475077720	-1.03271913612816	8.70032962931953
O	-0.00522146294569	-5.37575344512311	7.49842109936406
O	-1.24145723860636	-5.19185287124689	9.30201311041535
C	0.98816643733707	1.97129964492993	-3.49509055376775
N	0.22513786914721	0.87101629082861	-3.84568705941479
C	1.22428051417857	3.13396644695564	-4.47565447192549
C	1.93769957650736	4.27776573095910	-3.73605986541772
C	-0.11403292412664	3.67175091928307	-5.01958778299239
C	2.12718021234346	2.68944920858844	-5.64579763691452
H	3.06080600719558	2.24138379668074	-5.27812111617394
H	2.39459138831440	3.56868428924358	-6.24804133665026
H	1.63240398344591	1.97303254393181	-6.30952504447912
H	2.90695183996850	3.95927069791207	-3.33698208598345
H	1.34103603691945	4.64773134982601	-2.89438704251224
H	2.10240612777327	5.10624516835131	-4.43907965050220
H	0.07728671714262	4.56363582437805	-5.63177307317239
H	-0.78374189451546	3.96666288338322	-4.20001118039824
H	-0.63804220156510	2.94514692511448	-5.64960098675968
C	-0.32407778432177	0.41931807424298	-5.08745905831607
C	-1.70015791005386	0.54134460460750	-5.32049597146300
C	-2.26509409313547	0.02400937500864	-6.48645760007117
C	-1.46196746626634	-0.62327796807348	-7.42748980284872
C	-0.09320585227710	-0.76434785686384	-7.19083440301385

C	0.47287676673895	-0.25511170846266	-6.02147548440703
H	-2.31829254211889	1.05171250478736	-4.58142286600922
H	-3.33661393358077	0.12745736413205	-6.65985558366293
H	-1.90377770771488	-1.02611940706432	-8.33917484241799
H	0.53633522144604	-1.28484726090830	-7.91326582379685
H	1.53538805027194	-0.38759880961623	-5.81785289450545
H	0.09356526057954	0.22103593683844	-3.06949062009518

Table S21. Cartesian Coordinates (in Å) of *E*-**2**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.39588142818470	0.17220039084973	-0.13131487479969
C	-0.41456593143127	-0.92720787309078	0.08682367860433
C	0.07953262623779	-2.03428382113543	0.82238598292635
C	1.41921858937724	-1.99375791550703	1.27223813266517
C	2.24040857091675	-0.88697328123844	1.05254710845744
C	1.70873952540402	0.19465848532796	0.35394024629786
C	0.10767550877214	1.47320833331998	-0.86514086652209
N	2.30390370684608	1.42187802963083	-0.00642323527992
C	1.44365420387068	2.21637913089725	-0.70753944865268
C	3.66810097282708	1.79378296462076	0.32763784147960
C	-1.05262717845054	2.22598880412215	-0.18015035266091
C	-0.21210501609425	1.18986179422624	-2.34874985486772
C	1.81025910617437	3.47860503573953	-1.16610776406165
C	0.98775435970491	4.34349891720324	-1.88618072682667
C	1.29341321231661	5.62280126012391	-2.37415847825625
C	2.54662035356845	6.25315954705691	-2.19886903143542
C	0.20410179082998	6.32839215000195	-3.11722480782233
C	2.77571593413280	7.51093423476817	-2.70639673471391

C	0.54000001118458	7.65624611529552	-3.61984634076798
C	1.76460127920391	8.22116228142607	-3.42481860430776
O	-0.91709362451215	5.81479350153673	-3.29474226080317
H	-1.43115155380645	-0.96819761501948	-0.30640116493876
N	-0.66489387714845	-3.19553982449111	0.92170685732014
H	1.81889630767324	-2.86411934919469	1.79185538087581
H	3.26633640278467	-0.89837575095362	1.42010281717846
H	3.68374347654620	2.70282005653966	0.94344804919323
H	4.25673526258519	1.97246104191051	-0.58200705391265
H	4.13709820726711	0.98431419724221	0.89126954542376
H	-1.27867737627830	3.17297023119824	-0.68256869718719
H	-1.95742937566321	1.60456585082095	-0.20801222704746
H	-0.81895432910250	2.44018785256450	0.87034647093087
H	-1.10645582043994	0.55683880002705	-2.41676871774583
H	0.61606437779099	0.66095637363502	-2.83675105201377
H	-0.40691460867458	2.11337790302215	-2.90483672022603
H	-0.03166800600740	4.03602403653849	-2.12692305490739
H	2.82560343528607	3.80871255232813	-0.93771445357691
H	3.35849689604046	5.76358383379825	-1.66145314469954
N	4.08100026191263	8.13297197790499	-2.50763833336686
H	2.00355178883220	9.21332347240413	-3.80444232462513
H	-0.24370257317906	8.18218010841254	-4.16494722440722
O	4.94941165100551	7.50060477557734	-1.87942689047893
O	4.25825346964037	9.26938431333049	-2.97915258442134
C	-1.48208305033666	-3.62834658672256	1.81686091377854
N	-2.08157907402664	-4.85422353068043	1.63215319613445
C	-1.88310583551959	-2.90236462386609	3.13776126970097
C	-2.49358543845626	-1.52990587344698	2.79322915431633

C	-0.62175580347614	-2.71479234708697	4.00397166393399
C	-2.91831778610601	-3.67436118871597	3.97852892187700
H	-3.87141814244405	-3.82040717683231	3.44939601337292
H	-3.14807901326911	-3.08878462553969	4.87822904721161
H	-2.54258658095373	-4.64652749411539	4.33111596183905
H	-3.38482378981965	-1.63698521495435	2.15967832776993
H	-1.77936861504308	-0.88298647055962	2.27424330757345
H	-2.79671006789789	-1.02016369153560	3.71864041742708
H	-0.89517308478971	-2.23022971344587	4.95205139378312
H	0.12297545649848	-2.08427846563242	3.50805916386845
H	-0.15370026274369	-3.68027905764423	4.24092096014733
C	-1.97676016207743	-5.80065820817877	0.59434186626173
C	-2.74692274916201	-6.97146414842756	0.73881451909175
C	-2.71569839439866	-7.96834195425710	-0.22918912616603
C	-1.91529659873310	-7.82145871440384	-1.36524245256383
C	-1.15234587473708	-6.66366319024374	-1.51051378590700
C	-1.17208317284166	-5.65270641327501	-0.54739063973691
H	-3.37725139584005	-7.09772043280607	1.62311805177782
H	-3.32082426568376	-8.86544532968088	-0.09414467910447
H	-1.88933850476726	-8.60158798785232	-2.12600372764995
H	-0.52303957642546	-6.53428851297587	-2.39199044072694
H	-0.57664548339615	-4.75409384476094	-0.66611241240397
H	-2.71301417968227	-5.13827812513043	2.37188002837371

Table S22. Cartesian Coordinates (in Å) of *E′*-**2**(o), Tautomer 1.

Atom	*X*	*Y*	*Z*
C	0.18666397685162	3.74891819972234	-3.78455877925429

C	-1.11265205164572	4.15024537871467	-3.48312290228371
C	-2.14656122754789	3.21294780970715	-3.41388645744065
C	-1.86167526683300	1.86598545417569	-3.65343676527600
C	-0.56056965351466	1.45312538224085	-3.93095620445964
C	0.49107756099839	2.38974065671652	-3.99035061065186
N	1.78718227031659	2.04284831122421	-4.37452307195627
C	2.49808623827376	1.06652681751664	-3.93440644727469
C	3.81981289237826	0.74887305485352	-4.67232483981388
C	4.88972324129998	1.70530182651808	-4.10466563655271
C	3.64255580486449	1.00771804536147	-6.17511792628961
C	4.29010214355503	-0.70374757662191	-4.47272003582277
N	2.25858465695047	0.28434755438418	-2.80616198000354
H	-1.32383456360811	5.20844966774496	-3.32114514752532
H	0.99127262071786	4.48040355198634	-3.87058722766824
H	-3.16649618223673	3.53076067038641	-3.19658824337781
H	-2.66360892536133	1.12623234995011	-3.62421128877769
H	-0.34858966099390	0.40079733324831	-4.12465030497664
H	5.85721854989086	1.52747244063413	-4.59540670790820
H	4.60190240280435	2.74936792371900	-4.27839249755914
H	5.02717091980743	1.55883791766020	-3.02393632197661
H	4.59611746106113	0.85030364028910	-6.69768861558105
H	2.89759915495530	0.32728019453766	-6.61046943643350
H	3.30193923474774	2.03163667617538	-6.35693847917684
H	4.61145697241612	-0.91487214129110	-3.44136246405628
H	5.16801155349170	-0.88683430743286	-5.10542434857025
H	3.52343162131460	-1.43451750620141	-4.77014883914354
C	1.51972277460682	0.58297724377039	-1.64559792856840
C	1.42633057493195	1.89140377031510	-1.14573859427621

C	0.72482098588547	2.15314741137824	0.03403542653437
C	0.13305060523093	1.10905890559430	0.73007183179124
C	0.92325742564493	-0.48503010056162	-0.94854966225292
C	0.24400092638308	-0.19223550891182	0.22860440145399
C	-0.67724811116377	1.08058929758930	2.00730266613722
H	0.65769683273901	3.17856716039446	0.39984120164794
H	1.91469097204074	2.70353948396389	-1.67855128954801
H	0.99973815167904	-1.49860787051046	-1.34265549200671
N	-0.44360863476357	-1.07922491565810	1.08893849675769
C	-0.63922691181082	-2.48230038814516	0.76904165818191
C	-2.00181476984963	1.86039552457161	1.85326947654878
C	0.11919342583442	1.61802540696973	3.21216579258545
H	-2.61559765887349	1.77124584314909	2.75859567185743
H	-1.78578550032213	2.92404407413389	1.68799352634635
H	-2.58407778223116	1.49402232722997	0.99874854133700
H	-0.46651892058673	1.53074417190941	4.13555754541410
H	0.35814574209538	2.67852802838051	3.05740810445221
H	1.06039512381132	1.07031002277180	3.34531880548031
H	0.10175567371003	-3.12307416291340	1.26720591270638
H	-1.64450036573214	-2.79093524759440	1.07548848171331
H	-0.55136448647842	-2.61905123440324	-0.31338632362539
C	-0.96066800810487	-0.41875707676054	2.16668190145771
C	-1.65351113884033	-0.92029937538381	3.26266052638156
C	-1.79573352236057	-2.24025179291359	3.70005695284374
C	-2.52268206623093	-2.67528480647046	4.82412660119940
H	-2.12120519415747	-0.17445738546676	3.90679382887838
H	-1.26275515344323	-3.03657623629222	3.17498616086983
C	-2.49458280307914	-4.06186073662383	5.12440490852424

C	-3.30285936719657	-1.75684056298179	5.70415694487960
C	-3.97556143552351	-2.38503260623501	6.83421898967307
C	-3.92027823710628	-3.72556704291448	7.07527873657365
C	-3.16942939843096	-4.57282501307131	6.20719651608743
O	-3.38656440649962	-0.52552128136587	5.50494975498383
N	-3.11645333046423	-6.00811008181887	6.47310054129763
O	-2.46163781985473	-6.72834812121290	5.69990832060247
O	-3.73351660572724	-6.43423287708239	7.46352808711561
H	-1.93094271336780	-4.74651609929415	4.48923088307648
H	-4.43628481524361	-4.17704158093664	7.92111202668090
H	-4.54279759338331	-1.71797731230923	7.48321358820392
H	2.75848579127882	-0.59878758020928	-2.77753494018677

Table S23. Cartesian Coordinates (in Å) of *Z*-**1**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-2.28465702823062	-1.32192871128515	-4.986575257
C	-0.96215556851578	-1.74654067632949	-5.089736191
C	0.07827258020871	-0.81596977969261	-5.138625708
C	-0.22253142238041	0.54703613178148	-5.082039019
C	-1.54014587167920	0.97932120017359	-4.951263447
C	-2.59512345261584	0.04757163595033	-4.890861653
N	-3.94040345731747	0.42778438642996	-4.872225212
C	-4.47674682948641	1.32919004418157	-4.128652842
C	-5.91698581635208	1.78959033251629	-4.440523845
C	-6.84546182292109	1.36277896083677	-3.286099069
C	-6.40445448119395	1.14843936713077	-5.744630703
C	-5.96655637355330	3.32462073616693	-4.604248847

N	-3.91500529341542	1.96262937447527	-3.020057764
H	-0.74258521627137	-2.81378528367261	-5.146126571
H	-3.10421309841911	-2.04183396516574	-4.976498461
H	1.11251902517479	-1.14892175438094	-5.226613626
H	0.58047635898700	1.28445122571787	-5.130905016
H	-1.76527253856233	2.04543579653371	-4.906518163
H	-7.87697469439380	1.68049589733163	-3.493588591
H	-6.84557397607668	0.27085238310039	-3.168170322
H	-6.54488321844969	1.80499684560738	-2.326444549
H	-7.42977337948103	1.48348483386566	-5.956318458
H	-5.76408639822099	1.42501505502543	-6.5908113
H	-6.39874662239456	0.05537077068040	-5.676013594
H	-5.75806675203159	3.87149862702760	-3.671641461
H	-6.97499874939835	3.62701271294524	-4.91733269
H	-5.25849594084224	3.66976798845716	-5.369536401
C	-2.96717027863066	1.49690157979447	-2.090683425
C	-2.75791844683359	0.13307194074317	-1.839052037
C	-1.85099247869734	-0.27128392899477	-0.866311796
C	-1.14026391636617	0.67563887441167	-0.118594344
C	-2.25298182244024	2.44072579843326	-1.335044916
C	-1.35038596514580	2.03949685428846	-0.358304361
N	-0.21699179245295	0.25235670493120	0.877336171
H	-1.69362164971659	-1.33223437472578	-0.687397229
H	-3.31489094434877	-0.61657850063048	-2.39591124
H	-2.39877992121094	3.50569727382208	-1.526063341
H	-0.81113193733288	2.78475832193598	0.220872813
C	0.71647951412590	-0.79971367787320	0.701931196
C	-0.11742542827987	0.83341660901261	2.170468435

C	0.88050141632895	0.01181474196907	2.932191042
C	1.54011435863576	-0.84350016048821	1.945828743
C	0.89314951453344	-0.08047069316410	4.295094398
C	0.11561465290361	0.83137456813255	5.197528678
C	1.64352756375179	-1.16188431196928	5.01350879
O	0.83078334191226	-1.47722061647182	-0.305652993
O	-0.78203639208501	1.79135311876383	2.532836519
C	2.71430630610923	-1.53987834035956	1.881605669
C	3.88135776708111	-1.56699765027393	2.716466698
H	-0.64621887867195	0.25524454161095	5.747369349
H	0.78832377613118	1.24534724690392	5.966213902
H	-0.37385165510414	1.65054682829858	4.669442173
H	2.58465294988410	-0.78399335303193	5.443406784
H	1.04238331261657	-1.52468872523878	5.859770057
H	1.89530363829125	-2.00900932465855	4.368987945
H	2.78699454506402	-2.17580626121235	0.99269571
N	4.37413523318333	-0.47401782688761	3.453633004
C	4.71845541846581	-2.67066012799686	2.919768805
C	5.51389912627789	-0.87776221074069	4.118384729
C	4.02367721541890	0.92294059471968	3.264172712
C	5.74136823271514	-2.25533016969099	3.824894536
C	6.84402128092331	-2.90645699999532	4.409467437
C	7.69228918171938	-2.18278577128779	5.237249074
C	7.46223753754041	-0.81549053151866	5.496507746
C	6.37697554422759	-0.14416611457085	4.940287324
C	4.53702109774928	-4.04555388441748	2.368162057
H	3.49968679148848	1.33526333594534	4.138057301
H	4.93203710396965	1.51331276373988	3.084721956

H	3.36861235489401	1.02118513614922	2.39554189
H	6.20312115535644	0.91004539103845	5.157420917
H	8.14609196688570	-0.27317199788928	6.150195313
H	8.55153331599582	-2.67420488460794	5.694499728
H	7.03243005683226	-3.96263726983758	4.211515001
H	3.87761873834057	-4.05508446284578	1.491314361
H	4.09687140239664	-4.73091240942983	3.109539321
H	5.50128822319454	-4.47765163001851	2.066582596
H	-4.36957508979462	2.83029185077461	-2.750396439

Table S24. Cartesian Coordinates (in Å) of *E*-**1**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-0.89265902061575	5.51871655973281	4.68109914245631
C	-1.78415734069618	6.50098456647078	5.10800959256498
C	-2.84026604406997	6.18337774791087	5.96533540853046
C	-3.00060325974255	4.85868504370777	6.37858718820229
C	-2.11475838022069	3.86868707426225	5.95776714294940
C	-1.02547458217907	4.18403937175064	5.11854617836167
N	-0.22279845464965	3.18041779973902	4.58899937434034
C	0.88181430371629	2.66949928118701	4.99831232417223
C	1.67933421594477	3.06064420279378	6.28077660263114
C	0.78935582522679	2.82003959657733	7.51612206646079
C	2.06597925000110	4.55022425006969	6.19379138653078
C	2.97720626087635	2.25292861927209	6.47540281675791
N	1.46296353679901	1.65941816358616	4.25216790358653
H	-1.65452562471005	7.52662664887413	4.75842470371311
H	-0.08542591471370	5.76757016271164	3.99129362033186

H	-3.53877919668119	6.95375903850909	6.29216836244497
H	-3.83122916474544	4.58748347590413	7.03243022540654
H	-2.26047976304628	2.83177549552093	6.26280419753693
H	2.32784939447244	1.29075835215125	4.62944732870827
H	1.35059116475697	3.07006146088501	8.42790659006194
H	-0.11220210532985	3.43998785434510	7.49439457024403
H	0.48137085409827	1.76759277503442	7.58583652913472
H	2.64927902962131	4.83142619339766	7.08235905380940
H	2.68333928909373	4.75015612911733	5.30705447059738
H	1.18465622482812	5.19760813047735	6.15125038749072
H	2.79399813331773	1.17589456802897	6.60579136592365
H	3.47033802819989	2.59600984659435	7.39440443097855
H	3.69956327581266	2.40508389883385	5.65968635174407
C	1.06153509671627	1.03325216850174	3.06240499988512
C	-0.08988792761022	1.36258459263733	2.32757767062398
C	-0.39355803132629	0.66580408701687	1.16052603776354
C	0.43634897577743	-0.35877165889327	0.69476644857722
C	1.89189551782556	-0.00042252200796	2.58479933545608
C	1.59164570185440	-0.68586693827815	1.41789738306589
N	0.11328131512252	-1.05808103488257	-0.50134214887173
H	-1.28574373939956	0.93486656120268	0.59966527346667
H	-0.73776180934063	2.15669706998097	2.68215166291761
H	2.79334804712716	-0.27071925640645	3.14042381357449
H	2.24383279397245	-1.48507057647162	1.07485336885783
C	-0.32790493602496	-0.43301699432271	-1.69358895849026
C	0.20036737974410	-2.46860427304522	-0.64782401231153
C	-0.34612310682223	-2.79141707599582	-2.00726393120785
C	-0.45840837896170	-1.51529586753175	-2.71344137143107

C	-0.88796923722359	-4.00302700834727	-2.33048285052904
C	-0.74864284236202	-5.22999807504576	-1.47872858974759
C	-1.73883189819380	-4.19544214028895	-3.55019391635410
O	-0.49999428367600	0.76609548886976	-1.83623214484497
O	0.61373504484444	-3.21336401092089	0.22691961070318
C	-0.54417486082011	-1.12237239010663	-4.01955031332604
C	-0.37664474445417	-1.82035777880277	-5.26255763234079
H	-1.73807408815805	-5.54347358016094	-1.10798657173739
H	-0.38452465539299	-6.06588932788904	-2.09818552275647
H	-0.07924734875489	-5.09488732627762	-0.62829375293885
H	-1.17670181973686	-4.68282231386470	-4.36232283772788
H	-2.57766365966790	-4.86463635642822	-3.31036586197478
H	-2.13668825283561	-3.25653028158413	-3.94641749716676
H	-0.74505640015799	-0.05131319792114	-4.13219766382054
N	0.49846701988738	-2.90294534362526	-5.46954370938167
C	-1.03780585575348	-1.53071202132926	-6.46199318676352
C	0.39545824666229	-3.29827655005654	-6.78761886286726
C	1.59882794067357	-3.30009154798236	-4.60852457932117
C	-0.57727973970391	-2.47475318403893	-7.42893146874004
C	-0.87748996452444	-2.70079713961979	-8.78546963977321
C	-0.20178988441352	-3.70470337333273	-9.46685907185237
C	0.77242620520817	-4.49326024085499	-8.81978801813257
C	1.08735272988175	-4.30020938398537	-7.47762579269729
C	-2.08788826883950	-0.49239122378281	-6.67727419058903
H	1.42457270650618	-4.28196616352901	-4.14617969854032
H	2.52866538697048	-3.34323725920113	-5.19114251242231
H	1.72401602854079	-2.56432355307334	-3.81062560661426
H	1.83345249462568	-4.92420311248079	-6.98499965050469

H	1.28662424663482	-5.27428355316562	-9.38074189078815
H	-0.42312270659710	-3.88872206980900	-10.51856907647360
H	-1.62671224806708	-2.09367033438566	-9.29553877057476
H	-2.06158148701487	0.28830095456452	-5.90675318088872
H	-3.10127455097326	-0.92371295106871	-6.66377159322205
H	-1.96158708713381	-0.00342023942437	-7.65323084283794

Table S25. Cartesian Coordinates (in Å) of *Z′*-**1**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-8.52319983150046	1.10330279640908	0.10290220875715
C	-9.17251817432017	0.77008661070345	-1.08436103162907
C	-8.55843215243875	0.99918631460359	-2.31823017731869
C	-7.28123931462052	1.56385187602860	-2.35174717006851
C	-6.61749372129314	1.88600290536677	-1.16879869644057
C	-7.22944968781415	1.65800473204354	0.08147287931755
N	-6.63216113921769	2.05196464204766	1.28772612105995
C	-5.50891315945466	1.56272001975137	1.69336396041427
C	-4.94688573752108	2.11049877627117	3.02690670300822
C	-6.08807353960451	1.97324738995734	4.06282662375025
C	-4.61018413962423	3.60413618676841	2.86715437675812
C	-3.73065580166010	1.34979307644940	3.57588087660028
N	-4.93038965284949	0.44639335841673	1.07962644180662
H	-10.17342610612800	0.33754669309000	-1.04536112223024
H	-9.00699601129821	0.94621646903532	1.06740064096589
H	-9.07451177265149	0.74939466147801	-3.24551686752861
H	-6.79482995490420	1.75800059590083	-3.30899390681196
H	-5.62635074306639	2.34088629340586	-1.20065773322040

H	-5.58213013575544	-0.01400122242113	0.44063648272845
H	-5.75770660619375	2.37884328004805	5.02947397982706
H	-6.98028676256287	2.51483452635853	3.73266307450146
H	-6.35964215827130	0.91865930270966	4.21170041114915
H	-4.33244373173399	4.03108099073657	3.84105585138512
H	-3.76351306407844	3.76254314064893	2.18491058612909
H	-5.47532325670388	4.15523577443715	2.47947025422279
H	-3.91857500786143	0.26968598350969	3.63430324827051
H	-3.52459658518769	1.70655066853037	4.59436968560659
H	-2.82085131400659	1.50575091434815	2.98717850655434
C	-3.57745126741251	0.26231264410040	0.71224326437843
C	-2.72251563735718	1.34059413897973	0.44326372215896
C	-1.40501684928030	1.12292195602047	0.05414727244192
C	-0.92187728131567	-0.18341690736101	-0.09307078884521
C	-3.08820197160197	-1.04267420282385	0.55259840101579
C	-1.77639842177284	-1.26721264467524	0.15173259283769
N	0.42529207478224	-0.40126795953695	-0.49121309689231
H	-0.75144694581445	1.96893508498353	-0.14475267693680
H	-3.10097867839240	2.35975628470713	0.51906032490408
H	-3.74363391214583	-1.88856564133443	0.76358748669542
H	-1.41279887417362	-2.28434466641298	0.02988147779267
C	1.53202635644610	0.31768064964128	0.02589622991463
C	0.82912579898033	-1.36912763367582	-1.45199018490127
C	2.30216508070325	-1.17532608864924	-1.65835265496670
C	2.75042002265561	-0.28689208487911	-0.58574379119129
C	2.95095091014378	-1.53513813567057	-2.80558953972813
C	2.34763837777084	-2.41280892319472	-3.86192434589748
C	4.31733210349603	-1.01881268630887	-3.14390972652943

O	1.46244723051740	1.21166809470144	0.85352700525803
O	0.05682550403995	-2.14475410859823	-1.99183052757709
C	3.94691561175361	0.01152041400194	0.00483093020502
C	5.25185935425245	-0.57766874259059	-0.07800657091433
H	2.22018434174118	-1.84226488198126	-4.79625847214824
H	3.04911534281130	-3.22754542508814	-4.10420564912639
H	1.38558745053921	-2.83949178903083	-3.57577951363042
H	5.09353036826052	-1.77841191932869	-2.95993438277494
H	4.36441274011576	-0.78459368929222	-4.21730664243553
H	4.59163979394053	-0.12571175278374	-2.57474831575726
H	3.87979307376734	0.84852464413354	0.70825290399622
N	5.51240863544921	-1.94197785832046	-0.30407404888338
C	6.46750891550804	0.10364503608463	0.06149099662374
C	6.87974856402766	-2.12727069873550	-0.30784971613998
C	4.56731373214977	-3.03597469608700	-0.15995649998393
C	7.50592319079184	-0.86086950913266	-0.10759501303626
C	8.91174795267049	-0.78691120402945	-0.09453648622104
C	9.64876547918099	-1.95278397049551	-0.25360760252188
C	9.00967160132963	-3.19831979628046	-0.42758460713946
C	7.62209842175582	-3.30480688113110	-0.45287386341083
C	6.65249147016282	1.57115944085770	0.25990989767807
H	4.35885970269866	-3.52638226776247	-1.12141505967964
H	4.96771597018486	-3.78294613941523	0.53824200484722
H	3.62532071763218	-2.65575290819166	0.24156420071917
H	7.14021820053916	-4.27147372949839	-0.60016277999461
H	9.61521521274689	-4.09681634181583	-0.54998571980928
H	10.73818503276460	-1.91024919262850	-0.24318050806649
H	9.41493605813223	0.17113477244009	0.04283292355088

H	5.76207787766969	2.04579625350536	0.69108368269506
H	6.86662388553376	2.09061739654125	-0.68736751212005
H	7.49700594394358	1.77188050940916	0.93330477198189

Table S26. Cartesian Coordinates (in Å) of *E′*-**1**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-7.06358530928630	3.97746824772525	0.44823146208541
C	-8.02567174459571	4.97533922749533	0.59400283004447
C	-9.25173592650350	4.70117126895611	1.20373363039318
C	-9.51016640379521	3.40328001851586	1.65125784313564
C	-8.55763257291659	2.39709043573219	1.50513048068862
C	-7.30373438242773	2.67252131588186	0.92287784565239
N	-6.40400065762498	1.64144107314352	0.65848526336227
C	-5.38306255364884	1.21635534636089	1.31322637306359
C	-4.84228092738284	1.73945616726175	2.67292730582985
C	-5.99386550321654	1.58051064984132	3.69530047630320
C	-4.44700917144130	3.22476133989734	2.58551460404821
C	-3.64788342777869	0.93921294217816	3.22177471679598
N	-4.84006706061286	0.01950118183893	0.80366604450356
H	-7.81317707091375	5.97888607451931	0.22183480946450
H	-6.11843917625953	4.19149478165228	-0.05175312852171
H	-10.00246975875930	5.48389719694039	1.31324255694329
H	-10.46926932123150	3.16634797327188	2.11467982484260
H	-8.77348658344622	1.38044150378951	1.83562149890133
H	-5.50565263276130	-0.39434805406427	0.14783183601090
H	-5.64175403067673	1.90540970009799	4.68455719127077
H	-6.86787183139010	2.18414048211520	3.43224111769691

H	-6.30662639758359	0.53044020955982	3.77598524104751
H	-4.09230499408768	3.56229862025782	3.56966702028187
H	-3.63014089828788	3.38615004707183	1.86887642833236
H	-5.29078617209914	3.85993972358588	2.29701652613221
H	-3.86196714077546	-0.13569212992769	3.26646687288711
H	-3.44349297261559	1.28320149869339	4.24531646819938
H	-2.73107373335756	1.08260758445593	2.64112194573943
C	-3.49378137892976	-0.16456521511604	0.39838268709415
C	-2.64852238552502	0.90893173942478	0.08504978152448
C	-1.33901119622136	0.68548271931474	-0.32846254060673
C	-0.85576397785051	-0.62252896431294	-0.45605357208497
C	-3.00436296247132	-1.47147224693187	0.25784540666329
C	-1.70165029814245	-1.70250464260884	-0.16798131092175
N	0.48349793970301	-0.84760990286850	-0.87694654289189
H	-0.69221675519033	1.52797261676548	-0.56171498846121
H	-3.02912649803464	1.92876947198985	0.14030243495949
H	-3.65300112477482	-2.31280551469848	0.50484912185450
H	-1.33755352182223	-2.72130788559762	-0.27403254659963
C	1.59948884529547	-0.11636404624372	-0.39940636833647
C	0.86731837828304	-1.83223828955130	-1.82848171361042
C	2.33691525003047	-1.64529631092419	-2.06584259592619
C	2.80560200178379	-0.73315145514805	-1.02328365080824
C	2.96532513402920	-2.03354832741306	-3.21576199060669
C	2.34828744709194	-2.94716520175143	-4.23264295927708
C	4.32194724252338	-1.51827145106274	-3.59305736744304
O	1.54645218208480	0.79313048939546	0.41253859894315
O	0.08328431545934	-2.61522489368985	-2.34014818468896
C	4.01471404837571	-0.41895931493385	-0.46557119458525

C	5.31932583467055	-1.00391006702825	-0.55428607064943
H	2.26497922295722	-2.42947952663804	-5.20187814366947
H	3.02144662249101	-3.80197723918292	-4.41014527674800
H	1.36445996294536	-3.31884838664356	-3.94432382916036
H	5.10903920964910	-2.26248058448985	-3.39343879493778
H	4.35099970348435	-1.32122834344021	-4.67436804123964
H	4.59525007693553	-0.60337276207173	-3.05889341695906
H	3.96251443767799	0.43793155387121	0.21579036965530
N	5.59555982189383	-2.36707247682453	-0.76979641985529
C	6.52645571723005	-0.30531166155827	-0.42681858381430
C	6.96489734668121	-2.53526537522640	-0.76763816822206
C	4.66729405133977	-3.47040134127828	-0.58709864660502
C	7.57641451806606	-1.25838583197607	-0.58160482769414
C	8.98207714054541	-1.17116295163333	-0.56749880063354
C	9.73120041365276	-2.33087101462816	-0.70947490553095
C	9.10600427775085	-3.58592843358277	-0.86821578892520
C	7.72000403467719	-3.70664784644134	-0.89592028716351
C	6.67060042758182	1.16704936114784	-0.21325259080172
H	4.49298058579073	-4.01537361261959	-1.52573881665799
H	5.06258793642200	-4.17176517336537	0.16000882568767
H	3.70861247462741	-3.08658162107154	-0.23204918365083
H	7.24767011462085	-4.67991914230892	-1.03030762505714
H	9.72151179381127	-4.47935101181537	-0.97714692120352
H	10.82006103748180	-2.27623033499066	-0.69699992924051
H	9.47703374110616	-0.20727665655662	-0.44126515239707
H	6.12351523419718	1.50258828902259	0.68031552640248
H	6.29490239240919	1.75056564029204	-1.06585707750835
H	7.72396553908205	1.43610575015246	-0.07051301274595

Table S27. Cartesian Coordinates (in Å) of *Z*-**1**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-2.54022559511083	1.86396954461414	4.974804769
C	-3.48311368445641	2.26824991313569	4.032905728
C	-3.18579415334994	3.28720284192565	3.124772951
C	-1.93019409915332	3.89765419306377	3.173306979
C	-0.97280367278717	3.48245359551661	4.095770467
C	-1.25879370102272	2.44718564945378	5.008672177
N	-0.37785515607282	2.06669404842759	6.021369132
C	0.88411430442725	1.83548451235017	5.913889218
C	1.68600673479887	1.65783110182517	7.226755199
C	1.49660602408188	0.19328209662298	7.673791906
C	1.12683083477821	2.60102586900769	8.301412566
C	3.19134145286899	1.93758951854711	7.062629751
N	1.62093598466255	1.64542783443217	4.752544018
H	-4.46415315630655	1.79085891679494	4.015190953
H	-2.77551091575938	1.08684130894920	5.703264685
H	-3.92671957952774	3.60726326907684	2.39197189
H	-1.68849520166526	4.70246823861790	2.476981078
H	0.00470379916253	3.96508095393310	4.125799943
H	2.05129153536791	0.00414061681785	8.604330758
H	0.43525446906421	-0.01727893419826	7.854245179
H	1.86353257125808	-0.50914649235546	6.912162285
H	1.63218299009784	2.42004761885397	9.260513281
H	1.28257210796580	3.65341497075354	8.026031699
H	0.05114441821639	2.44695319029890	8.430882747

H	3.70236393721241	1.19021603368830	6.43661051
H	3.67551322472921	1.89029793193137	8.046708516
H	3.38602295800070	2.94117040863705	6.656249145
C	1.21079433433485	1.21819174163279	3.471631396
C	0.13150609075585	0.34562494474630	3.278240938
C	-0.19015603032257	-0.10458064585924	2.002266993
C	0.55867098749393	0.30611955784380	0.89119398
C	1.96158908698502	1.62121192748702	2.357650761
C	1.64158975430413	1.17502270260154	1.080666493
N	0.22977189499824	-0.15146533024713	-0.410579968
H	-1.03397823648686	-0.77707343439429	1.868113826
H	-0.45301323245550	0.00463513612499	4.129955048
H	2.79922855693562	2.30859954669694	2.491969604
H	2.23618923994837	1.49766805187834	0.229488472
C	-1.06896836238691	-0.32555951149181	-0.914316573
C	1.19614449034103	-0.54073776928039	-1.416341503
C	0.43212851086072	-0.90027017108211	-2.616841983
C	-0.89957588384949	-0.81543603491107	-2.321926556
O	-2.11953747197549	-0.12373847765036	-0.327810428
O	2.40220178680647	-0.57043579626107	-1.217814134
C	-1.94899182897093	-1.23911909002534	-3.181251676
C	0.94539320480391	-1.51369295518213	-3.910380383
C	-1.56010594094421	-1.57743071570280	-4.448758514
C	-0.16465490922639	-1.24281992788392	-4.996876044
C	2.30685219887442	-0.92078178054040	-4.30894222
C	1.11219851224312	-3.03214188605838	-3.667338701
N	-2.28423887037998	-2.20437459459384	-5.427493695
C	-0.14790007076340	-2.07546515310056	-6.273817569

C	-0.21493077741235	0.25491029042643	-5.408182666
C	-1.44666642359352	-2.57411603458045	-6.496703882
C	0.83257467267884	-2.30309137166496	-7.229963266
C	-1.77639190903648	-3.31482470420952	-7.629068762
C	-0.76469769389879	-3.55400686167846	-8.567005989
C	0.52336508357192	-3.05519273626752	-8.374643699
C	-3.65780987653982	-2.63791457591765	-5.277666996
H	-2.96134565870639	-1.35233577933686	-2.797140967
H	2.26667868591555	0.16794050498540	-4.432202929
H	3.03815703715146	-1.12750202355496	-3.520451847
H	2.67620651175801	-1.36525079343351	-5.241447624
H	1.48297719363191	-3.53914432267855	-4.567867953
H	0.16054346692033	-3.49846375954888	-3.377999227
H	1.83430820211547	-3.19971073078004	-2.85851186
H	-0.29614148836605	0.90107597658626	-4.525457194
H	-1.08173063477802	0.43782754556764	-6.055418042
H	0.68506845514977	0.53001647566743	-5.969888668
H	1.83875340519392	-1.90520345558083	-7.105336864
H	1.29708322230562	-3.24828934225573	-9.117567331
H	-0.99329225574538	-4.13728067707850	-9.459301819
H	-2.78024902144320	-3.70765325462832	-7.78755601
H	-4.14360549035974	-2.67334396620684	-6.258942794
H	-3.72210402171217	-3.63335825741712	-4.811508082
H	-4.20264413496817	-1.92090547397479	-4.654483233
H	2.62599520676261	1.73748924209160	4.860059615

Table S28. Cartesian Coordinates (in Å) of *E*-**1**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-0.52310776387785	5.63861943008876	4.83196277303047
C	-1.39160007831360	6.61102796790885	5.32403585823049
C	-2.47534521046167	6.25857880864328	6.13191419519052
C	-2.68687212291587	4.90970159761977	6.42782949334479
C	-1.82495095582725	3.92945038388436	5.94036349826401
C	-0.70776438991360	4.27633067314970	5.15078293588407
N	0.07121791750342	3.29362018933002	4.55411951587726
C	1.15773737406886	2.71979681056233	4.93055834787484
C	1.95206950192926	2.98989594887136	6.24597131692231
C	1.03340875244797	2.71376014885474	7.45235340658708
C	2.40756340610335	4.46240507079388	6.25978835658542
C	3.20775418708658	2.11097492080569	6.40512079890293
N	1.71843026902939	1.75723471178814	4.11349288910791
H	-1.22126026023208	7.65758266838946	5.06547322913212
H	0.30525564759144	5.91770364651726	4.17982591436558
H	-3.15547624057673	7.02178029042601	6.51038009399560
H	-3.53932385406991	4.61280571220247	7.04129914001214
H	-2.00927516224184	2.87588702965867	6.15380797231687
H	2.56780600884774	1.33420141081368	4.46802140449735
H	1.58840973977106	2.88880168931803	8.38528745646593
H	0.15678508937470	3.36887779372018	7.45399383105823
H	0.68381245329638	1.67206841667211	7.45634217340569
H	2.99370526720064	4.65806517860507	7.16918389843915
H	3.04210030802771	4.69066093819522	5.39216065922107
H	1.55674444146448	5.15078897587869	6.25248222204160
H	2.97208225524894	1.03748020366720	6.45397486269868
H	3.69755213216550	2.36485492550696	7.35439278466365

H	3.95322901971309	2.28611294887048	5.61504288679049
C	1.31460337892319	1.24076074423110	2.87009951398205
C	0.18321004334459	1.66154799706426	2.15201847689779
C	-0.12766741645087	1.06787755440988	0.93037512688264
C	0.68038729932225	0.06428428059246	0.38603734595666
C	2.12039771619094	0.22605464088988	2.31819353118186
C	1.81826387226651	-0.34922844372384	1.09299446827551
N	0.35920981021217	-0.52910432968583	-0.86221925448661
H	-1.00771459831818	1.40510589324985	0.38704093428122
H	-0.44799730767909	2.44171241414083	2.56355329191819
H	3.00685029296647	-0.11521492527978	2.85916399235257
H	2.45537136841533	-1.13344788369557	0.69052167246358
C	-0.11894308330588	0.15195153084952	-1.99160324145170
C	0.43764315276502	-1.94551118712004	-1.14511121500265
C	0.04460943025884	-2.11575256086450	-2.55001273895912
C	-0.32131515420744	-0.89614718480490	-3.04588797233755
O	-0.32964032622543	1.34951746470263	-2.09405142609096
O	0.75111403823374	-2.78355533389371	-0.31189286403773
C	-0.91074797660038	-0.68319314503170	-4.32166451727757
C	-0.18906855824496	-3.41122476395594	-3.31152911184437
C	-0.92539506873938	-1.77634525445612	-5.14421570626006
C	-0.10998670361528	-3.04269976979435	-4.84272664486709
C	0.83889382034967	-4.48485919829592	-2.91850553782049
C	-1.60403341782283	-3.91457378772855	-2.94196729598531
N	-1.59056158091575	-1.94684698631189	-6.32951805600602
C	-0.70297994914064	-4.01648778788638	-5.85469756815138
C	1.34675450521903	-2.72930114649141	-5.28376504630475
C	-1.53033071652391	-3.29289838988823	-6.73627837641489

C	-0.48280770234589	-5.36595938043708	-6.09469325768076
C	-2.16122867867461	-3.89009945072656	-7.82496342172304
C	-1.94470100099725	-5.25778943644030	-8.03237158008770
C	-1.11601489480638	-5.98926517554206	-7.18200150233650
C	-2.43701446516067	-0.94481280538422	-6.94305428290250
H	-1.38075399159580	0.27021937262372	-4.55670265245189
H	1.87021415229630	-4.16066735333235	-3.10114422420272
H	0.75342507380542	-4.69521018456861	-1.84731628025763
H	0.66380009471652	-5.41966768409814	-3.46516267049840
H	-1.83816423980914	-4.85403888081464	-3.45968183588215
H	-2.37361911105917	-3.17610666190249	-3.20490642684932
H	-1.66018578388945	-4.09635192024334	-1.86142369773163
H	1.80302421790154	-1.98243654445741	-4.62269468800435
H	1.35302022024364	-2.33869444576775	-6.30909483284029
H	1.95690999447962	-3.63965460230624	-5.26908565074867
H	0.17526593288143	-5.94878135437687	-5.45138962779234
H	-0.95654347620475	-7.05243370168550	-7.36123046795756
H	-2.43190252260667	-5.75221525779915	-8.87317316567959
H	-2.80987049638069	-3.32620907011937	-8.49478123303403
H	-2.47507497189603	-1.10550523025280	-8.02604751894404
H	-3.46189294358400	-0.97614042188164	-6.54161430193543
H	-2.01750201043185	0.05032725754869	-6.76177737625960

Table S29. Cartesian Coordinates (in Å) of *Z′*-**1**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-8.33214366065714	1.48171973705850	0.67735811244569
C	-8.98863973140274	1.28040388912725	-0.53535573915348

C	-8.37214690537575	1.62104163543360	-1.74208586499338
C	-7.08553636682314	2.16457667668116	-1.72214558111150
C	-6.41558310303646	2.35641669112961	-0.51463282345882
C	-7.02938547938573	2.01526427133963	0.70891883414341
N	-6.42383453469304	2.27743038215527	1.94572208718301
C	-5.31612508403398	1.71701904839382	2.30247533711611
C	-4.73506122133234	2.12816025571262	3.67663414733100
C	-5.89062539429483	1.99344358363409	4.69611953388125
C	-4.29996062158551	3.60461480390874	3.62845492843999
C	-3.57584050347487	1.25104992118289	4.17236172409654
N	-4.77114483007957	0.64994951449594	1.58558890605608
H	-9.99656637888906	0.86246904236665	-0.53685274151414
H	-8.81715030866578	1.23638785789890	1.62270029282758
H	-8.89290771788862	1.47298587643846	-2.68843071769208
H	-6.59612812143883	2.44415729946417	-2.65651661779918
H	-5.41632695936123	2.79434200651355	-0.50369079797241
H	-5.42472555136843	0.29172063184610	0.88595578627434
H	-5.54080518034858	2.30482557406936	5.69055828405617
H	-6.74250108214803	2.61546452071246	4.40385418184627
H	-6.23338825853650	0.95163904267501	4.76673370238288
H	-4.00501809232367	3.94032670011359	4.63265265495193
H	-3.43827559101866	3.75693187046234	2.96417631713897
H	-5.12419310404122	4.23784959835504	3.27847852571632
H	-3.83478835827610	0.18440226600049	4.14828508856938
H	-3.35582887752508	1.51642780943230	5.21567426279893
H	-2.65326988119449	1.39015982244710	3.59976094083155
C	-3.41486108753008	0.43847543844925	1.23055563551436
C	-2.51921479334223	1.49877506539802	1.03842400823415

C	-1.20258153751284	1.25827086412176	0.65730826916501
C	-0.75829073224600	-0.05353634401686	0.44453630399889
C	-2.96799575709171	-0.87047984409464	1.00261336494687
C	-1.65613626372042	-1.11740219135313	0.61329230534632
N	0.58208699918527	-0.30285484676704	0.05860042787122
H	-0.51817541386469	2.09187610935410	0.51735403049114
H	-2.86428876404234	2.52446875175014	1.16832792164941
H	-3.65623760838273	-1.70327708375512	1.15289007434129
H	-1.32452399768242	-2.13871675581479	0.44116511571799
C	1.71216200600381	0.36208687876114	0.55853953897594
C	0.98903190941177	-1.26915528287776	-0.94288249216214
C	2.45404701351441	-1.22437268585504	-0.99580684645957
C	2.88843642851614	-0.24550807135758	-0.14545747596782
O	1.73086613055966	1.25316035415524	1.39233048228206
O	0.19830076520521	-1.93211643602394	-1.59767255893962
C	4.23303523320567	0.20075973169494	-0.04189405190851
C	3.38182216033911	-1.92052581839579	-1.97956800134419
C	5.14889122894611	-0.55201530917611	-0.72648255676615
C	4.80760343604011	-1.93257599358375	-1.30674056224242
C	2.88573131136464	-3.33629980679185	-2.31584719109966
C	3.39706907904032	-1.07557918269766	-3.27494914322805
N	6.46154563028022	-0.26915248022993	-0.99123012226764
C	6.02365213115554	-2.18402090583713	-2.19068735460693
C	4.87363514234611	-2.92772557378618	-0.11510144993622
C	6.98515704278692	-1.19122139597464	-1.91781237312250
C	6.35143865169967	-3.21592706725180	-3.05969616053260
C	8.24378395780886	-1.18847242932463	-2.51392916445498
C	8.54196685089969	-2.22390725391609	-3.40793833261846

C	7.61182381083536	-3.22718643235889	-3.67818138507146
C	7.13944627336882	0.93959233370052	-0.57030427736934
H	4.46573038513641	1.12587904307039	0.48257374984033
H	2.79306204960785	-3.96883269703216	-1.42517611005827
H	1.89153494125777	-3.27544945285515	-2.77091254059237
H	3.55672481897677	-3.83082173932555	-3.02930459322363
H	4.05305571924317	-1.52445124916611	-4.03222881810447
H	3.74555515256359	-0.05177876806225	-3.08137173351789
H	2.38337598836265	-1.01853531858122	-3.69057003681942
H	4.05483848819121	-2.74706086734556	0.59227024337449
H	5.82633178541167	-2.81403316815193	0.41713879360438
H	4.81303950425022	-3.96134235332652	-0.47411748769680
H	5.64520870104719	-4.01863493214071	-3.26773599232580
H	7.86346715993708	-4.02806635960369	-4.37315157520282
H	9.51740191541974	-2.24260224671714	-3.89453323043185
H	8.97721897251955	-0.40970545997327	-2.30730897399192
H	8.21431126570888	0.74837315010500	-0.47999956936514
H	6.98235196812944	1.76318907889491	-1.28386059699329
H	6.76546484633826	1.24725267501756	0.41178172867570

Table S30. Cartesian Coordinates (in Å) of *E′*-**1**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-6.79935194348848	4.26990719001254	1.27138886784872
C	-7.73605884725582	5.27548580171750	1.50372258030648
C	-8.97136323172008	4.98021906877076	2.08437379937372
C	-9.26482617535000	3.65439250140160	2.41309688864143
C	-8.33784892667937	2.64099912231109	2.17954564752302

C	-7.07417578476558	2.93354963335805	1.62626556185346
N	-6.20229938896007	1.90810272810796	1.26973455783100
C	-5.19766917426899	1.38909520211295	1.88299465487027
C	-4.64202912987284	1.77655013608065	3.28191996778161
C	-5.80455359315428	1.60715273197323	4.28924159114902
C	-4.16615432738555	3.24092446058521	3.30326900827291
C	-3.49587266878288	0.87411437117319	3.77165131735100
N	-4.69257289453116	0.23028172038995	1.26648313118847
H	-7.49601167925522	6.30250844866193	1.22336792250388
H	-5.84750303262931	4.50249767410696	0.79275136752941
H	-9.70251359553244	5.76911095293777	2.26152590603135
H	-10.23159832478960	3.40189525186744	2.85191416739815
H	-8.58092991246253	1.60493856446097	2.41821657519134
H	-5.35347113402873	-0.07487897109158	0.54880897910063
H	-5.43828400765876	1.83800365371009	5.29964849692980
H	-6.64278526126510	2.27600732566542	4.07236900150666
H	-6.17536297841308	0.57303974839584	4.29263242963591
H	-3.79848777953632	3.48770230979196	4.30952344557009
H	-3.33875740388157	3.40833496856338	2.60042522020622
H	-4.97397505848991	3.93903732820751	3.05983616087479
H	-3.76607761555061	-0.18818772008068	3.72883934441176
H	-3.28371986446521	1.12459654715377	4.82055360148470
H	-2.56811060572266	1.01482646100011	3.20831131372242
C	-3.33889023795103	0.02765217672020	0.87894889431381
C	-2.46092138543709	1.09218331471502	0.63671404538414
C	-1.14922799951422	0.85588062124457	0.23537241123688
C	-0.69371138115701	-0.45640705361976	0.05304355182788
C	-2.88086690370918	-1.28182390883638	0.68148110305928

C	-1.57435498892730	-1.52537731829365	0.27184165227362
N	0.64222585650733	-0.70131997068598	-0.35209098778558
H	-0.47767704035132	1.69231777248812	0.05522318023896
H	-2.81705635744332	2.11741844019371	0.73906215677785
H	-3.55620501261353	-2.11680484780029	0.87243718889759
H	-1.23303369037122	-2.54734407837854	0.12375849969157
C	1.77384568548767	-0.01376119837066	0.11145553224413
C	1.04019466718904	-1.68518359547097	-1.33964640716582
C	2.50361786019868	-1.62538721386111	-1.42268861288391
C	2.94327251541925	-0.62413120717627	-0.60184615420976
O	1.79887682251987	0.89494258000264	0.92590695867925
O	0.24420780103592	-2.37123544727364	-1.96343137652472
C	4.28482514358682	-0.16192553336506	-0.53294592104711
C	3.41994239967136	-2.33306312846620	-2.40901402530019
C	5.19571028364702	-0.91932617496021	-1.21872341816821
C	4.85866321608050	-2.31494826346637	-1.76449712481978
C	2.93287969538971	-3.76128686623772	-2.70394540490206
C	3.40041659878050	-1.51646510268475	-3.72238477246001
N	6.50055691124159	-0.62893475442365	-1.51238050959323
C	6.06041760206872	-2.57100110590433	-2.66657580907468
C	4.95970557627652	-3.28442284353732	-0.55421973203411
C	7.01667838562434	-1.56363603524256	-2.43055561506172
C	6.38236821776199	-3.61556240385038	-3.52255145738704
C	8.26392661774759	-1.56004921825446	-3.05013688528356
C	8.55602701464718	-2.60926794226380	-3.92990329186010
C	7.63112250011476	-3.62631615955151	-4.16417324085262
C	7.17242271182360	0.59506823997352	-1.12764453285281
H	4.51714507702627	0.77628300933503	-0.03199795281654

H	2.86541402399148	-4.37440162861674	-1.79759670540826
H	1.92905969367895	-3.72103824503167	-3.13975233465707
H	3.59488160667657	-4.26471586649286	-3.41950462377384
H	4.04697102573014	-1.97403901458035	-4.48255420280227
H	3.74072633356583	-0.48489608472556	-3.55738562545317
H	2.37837676421006	-1.47946990087847	-4.11928562779674
H	4.15356694572482	-3.09767324906800	0.16595518656707
H	5.92171721721886	-3.14899058949203	-0.04446327904450
H	4.90366183579947	-4.32596703418598	-0.89039229271402
H	5.68021804787013	-4.42850808576887	-3.70306684526212
H	7.87778426751086	-4.43744891656873	-4.84897053988075
H	9.52244497429613	-2.62761955151962	-4.43420044136911
H	8.99311417565552	-0.77028798725673	-2.87220622926027
H	8.25174744068767	0.41970938708247	-1.06329735303418
H	6.98515319914692	1.40550111667629	-1.84899453632101
H	6.82042262576181	0.91287265638405	-0.14058799841935

Table S31. Cartesian Coordinates (in Å) of *Z*-**2**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-0.08161613836684	3.04096535117599	-4.15968552926017
C	-1.40109271732665	3.44233308731531	-3.96504722464278
C	-2.40895497109488	2.49475163232336	-3.76805608927273
C	-2.07652771997269	1.13741596786730	-3.77036871749997
C	-0.75599513847367	0.72888042431550	-3.94124910824570
C	0.26984080144409	1.67741238940752	-4.12938959652732
N	1.58609540352689	1.31946090701791	-4.41845090978903
C	2.30873424518208	0.43656064365358	-3.82211469322774

C	3.65506881408934	0.05769052633081	-4.48796172046095
C	4.66770630734158	1.15752458520079	-4.10689236976921
C	3.47927976781173	0.02422595276519	-6.01305813354952
C	4.20203720647768	-1.30513503875018	-4.02585286825092
N	2.06757605852114	-0.17962082011098	-2.60203302158467
H	-1.64770544997588	4.50526315181137	-3.98504532162195
H	0.70455772860821	3.77478595653567	-4.34202692518633
H	-3.44416419357471	2.80900319370647	-3.63210976612799
H	-2.85597008626634	0.38555144084175	-3.63398260611110
H	-0.50743936333296	-0.33303079628872	-3.94465364178338
H	5.65091830586711	0.94015548081287	-4.54867039184771
H	4.32913308043024	2.13312892226570	-4.47627173015827
H	4.79370437772351	1.22580451618748	-3.01691319528836
H	4.44868654811357	-0.15126459085394	-6.50019298564100
H	2.79434262260882	-0.78012003124470	-6.31610868825490
H	3.06446931247572	0.96971640868152	-6.37587084401283
H	4.50872899625426	-1.30974538816007	-2.96896338274949
H	5.10285900288398	-1.54669380395644	-4.60499751514211
H	3.48414579466835	-2.12108519893652	-4.19663734623109
C	1.27550241466380	0.24521222926014	-1.51215408109438
C	1.12198293403848	1.60032795445291	-1.19792784881297
C	0.36294191140852	1.97868399342634	-0.08250878541593
C	-0.21088146162217	1.01264934141721	0.72655822630472
C	0.70003720822653	-0.74957997952613	-0.69641183160044
C	-0.03971512452819	-0.34903705943184	0.41379760499338
C	-1.13699158339710	1.13156486369465	1.92414890525928
H	0.24173178636336	3.03918788034375	0.14454749942993
H	1.59841551646162	2.35651450531040	-1.81707316690207

H	0.82209955623372	-1.80245087375811	-0.95399258895706
N	-0.71299141405844	-1.14819984634376	1.33699758768726
C	-1.00861432958145	-0.32815190510832	2.52716437129136
C	-0.44038120695567	-2.56580767405446	1.46441985671723
C	-2.57181350244198	1.37788839537097	1.41361837414353
C	-0.75966036153390	2.22112499478767	2.92856740536200
O	-2.29923056476311	-0.73369980036662	3.05543051769802
C	0.09563740661526	-0.47533396076727	3.53249383034369
C	-0.04949307564583	-1.11456040311414	4.70461146330479
C	-2.43069605241999	-1.41486488797774	4.22180160754277
C	-1.34277664036964	-1.63291439273425	5.09982906359054
C	-3.71426803688474	-1.87994173242845	4.53786526716210
C	-1.57125094511007	-2.32941451579721	6.28927390460544
C	-3.92811792153688	-2.56745977332063	5.72448665417751
C	-2.85159841559578	-2.78767279054551	6.58971894098817
N	-3.07562041375681	-3.52039266617096	7.84778042100904
O	-4.22507207200605	-3.91114100415635	8.09025813051772
O	-2.10123678255382	-3.70391328122907	8.58979188998982
H	-3.28600693911118	1.44223204014546	2.24404089844290
H	-2.59269617237522	2.32569745929498	0.86063243275477
H	-2.89885867382148	0.58067958875905	0.73583087820880
H	-1.40576154748104	2.17437417968390	3.81620511599091
H	-0.89795351573123	3.21151979874754	2.47450165069032
H	0.28352595029757	2.14888196396114	3.25812651717898
H	1.06478736753426	-0.09340498899463	3.20984045071604
H	0.79837172116514	-1.25497005878499	5.37779374188627
H	-0.75730189217554	-2.51692646614619	6.98810901613783
H	-4.91475504634970	-2.93846646627056	5.99274639528461

H	-4.52969832762305	-1.69166451317664	3.84077544030415
H	0.60399049312918	-2.78940895753066	1.74489149058014
H	-1.10583812913355	-2.99693084956671	2.22019803337618
H	-0.66012593203455	-3.06622280567550	0.51219482791032
H	2.61196721881704	-1.01794340559394	-2.42638178656047

Table S32. Cartesian Coordinates (in Å) of *E*-**2**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	1.53995015201058	0.19556246311425	-0.41421102116100
C	1.13967165146714	-0.35516265659419	0.78642568287706
C	-0.08049263392165	0.05068298438989	1.37945618190803
C	-0.86683763826119	1.01553262548310	0.73051683468962
C	-0.45872552000857	1.56983826567720	-0.49036412613928
C	0.74477429736720	1.15856060174510	-1.05327732889115
C	2.81391563951190	-0.00116166051123	-1.21850138308165
C	2.37844771530558	0.62178368747943	-2.60997769445833
N	1.36128629904934	1.57674320221623	-2.24477771648301
C	3.27946582162781	-1.45247274168122	-1.33790085869380
C	3.93112600535103	0.84448591510309	-0.57319522082602
C	0.62264909546103	2.30996722803802	-3.25472525371678
O	1.71695120293837	-0.50944628055301	-3.35735788783759
C	3.47103368021686	1.23311589318158	-3.42815389673781
C	1.79272282572222	-0.62121127913077	-4.69715208141289
C	3.62662488228519	1.00017672273440	-4.74393141772235
C	2.75150816450954	0.09520742874300	-5.45670062348429
C	0.91264652220547	-1.51841873179103	-5.32426044503181
C	2.80687867206564	-0.10683632527789	-6.83806530611613
C	0.97996727646251	-1.71095767128425	-6.69574654946930
C	1.92736608306146	-1.00066456613333	-7.44319277625389

H	1.75940686998935	-1.10849348675589	1.28187209090794
N	-0.41432323981661	-0.56771697428719	2.60069271751751
H	-1.80339556416601	1.31814163607106	1.18659116717294
H	-1.09684910764617	2.30473123140350	-0.98078555515144
H	4.13597244902603	-1.53436299283781	-2.02128059181318
H	3.60854871155453	-1.81640779463856	-0.35495166751247
H	2.48296092696131	-2.10926712914964	-1.70016233427997
H	3.66272822669949	1.90777369540017	-0.52703114522208
H	4.87978883164545	0.73835325086528	-1.11710808846694
H	4.09417725259486	0.49783911747261	0.45502403887785
H	-0.21691496090355	1.72559286679138	-3.66859161164254
H	0.22187825671038	3.23561999668695	-2.82218546706539
H	1.30008322203425	2.58553807485741	-4.07015740595058
H	4.41871755878699	1.50259989283988	-5.30268472664264
H	4.11509945461532	1.93982660443661	-2.90873296860160
H	3.53343364672890	0.42625447835743	-7.44983464473467
N	1.99776708642579	-1.20369265422318	-8.89825609397928
H	0.31038428476214	-2.40230165341524	-7.20274497783964
H	0.18734866339935	-2.05601051253508	-4.71480994110130
O	1.20829197050080	-2.01101133920933	-9.40734296081826
O	2.84317577504284	-0.55638846167558	-9.53215732580597
C	-1.49307064995096	-0.40000684774470	3.44485269077812
H	0.26742847406839	-1.25170757328977	2.90566244671067
C	-1.46131915204542	-1.30274260637825	4.71721265678145
N	-2.40171088424363	0.45271302739243	3.12579258095554
C	-1.46782630480501	-0.40500909505841	5.97033124559465
C	-2.70609643677846	-2.21173744428154	4.71792794608809
C	-0.22010013829628	-2.21210930587595	4.80384593162009

C	-3.57569966140176	0.83057319144031	3.76490704908581
C	-3.60386666540716	1.95662156151766	4.61523957705608
C	-4.80535580813154	2.41944112947484	5.14830430495786
C	-6.01346186388015	1.78933856004220	4.84022586642050
C	-6.00214222543523	0.69317459941590	3.97425055093142
C	-4.80604339187867	0.22257003374584	3.43588392676287
H	-2.66704128785341	2.46801520912133	4.83973129588354
H	-4.79626028208875	3.28886856362014	5.80803010651923
H	-6.95176361208302	2.15763092225979	5.25522576676228
H	-6.93794782455171	0.19915685718439	3.70711560298532
H	-4.80661827566867	-0.61800937541388	2.74081934069740
H	-1.42471068751203	-1.03221211050346	6.87237792661113
H	-2.37406310293530	0.20551797923032	6.02851847614401
H	-0.59862426253646	0.26720041397491	5.98343804931521
H	-2.68212119210125	-2.86794738285356	5.59991572091032
H	-2.73501377300560	-2.84814859185369	3.82244461883533
H	-3.63314330089496	-1.63119608268048	4.75544546272893
H	-0.28160233841732	-2.80490955930387	5.72604929529392
H	-0.16127759829178	-2.93328182141505	3.97465834066045
H	0.72023673675324	-1.64374720317060	4.86152160310387

Table S33. Cartesian Coordinates (in Å) of *Z′*-**2**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	0.89767633769961	0.10936544072110	-0.79151085138827
C	0.14467455755034	1.22609396694799	-0.47817797963068
C	-1.26199855888611	1.14061845299571	-0.49282704188386
C	-1.87381932112248	-0.06765789384490	-0.84611142256067

C	-1.12006199342345	-1.21178979564407	-1.13463665939154
C	0.27003815286665	-1.10712109636398	-1.10802072476121
C	2.40084557616544	-0.06900500673839	-0.91862385999451
C	2.51326553066797	-1.64971438911102	-0.86981424152862
N	1.23100198841775	-2.08829877427453	-1.37786304499771
C	3.22237191914025	0.61725982592576	0.17275030758216
C	2.83503320317006	0.46336402271125	-2.29990462643183
C	0.88278584062137	-3.49564695926670	-1.42300300724855
O	2.57594421901471	-1.99835791317538	0.58945117698367
C	3.66013613128090	-2.25036975365075	-1.61823959762550
C	3.31526792504600	-3.02563194450801	1.05384531068461
C	4.47559556755493	-3.18339032827654	-1.09538935686294
C	4.30852172011055	-3.65327550837358	0.26264486348968
C	3.09812656498263	-3.43030211147383	2.38049854511054
C	5.06887339045773	-4.68230024671569	0.82423127626261
C	3.86129949775997	-4.45164069779231	2.92617957600848
C	4.84081541211452	-5.07137569404717	2.14119261665615
H	0.61464555742856	2.17065963257075	-0.19944227982930
N	-2.02320092194291	2.31403911872835	-0.21452151567598
H	-2.96127682972214	-0.11486568073575	-0.89682952657496
H	-1.61974461322527	-2.14799053048150	-1.38218750251690
H	4.28640384764143	0.35862531370533	0.08143120061588
H	3.13871907482185	1.70729452522752	0.06689717443174
H	2.88318530971278	0.34157329286670	1.17578111896587
H	2.31033704518443	-0.04669918188511	-3.11827988713188
H	3.91819909386729	0.35563947750738	-2.44813911831981
H	2.59321253644496	1.53155532560121	-2.36439850134174
H	0.49065481871968	-3.86245331574837	-0.45925269377612

H	0.12380938711666	-3.66800291313500	-2.19691585859101
H	1.77081783286251	-4.07892460432291	-1.68925711431624
H	5.27922203438696	-3.61241911482788	-1.69717383976255
H	3.77487080637333	-1.92749451143878	-2.65110403313375
H	5.84141304625307	-5.18437299608643	0.24347796175678
N	5.64908079882399	-6.15682915176590	2.71995547553175
H	3.71320035525286	-4.78093721460753	3.95237467500067
H	2.32940148694177	-2.92700994437887	2.96556274852110
O	5.42754878860150	-6.47664446332939	3.89542864709990
O	6.50430172477422	-6.68778983965772	1.99798964489090
C	-3.14812778500656	2.45935126460276	0.59025978975667
H	-2.01659402118495	2.99550347256633	-0.97682240208055
C	-3.26681567316533	1.71971445674127	1.94303521169858
N	-4.07494028801800	3.31284837798419	0.29965070349697
C	-3.80581061141099	2.72837902331205	2.97947168316049
C	-4.29179014514878	0.57488090325973	1.81035753369165
C	-1.93204947194666	1.17039877833513	2.47177796710315
C	-4.10355710094027	3.98472331415694	-0.92891921395233
C	-4.41789830908212	3.31804628772676	-2.13214523762142
C	-4.52798300194814	4.02476911136921	-3.32886032121388
C	-4.31943848378269	5.40576910208537	-3.35995566315657
C	-4.00709166465844	6.07546550233644	-2.17410014630571
C	-3.90527396517821	5.37863238534993	-0.97118734109462
H	-4.59957242338200	2.24217711704535	-2.10803078211075
H	-4.78388300966797	3.49077705008001	-4.24555993857187
H	-4.40934833975916	5.95576648030713	-4.29693805283249
H	-3.84987924565239	7.15524831760618	-2.18327827539067
H	-3.68104643676072	5.90149160591525	-0.04082718739967

H	-3.93858166774900	2.22168295704351	3.94588470882490
H	-4.76432479698226	3.14843538795603	2.66004637219396
H	-3.10330838904205	3.56069180766188	3.12276976829009
H	-4.47046647110445	0.12065082713355	2.79533075595474
H	-3.93802007251768	-0.21928639379628	1.14053191983318
H	-5.24789041303008	0.95507627960575	1.42876914056145
H	-2.08101824893417	0.80741099458676	3.49822550990970
H	-1.54715023217637	0.33338966530608	1.88008879124230
H	-1.15933757327744	1.95022610387165	2.50235667169635

Table S34. Cartesian Coordinates (in Å) of *E′*-**2**(c), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-4.37086933059422	5.04855792888304	0.98996650612396
C	-5.26096307811787	6.08088707772793	1.28178506647113
C	-6.58229429281218	5.80414991840887	1.63937294841434
C	-7.00743588077329	4.47489801193654	1.68323324868229
C	-6.12752487287593	3.43576993997877	1.38846859691832
C	-4.78216957587563	3.70255185841926	1.06112137563088
N	-3.93760255477877	2.67756481325758	0.63885710425575
C	-3.07385176573368	1.97106201143849	1.27767862359295
C	-2.71318736881902	2.05143461401858	2.78681710741512
C	-4.01665000997768	1.77080121561205	3.57282100384690
C	-2.18722859415762	3.44892177110376	3.16097598105769
C	-1.68700296423584	0.99794927710441	3.23918535772948
N	-2.55842341794304	0.89224605238433	0.53394004880142
H	-4.91549067466139	7.11452164633263	1.22600659848041
H	-3.34784193940465	5.27151689823813	0.68504185986520

H	-7.27554797437124	6.61428665669777	1.86569167812410
H	-8.04154665757601	4.24086246893639	1.94142087407275
H	-6.47078233605150	2.40070088252243	1.40417713209368
H	-3.12913216372292	0.77147775922005	-0.30566685871363
H	-3.79488859022651	1.78098285538732	4.64929999341575
H	-4.78864229654353	2.52200606165321	3.37929313842289
H	-4.42277470534246	0.78150576143949	3.32115968533226
H	-1.96290885934661	3.47511515418479	4.23692312192116
H	-1.25892707017985	3.68733234341165	2.62425866170797
H	-2.92005582381395	4.23488562326982	2.95136179876287
H	-1.99759229452838	-0.01784328150815	2.96548108140889
H	-1.60730093499489	1.04108604647623	4.33454826853415
H	-0.68780263898436	1.17263588038945	2.82753733069706
C	-1.17533607004302	0.66430543932175	0.28238253442793
C	-0.23605138867448	1.70186724133594	0.32691645118336
C	1.11551178552351	1.44437169031248	0.04937015691931
C	1.51289050203474	0.16692157816737	-0.30644332569502
C	-0.78350597156939	-0.63829594715919	-0.07791486014157
C	0.55964210281734	-0.86903706878026	-0.36905399198653
C	2.88856566870407	-0.40937246670725	-0.59230127198809
H	1.83834573249860	2.26152936645929	0.08979105179721
H	-0.56810874812769	2.71653491866135	0.54412175920511
H	-1.52758846916848	-1.43420253165208	-0.10363578925110
N	1.16924034210980	-2.06863562642275	-0.72840938363152
C	2.48764398692929	-1.76254478118155	-1.31543728401801
C	0.39920900796566	-3.20788496782419	-1.18922146428907
C	3.58884487053314	-0.70591381913713	0.74972349271311
C	3.79270176751007	0.47502711447110	-1.45239869737647

O	3.42023873344234	-2.80080734696267	-0.91622300165611
C	2.36533844527126	-1.64237719482495	-2.80630570848509
C	2.88762745386949	-2.53175023070563	-3.66657915327932
C	3.91033149595194	-3.71975037656260	-1.78688057943860
C	3.68817723757984	-3.63682999601513	-3.18156431463866
C	4.67794592267745	-4.75694916042944	-1.24074226101326
C	4.24595393541523	-4.61587165096064	-4.00797683801253
C	5.22947907996899	-5.72093027483798	-2.07340930001337
C	5.00615760413493	-5.64148342383510	-3.45168142126927
N	5.58854916475385	-6.66554484696874	-4.33677002614129
O	6.26506547605584	-7.56086269078973	-3.81430693065328
O	5.36732017729535	-6.57117724221052	-5.55128399291529
H	4.57817706648831	-1.15318093515761	0.59294286420532
H	3.71617996291298	0.23633333844842	1.29819502100308
H	2.99598408749525	-1.38769094676596	1.37094832508420
H	4.72011249715149	-0.05281348785943	-1.71457658660085
H	4.07615078057941	1.37660699113081	-0.89276062966092
H	3.30726796641449	0.79870980953630	-2.38064353887082
H	1.74472521184717	-0.81540000316505	-3.15310479685029
H	2.71891165229878	-2.44003295312227	-4.74118808014043
H	4.09456199679271	-4.58506735019267	-5.08598364420130
H	5.83010585341116	-6.53545262028594	-1.67488223103169
H	4.83086898674906	-4.78890010017665	-0.16284312625928
H	-0.20402894231589	-2.99220770888789	-2.08801529502604
H	1.07784900432990	-4.03761659368974	-1.41336355589603
H	-0.27459130317149	-3.54145739149889	-0.38925890917324

Table S35. Cartesian Coordinates (in Å) of *Z*-**2**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	0.18666350449790	3.74891868745354	-3.78456364258512
C	-1.11265233447598	4.15024617478349	-3.48312740048715
C	-2.14656134062240	3.21294862569685	-3.41388810252107
C	-1.86167509393688	1.86598574815676	-3.65343578945747
C	-0.56056963835033	1.45312564486353	-3.93095551829624
C	0.49107731311836	2.38974097065098	-3.99035269272541
N	1.78718209030622	2.04284810509040	-4.37452508872097
C	2.49808577865562	1.06652700065495	-3.93440723448089
C	3.81981304752406	0.74887188758433	-4.67232434523754
C	4.88972484742699	1.70529602673020	-4.10465990973265
C	3.64255958075235	1.00772253066645	-6.17511685595553
C	4.29009750744264	-0.70375074562847	-4.47272321958530
N	2.25858314088393	0.28434863513356	-2.80616231688259
H	-1.32383488848257	5.20845078644895	-3.32115177718539
H	0.99127186171490	4.48040409789057	-3.87059450531800
H	-3.16649614538236	3.53076173896332	-3.19658964680918
H	-2.66360842442108	1.12623238560400	-3.62420806936075
H	-0.34858943094916	0.40079724352359	-4.12464755217906
H	5.85722083401820	1.52746559827884	-4.59539927247480
H	4.60190737758601	2.74936344855000	-4.27838450395488
H	5.02716979415274	1.55882846428740	-3.02393074407969
H	4.59612187503028	0.85030792286454	-6.69768630559723
H	2.89760232660727	0.32728764094904	-6.61047200786448
H	3.30194515053804	2.03164231270538	-6.35693468905179
H	4.61145181023074	-0.91487904557130	-3.44136625068191
H	5.16800659022664	-0.88683825325277	-5.10542779875366
H	3.52342459472688	-1.43451726530724	-4.77015397260371

C	1.51972134423836	0.58297908076201	-1.64559836643811
C	1.42632854329735	1.89140556276644	-1.14573903014597
C	0.72481929081389	2.15314862871597	0.03403531551741
C	0.13304972315292	1.10905987560419	0.73007202234741
C	0.92325666141080	-0.48502860909822	-0.94854985485353
C	0.24400046241735	-0.19223441400029	0.22860449389859
C	-0.67724875511330	1.08058987724529	2.00730301429396
H	0.65769461010817	3.17856828973591	0.39984127067212
H	1.91468849853950	2.70354143901485	-1.67855188878398
H	0.99973778706467	-1.49860636209352	-1.34265564701382
N	-0.44360833165448	-1.07922424503723	1.08893879296734
C	-0.63922590741941	-2.48229982891155	0.76904198854464
C	-2.00181588098998	1.86039533268454	1.85326996547734
C	0.11919251014199	1.61802658694245	3.21216609379385
H	-2.61559858133970	1.77124541960842	2.75859626464442
H	-1.78578722628903	2.92404399087676	1.68799391130719
H	-2.58407888787163	1.49402172599416	0.99874919787598
H	-0.46651990107949	1.53074535324399	4.13555783253628
H	0.35814439376290	2.67852927534509	3.05740818392065
H	1.06039443784639	1.07031165413103	3.34531934306258
H	0.10175727827956	-3.12307321580528	1.26720584468324
H	-1.64449903661389	-2.79093530315955	1.07548925914232
H	-0.55136395553234	-2.61905050894615	-0.31338605627337
C	-0.96066777987164	-0.41875664764620	2.16668233591662
C	-1.65351053438557	-0.92029926866865	3.26266102696790
C	-1.79573253446712	-2.24025178941539	3.70005727348207
C	-2.52268102306797	-2.67528512934912	4.82412683231398
H	-2.12120491294008	-0.17445754024254	3.90679440906104

H	-1.26275400417511	-3.03657604372184	3.17498634451973
C	-2.49458147425784	-4.06186108197987	5.12440502474500
C	-3.30285855257698	-1.75684116551388	5.70415725331127
C	-3.97556053883409	-2.38503347772191	6.83421919435813
C	-3.92027703084184	-3.72556791967900	7.07527883472719
C	-3.16942791665426	-4.57282561577921	6.20719659176958
O	-3.38656396517955	-0.52552190459047	5.50495011408368
N	-3.11645142964397	-6.00811070285639	6.47310052307408
O	-2.46163599147136	-6.72834854146863	5.69990805516447
O	-3.73351466368128	-6.43423376738477	7.46352797543728
H	-1.93094114920933	-4.74651624564480	4.48923100004127
H	-4.43628354709049	-4.17704265229286	7.92111206003817
H	-4.54279693446062	-1.71797837743307	7.48321379714722
H	2.75848317681953	-0.59878710200162	-2.77753438475273

Table S36. Cartesian Coordinates (in Å) of *E*-**2**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-0.08275782931466	0.08004415108507	0.82635363755075
C	0.03057735184772	1.06100853920316	-0.13806370922570
C	0.18857743964888	0.69979495110173	-1.49777602425900
C	0.22820693828120	-0.66402608799044	-1.84487703410472
C	0.11303587347616	-1.65546788041140	-0.86668438255390
C	-0.04176554015055	-1.27121650598381	0.46121531136735
C	-0.25910321396922	0.19380399381919	2.33219324656866
N	-0.17973509085555	-2.05704410578666	1.62332997017040
C	-0.30993888271334	-1.28677185075573	2.74414670064542
C	-0.18208062871549	-3.51015808751459	1.62774285840667

C	-1.57798915057090	0.92475128193659	2.66235868686873
C	0.95132389255901	0.91820732456197	2.95924623551536
C	-0.45690276419184	-1.84285255885964	4.01040454109441
C	-0.59735510913625	-1.12039221218676	5.19576766167601
C	-0.74696929874066	-1.61601864428619	6.49799465684343
C	-0.77700056192785	-2.99376675784425	6.81835516081354
C	-0.87970024919565	-0.59732551567183	7.58582236308790
C	-0.92691901602678	-3.40598994480257	8.12102337846480
C	-1.03375772372382	-1.13002609317913	8.93554095343005
C	-1.05662273365427	-2.46781581023363	9.19218401083776
O	-0.85949926898132	0.62613523048121	7.35291162810662
H	-0.00197953863528	2.11756521598044	0.14182971309602
N	0.29552594478202	1.75583496442977	-2.41360371258861
H	0.35006826576912	-0.93132685257432	-2.88907132695931
H	0.14822183892770	-2.70108792689868	-1.17073029956957
H	-1.12490006964829	-3.89577805827763	2.03768723811815
H	0.65106932906536	-3.89904891536269	2.22840347705539
H	-0.07299278133246	-3.87610592368205	0.60464465344672
H	-1.73672768742076	1.00922303905206	3.74295470665985
H	-1.54921680273902	1.93995444390157	2.24510243617193
H	-2.43881273230285	0.40261662739278	2.22647023935275
H	1.02348630566356	1.93444005112190	2.54956017030382
H	1.88721903712378	0.39303375201962	2.73189157840719
H	0.85692831308884	0.99944222570718	4.04749862218432
H	-0.59849340642634	-0.02938348514673	5.16049788537506
H	-0.46149051557421	-2.93297712421974	4.07154854748601
H	-0.68265016434360	-3.75848774584293	6.04773411312735
N	-0.95394557441302	-4.83639369012506	8.41770873162105

H	-1.17239692591208	-2.85415791203342	10.20347827898420
H	-1.13120839903709	-0.39935419539313	9.73836190478319
O	-0.84018608600467	-5.63870207459072	7.47408885655898
O	-1.08991801851408	-5.17733398123223	9.60467535591770
C	0.44591247465352	1.76396568189603	-3.79177278443933
H	0.25151133925357	2.67251841822740	-1.98437854463112
N	0.51580083853912	0.63852980493254	-4.40591253627480
C	0.50931938971629	3.18928552979114	-4.42060327804560
C	0.41976836705299	4.32888595251943	-3.38678335188746
C	-0.66846993658025	3.35533241283328	-5.40138196859562
C	1.84563427135707	3.34710866930935	-5.17263699364018
H	2.70180329852547	3.22077175272450	-4.49534278436216
H	1.90483406669400	4.35478804117506	-5.60807218691710
H	1.94338034429150	2.62302723012055	-5.98732628484689
H	1.25229778876105	4.31853957681985	-2.66738736472153
H	-0.53651203516790	4.33802908612938	-2.84247169347561
H	0.48102354402628	5.28842925658206	-3.91629242374196
H	-0.65035826273858	4.36818257859581	-5.82820856870909
H	-1.63312855862324	3.22044457809761	-4.89258343935372
H	-0.61390364726110	2.64058657143494	-6.22847200118186
C	0.65415815774245	0.34024572549945	-5.75921200980527
C	-0.47908207439668	0.10369530524848	-6.56401523262666
C	-0.33893310490779	-0.32833377155600	-7.88172111733936
C	0.92653149186020	-0.55266292643142	-8.42849522048832
C	2.05451994179536	-0.35183734528838	-7.62954931847125
C	1.92535527051897	0.07929003725731	-6.31059607666600
H	-1.47066294134176	0.25334429731565	-6.13524721208794
H	-1.23223970802256	-0.49734116276305	-8.48513741183524

H	1.03170694524337	-0.89487084170106	-9.45794614356032
H	3.05041579561150	-0.53915412668053	-8.03428922800975
H	2.80809117733573	0.21234981700238	-5.68408384512269

Table S37. Cartesian Coordinates (in Å) of *Z′*-**2**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-0.07358811889789	0.28345187305406	-0.12390421729767
C	-0.96578381349045	-0.74545287480564	0.11852092226012
C	-0.57120191116906	-1.82821561661436	0.93041471594294
C	0.72483605871237	-1.84863851044957	1.46906468179900
C	1.62214257575183	-0.80056484926335	1.25190344014556
C	1.20500178381669	0.25843763753396	0.44884334746684
C	-0.23439834502895	1.55090153165995	-0.94701500223806
N	1.89803317738884	1.42096281244059	0.06073028409540
C	1.13471297505182	2.21989847693786	-0.74670212536737
C	3.25654809683666	1.73661915342672	0.46806764249235
C	-1.38175327609383	2.41526769500866	-0.38066686842963
C	-0.48539655928968	1.19419235875532	-2.42835553275379
C	1.60882068421119	3.42336434509681	-1.25332548486809
C	0.88781618901723	4.28712847544744	-2.08083667432069
C	1.30169229160092	5.50962552434805	-2.62257898565204
C	2.57719330120780	6.08123007338088	-2.39709576341657
C	0.30897328743035	6.22505276022640	-3.48532126051518
C	2.91190253484216	7.28679188007970	-2.96385634893199
C	0.75610521230156	7.49777300897330	-4.04267049822917
C	1.99576737117470	8.00466057410164	-3.79527204941890
O	-0.82427235267163	5.76245368460952	-3.71178696906504

H	-1.97531454222541	-0.73052410752844	-0.29586110734906
N	-1.48248603581121	-2.88977645621031	1.12786167460423
H	1.04141333223596	-2.70857866487278	2.05802403077410
H	2.61967031674758	-0.84735037232905	1.68711086568309
H	3.28640172131845	2.68807694173477	1.01537915902157
H	3.91828770795198	1.80933332799402	-0.40543796313320
H	3.63224222367984	0.94830374675272	1.12388027374940
H	-1.50725584428776	3.34356450508624	-0.94799334761538
H	-2.32466521802396	1.85573761544486	-0.43550272933023
H	-1.20046005939762	2.67396715370406	0.66993512265632
H	-1.41363707719898	0.61442830590608	-2.51374820564777
H	0.33363913946460	0.58670388021663	-2.83314441688309
H	-0.58897605403395	2.09080704825731	-3.04906504207620
H	-0.13042306022932	4.02239917183088	-2.37171384411237
H	2.62603776024127	3.70829410246004	-0.97797455462345
H	3.32039792425365	5.58526532106560	-1.77321703061385
N	4.23768611602236	7.84968640577915	-2.71075117840961
H	2.31936967829735	8.95524993233579	-4.21618846612649
H	0.04384185935458	8.02950307079412	-4.67330442636039
O	5.02177237175348	7.21238891065456	-1.98618457832895
O	4.51057419848834	8.94099705614795	-3.23694728346014
C	-1.52233984201874	-3.80586765998532	2.18766572761345
H	-1.79373606893791	-3.31703442369028	0.25227659077806
N	-1.70182068337971	-5.06576630620665	1.98021577184583
C	-1.58255432157683	-3.31750037892873	3.65412449767487
C	-1.59821641814115	-1.79100798569316	3.82275939171398
C	-0.41121078660894	-3.92780715066615	4.44516477040779
C	-2.90609493303742	-3.86451635870234	4.23893640070032

H	-3.77348043673984	-3.44985941911934	3.70644456861860
H	-2.98782135288905	-3.57723973159767	5.29649954412222
H	-2.94423421571665	-4.95560732708123	4.16011365975800
H	-2.38104358031688	-1.32229867766654	3.21218926318206
H	-0.64224667439302	-1.31903412103366	3.57239979777116
H	-1.81232725486995	-1.55565982833516	4.87421121735486
H	-0.51075022783416	-3.68157511371207	5.51151441995108
H	0.56027376517313	-3.54043385552286	4.10680701701851
H	-0.40214355746759	-5.01914646888046	4.33929434978091
C	-1.64872738935080	-5.62502879238208	0.69407390040085
C	-2.79089994801809	-6.25787169583649	0.16831522398799
C	-2.74539631139847	-6.88177347825714	-1.07710331762343
C	-1.55994468571896	-6.90676603066109	-1.81617014165329
C	-0.41676323412748	-6.29570529856735	-1.29614387576823
C	-0.45671038212191	-5.65506742324526	-0.05830715630888
H	-3.70785903561943	-6.25511596843264	0.75835563346591
H	-3.64245540990684	-7.36374922837962	-1.46835931451157
H	-1.52439856466727	-7.40786250875786	-2.78358371279923
H	0.51852947821576	-6.31983839678363	-1.85748449684694
H	0.44310745016433	-5.19428728104737	0.35247506324860

Table S38. Cartesian Coordinates (in Å) of *E′*-**2**(o), Tautomer 2.

Atom	*X*	*Y*	*Z*
C	-4.25161050865004	5.31761535248021	1.78265852775089
C	-5.08076477532846	6.35401839757702	2.20845993010473
C	-6.41061060443357	6.10659642811732	2.55494805464740
C	-6.90744403987772	4.80528714529052	2.45171039580425
C	-6.08898736886153	3.76309855521900	2.02126825407397

C	-4.73644557408159	3.99762467933645	1.70436348038716
N	-3.95267396552783	2.98339148286906	1.15041571727953
C	-3.11265141286668	2.17729097355007	1.69111660043527
C	-2.72469249279373	2.06745480524026	3.19116699873323
C	-4.02915600325674	1.77152855668816	3.96957311838162
C	-2.11483586346569	3.38289926092942	3.70934487190405
C	-1.75258350125162	0.91476724244544	3.49752422026925
N	-2.65603612939122	1.16524751114399	0.81465334129863
H	-4.68114319958697	7.36769901424248	2.26473457212195
H	-3.22179846059748	5.52138934890746	1.48735186013199
H	-7.05657304626476	6.92024898373912	2.88441941640995
H	-7.94897485667342	4.59700054386763	2.70123193049601
H	-6.48834019423217	2.75341397776763	1.92002862676635
H	-3.26182272146636	1.15188565924685	-0.00893087064207
H	-3.78966227341045	1.64527015311344	5.03468150618756
H	-4.75756493282555	2.58318545846233	3.88068665959951
H	-4.49752259297803	0.84258295470762	3.61650168836621
H	-1.87791020118241	3.27534083703186	4.77727889639706
H	-1.17964706485079	3.62959516695157	3.18831545241892
H	-2.80317564816706	4.22732423318529	3.60113815883605
H	-2.12582130371740	-0.04529377439022	3.12016498443200
H	-1.64989903808412	0.82894141934491	4.58806933295186
H	-0.75091472227717	1.08002481368496	3.08722606654281
C	-1.29669617398288	0.93092661920944	0.48543193647211
C	-0.30233835417751	1.90266172260702	0.67886920401576
C	1.02757987355646	1.64960857687993	0.32365249448595
C	1.35980678424329	0.43570199934907	-0.25873759859594
C	-0.96768214597524	-0.30589710074050	-0.09966146002525

C	0.35644605839610	-0.51961372038156	-0.46561345895229
C	2.67871290151805	-0.11418910354990	-0.75622241487101
H	1.78467629318616	2.41878033824751	0.48416084640618
H	-0.58072133949161	2.87465593534142	1.08396952613253
H	-1.74984920707811	-1.05024587037064	-0.24517676089842
N	0.92880424910176	-1.66779663158315	-1.05912425269293
C	0.17672851218011	-2.89080844510648	-1.28064338829577
C	3.69530594741655	-0.27913359107832	0.39462384325911
C	3.28034922638867	0.75547075545355	-1.87753534839843
H	4.62200844587572	-0.74305798237723	0.03406974068530
H	3.94455849593268	0.70563105665943	0.81169742722301
H	3.28724331559748	-0.89999072781112	1.20177283406130
H	4.20037083446226	0.30360150138340	-2.26867950980667
H	3.52756370136832	1.75087017257922	-1.48545659225614
H	2.57497416803992	0.87996022896497	-2.70844943294552
H	-0.18263983891688	-2.96690357770995	-2.31634934711846
H	0.80983540041781	-3.75579309800670	-1.05514216791401
H	-0.68623961303494	-2.90911588967628	-0.60790733876516
C	2.26189012844905	-1.48771015542656	-1.29864978880462
C	3.17635772096718	-2.33990183231316	-1.90551566313853
C	2.95795840895646	-3.49738596258721	-2.65911734234721
C	3.94627055543707	-4.31458106358567	-3.23798707455161
H	4.22299440753106	-2.04378072179676	-1.82168012100106
H	1.93338714236272	-3.80096156056334	-2.88663468412919
C	3.50934023582572	-5.41725845767068	-4.01789312027795
C	5.41037227505951	-4.07224613757527	-3.07893117485544
C	6.28513489670950	-5.01037842004095	-3.77084304720412
C	5.81281210215098	-6.05748892865821	-4.50454226331227

C	4.40599604715127	-6.26080439844497	-4.62805850120869
O	5.87851836074615	-3.13154395846936	-2.40164461711268
N	3.90943073900162	-7.38652015574756	-5.41670821281644
O	2.68045131456856	-7.54784193907179	-5.50637839863544
O	4.74853286532748	-8.12526901051200	-5.95789846059783
H	2.44281703524389	-5.60971773049491	-4.14165942799648
H	6.48298168222206	-6.75259186641922	-5.00767243460710
H	7.35522304336608	-4.83476604965541	-3.66183924069471

Table S39. Cartesian Coordinates (in Å) of [**1**(o)]$^{\bullet-}$.

Atom	*X*	*Y*	*Z*
C	-1.61533132831239	4.73699173129920	3.39257828674069
C	-1.70210676817715	5.39598064349902	2.17036129110046
C	-0.64304608139294	5.34045600056928	1.25994361281981
C	0.50581348066983	4.62607552345380	1.60271823035526
C	0.61222957790783	3.97354163713649	2.82966635340052
C	-0.45787451871597	4.01495182321956	3.74027874383145
N	-0.41489240556370	3.39830252940351	4.99764429886011
C	0.55873959051859	2.53814684344118	5.53553571892467
C	0.87666734118476	2.82396357797007	7.01908719673657
C	-0.40731391973315	2.71010809674848	7.87171500301724
C	1.46263239056930	4.24308507409310	7.16270880446954
C	1.89285407838915	1.80616990469110	7.54894393046933
N	1.19027096685083	1.58439967273534	4.93973073991643
H	-2.61297807637556	5.94260993415837	1.92068513732419
H	-2.45844039110696	4.76399412691378	4.08813182573469
H	-0.71958896634113	5.83411242252356	0.29116274992271
H	1.33833408864976	4.56423933824268	0.90056791648301

H	1.51672041435698	3.42307017630077	3.07608293389254
H	-0.16138091783138	2.84321673181501	8.93509494707901
H	-1.16011900410039	3.47648829278478	7.62915396512799
H	-0.87520526493123	1.72387273894552	7.75167114900159
H	1.68511200662815	4.46200760835298	8.21785934036060
H	2.39635474800156	4.33540185018604	6.59182585521553
H	0.77048854413861	5.01401997618263	6.79720571181474
H	1.51565247198577	0.78095377868733	7.45520100023119
H	2.10281580157351	2.01165547612687	8.60957332687384
H	2.83103710063057	1.85584986085396	6.98556218918581
C	0.91153934431956	1.00771017743103	3.69990510803296
C	-0.37766667782968	0.86929934441831	3.13765862437295
C	-0.57986828511467	0.15837080399164	1.96297784652574
C	0.50445974102800	-0.41308253643879	1.26531271838044
C	1.98258864869472	0.40083313079767	3.01109947650426
C	1.79721272809544	-0.26952426539704	1.81051889649212
N	0.29060507186903	-1.11317127452096	0.06472034789584
H	-1.58226733755476	0.06280688550800	1.55458015774039
H	-1.23864282394116	1.29695031554421	3.65058616346854
H	2.98050740416794	0.47611230464705	3.44631354396165
H	2.64503756611904	-0.72294939947753	1.30504361720076
C	-0.70845115151690	-0.77027370290652	-0.92615835741885
C	1.02713915372636	-2.24499937010741	-0.36295970116800
C	0.39959670212227	-2.72491127476708	-1.63463484880509
C	-0.56058169394698	-1.70762588971956	-2.03060281410962
C	0.60142111243672	-3.99719347825635	-2.12823894434244
C	1.69412742841795	-4.91816534024312	-1.66461246633501
C	-0.31183701748755	-4.62212903075118	-3.14191014616476

O	-1.47321817560055	0.18821300502497	-0.80660214166219
O	1.96391630828378	-2.72074912969247	0.27604258159813
C	-1.30424026785450	-1.44599006520005	-3.19549903298629
C	-1.14254273721595	-1.82192406812143	-4.55389214327832
H	1.26946885279086	-5.82978478774139	-1.20613823889636
H	2.28168973891322	-5.26954034435341	-2.53298623341549
H	2.36843427953760	-4.45349453459707	-0.94316655006089
H	0.19766636498242	-4.81285836845473	-4.10271774216982
H	-0.63960651636954	-5.61027262676737	-2.77301064336395
H	-1.20188821111161	-4.02261385630414	-3.34903841004125
H	-2.13882931196191	-0.76010413124634	-3.02292563702935
N	0.08266105400742	-2.18511486140237	-5.16269341756347
C	-2.15028911548850	-1.89218369789912	-5.54252384823155
C	-0.14195278917196	-2.48369342521715	-6.49125847359091
C	1.40401400119273	-1.89189744895739	-4.64526616716864
C	-1.54066536699284	-2.32008670546846	-6.75323908355446
C	-2.01701138716709	-2.59134756813474	-8.05264383748403
C	-1.11558079288240	-2.98003525288288	-9.04454544016402
C	0.25745434556798	-3.10772988073966	-8.77167057449085
C	0.76062041288778	-2.85925625769064	-7.48637226644565
C	-3.61044423271567	-1.66191033830568	-5.33248917628169
H	1.97983547010754	-2.80734972624958	-4.44420339083684
H	1.96140525533464	-1.27598257523058	-5.36807658034784
H	1.30768248762854	-1.33998777093062	-3.70754278781137
H	1.82449390651362	-2.97474320983066	-7.27276224200864
H	0.94170194265035	-3.40961453718049	-9.56656964297342
H	-1.48132499629900	-3.18772482855079	-10.05259766242950
H	-3.07985632033308	-2.49178525962629	-8.28298365553231

H	-3.80335569815962	-1.06056794538892	-4.43473504375523
H	-4.17307076047949	-2.60447756203881	-5.21225941462915
H	-4.05689059377663	-1.13246191565282	-6.18847928902525
H	-1.03263801989673	3.82534290474433	5.68256070450929

Table S40. Cartesian Coordinates (in Å) of [**1**(c)]$^{\bullet-}$.

Atom	*X*	*Y*	*Z*
C	-1.36015231954010	4.97440402030607	3.75838241797500
C	-1.57301310892001	5.72470957703338	2.60591870222881
C	-0.64178285058734	5.70039983101135	1.56462745487013
C	0.50865029824303	4.92310814508827	1.70463361798657
C	0.74097370669391	4.17762268682017	2.85939572434566
C	-0.20101532179040	4.18871591575800	3.90165314565365
N	-0.02845468781881	3.47934012924345	5.09772707937338
C	0.97388875816557	2.55796182531364	5.45600452359205
C	1.46375431696345	2.72838024812451	6.91215698058687
C	0.28107659452015	2.56551459914910	7.89323748917638
C	2.09205755178823	4.12462066523333	7.09162100146093
C	2.51125026534781	1.66060883463673	7.24588235019103
N	1.49870220005529	1.63385298705032	4.73380273344822
H	-2.48404886509424	6.31862311143432	2.51483184719922
H	-2.10668508034966	4.97838895897290	4.55707615578042
H	-0.81874042993523	6.26757116568416	0.65066195137048
H	1.24098353045402	4.88259219326122	0.89734052598766
H	1.64268761381089	3.57680634171769	2.94517675923415
H	0.64717459867652	2.61522251549946	8.92881998929596
H	-0.47950494024364	3.35564550541141	7.79366496060033

H	-0.21596746176619	1.59617060495211	7.75422832873008
H	2.43835332371012	4.25825328283246	8.12739088101450
H	2.95622445196205	4.24929696781405	6.42535215731986
H	1.38036513649013	4.93143281318925	6.86807539275933
H	2.10347253445892	0.65056877624217	7.12184363099070
H	2.84575208000631	1.78412902992072	8.28708183946593
H	3.37963779679135	1.73931786563179	6.58264300004010
C	1.07752484555099	1.16380311256574	3.48287709001945
C	-0.26322638465222	1.09372428087466	3.05288671179982
C	-0.60602067595953	0.48857262513587	1.85042152604522
C	0.38419976571067	-0.03255693053411	0.98691552524461
C	2.05474670306313	0.60351568910626	2.63806866624155
C	1.73063651373715	0.04794446624555	1.40778754593922
N	0.04214615678803	-0.61316247257369	-0.23676653846515
H	-1.64630226636746	0.44494660465536	1.54055938266075
H	-1.05607262307961	1.48636827807689	3.68995303078914
H	3.09457007287775	0.62471147024679	2.96990533298582
H	2.50562849190568	-0.37927871613815	0.77814963250347
C	-1.13286619168153	-0.30635285150584	-1.00463987356541
C	0.83650957056935	-1.63441158416384	-0.94016567697045
C	0.14827500697876	-1.88430810087132	-2.16611459023343
C	-1.03379617638448	-1.11942491176563	-2.19627140370502
O	-2.01362411192416	0.50905344186686	-0.67836460687490
O	1.85830625236619	-2.14977879692821	-0.44372928142279
C	-2.00398405667704	-1.24200569472959	-3.23237577632531
C	0.40696429271336	-2.98142918608059	-3.18598384533809
C	-1.64680909492006	-1.97635533268733	-4.32412519859761
C	-0.22028586599260	-2.48289032661976	-4.55717737470036

C	1.90735477638736	-3.29395355368231	-3.30644324845434
C	-0.32105384693641	-4.26176061751591	-2.71615292976795
N	-2.45383176258475	-2.40570782915104	-5.38834142336986
C	-0.45793006425804	-3.50908990204485	-5.66352660725496
C	0.60575536093472	-1.31188710637309	-5.15118886324560
C	-1.79427938522965	-3.38166014269986	-6.12341227433316
C	0.39421872080019	-4.39161886929924	-6.31045975168812
C	-2.28059294108306	-4.16104363935771	-7.17972198652074
C	-1.40413393493539	-5.06048407454533	-7.79781115426992
C	-0.07781195820201	-5.17869395601411	-7.37732182418405
C	-3.86966974774002	-2.15154084092817	-5.44578120834547
H	-2.99575461468418	-0.80756762303154	-3.09737929238452
H	2.48597132016952	-2.42204617876196	-3.63550140978712
H	2.29430832423241	-3.57195796670635	-2.31960955552351
H	2.09044986939476	-4.12491163622630	-4.00254007559275
H	-0.18530934520669	-5.08991780813955	-3.42834757116880
H	-1.39777595845236	-4.07751618559278	-2.60200401077835
H	0.07799788896038	-4.57026901245702	-1.74103154045215
H	0.76303970675355	-0.53777064804181	-4.38902522833832
H	0.06925541090528	-0.86789754672109	-6.00039542369226
H	1.58220196400344	-1.65930672302745	-5.51414239231122
H	1.43452035194730	-4.48143486018568	-5.99747254376317
H	0.59305826175974	-5.88248515192595	-7.87189628361140
H	-1.77045128184082	-5.67882897047731	-8.61991965748046
H	-3.31444803629321	-4.08150486792071	-7.51826936243393
H	-4.23900872051702	-2.31158171296535	-6.46588061357975
H	-4.44120322340853	-2.79866366829380	-4.75541217119152
H	-4.06568518904834	-1.10667212651286	-5.17318012162313

H	-0.54135586254267	3.87382955709115	5.88113060643857

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