SUPPLEMENTARY INFORMATION

# Ratiometric temperature sensing with fluorescent thermochromic switches

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## Experimental Procedures

***Materials and Methods.*** Chemicals were purchased from commercial sources and used as received. $H_2O$ (18.2 MΩ cm) was purified with a Barnstead International NANOpure DIamond Analytical system. Compounds **1Cl**, **3Cl** and **5**–**11** were prepared accordingly to literature procedures.[S1–S6] Electrospray ionization mass spectra (ESIMS) were recorded with a Bruker micrOTO-Q II spectrometer. Nuclear magnetic resonance (NMR) spectra were recorded with a Bruker Avance 400 spectrometer. Absorption spectra were recorded in aerated quartz cells (path length = 1.0 cm) with a Varian Cary 100 Bio spectrometer, equipped with an Agilent Technology Cary Dual cell Peltier accessory. Emission spectra were recorded in aerated quartz cells (path length = 1.0 cm) with a Varian Cary Eclipse spectrometer equipped with a Varian Cary Single cell Peltier accessory. Fluorescence quantum yields were calculated against 9,10-diphenylanthracene (**1Cl** and **2Cl**), cresyl violet (**1OpH** and **2OpH**), quinine sulfate (**3Cl** and **4Cl**) and rhodamine 6G (**3OpH** and **4OpH**). Fluorescence images were recorded with a Leica SP5 confocal laser-scanning microscope.

***Synthesis of 2Cl and 4Cl.*** Trifluoroacetic acid (TFA, 450 μL, 5.72 mmol) was added dropwise to a solution of **5** (250 mg, 0.87 mmol) and either **6** (216 mg, 0.88 mmol) or **7** (184 mg, 0.88 mmol) in EtOH (10 mL). The mixture was heated under reflux for 24 hours. After cooling down to ambient temperature, the solvent was distilled off under reduced pressure and the residue was dissolved in $CH_2Cl_2$ (5 mL). Addition of $Et_2O$ (200 mL) and refrigeration for 12 hours caused the formation of a precipitate. After filtration, the solid residue was dissolved in aqueous $NaHCO_3$ (5% w/v, 20 mL) and stirred for 1 hour at ambient temperature. The aqueous mixture were extracted with EtOAc (3 × 40 mL). The organic phase was dried over anhydrous $Na_2SO_4$, filtered and the solvent was distilled off under reduced pressure to give either **2Cl** (68%, 264 mg), as a green solid, or **4Cl** (35%, 125 mg), as a red solid. **2Cl**: ESIMS: *m/z* = 431.2338 [$M^+$] (*m/z* calcd for $C_{27}H_{31}N_2O_3^+$ 431.2335); $^1$H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.18 (s, 3H), 1.20–1.26 (t, 6H), 1.46 (s, 3H), 3.37–3.47 (m, 4H), 3.60–3.68 (m, 2H), 3.77–3.81 (m, 1H), 4.10–4.16 (m,1H), 6.51 (s, 1H), 6.55–6.61 (d, 9 Hz, 1H), 6.65–6.71 (m, 1H), 6.77–6.86 (m, 2H), 6.90–6.97 (t, 7 Hz, 1H), 7.05–7.11 (d, 7 Hz, 1H), 7.14–7.19 (m, 1H), 7.25–7.29 (m, 1H), 7.60 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ (ppm) = 161.2, 155.8, 150.8, 150.6, 139.9, 139.4, 128.9, 128.0, 127.5, 126,7, 122.4, 121.5, 117.0, 112.0, 110.1, 109.0, 108.8, 97.1, 63.5, 50.2, 47.9, 44.8, 28.5, 20.4, 12.5. **4Cl**: ESIMS: *m/z* = 395.2111 [$M^+$] (*m/z* calcd for $C_{27}H_{27}N_2O^+$ 395.2123); $^1$H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.27(s, 3H), 1.54 (s, 3H), 3.54–3.59 (m,1 H) 3.67–3.76 (m, 2H), 3.88 (s, 3H), 4.11–4.16 (m, 1H), 6.32–6.38 (d, 16 Hz, 1H), 6.84–6.88 (d, 8 Hz, 1H), 6.96-7.02 (t, 7 Hz, 1H), 7.06 (s, 1H), 7.10–7.16 (m, 2H), 7.18–7.25 (t, 8 Hz, 1H), 7.35–7.45 (m, 2H), 7.48–7.55 (d, 7 Hz, 1H), 7.64–7.67 (d, 9 Hz, 1H), 8.10–8.16 (d, 8 Hz, 1H), 8.20 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ (ppm) = 150.8, 141.5, 140.9, 140.0, 133.1, 127.7, 127.6, 126.0, 124.7, 123.1, 122.9, 122.8, 122.5, 121.6, 120.4, 119.1, 118.9, 112.1, 110.2, 108.6, 108.5, 63.6, 50.2, 48.0, 29.2, 28.6, 20.4.

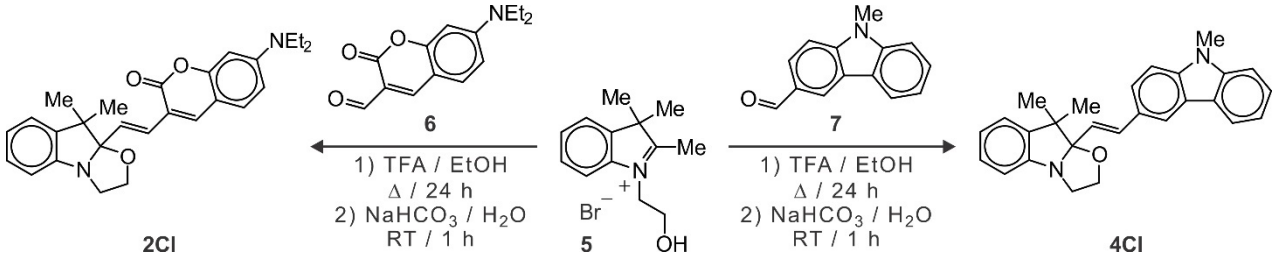


Fig. S1 Synthesis of **2Cl** and **4Cl**.

***Preparation of Doped Alginate Beads.*** A $CH_2Cl_2$ solution of **2Cl** (17 μM, 500 μL ) was mixed with a $CH_2Cl_2$ solution of an amphiphilic polymer (Pluronic 123, 2.5 mg $mL^{-1}$, 1 mL) and stirred for 15 minutes at ambient temperature. The solvent was distilled off under reduced pressure and the residue was dissolved in an aqueous solution of sodium alginate (4% w/v, 2 mL). Droplets of the resulting solution were added to an aqueous solution of $CaCl_2$ (0.24 M, 750 μL) with a syringe through a 25-gauge needle. Beads with diameters of a few millimeters formed upon contact of the droplets with the $CaCl_2$ solution. After 2 minutes, individual beads were suspended in $H_2O$ (500 μL) and transferred into either a glass dish for imaging experiments or a quartz cuvette for spectroscopic measurements. The sample was cooled down with ice or warmed up with a heating plate, while monitoring its temperature with a digital thermometer.

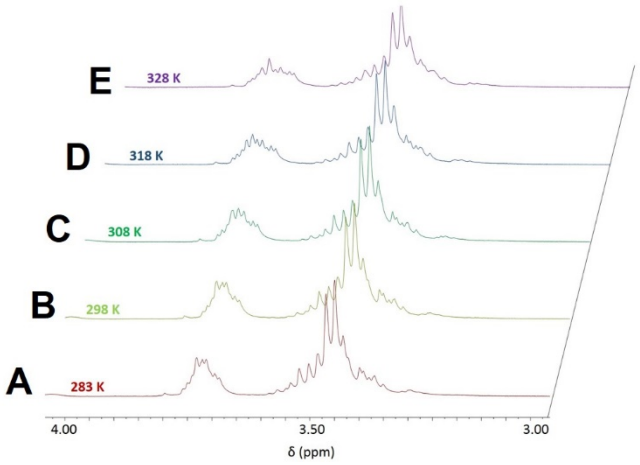


Fig. S2 Partial $^{1}$H NMR spectra (400 MHz, 15 mM, $CD_3CN$) of **2** at 283 (**A**), 298 (**B**), 308 (**C**), 318 (**D**) and 328 K (**E**).

Table S1 Photophysical [a] and thermodynamic [b] parameters for **1**–**4** in MeCN/$H_2O$ (1:1 v/v).

| | Cl | | | OpH | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $\lambda_{Ab}$ (nm) | $\lambda_{Em}$ (nm) | $\phi$ | $\lambda_{Ab}$ (nm) | $\lambda_{Em}$ (nm) | $\phi$ | $K_{Eq}$ | $\Delta H$ (kcal mol$^{-1}$) | $T\Delta S$ (kcal mol$^{-1}$) |
| **1** | 412 | 475 | 0.01 | 587 | 650 | 0.02 | $1\cdot10^{-8}$ | –4.3 | –15.0 |
| **2** | 412 | 489 | 0.98 | 575 | 660 | 0.15 | $3\cdot10^{-7}$ | –12.7 | –21.7 |
| **3** | 240; 287 | — | — | 504 | — | — | $7\cdot10^{-8}$ | –0.3 | –10.0 |
| **4** | 240; 287 | 383 | 0.18 | 490 | 596 | 0.02 | $8\cdot10^{-7}$ | –5.7 | –14.0 |

[a] Wavelengths at the absorption ($\lambda_{Ab}$) and emission ($\lambda_{Em}$) maxima and fluorescence quantum yield ($\phi$). [b] Constant ($K_{Eq}$), enthalpic ($\Delta H$) and entropic ($T\Delta S$) terms for the equilibrium between the ring-closed isomer and the corresponding protonated form at 298 K.

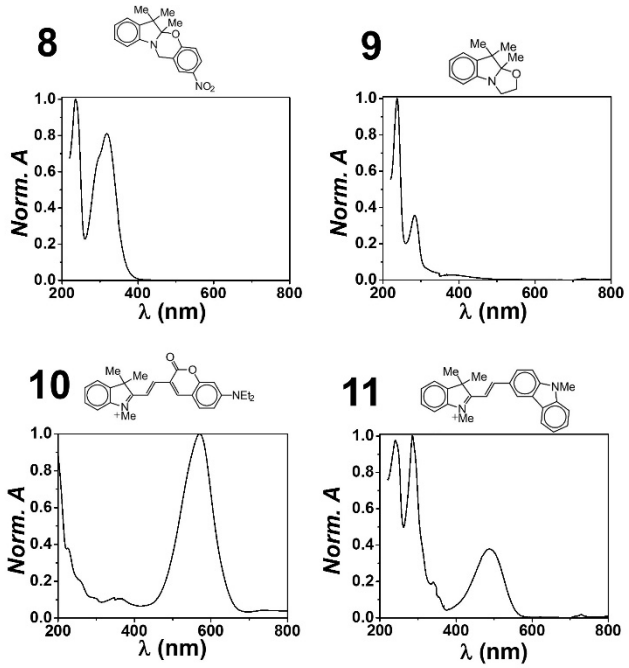


Fig. S3 Normalized absorption spectra of **8** and **9** as well as of the hexafluorophosphate salts of **10** and **11** in MeCN at 293 K.

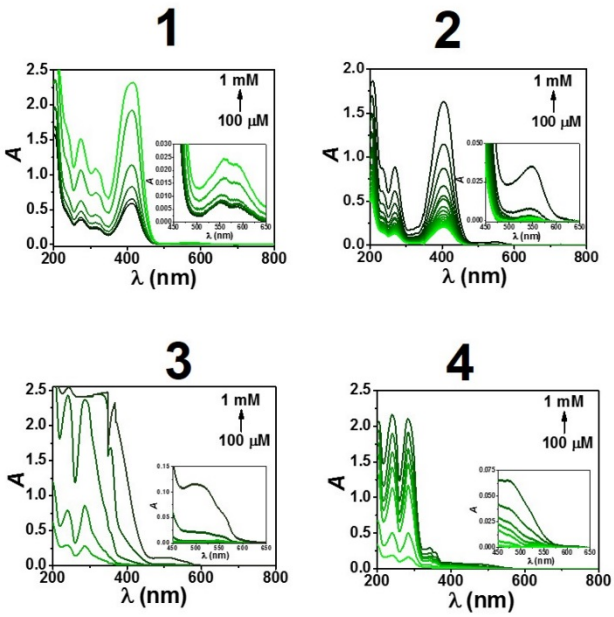


Fig. S4 Absorption spectra of **1**–**4** in MeCN recorded over a range of concentrations (10 µM–1 mM) at 293 K.

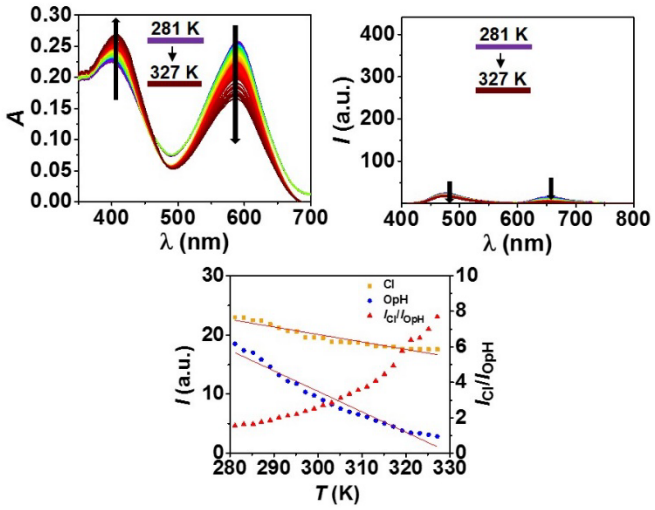


Fig. S5 Absorption (left) and emission (right, $\lambda_{Ex}$ = 400 and 587 nm) spectra of **1** (138 μM) in MeCN/$H_2O$ (1:1 v/v) at temperatures ranging from 281 to 327 K together with the temperature dependence (bottom) of the emission intensities of **Cl** and **OpH** and their ratio.

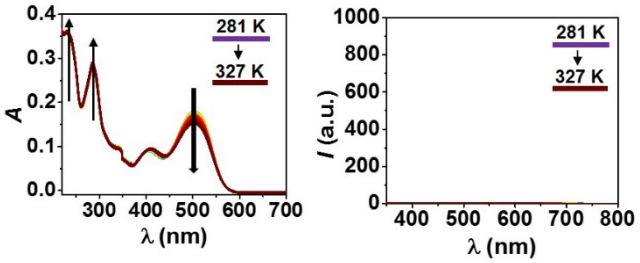


Fig. S6 Absorption (left) and emission (right, $\lambda_{Ex}$ = 286 and 504 nm) spectra of **3** (32 μM) in MeCN/$H_2O$ (1:1 v/v) at temperatures ranging from 281 to 327 K.

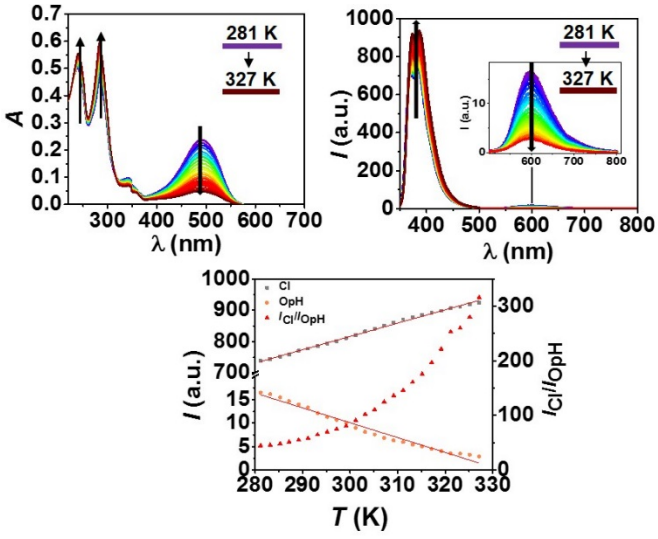


Fig. S7 Absorption (left) and emission (right, $\lambda_{Ex}$ = 286 and 490 nm) spectra of **4** (100 μM) in MeCN/$H_2O$ (1:1 v/v) at temperatures ranging from 281 to 327 K together with the temperature dependence (bottom) of the emission intensities of **Cl** and **OpH** and their ratio.

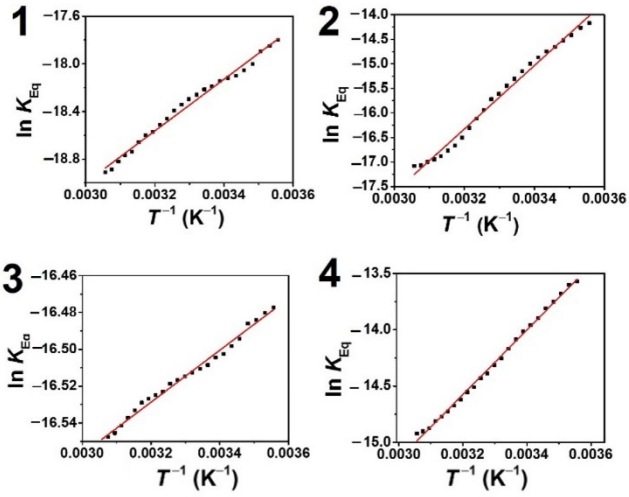


Fig. S8 Logarithmic plot of $K_{Eq}$ for **1**–**4** in MeCN/$H_2O$ (1:1 v/v) against the inverse of temperature (281–327 K).

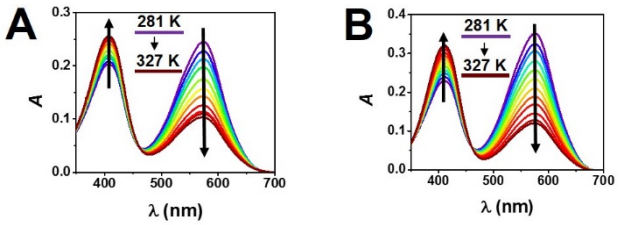


Fig. S9 Absorption spectra of **2** (16 μM) in mixtures of MeCN and $H_2O$ with relative amounts varying from 4:1 (**A**) to 3:2 (**B**) (v/v) at temperatures ranging from 281 to 327 K.

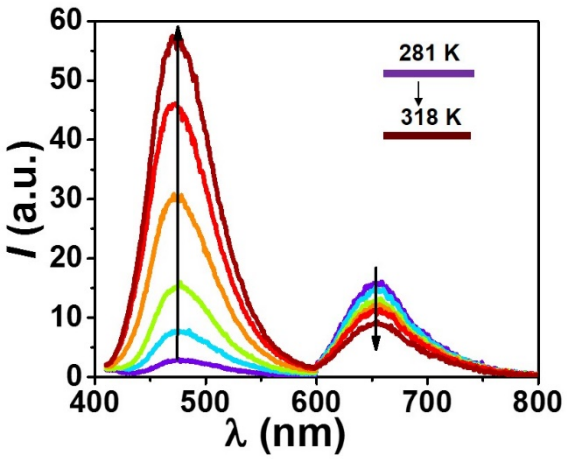


Fig. S10 Emission spectra ($\lambda_{Ex}$ = 415 and 575 nm) of an alginate bead, doped with **2**, suspended in $H_2O$ at temperatures ranging from 281 to 318 K.

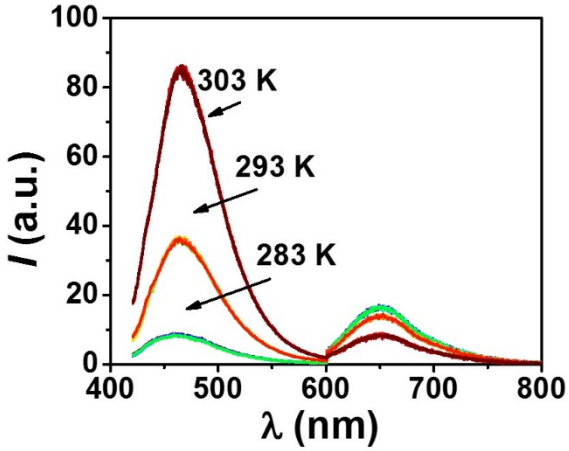


Fig. S11 Emission spectra ($\lambda_{Ex}$ = 415 and 575 nm) of an alginate bead, doped with **2**, suspended in $H_2O$ recorded sequentially at each temperature over the course of 10 min with intervals of 1 min.

## DFT Calculations

***Methods.*** The structure adopted by the ring-closed isomer of **8** in the solid state[S6] was optimized with the restricted M062X functional[S7] and the 6-311+G(d,p) basis set implemented in Gaussian 09.[S8] The frequencies of the optimized geometry were calculated at the same level of theory and no imaginary frequencies were found.

The length of the [C–O] bond at the junction of the two heterocycles within the optimized geometry was increased in ten consecutive steps of 0.150 Å each. At each step, the [C–O] bond was constrained and the remaining coordinates were optimized at the same level of theory. The optimized energy at each step was plotted, relative to that of the initial step, against the [C–O] bond length to build a profile (*Scan 1* in Fig. S12) of the ring-opening process. The dihedral angle about the [N–C] bond linking the 3*H*-indolium cation to the 4-nitrophenolate anion of the final geometry of *Scan 1* was rotated in ten consecutive steps of 21.09º each. At each step, this dihedral angle was constrained and the remaining coordinates were optimized. The optimized energy at each step was plotted, relative to that of the initial step of *Scan 1*, against the [N–C] bond dihedral angle to reconstruct a profile (*Scan 2* in Fig. S12) of the conformational change. The distance between the carbon and oxygen atoms of the cleaved bond in the final geometry of *Scan 2* was decreased in ten consecutive steps of 0.349 Å each. At each step, the [C–O] distance was constrained and the remaining coordinates were optimized. The optimized energy at each step was plotted, relative to that of the initial step of *Scan 1*, against the [C–O] distance to build a profile (*Scan 3* in Fig. S12) of the ring-closing process.

The initial and final geometries of each scan were optimized again at the same level of theory, allowing all coordinates to relax, with the polarizable continuum model (PCM) for either acetonitrile or water, using the integral equation formalism (IEF) variant.[S9] The frequencies of the optimized geometries were calculated and no imaginary frequencies were found. Using the same solvation models, the geometry with the highest energy of each scan was optimized to a transition state and subjected to frequency calculations. In all instances, one imaginary frequency was found The relative free energies of the minima and transition states were then estimated from the frequency calculations and compiled into a single plot (Fig. S13) to reconstruct a profile of the ring-opening and -closing processes associated with **8**.

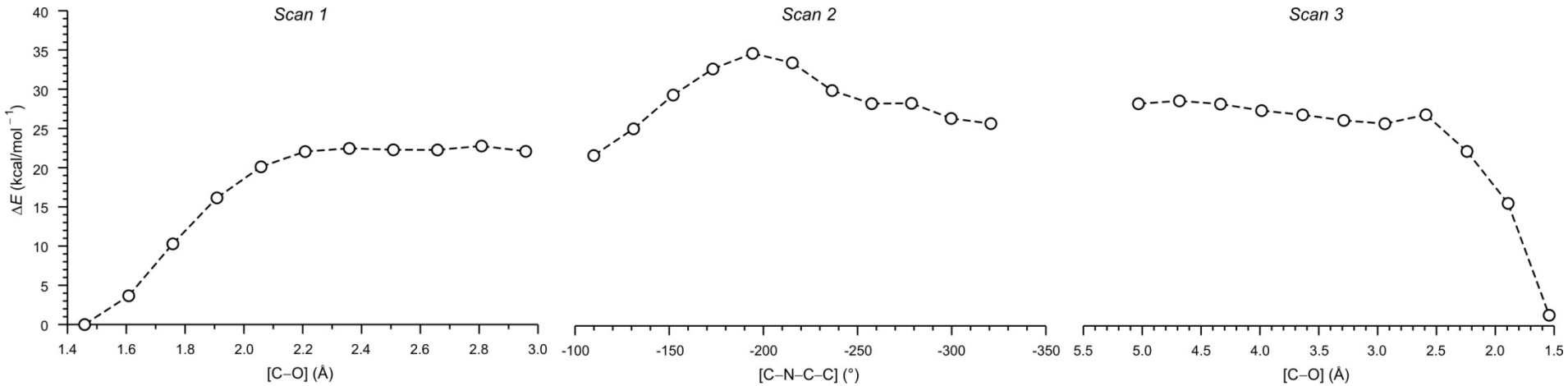


Fig. S12 Simulated energy profiles for the ring-opening (*Scan 1*), rotation (*Scan 2*) and ring-closing (*Scan 3*) steps associated with **8**.

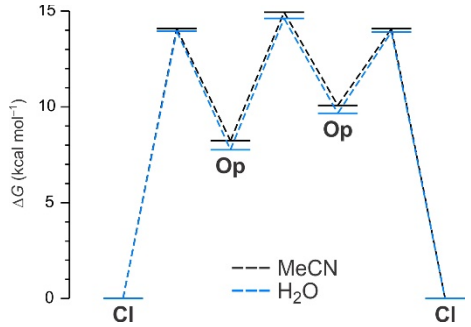


Fig. S13 Simulated free-energy profiles for the ring-opening, rotation and ring-closing steps associated with the **8** in acetonitrile and water.

**Coordinates of the Geometries Optimized from the Initial Structures of *Scan 1***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | 1.114535000 | –0.033268000 | 1.244452000 |
| C | 1.724817000 | 1.018178000 | 0.531707000 |
| C | 1.492914000 | 2.383712000 | 0.614718000 |
| H | 0.730129000 | 2.797455000 | 1.262974000 |
| C | 2.282041000 | 3.228403000 | –0.173934000 |
| H | 2.115141000 | 4.298261000 | –0.127319000 |
| C | 3.264717000 | 2.721452000 | –1.017027000 |
| H | 3.858877000 | 3.395217000 | –1.622234000 |
| C | 3.480340000 | 1.339234000 | –1.093138000 |
| H | 4.240249000 | 0.937528000 | –1.755606000 |
| C | 2.703751000 | 0.497089000 | –0.322369000 |
| C | 2.734369000 | –1.011752000 | –0.166443000 |
| C | 1.335819000 | –1.240245000 | 0.471649000 |
| O | 0.395826000 | –1.287635000 | –0.650071000 |
| C | –0.860531000 | –0.846355000 | –0.452838000 |
| C | –1.778226000 | –1.095857000 | –1.482053000 |
| H | –1.441543000 | –1.632212000 | –2.360047000 |
| C | –3.084069000 | –0.666464000 | –1.366600000 |
| H | –3.806248000 | –0.852561000 | –2.149473000 |
| C | –3.461531000 | 0.017507000 | –0.213701000 |
| C | –2.564896000 | 0.283305000 | 0.810946000 |
| H | –2.890798000 | 0.830191000 | 1.687275000 |
| C | –1.251455000 | –0.146576000 | 0.701025000 |
| C | –0.227503000 | 0.114885000 | 1.778968000 |
| H | –0.346089000 | 1.116157000 | 2.192807000 |
| H | –0.358082000 | –0.585726000 | 2.608586000 |
| C | 3.838913000 | –1.391396000 | 0.833828000 |
| H | 4.803639000 | –1.070371000 | 0.435943000 |
| H | 3.874076000 | –2.473244000 | 0.985109000 |
| H | 3.685303000 | –0.904848000 | 1.799669000 |
| C | 2.937904000 | –1.768997000 | –1.475746000 |
| H | 3.954826000 | –1.598492000 | –1.836679000 |
| H | 2.236054000 | –1.441973000 | –2.241392000 |
| H | 2.816357000 | –2.844881000 | –1.323109000 |
| C | 1.145154000 | –2.511588000 | 1.272326000 |
| H | 0.093447000 | –2.641170000 | 1.537105000 |
| H | 1.737195000 | –2.479528000 | 2.186687000 |
| H | 1.449833000 | –3.371332000 | 0.673293000 |
| N | –4.840274000 | 0.480275000 | –0.083561000 |
| O | –5.613703000 | 0.244251000 | –0.993070000 |
| O | –5.154021000 | 1.080138000 | 0.927840000 |

*Water*

| | | | |
|---|---|---|---|
| N | 1.114474000 | –0.033062000 | 1.244197000 |
| C | 1.724809000 | 1.018285000 | 0.531548000 |
| C | 1.492981000 | 2.383892000 | 0.614628000 |
| H | 0.730255000 | 2.797638000 | 1.262960000 |
| C | 2.282315000 | 3.228586000 | –0.173904000 |
| H | 2.115528000 | 4.298463000 | –0.127171000 |

| | | | |
|---|---|---|---|
| C | 3.265131000 | 2.721609000 | –1.016893000 |
| H | 3.859515000 | 3.395373000 | –1.621896000 |
| C | 3.480706000 | 1.339326000 | –1.093055000 |
| H | 4.240877000 | 0.937651000 | –1.755246000 |
| C | 2.703872000 | 0.497153000 | –0.322483000 |
| C | 2.734389000 | –1.011703000 | –0.166545000 |
| C | 1.335814000 | –1.240100000 | 0.471492000 |
| O | 0.395779000 | –1.287067000 | –0.650430000 |
| C | –0.860688000 | –0.846218000 | –0.452920000 |
| C | –1.778499000 | –1.096053000 | –1.481996000 |
| H | –1.442052000 | –1.632682000 | –2.359920000 |
| C | –3.084369000 | –0.666836000 | –1.366415000 |
| H | –3.806523000 | –0.853359000 | –2.149202000 |
| C | –3.461694000 | 0.017332000 | –0.213531000 |
| C | –2.564957000 | 0.283359000 | 0.811047000 |
| H | –2.890603000 | 0.830240000 | 1.687461000 |
| C | –1.251500000 | –0.146388000 | 0.700995000 |
| C | –0.227538000 | 0.115093000 | 1.778929000 |
| H | –0.346169000 | 1.116307000 | 2.192832000 |
| H | –0.358100000 | –0.585598000 | 2.608441000 |
| C | 3.838833000 | –1.391424000 | 0.833822000 |
| H | 4.803629000 | –1.070707000 | 0.435861000 |
| H | 3.873674000 | –2.473247000 | 0.985187000 |
| H | 3.685253000 | –0.904867000 | 1.799670000 |
| C | 2.938134000 | –1.769104000 | –1.475741000 |
| H | 3.955009000 | –1.598378000 | –1.836670000 |
| H | 2.236252000 | –1.442499000 | –2.241565000 |
| H | 2.816906000 | –2.844974000 | –1.322799000 |
| C | 1.144844000 | –2.511471000 | 1.271967000 |
| H | 0.093083000 | –2.641011000 | 1.536522000 |
| H | 1.736630000 | –2.479485000 | 2.186492000 |
| H | 1.449764000 | –3.371171000 | 0.673001000 |
| N | –4.840267000 | 0.479958000 | –0.083356000 |
| O | –5.613962000 | 0.243979000 | –0.992787000 |
| O | –5.154275000 | 1.079926000 | 0.927974000 |

**Coordinates of the Transition State for Ring Opening Optimized from the Structures with Highest Energy of *Scan 1***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | 1.056206000 | –0.285167000 | 1.296179000 |
| C | 1.500709000 | 0.844230000 | 0.549615000 |
| C | 1.021193000 | 2.142302000 | 0.590765000 |
| H | 0.192824000 | 2.431317000 | 1.225566000 |
| C | 1.649459000 | 3.071163000 | –0.239800000 |
| H | 1.304460000 | 4.097838000 | –0.240004000 |
| C | 2.706166000 | 2.698802000 | –1.069822000 |
| H | 3.172630000 | 3.440927000 | –1.706000000 |
| C | 3.165084000 | 1.380031000 | –1.095155000 |
| H | 3.984555000 | 1.092795000 | –1.744798000 |
| C | 2.545930000 | 0.450955000 | –0.276546000 |
| C | 2.811712000 | –1.017319000 | –0.054226000 |
| C | 1.650598000 | –1.386246000 | 0.857098000 |
| O | 0.071774000 | –1.943495000 | –0.479266000 |

| | | | |
|---|---|---|---|
| C | –0.950775000 | –1.176080000 | –0.440537000 |
| C | –1.852216000 | –1.104903000 | –1.549446000 |
| H | –1.623096000 | –1.711659000 | –2.417304000 |
| C | –2.979950000 | –0.324830000 | –1.519511000 |
| H | –3.661883000 | –0.299633000 | –2.359294000 |
| C | –3.247228000 | 0.456508000 | –0.387350000 |
| C | –2.378055000 | 0.455111000 | 0.704704000 |
| H | –2.596881000 | 1.087243000 | 1.557609000 |
| C | –1.259242000 | –0.348471000 | 0.701557000 |
| C | –0.299351000 | –0.326030000 | 1.861393000 |
| H | –0.449326000 | 0.548806000 | 2.493955000 |
| H | –0.373334000 | –1.208041000 | 2.495396000 |
| C | 4.117751000 | –1.205089000 | 0.753879000 |
| H | 4.949294000 | –0.821226000 | 0.160920000 |
| H | 4.295454000 | –2.263373000 | 0.954928000 |
| H | 4.083707000 | –0.660434000 | 1.699705000 |
| C | 2.878424000 | –1.835580000 | –1.345780000 |
| H | 3.758636000 | –1.522486000 | –1.911284000 |
| H | 1.984277000 | –1.686938000 | –1.946566000 |
| H | 2.983076000 | –2.899555000 | –1.123012000 |
| C | 1.590748000 | –2.702542000 | 1.542774000 |
| H | 0.601894000 | –2.931962000 | 1.926927000 |
| H | 2.306132000 | –2.686672000 | 2.371298000 |
| H | 1.885146000 | –3.484385000 | 0.844110000 |
| N | –4.421398000 | 1.281178000 | –0.353004000 |
| O | –5.164807000 | 1.286560000 | –1.326295000 |
| O | –4.643033000 | 1.953121000 | 0.647124000 |

*Water*

| | | | |
|---|---|---|---|
| N | 1.056984000 | –0.284035000 | 1.295552000 |
| C | 1.502414000 | 0.844760000 | 0.548933000 |
| C | 1.024165000 | 2.143321000 | 0.590349000 |
| H | 0.196759000 | 2.433073000 | 1.226099000 |
| C | 1.652734000 | 3.071571000 | –0.240782000 |
| H | 1.308807000 | 4.098617000 | –0.240724000 |
| C | 2.708685000 | 2.698189000 | –1.071349000 |
| H | 3.175566000 | 3.439871000 | –1.707751000 |
| C | 3.166545000 | 1.378969000 | –1.096727000 |
| H | 3.985711000 | 1.091064000 | –1.746440000 |
| C | 2.546872000 | 0.450450000 | –0.277843000 |
| C | 2.811725000 | –1.017947000 | –0.054913000 |
| C | 1.648878000 | –1.386148000 | 0.854645000 |
| O | 0.075236000 | –1.936772000 | –0.484020000 |
| C | –0.949290000 | –1.171841000 | –0.442482000 |
| C | –1.851904000 | –1.101803000 | –1.550495000 |
| H | –1.622064000 | –1.706884000 | –2.419340000 |
| C | –2.981723000 | –0.324822000 | –1.518681000 |
| H | –3.664384000 | –0.300708000 | –2.357897000 |
| C | –3.249893000 | 0.454461000 | –0.385315000 |
| C | –2.379546000 | 0.454013000 | 0.706016000 |
| H | –2.598783000 | 1.084723000 | 1.559856000 |
| C | –1.258646000 | –0.346555000 | 0.701053000 |

| | | | |
|---|---|---|---|
| C | –0.298392000 | –0.323304000 | 1.860760000 |
| H | –0.447900000 | 0.552357000 | 2.492244000 |
| H | –0.373214000 | –1.204373000 | 2.495967000 |
| C | 4.115885000 | –1.205077000 | 0.756617000 |
| H | 4.948665000 | –0.821306000 | 0.165361000 |
| H | 4.293285000 | –2.263213000 | 0.958635000 |
| H | 4.079276000 | –0.659983000 | 1.702087000 |
| C | 2.882103000 | –1.837000000 | –1.345634000 |
| H | 3.764220000 | –1.524809000 | –1.908643000 |
| H | 1.990020000 | –1.688440000 | –1.949512000 |
| H | 2.985781000 | –2.900845000 | –1.121740000 |
| C | 1.587103000 | –2.702512000 | 1.540118000 |
| H | 0.597647000 | –2.930866000 | 1.923481000 |
| H | 2.301466000 | –2.687195000 | 2.369483000 |
| H | 1.881755000 | –3.484666000 | 0.841927000 |
| N | –4.425973000 | 1.275808000 | –0.348943000 |
| O | –5.170426000 | 1.280689000 | –1.321658000 |
| O | –4.648889000 | 1.945935000 | 0.652203000 |

**Coordinates of the Geometries Optimized from the Final Structures of *Scan 1***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | 1.024200000 | –0.439162000 | 1.020765000 |
| C | 1.459911000 | 0.739571000 | 0.333530000 |
| C | 0.828361000 | 1.967484000 | 0.237437000 |
| H | –0.134296000 | 2.160444000 | 0.690358000 |
| C | 1.498127000 | 2.954594000 | –0.484125000 |
| H | 1.043173000 | 3.931590000 | –0.589447000 |
| C | 2.738660000 | 2.704842000 | –1.071967000 |
| H | 3.232157000 | 3.492540000 | –1.627847000 |
| C | 3.353730000 | 1.458302000 | –0.951227000 |
| H | 4.321181000 | 1.272148000 | –1.403755000 |
| C | 2.696778000 | 0.471247000 | –0.236237000 |
| C | 3.082340000 | –0.947734000 | 0.089738000 |
| C | 1.904964000 | –1.388809000 | 0.922242000 |
| O | –0.495591000 | –2.278767000 | –0.580141000 |
| C | –1.371337000 | –1.380640000 | –0.511230000 |
| C | –2.412261000 | –1.221140000 | –1.497786000 |
| H | –2.413835000 | –1.907286000 | –2.336753000 |
| C | –3.375507000 | –0.256179000 | –1.387636000 |
| H | –4.153346000 | –0.157754000 | –2.134035000 |
| C | –3.365403000 | 0.624415000 | –0.289266000 |
| C | –2.363926000 | 0.531402000 | 0.685936000 |
| H | –2.373852000 | 1.226426000 | 1.518171000 |
| C | –1.389685000 | –0.430019000 | 0.585349000 |
| C | –0.315626000 | –0.553344000 | 1.630169000 |
| H | –0.401526000 | 0.231632000 | 2.383609000 |
| H | –0.353335000 | –1.521688000 | 2.127159000 |
| C | 4.393363000 | –1.032016000 | 0.888143000 |
| H | 5.206769000 | –0.656617000 | 0.264905000 |
| H | 4.617409000 | –2.065521000 | 1.156793000 |
| H | 4.342388000 | –0.428711000 | 1.796014000 |
| C | 3.142346000 | –1.831022000 | –1.173997000 |

| | | | |
|---|---|---|---|
| H | 3.927506000 | –1.449923000 | –1.828952000 |
| H | 2.190271000 | –1.810078000 | –1.706823000 |
| H | 3.381232000 | –2.862864000 | –0.910289000 |
| C | 1.753182000 | –2.738540000 | 1.506922000 |
| H | 0.907025000 | –3.223105000 | 1.009558000 |
| H | 1.544934000 | –2.678383000 | 2.576868000 |
| H | 2.657929000 | –3.322821000 | 1.354766000 |
| N | –4.372013000 | 1.621535000 | –0.168878000 |
| O | –5.240896000 | 1.698602000 | –1.035169000 |
| O | –4.348242000 | 2.382118000 | 0.797628000 |

*Water*

| | | | |
|---|---|---|---|
| N | 1.023805000 | –0.440691000 | 1.015350000 |
| C | 1.460692000 | 0.738355000 | 0.329435000 |
| C | 0.829205000 | 1.966267000 | 0.232575000 |
| H | –0.133730000 | 2.159406000 | 0.684826000 |
| C | 1.499951000 | 2.953499000 | –0.487992000 |
| H | 1.045234000 | 3.930571000 | –0.593691000 |
| C | 2.741392000 | 2.703887000 | –1.074033000 |
| H | 3.235713000 | 3.491673000 | –1.629062000 |
| C | 3.356626000 | 1.457509000 | –0.952076000 |
| H | 4.325047000 | 1.271636000 | –1.402636000 |
| C | 2.698680000 | 0.470360000 | –0.238098000 |
| C | 3.084688000 | –0.948055000 | 0.089781000 |
| C | 1.904912000 | –1.390206000 | 0.918258000 |
| O | –0.502421000 | –2.279953000 | –0.583885000 |
| C | –1.376870000 | –1.380746000 | –0.512884000 |
| C | –2.420124000 | –1.220825000 | –1.496999000 |
| H | –2.424413000 | –1.907224000 | –2.335768000 |
| C | –3.382582000 | –0.255402000 | –1.384693000 |
| H | –4.162190000 | –0.156978000 | –2.129225000 |
| C | –3.369163000 | 0.625380000 | –0.286443000 |
| C | –2.364985000 | 0.532025000 | 0.686307000 |
| H | –2.372358000 | 1.227227000 | 1.518414000 |
| C | –1.391432000 | –0.429764000 | 0.583538000 |
| C | –0.315263000 | –0.553824000 | 1.626288000 |
| H | –0.399242000 | 0.231187000 | 2.379863000 |
| H | –0.353034000 | –1.521895000 | 2.123790000 |
| C | 4.391673000 | –1.029331000 | 0.895457000 |
| H | 5.207727000 | –0.653450000 | 0.276019000 |
| H | 4.615676000 | –2.062109000 | 1.166929000 |
| H | 4.334463000 | –0.424828000 | 1.802149000 |
| C | 3.153177000 | –1.831486000 | –1.173187000 |
| H | 3.940855000 | –1.448927000 | –1.824237000 |
| H | 2.204040000 | –1.812446000 | –1.711353000 |
| H | 3.392937000 | –2.862770000 | –0.908246000 |
| C | 1.752142000 | –2.739749000 | 1.503113000 |
| H | 0.899736000 | –3.220992000 | 1.013587000 |
| H | 1.553780000 | –2.678389000 | 2.574981000 |
| H | 2.653037000 | –3.327828000 | 1.343185000 |
| N | –4.374917000 | 1.622458000 | –0.163670000 |
| O | –5.246233000 | 1.699861000 | –1.027865000 |

| | | | |
|---|---|---|---|
| O | –4.348973000 | 2.383333000 | 0.802695000 |

**Coordinates of the Transition State for the Conformational Change Optimized from the Structures with Highest Energy of *Scan 2***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | –1.167884000 | –0.835063000 | –0.102240000 |
| C | –1.238148000 | 0.453527000 | 0.549201000 |
| C | –0.253631000 | 1.211758000 | 1.168160000 |
| H | 0.775795000 | 0.900356000 | 1.235486000 |
| C | –0.648027000 | 2.432361000 | 1.714331000 |
| H | 0.097278000 | 3.047609000 | 2.202959000 |
| C | –1.967446000 | 2.873998000 | 1.643657000 |
| H | –2.237735000 | 3.828632000 | 2.077793000 |
| C | –2.941037000 | 2.095311000 | 1.021616000 |
| H | –3.970566000 | 2.430951000 | 0.968205000 |
| C | –2.561664000 | 0.880988000 | 0.476546000 |
| C | –3.386610000 | –0.158342000 | –0.229099000 |
| C | –2.341139000 | –1.191846000 | –0.533454000 |
| O | 1.241048000 | –1.842488000 | 2.206654000 |
| C | 1.895144000 | –1.269831000 | 1.304388000 |
| C | 3.208022000 | –0.707744000 | 1.522905000 |
| H | 3.642580000 | –0.822298000 | 2.509119000 |
| C | 3.879606000 | –0.029812000 | 0.543120000 |
| H | 4.855933000 | 0.397559000 | 0.733895000 |
| C | 3.305188000 | 0.117878000 | –0.735001000 |
| C | 2.048621000 | –0.434636000 | –1.014330000 |
| H | 1.628472000 | –0.320003000 | –2.007091000 |
| C | 1.355364000 | –1.100792000 | –0.034505000 |
| C | 0.024589000 | –1.714648000 | –0.318482000 |
| H | –0.032814000 | –2.028959000 | –1.360681000 |
| H | –0.122490000 | –2.579850000 | 0.330644000 |
| C | –4.001661000 | 0.364514000 | –1.541081000 |
| H | –4.718108000 | 1.151634000 | –1.300944000 |
| H | –4.530733000 | –0.434874000 | –2.062963000 |
| H | –3.235526000 | 0.777013000 | –2.199517000 |
| C | –4.472571000 | –0.752225000 | 0.688346000 |
| H | –5.174686000 | 0.039801000 | 0.953160000 |
| H | –4.037740000 | –1.154832000 | 1.604508000 |
| H | –5.023545000 | –1.541769000 | 0.174979000 |
| C | –2.598282000 | –2.455631000 | –1.260432000 |
| H | –2.166555000 | –3.307844000 | –0.732143000 |
| H | –2.133473000 | –2.406987000 | –2.251080000 |
| H | –3.667309000 | –2.609893000 | –1.387573000 |
| N | 4.008386000 | 0.817837000 | –1.753450000 |
| O | 5.111345000 | 1.295246000 | –1.494841000 |
| O | 3.495577000 | 0.930160000 | –2.865833000 |

*Water*

| | | | |
|---|---|---|---|
| N | –1.167982000 | –0.832971000 | –0.105751000 |
| C | –1.238355000 | 0.455895000 | 0.545002000 |
| C | –0.253168000 | 1.216626000 | 1.159938000 |
| H | 0.777228000 | 0.907593000 | 1.223483000 |

| | | | |
|---|---|---|---|
| C | –0.647866000 | 2.437022000 | 1.706477000 |
| H | 0.098044000 | 3.054163000 | 2.191823000 |
| C | –1.968332000 | 2.876190000 | 1.639889000 |
| H | –2.238957000 | 3.830704000 | 2.074075000 |
| C | –2.942499000 | 2.095293000 | 1.021457000 |
| H | –3.972730000 | 2.429196000 | 0.970880000 |
| C | –2.562797000 | 0.881205000 | 0.476013000 |
| C | –3.388053000 | –0.159562000 | –0.227121000 |
| C | –2.341844000 | –1.191410000 | –0.534302000 |
| O | 1.232108000 | –1.838135000 | 2.205432000 |
| C | 1.890276000 | –1.267571000 | 1.304466000 |
| C | 3.203392000 | –0.707890000 | 1.527095000 |
| H | 3.634486000 | –0.822057000 | 2.514877000 |
| C | 3.879796000 | –0.032293000 | 0.549010000 |
| H | 4.856246000 | 0.393318000 | 0.742991000 |
| C | 3.310044000 | 0.115075000 | –0.731191000 |
| C | 2.053213000 | –0.435370000 | –1.014325000 |
| H | 1.636309000 | –0.320984000 | –2.008456000 |
| C | 1.355308000 | –1.099258000 | –0.036329000 |
| C | 0.024613000 | –1.711268000 | –0.325220000 |
| H | –0.031142000 | –2.020029000 | –1.369129000 |
| H | –0.123686000 | –2.580199000 | 0.318580000 |
| C | –4.007918000 | 0.362078000 | –1.537343000 |
| H | –4.725043000 | 1.147903000 | –1.295043000 |
| H | –4.537147000 | –0.438473000 | –2.057230000 |
| H | –3.244446000 | 0.775533000 | –2.198240000 |
| C | –4.470591000 | –0.755090000 | 0.693424000 |
| H | –5.173539000 | 0.035826000 | 0.959374000 |
| H | –4.032684000 | –1.156401000 | 1.608676000 |
| H | –5.021223000 | –1.545973000 | 0.181763000 |
| C | –2.598585000 | –2.455096000 | –1.261291000 |
| H | –2.166193000 | –3.307117000 | –0.733214000 |
| H | –2.133965000 | –2.405883000 | –2.252014000 |
| H | –3.667500000 | –2.609872000 | –1.388248000 |
| N | 4.018004000 | 0.812641000 | –1.747587000 |
| O | 5.121299000 | 1.288075000 | –1.485806000 |
| O | 3.509451000 | 0.925330000 | –2.861953000 |

**Coordinates of the Geometries Optimized from the Final Structures of *Scan 2***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | –1.035083000 | –0.092853000 | 1.022494000 |
| C | –1.637446000 | 0.743272000 | 0.028414000 |
| C | –1.359448000 | 2.070482000 | –0.243582000 |
| H | –0.606954000 | 2.627283000 | 0.305791000 |
| C | –2.110596000 | 2.651688000 | –1.265005000 |
| H | –1.937362000 | 3.689061000 | –1.523327000 |
| C | –3.078630000 | 1.922184000 | –1.957508000 |
| H | –3.643524000 | 2.405262000 | –2.745473000 |
| C | –3.333602000 | 0.583978000 | –1.652119000 |

| | | | |
|---|---|---|---|
| H | –4.090280000 | 0.026936000 | –2.192889000 |
| C | –2.594859000 | –0.005183000 | –0.639799000 |
| C | –2.608455000 | –1.398533000 | –0.064340000 |
| C | –1.549844000 | –1.284471000 | 1.006692000 |
| O | 1.300279000 | 2.940211000 | 1.595521000 |
| C | 1.854522000 | 1.972618000 | 1.019728000 |
| C | 3.064479000 | 2.120850000 | 0.244641000 |
| H | 3.494327000 | 3.113960000 | 0.184395000 |
| C | 3.650808000 | 1.071054000 | –0.405914000 |
| H | 4.553808000 | 1.209767000 | –0.986607000 |
| C | 3.074962000 | –0.211456000 | –0.327996000 |
| C | 1.908515000 | –0.418147000 | 0.416982000 |
| H | 1.487339000 | –1.417405000 | 0.455589000 |
| C | 1.309733000 | 0.626382000 | 1.077936000 |
| C | 0.054100000 | 0.405362000 | 1.881382000 |
| H | 0.188638000 | –0.310738000 | 2.690229000 |
| H | –0.278806000 | 1.353262000 | 2.306209000 |
| C | –2.183894000 | –2.448380000 | –1.109898000 |
| H | –2.913046000 | –2.440099000 | –1.921567000 |
| H | –2.168309000 | –3.448248000 | –0.673390000 |
| H | –1.199890000 | –2.220179000 | –1.524028000 |
| C | –3.962181000 | –1.767319000 | 0.568072000 |
| H | –4.720842000 | –1.789637000 | –0.215916000 |
| H | –4.257797000 | –1.034423000 | 1.320701000 |
| H | –3.914303000 | –2.755669000 | 1.029006000 |
| C | –1.177580000 | –2.379317000 | 1.933521000 |
| H | –1.672750000 | –2.212170000 | 2.895869000 |
| H | –0.102817000 | –2.423759000 | 2.108009000 |
| H | –1.516240000 | –3.335076000 | 1.538322000 |
| N | 3.676705000 | –1.305371000 | –1.009204000 |
| O | 4.708135000 | –1.112853000 | –1.649303000 |
| O | 3.150298000 | –2.415052000 | –0.941432000 |

*Water*

| | | | |
|---|---|---|---|
| N | –1.033441000 | –0.094690000 | 1.021438000 |
| C | –1.636511000 | 0.741081000 | 0.027550000 |
| C | –1.358140000 | 2.067917000 | –0.245964000 |
| H | –0.605169000 | 2.624946000 | 0.302412000 |
| C | –2.110078000 | 2.648870000 | –1.267004000 |
| H | –1.936698000 | 3.686007000 | –1.526219000 |
| C | –3.079403000 | 1.919404000 | –1.957789000 |
| H | –3.645021000 | 2.402231000 | –2.745389000 |
| C | –3.334952000 | 0.581658000 | –1.650786000 |
| H | –4.092785000 | 0.024596000 | –2.189906000 |
| C | –2.595412000 | –0.007118000 | –0.638795000 |

| | | | |
|---|---|---|---|
| C | –2.609842000 | –1.399787000 | –0.061713000 |
| C | –1.549501000 | –1.285849000 | 1.007545000 |
| O | 1.302874000 | 2.939693000 | 1.599809000 |
| C | 1.856191000 | 1.973231000 | 1.020822000 |
| C | 3.065508000 | 2.123636000 | 0.245294000 |
| H | 3.495570000 | 3.116800000 | 0.187399000 |
| C | 3.651837000 | 1.075425000 | –0.407837000 |
| H | 4.554700000 | 1.215773000 | –0.988331000 |
| C | 3.075898000 | –0.207170000 | –0.332935000 |
| C | 1.909741000 | –0.415856000 | 0.412333000 |
| H | 1.488736000 | –1.415238000 | 0.449325000 |
| C | 1.310960000 | 0.627060000 | 1.075764000 |
| C | 0.055839000 | 0.403847000 | 1.879693000 |
| H | 0.192053000 | –0.312777000 | 2.687766000 |
| H | –0.278006000 | 1.350750000 | 2.305940000 |
| C | –2.188436000 | –2.451328000 | –1.106858000 |
| H | –2.919433000 | –2.443198000 | –1.916872000 |
| H | –2.173053000 | –3.450557000 | –0.668930000 |
| H | –1.205014000 | –2.224618000 | –1.523158000 |
| C | –3.962976000 | –1.766298000 | 0.573313000 |
| H | –4.723100000 | –1.787292000 | –0.209286000 |
| H | –4.255786000 | –1.033102000 | 1.326727000 |
| H | –3.915616000 | –2.754751000 | 1.034039000 |
| C | –1.177687000 | –2.380003000 | 1.935138000 |
| H | –1.670684000 | –2.209852000 | 2.898076000 |
| H | –0.102686000 | –2.426679000 | 2.107397000 |
| H | –1.519608000 | –3.335532000 | 1.542213000 |
| N | 3.678388000 | –1.299317000 | –1.015857000 |
| O | 4.710388000 | –1.105261000 | –1.655019000 |
| O | 3.152467000 | –2.409381000 | –0.951142000 |

**Coordinates of the Transition State for Ring Closing Optimized from the Structures with Highest Energy of *Scan 3***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | –1.175121000 | –0.630040000 | 1.130992000 |
| C | –1.567994000 | 0.645020000 | 0.630651000 |
| C | –1.223820000 | 1.897532000 | 1.109589000 |
| H | –0.561691000 | 2.029354000 | 1.956291000 |
| C | –1.762300000 | 2.996655000 | 0.439278000 |
| H | –1.517301000 | 3.995111000 | 0.780084000 |
| C | –2.602745000 | 2.830544000 | –0.660848000 |
| H | –3.003544000 | 3.702386000 | –1.163155000 |
| C | –2.927949000 | 1.554509000 | –1.126012000 |
| H | –3.578690000 | 1.428783000 | –1.984385000 |
| C | –2.396077000 | 0.458155000 | –0.468917000 |
| C | –2.566437000 | –1.022927000 | –0.699704000 |
| C | –1.573124000 | –1.587891000 | 0.304786000 |
| O | 0.276066000 | –1.701897000 | –0.770790000 |
| C | 1.199099000 | –0.939780000 | –0.319984000 |
| C | 2.286089000 | –0.535654000 | –1.158116000 |
| H | 2.282979000 | –0.888375000 | –2.182521000 |
| C | 3.312306000 | 0.244912000 | –0.690360000 |
| H | 4.137341000 | 0.523394000 | –1.332752000 |

| | | | |
|---|---|---|---|
| C | 3.286364000 | 0.694182000 | 0.636741000 |
| C | 2.227933000 | 0.362723000 | 1.484038000 |
| H | 2.221607000 | 0.743501000 | 2.498872000 |
| C | 1.207463000 | –0.447528000 | 1.037247000 |
| C | 0.045253000 | –0.777969000 | 1.935666000 |
| H | 0.075447000 | –1.797259000 | 2.317120000 |
| H | –0.007847000 | –0.106240000 | 2.792359000 |
| C | –2.310341000 | –1.456283000 | –2.144962000 |
| H | –3.090741000 | –1.030930000 | –2.779507000 |
| H | –2.358817000 | –2.543494000 | –2.235739000 |
| H | –1.334963000 | –1.116745000 | –2.485384000 |
| C | –3.980887000 | –1.470613000 | –0.260514000 |
| H | –4.714411000 | –0.967487000 | –0.892355000 |
| H | –4.178003000 | –1.206140000 | 0.780444000 |
| H | –4.097868000 | –2.548871000 | –0.385565000 |
| C | –1.527940000 | –3.039046000 | 0.618611000 |
| H | –2.387174000 | –3.275911000 | 1.254288000 |
| H | –0.614395000 | –3.331140000 | 1.126696000 |
| H | –1.611919000 | –3.608513000 | –0.305908000 |
| N | 4.353079000 | 1.518057000 | 1.129989000 |
| O | 5.265526000 | 1.816313000 | 0.369423000 |
| O | 4.317656000 | 1.896877000 | 2.294517000 |

*Water*

| | | | |
|---|---|---|---|
| N | –1.175888000 | –0.628776000 | 1.130452000 |
| C | –1.569680000 | 0.645657000 | 0.629683000 |
| C | –1.226912000 | 1.898545000 | 1.108721000 |
| H | –0.566041000 | 2.030819000 | 1.956358000 |
| C | –1.765520000 | 2.997184000 | 0.437585000 |
| H | –1.521719000 | 3.995908000 | 0.778496000 |
| C | –2.604953000 | 2.830201000 | –0.663213000 |
| H | –3.006069000 | 3.701636000 | –1.165990000 |
| C | –2.929014000 | 1.553758000 | –1.128291000 |
| H | –3.579347000 | 1.427379000 | –1.986863000 |
| C | –2.396738000 | 0.457920000 | –0.470617000 |
| C | –2.566310000 | –1.023435000 | –0.700535000 |
| C | –1.570916000 | –1.587056000 | 0.302776000 |
| O | 0.272966000 | –1.693781000 | –0.774533000 |
| C | 1.197656000 | –0.934916000 | –0.321137000 |
| C | 2.285817000 | –0.532090000 | –1.158367000 |
| H | 2.282045000 | –0.882814000 | –2.183462000 |
| C | 3.314049000 | 0.244891000 | –0.689072000 |
| H | 4.139842000 | 0.522199000 | –1.330989000 |
| C | 3.288911000 | 0.691727000 | 0.638868000 |
| C | 2.229303000 | 0.361341000 | 1.485386000 |
| H | 2.223301000 | 0.740413000 | 2.500851000 |
| C | 1.206806000 | –0.445433000 | 1.037099000 |
| C | 0.044167000 | –0.775066000 | 1.935512000 |
| H | 0.074907000 | –1.793713000 | 2.318633000 |
| H | –0.009303000 | –0.102193000 | 2.791250000 |
| C | –2.314206000 | –1.458119000 | –2.145963000 |
| H | –3.096557000 | –1.033833000 | –2.778797000 |

| | | | |
|---|---|---|---|
| H | –2.362793000 | –2.545450000 | –2.235398000 |
| H | –1.339998000 | –1.118613000 | –2.489762000 |
| C | –3.979577000 | –1.471284000 | –0.257221000 |
| H | –4.714715000 | –0.968949000 | –0.887792000 |
| H | –4.174012000 | –1.205898000 | 0.784002000 |
| H | –4.096467000 | –2.549692000 | –0.380931000 |
| C | –1.523546000 | –3.038157000 | 0.616721000 |
| H | –2.381931000 | –3.275956000 | 1.253131000 |
| H | –0.609374000 | –3.328821000 | 1.124599000 |
| H | –1.607595000 | –3.608031000 | –0.307528000 |
| N | 4.357431000 | 1.511790000 | 1.133696000 |
| O | 5.270971000 | 1.809336000 | 0.373878000 |
| O | 4.323118000 | 1.888644000 | 2.298967000 |

**Coordinates of the Geometries Optimized from the Final Structures of *Scan 3***

*Acetonitrile*

| | | | |
|---|---|---|---|
| N | –1.240941000 | –0.386009000 | 1.136369000 |
| C | –1.799455000 | 0.802302000 | 0.624607000 |
| C | –1.712380000 | 2.095712000 | 1.119446000 |
| H | –1.125788000 | 2.335297000 | 1.997950000 |
| C | –2.412730000 | 3.101151000 | 0.443584000 |
| H | –2.355492000 | 4.119192000 | 0.810928000 |
| C | –3.169292000 | 2.819757000 | –0.688615000 |
| H | –3.697897000 | 3.616211000 | –1.198022000 |
| C | –3.240229000 | 1.508973000 | –1.178136000 |
| H | –3.822418000 | 1.285058000 | –2.066175000 |
| C | –2.549017000 | 0.510607000 | –0.520986000 |
| C | –2.471111000 | –0.980790000 | –0.788435000 |
| C | –1.202448000 | –1.331846000 | 0.037741000 |
| O | –0.068124000 | –1.027146000 | –0.836604000 |
| C | 1.083404000 | –0.616430000 | –0.273248000 |
| C | 2.196919000 | –0.532320000 | –1.119824000 |
| H | 2.081370000 | –0.809545000 | –2.159871000 |
| C | 3.413252000 | –0.108040000 | –0.626424000 |
| H | 4.283520000 | –0.039633000 | –1.264412000 |
| C | 3.503697000 | 0.234142000 | 0.720502000 |
| C | 2.410135000 | 0.167588000 | 1.571521000 |
| H | 2.514543000 | 0.454950000 | 2.610645000 |
| C | 1.185341000 | –0.258829000 | 1.081612000 |
| C | –0.042381000 | –0.348757000 | 1.955359000 |
| H | –0.006931000 | –1.250513000 | 2.573221000 |
| H | –0.095110000 | 0.497991000 | 2.639547000 |
| C | –2.355357000 | –1.343097000 | –2.266427000 |
| H | –3.297564000 | –1.112801000 | –2.769107000 |
| H | –2.167391000 | –2.413299000 | –2.388640000 |
| H | –1.554830000 | –0.788600000 | –2.753705000 |
| C | –3.704716000 | –1.666115000 | –0.177532000 |
| H | –4.602637000 | –1.279353000 | –0.663558000 |
| H | –3.780187000 | –1.467695000 | 0.893967000 |
| H | –3.669178000 | –2.747100000 | –0.334786000 |
| C | –1.050873000 | –2.770398000 | 0.486452000 |
| H | –1.804597000 | –3.018981000 | 1.233245000 |

| | | | |
|---|---|---|---|
| H | –0.060298000 | –2.933042000 | 0.916914000 |
| H | –1.158132000 | –3.435486000 | –0.372026000 |
| N | 4.785484000 | 0.688808000 | 1.251731000 |
| O | 5.733594000 | 0.749406000 | 0.491121000 |
| O | 4.848356000 | 0.985951000 | 2.430278000 |

*Water*

| | | | |
|---|---|---|---|
| N | –1.240837000 | –0.385761000 | 1.136198000 |
| C | –1.799436000 | 0.802426000 | 0.624517000 |
| C | –1.712469000 | 2.095876000 | 1.119446000 |
| H | –1.125943000 | 2.335435000 | 1.998008000 |
| C | –2.413069000 | 3.101277000 | 0.443681000 |
| H | –2.355977000 | 4.119293000 | 0.811134000 |
| C | –3.169790000 | 2.819832000 | –0.688454000 |
| H | –3.698671000 | 3.616219000 | –1.197697000 |
| C | –3.240650000 | 1.509009000 | –1.178052000 |
| H | –3.823154000 | 1.285042000 | –2.065874000 |
| C | –2.549136000 | 0.510679000 | –0.521070000 |
| C | –2.471110000 | –0.980727000 | –0.788517000 |
| C | –1.202410000 | –1.331669000 | 0.037621000 |
| O | –0.068059000 | –1.026479000 | –0.836795000 |
| C | 1.083563000 | –0.616249000 | –0.273279000 |
| C | 2.197190000 | –0.532472000 | –1.119799000 |
| H | 2.081877000 | –0.809963000 | –2.159807000 |
| C | 3.413540000 | –0.108384000 | –0.626327000 |
| H | 4.283799000 | –0.040396000 | –1.264360000 |
| C | 3.503846000 | 0.233974000 | 0.720613000 |
| C | 2.410183000 | 0.167629000 | 1.571616000 |
| H | 2.514331000 | 0.454945000 | 2.610769000 |
| C | 1.185387000 | –0.258633000 | 1.081625000 |
| C | –0.042336000 | –0.348565000 | 1.955376000 |
| H | –0.006859000 | –1.250378000 | 2.573101000 |
| H | –0.095032000 | 0.498100000 | 2.639631000 |
| C | –2.355573000 | –1.343191000 | –2.266501000 |
| H | –3.297762000 | –1.112683000 | –2.769096000 |
| H | –2.167969000 | –2.413474000 | –2.388510000 |
| H | –1.554953000 | –0.789027000 | –2.754047000 |
| C | –3.704615000 | –1.666176000 | –0.177526000 |
| H | –4.602570000 | –1.279700000 | –0.663713000 |
| H | –3.780116000 | –1.467763000 | 0.893979000 |
| H | –3.668762000 | –2.747147000 | –0.334639000 |
| C | –1.050476000 | –2.770185000 | 0.486176000 |
| H | –1.803964000 | –3.018897000 | 1.233159000 |
| H | –0.059803000 | –2.932720000 | 0.916435000 |
| H | –1.157989000 | –3.435248000 | –0.372286000 |
| N | 4.785467000 | 0.688502000 | 1.251795000 |
| O | 5.733802000 | 0.749190000 | 0.491310000 |
| O | 4.848611000 | 0.985733000 | 2.430367000 |

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