# Development of a New Dual Polarity and Viscosity Probe Based on the Foldamer Concept

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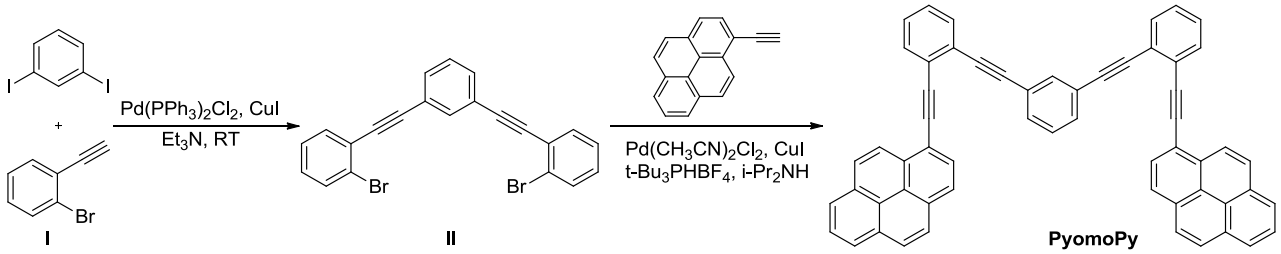
**General Information**

Sonogashira couplings were carried out in dry glassware under positive pressure of argon. All commercially available reagents and solvents used in extraction and purification, (triethylamine, diisopropylamine, dichlorometane, hexane and ethyl acetate) were obtained from standard chemical suppliers and used without further purification. Compound **I** was also commercially available. TLC was performed on aluminium-backed plates coated with silica gel 60 (230-240 mesh) with $F_{254}$ indicator. The spots were visualized with UV light (254 nm) and/or staining with Ce/Mo reagent or phosphomolybdic acid solution and subsequent heating.

NMR Spectra were measured at room temperature. $^{1}H$ NMR spectra were recorded at 300 or 600 MHz. Chemical shifts are reported in ppm using residual solvent peak as reference ($CHCl_3$: $\delta$ 7.26). Data are reported as follows: chemical shift, multiplicity (s: singlet, d: doublet, m: multiplet, dd: doublet of doublets), coupling constant (*J* in Hz) and integration. $^{13}C$-NMR spectra were recorded at 75.4 or 151 MHz using broadband proton decoupling and chemical shifts are reported in ppm using residual solvent peaks as reference ($CDCl_3$: $\delta$ 77.16). Carbon multiplicities were assigned by DEPT techniques.

High resolution mass spectra (HRMS) were recorded on a Micromass AutoSpec using EI at 70eV.

*Synthesis of* ***PyomoPy*****:**




**Compound II:** 1,3-diiodobenzene (231 mg, 0.7 mmol), $Pd(PPh_3)_2Cl_2$ (48mg, 0.07 mmol) and CuI (13mg, 0.07 mmol) were carefully deoxygenated and suspended in $Et_3N$ (5 mL). After 10 minutes, a solution of the comercial alkyne **I** (300 mg, 1.7 mmol) in 2 mL of $Et_3N$ was added dropwise over 10 minutes and the reaction mixture was stirred overnight at room temperature under argon atmosphere. The mixture was then diluted with $CH_2Cl_2$ (3 x 15 mL), washed with saturated $NH_4Cl$ (3 x 15 mL), dried over anhydrous $Na_2SO_4$ and the solvent was removed. The residue was purified by flash chromatography ($CH_2Cl_2$:Hexane, 1:4) to give the corresponding coupling product **II** (250 mg, 82%) as a pale brown solid.

**$^1$H-NMR** (300 MHz, $CDCl_3$): δ = 7.70 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.49-7.43 (m, 4H), 7.26 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 2H), 7.12 – 7.05 (m, 2H).

**$^{13}$C-NMR** (75 MHz, $CDCl_3$): δ = 134.7 (CH), 133.4 (CH), 132.6 (CH), 131.9 (CH), 129.7 (CH), 128.7 (CH), 127.2 (CH), 125.8 (C), 125.2 (C), 123.5 (C), 93.1 (C), 88.8 (C).

**HRMS** (EI, 70 eV) *m/z* calcd. for $C_{22}H_{12}Br_2$ $[M]^+$: 433.9306; found: 433.9317, $[M+2]^+$: 435.9285; found: 435.9287.

**PyomoPy:** Compound **I** (93 mg, 0.2 mmol), $Pd(CH_3CN)_2Cl_2$ (5 mg, 0.02 mmol), CuI (4 mg, 0.02 mmol) and *t*$Bu_3PHBF_4$ (12 mg, 0.04 mmol) were carefully deoxygenated and suspended in a mixture of dioxane (3 mL) and *i*$Pr_2NH$ (3 mL). After 10 mintues, a solution of 1-ethynylpyrene (116 mg, 0.5 mmol) in 2 mL of *i*$Pr_2NH$ was added dropwise over 10 minutes and the reaction mixture was stirred under argon atmosphere at 80ºC for 18h. The mixture was then diluted with $CH_2Cl_2$, washed with saturated $NH_4Cl$ (3 x 15 mL), dried over anhydrous $Na_2SO_4$ and the solvent was removed. The residue was purified by flash chromatography ($CH_2Cl_2$:Hexane, 1:4) to give the corresponding coupling product **PyomoPy** (110 mg, 76%) as a brown solid.

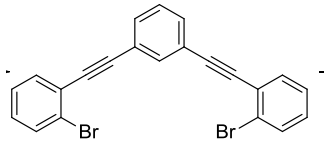
**$^1$H-NMR** (600 MHz, $CDCl_3$): δ = δ 8.37 (d, *J* = 8.9 Hz, 2H), 8.21 (s, 1H), 8.04 (d, *J* = 7.5 Hz, 2H), 7.96 (d, *J* = 2.8 Hz, 2H), 7.94 (d, *J* = 4.1 Hz, 2H), 7.81 (d, *J* = 9.0 Hz, 2H), 7.78 (d, *J* = 8.8 Hz, 2H), 7.77 – 7.70 (m, 6H), 7.67 (d, *J* = 7.7 Hz, 2H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.42 – 7.38 (m, 3H), 7.36 (dd, *J* = 14.4, 6.9 Hz, 2H).

**$^{13}$C-NMR** (151 MHz, $CDCl_3$): δ = 135.8 (CH), 132.4 (CH), 132.2 (CH), 132.1 (CH), 131.6 (C), 131.2 (C), 131.1 (C), 129.4 (CH), 128.77 (CH), 128.75 (CH), 128.4 (CH), 128.03 (CH), 127.96 (CH), 127.2 (CH), 126.5 (C), 125.95 (CH), 125.94 (CH), 125.4 (CH), 125.29 (CH), 125.27 (C), 124.18 (CH), 124.15 (C), 124.10 (C), 123.9 (C), 117.2 (C), 93.7 (C), 93.2 (C), 92.8 (C), 89.8 (C).

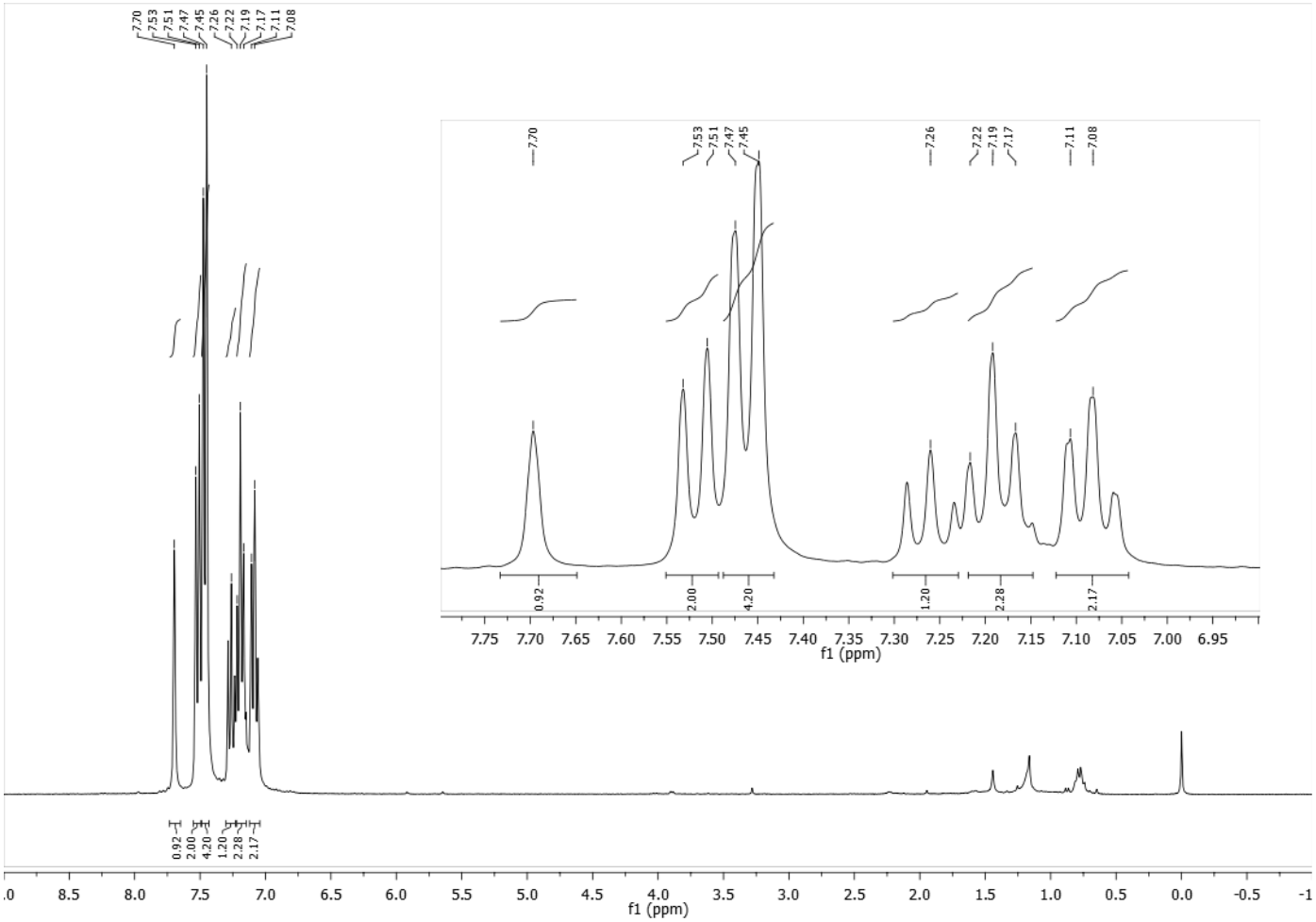
**HRMS** (ESI) *m/z* calcd. for $C_{58}H_{31}$ $[M^+ + 1]$: 727.2426; found: 727.2405.

Copies of $^{1}$H-NMR and $^{13}$C-NMR of compounds **II** and **PyomoPy**

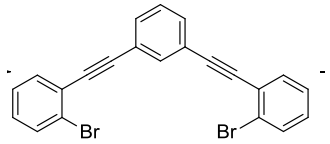
**$^{1}$H-NMR** ($CDCl_3$, 300 MHz)



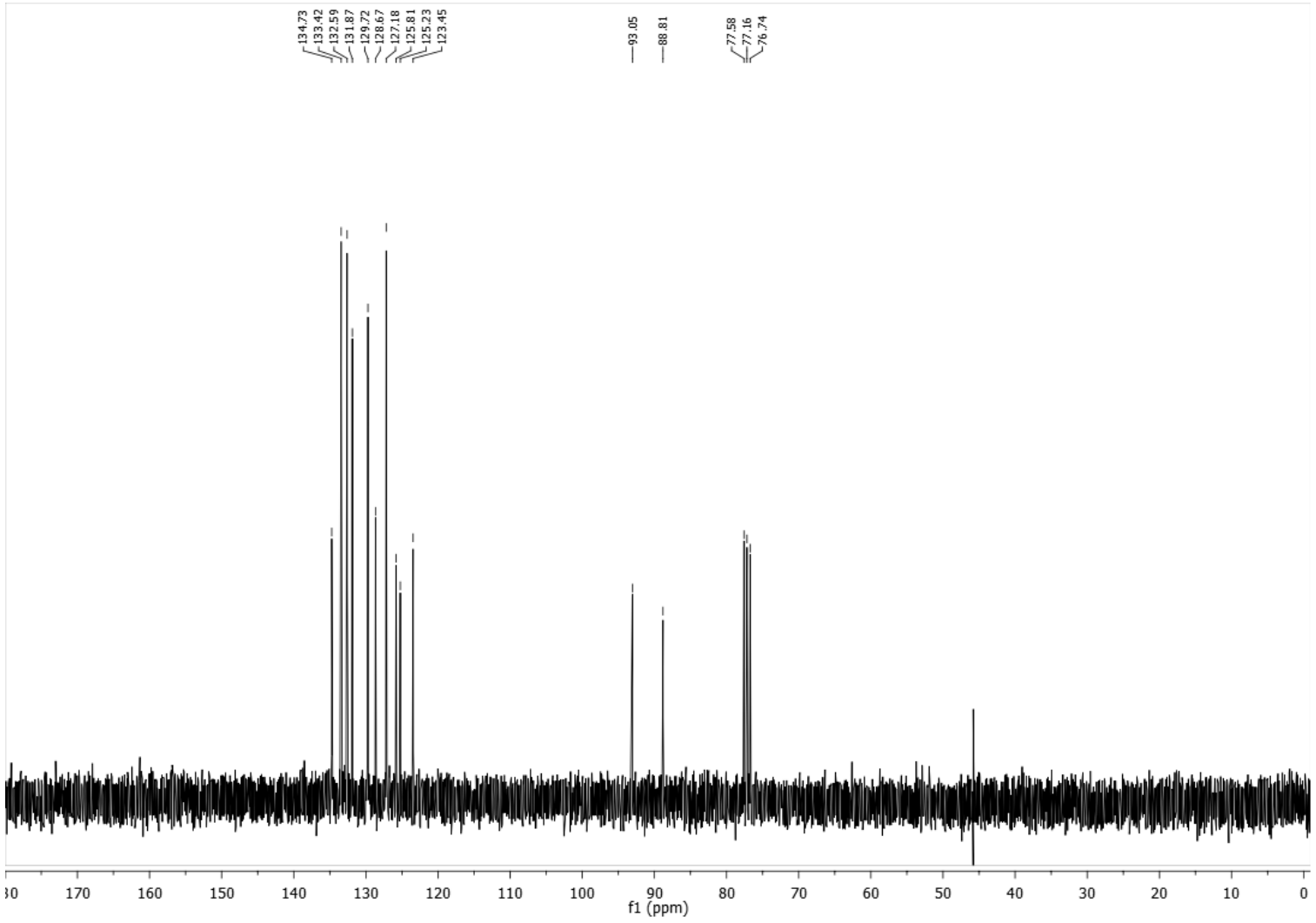

**II**



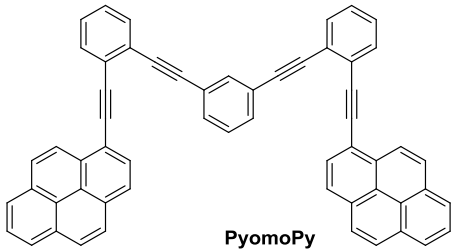
**$^{13}$C-NMR** ($CDCl_3$, 75 MHz)

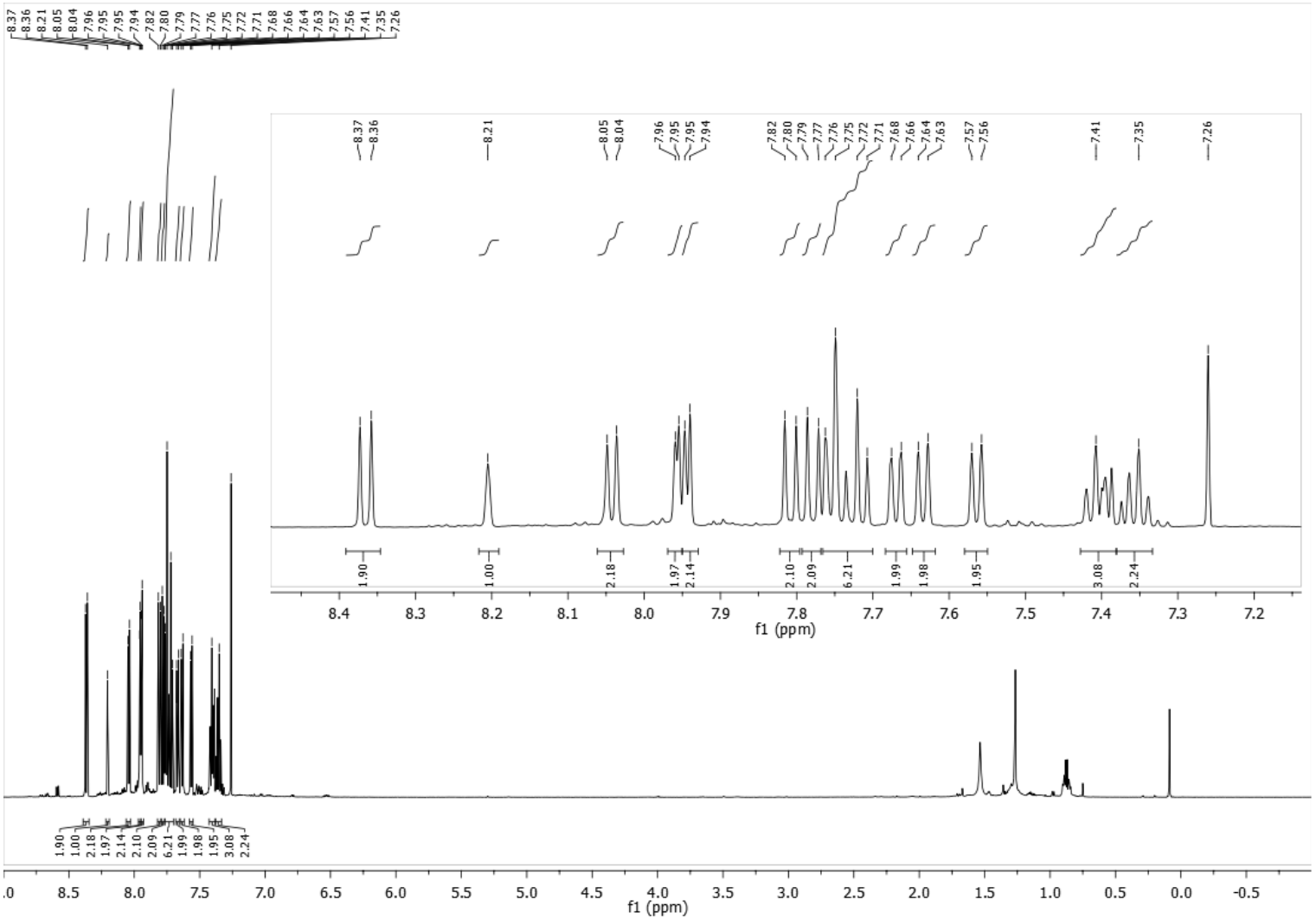



**II**

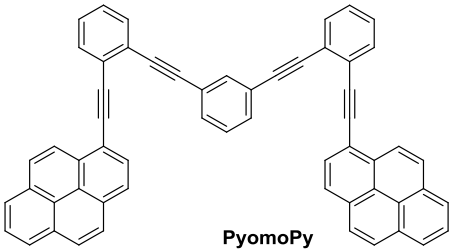


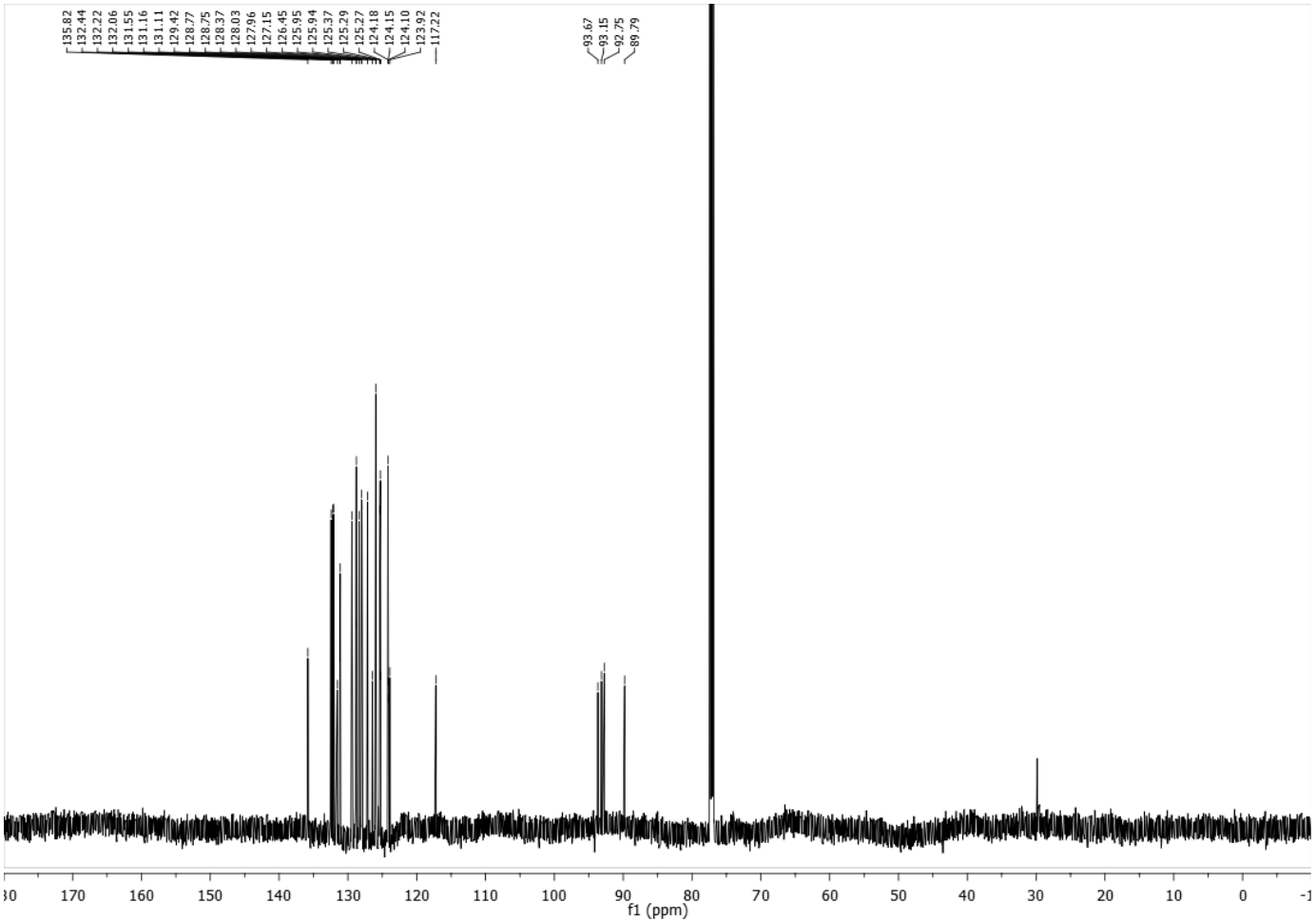
**$^1$H-NMR** ($CDCl_3$, 600 MHz)



**$^{13}$C-NMR** ($CDCl_3$, 151 MHz)



**Absorption and Steady State Fluorescence**

Absorption spectra were recorded at 25 °C with a Perkin-Elmer Lambda 650 UV/vis spectrophotometer equipped with a Peltier temperature-controlled cell holder. Steady-state fluorescence emission spectra were collected on a JASCO FP-6500 spectrofluorometer equipped with a 450 W xenon lamp for excitation, with temperature controller ETC-273T at 25 °C. All experiments were performed using 5x10-mm quartz cuvettes.

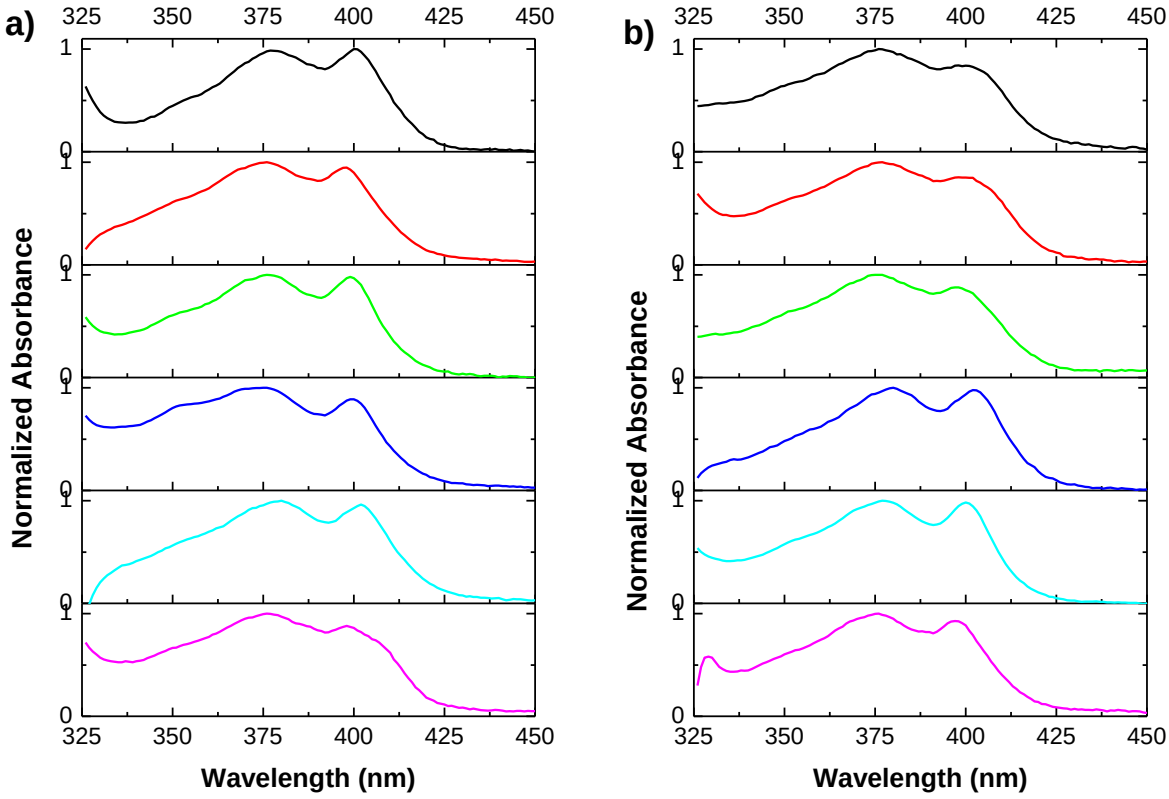



**Figure S1**. Normalized absorption spectra of **PyomoPy** in different solvents ($2\times10^{-6}$ M): (a) n-hexane (magenta), toluene (cyan), 1,4-dioxane (blue), THF (green), ethyl-acetate (red), $CH_2Cl_2$ (black). (b) acetone (magenta), DMF (cyan), DMSO (blue), acetonitrile (green), ethanol (red), methanol (black).

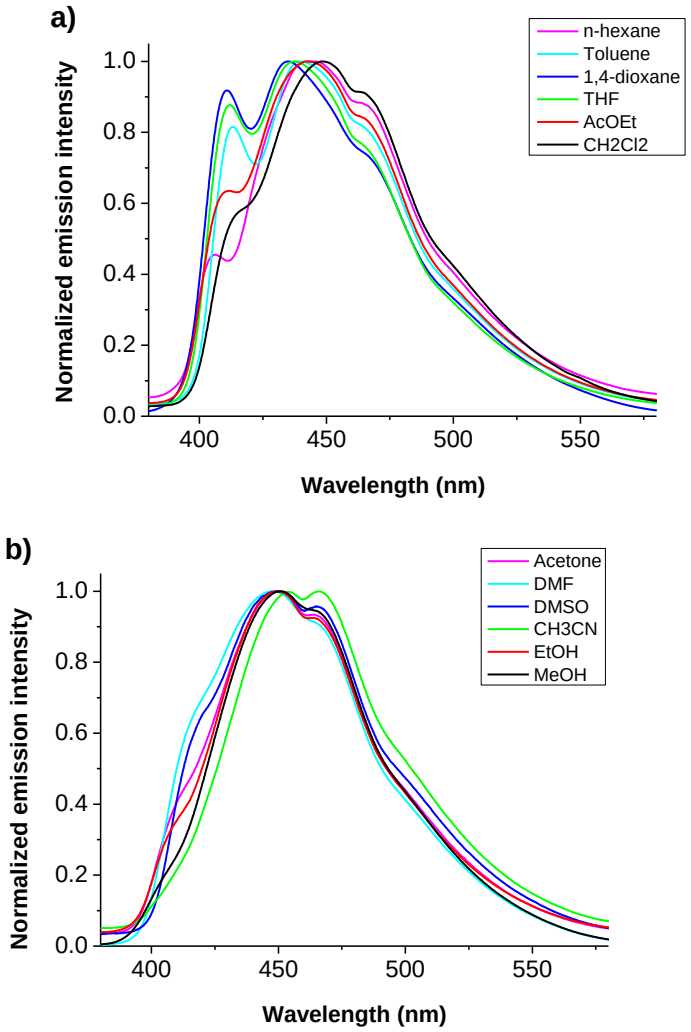



**Figure S2**. Normalized emission spectra of **PyomoPy** in different solvents ($2\times10^{-6}$ M): (a) *n*-hexane (magenta), toluene (cyan), 1,4-dioxane (blue), THF (green), ethyl acetate (red), $CH_2Cl_2$ (black). (b) acetone (magenta), DMF (cyan), DMSO (blue), acetonitrile (green), ethanol (red), methanol (black). $\lambda_{ex}$ = 375 nm.

**Computational Details**

The emission spectra were theoretically modeled in the frame of Time Dependent Density Functional Theory (TD-DFT). To this aim, the equilibrium geometries of the $S_1$ states were optimized using the long-range corrected version of the hybrid functional B3LYP, at TD-CAMB3LYP/6-31G* level of theory.[1] The default grid values as implemented in Gaussian09 had been used during the DFT optimizations. The importance of dispersion for the modeling of the structure of these compounds was evaluated by reoptimizing the first singlet excited states of the species presenting the largest overlap between the pirene macrocycles after including Empirical Dispersion Correction (D3).[2] The comparison of the geometries calculated with and without including dispersion corrections revealed very small differences between the two optimized geometries.

Final vertical emission energies on TD-CAMB3LYP/6-31G* geometries were calculated with the more flexible triple-ξ quality basis set 6-311+G**.[3] The effect of including the dispersion correction in the emission energies was also found to be very small, amounting at most to ca. 3kcal/mol. As expected, due to the important charge transfer character of the transitions the performance of standard pure and hybrid functionals, such as BLYP[4] and B3LYP[5], was found to be very poor, leading to important underestimation of the emission energies that amounted up to 1 eV. Finally, bulk n-hexane and methanol solvent effects were estimated by using Polarizable Continuum Model (PCM).[6] All the calculations have been performed with Gaussian09 program suite.[7]

**Table S1**. Relative stabilities of the different conformers of PyomoPy taking the most stable one A (VI) as a reference.

| | ΔE (kcal/mol) |
|---|---|
| D (I) | 1.37 |
| C (II) | 0.67 |
| B (III) | 1.09 |
| A (IV) | 2.86 |
| A (V) | 0.62 |
| A (VI) | 0 |
| A (VII) | 1.51 |
| A (VIII) | 0.20 |
| A (IX) | 2.73 |

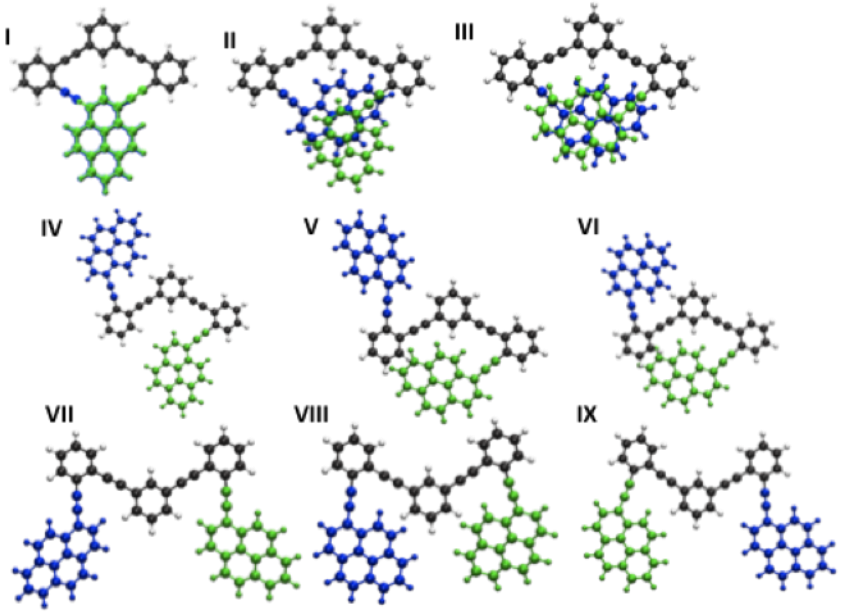


**Table S2**. TD-CAM-B3LYP/6-311+G** calculated emission energies ($E_{emiss}$) and oscillator strenghts ($f$) at the $S_1$ minimum for the different conformers of PyomoPy (conformer labeling as referred in Table S1).

| | Gas Phase | | Hexane | | Methanol | |
|---|---|---|---|---|---|---|
| | $E_{emiss}$ (nm) | f | $E_{emiss}$ (nm) | f | $E_{emiss}$ (nm) | f |
| D (I) | 479.21 | 0.0725 | 483.98 | 0.1009 | 482.62 | 0.0976 |
| C (II) | 435.93 | 0.5337 | 445.82 | 0.7252 | 442.93 | 0.7065 |
| B (III) | 445.05 | 0.3643 | 452.74 | 0.5209 | 449.29 | 0.5015 |
| A (IV) | 433.06 | 0.9010 | 445.52 | 1.0530 | 442.77 | 1.0389 |
| A (V) | 435.43 | 0.5488 | 445.71 | 0.7544 | 443.04 | 0.7372 |
| A (VI) | 435.71 | 0.5255 | 445.83 | 0.7278 | 443.17 | 0.7102 |
| A (VII) | 425.86 | 1.1404 | 439.94 | 1.3212 | 437.35 | 1.3046 |
| A (VIII) | 430.59 | 0.6661 | 442.66 | 0.8521 | 440.12 | 0.8345 |
| A (IX) | 432.79 | 0.7076 | 445.14 | 0.8890 | 442.52 | 0.8717 |

**Table S3.** Cartesian coordinates (in Angstroms) of the optimized $S_1$ minimum for the different conformers of PyomoPy.

| Atom | X | Y | Z |
|---|---|---|---|
| | | D (I) | |
| C | -6.411239 | 0.515181 | -1.683331 |
| C | -5.723993 | -0.637372 | -2.035029 |
| C | -4.314585 | -0.656936 | -2.064754 |
| C | -3.600544 | 0.522777 | -1.712814 |
| C | -4.313463 | 1.694820 | -1.341284 |
| C | -5.724072 | 1.664547 | -1.326501 |
| C | -3.580996 | -1.820501 | -2.415619 |
| C | -2.178033 | 0.519431 | -1.703910 |
| C | -1.476039 | -0.668078 | -2.047550 |
| C | -2.209809 | -1.821171 | -2.409781 |
| C | -0.056861 | -0.662276 | -2.003909 |
| H | 0.479698 | -1.570668 | -2.259251 |
| C | 0.634892 | 0.468139 | -1.647742 |
| C | -0.034037 | 1.653888 | -1.286907 |
| C | -1.469056 | 1.690305 | -1.322485 |
| C | -2.204154 | 2.847523 | -0.974290 |
| C | -3.574871 | 2.850976 | -0.979506 |
| H | -4.117064 | 3.750653 | -0.702950 |
| H | -1.656806 | 3.739585 | -0.689938 |
| H | -4.127118 | -2.717977 | -2.691207 |
| H | -7.496818 | 0.511025 | -1.670199 |
| H | -6.267327 | -1.536639 | -2.310076 |
| H | -6.265853 | 2.563921 | -1.048729 |
| H | -1.663229 | -2.721382 | -2.675425 |
| H | 1.719380 | 0.460080 | -1.624405 |
| C | -6.411374 | -0.515047 | 1.682989 |
| C | -5.724217 | -1.664463 | 1.326286 |
| C | -4.313615 | -1.694784 | 1.341174 |
| C | -3.600685 | -0.522748 | 1.712706 |
| C | -4.314709 | 0.657005 | 2.064533 |
| C | -5.724115 | 0.637498 | 2.034680 |
| C | -3.575029 | -2.850982 | 0.979500 |
| C | -2.178176 | -0.519452 | 1.703923 |
| C | -1.469210 | -1.690371 | 1.322623 |
| C | -2.204315 | -2.847574 | 0.974390 |
| C | -0.034196 | -1.654000 | 1.287175 |
| C | 0.634759 | -0.468256 | 1.647976 |
| C | -0.056985 | 0.662208 | 2.004024 |
| C | -1.476159 | 0.668041 | 2.047559 |
| C | -2.209922 | 1.821178 | 2.409689 |
| C | -3.581106 | 1.820558 | 2.415417 |
| H | -4.127225 | 2.718061 | 2.690923 |
| H | -1.663324 | 2.721375 | 2.675339 |
| H | -4.117229 | -3.750650 | 0.702931 |
| H | -7.496951 | -0.510855 | 1.669758 |
| H | -6.266016 | -2.563822 | 1.048501 |
| H | -6.267436 | 1.536799 | 2.309638 |
| H | -1.656972 | -3.739668 | 0.690127 |
| H | 1.719248 | -0.460241 | 1.624706 |
| H | 0.479583 | 1.570596 | 2.259351 |

| | | | |
|---|---|---|---|
| C | 0.713173 | -2.786064 | 0.910594 |
| C | 1.373650 | -3.754907 | 0.588040 |
| C | 2.140682 | -4.888921 | 0.229956 |
| C | 3.526943 | -4.778133 | -0.049589 |
| C | 1.534187 | -6.154292 | 0.153783 |
| C | 4.251496 | -5.930655 | -0.378532 |
| C | 2.268502 | -7.278112 | -0.177103 |
| H | 0.474028 | -6.234407 | 0.368870 |
| C | 3.634163 | -7.168431 | -0.442135 |
| H | 5.311265 | -5.833738 | -0.588402 |
| H | 1.779611 | -8.245885 | -0.226381 |
| H | 4.213646 | -8.048939 | -0.699863 |
| C | 4.185592 | -3.516695 | -0.015364 |
| C | 4.766812 | -2.456187 | -0.009509 |
| C | 5.471291 | -1.214728 | -0.004869 |
| C | 4.778755 | 0.000081 | -0.000016 |
| C | 6.873291 | -1.204076 | -0.006804 |
| C | 5.471451 | 1.214803 | 0.004628 |
| H | 3.694483 | 0.000170 | 0.000180 |
| C | 7.562413 | -0.000092 | -0.000465 |
| H | 7.408935 | -2.146991 | -0.011125 |
| C | 6.873447 | 1.203979 | 0.006104 |
| H | 8.647717 | -0.000165 | -0.000634 |
| H | 7.409197 | 2.146836 | 0.010274 |
| C | 4.767075 | 2.456319 | 0.009485 |
| C | 4.185706 | 3.516743 | 0.015489 |
| C | 3.527002 | 4.778156 | 0.049822 |
| C | 2.140737 | 4.888878 | -0.229676 |
| C | 4.251513 | 5.930710 | 0.378749 |
| C | 1.534169 | 6.154213 | -0.153416 |
| C | 3.634115 | 7.168447 | 0.442441 |
| H | 5.311293 | 5.833836 | 0.588584 |
| C | 2.268433 | 7.278062 | 0.177480 |
| H | 0.473997 | 6.234266 | -0.368461 |
| H | 4.213563 | 8.048971 | 0.700194 |
| H | 1.779492 | 8.245806 | 0.226810 |
| C | 1.373719 | 3.754869 | -0.587826 |
| C | 0.713303 | 2.785977 | -0.910357 |

| Atom | X | Y | Z |
|---|---|---|---|
| | | C (II) | |
| C | 5.946741 | 5.242237 | -2.242403 |
| C | 4.694545 | 5.728732 | -1.891214 |
| C | 3.655672 | 4.855076 | -1.560560 |
| C | 3.893695 | 3.455767 | -1.586865 |
| C | 5.175777 | 2.966601 | -1.946684 |
| C | 6.186759 | 3.875359 | -2.270472 |
| C | 2.348097 | 5.326215 | -1.193103 |
| C | 2.846643 | 2.544498 | -1.252610 |
| C | 1.566794 | 3.043482 | -0.894590 |
| C | 1.355616 | 4.464220 | -0.876603 |
| C | 0.551782 | 2.138655 | -0.569579 |
| H | -0.428753 | 2.512280 | -0.289077 |
| C | 0.784279 | 0.776694 | -0.595666 |
| C | 2.039588 | 0.263607 | -0.944190 |
| C | 3.089049 | 1.146843 | -1.278503 |
| C | 4.396260 | 0.681029 | -1.648254 |
| C | 5.386595 | 1.545693 | -1.965142 |
| H | 6.369295 | 1.175656 | -2.243839 |
| H | 4.568535 | -0.389428 | -1.668978 |
| H | 2.174151 | 6.398419 | -1.176128 |
| H | 6.742641 | 5.935212 | -2.496936 |
| H | 4.511191 | 6.799327 | -1.871101 |
| H | 7.167696 | 3.498706 | -2.546258 |
| H | 0.371216 | 4.831395 | -0.601057 |
| H | -0.005821 | 0.083832 | -0.330963 |
| C | 1.773980 | -3.566368 | 3.091623 |
| C | 0.646724 | -3.373755 | 2.310496 |
| C | -0.059499 | -2.151902 | 2.356437 |
| C | 0.403635 | -1.113918 | 3.209284 |
| C | 1.559446 | -1.324158 | 4.013950 |
| C | 2.226939 | -2.560917 | 3.936961 |
| C | -1.219244 | -1.922177 | 1.575414 |
| C | -0.280553 | 0.130893 | 3.253685 |
| C | -1.422680 | 0.337384 | 2.437678 |
| C | -1.879813 | -0.715623 | 1.620521 |
| C | -2.085847 | 1.629267 | 2.466024 |
| C | -1.597478 | 2.629428 | 3.363132 |
| C | -0.510743 | 2.404631 | 4.151493 |
| C | 0.190901 | 1.159899 | 4.117274 |
| C | 1.331104 | 0.923512 | 4.911198 |
| C | 1.999729 | -0.275199 | 4.864031 |
| H | 2.880225 | -0.435197 | 5.479215 |
| H | 1.681597 | 1.715344 | 5.567239 |
| H | -1.579923 | -2.717541 | 0.931050 |
| H | 2.309917 | -4.508813 | 3.039277 |
| H | 0.295680 | -4.157669 | 1.646529 |
| H | 3.110338 | -2.719074 | 4.548997 |
| H | -2.768691 | -0.557270 | 1.017245 |
| H | -2.111404 | 3.584020 | 3.391210 |
| H | -0.151787 | 3.182064 | 4.819554 |
| C | -3.153430 | 1.907458 | 1.640130 |
| C | -4.106217 | 2.161301 | 0.898068 |
| C | -5.202677 | 2.498288 | 0.117992 |
| C | -5.722451 | 1.625163 | -0.898948 |

| | | | |
|---|---|---|---|
| C | -5.859670 | 3.740510 | 0.339811 |
| C | -6.875882 | 2.018610 | -1.602285 |
| C | -6.975919 | 4.093660 | -0.374227 |
| H | -5.458237 | 4.400329 | 1.101473 |
| C | -7.496184 | 3.223608 | -1.352268 |
| H | -7.264295 | 1.349504 | -2.362781 |
| H | -7.462000 | 5.044806 | -0.181807 |
| H | -8.381117 | 3.504118 | -1.914000 |
| C | -5.104565 | 0.401896 | -1.225702 |
| C | -4.613774 | -0.654460 | -1.575271 |
| C | -4.085666 | -1.901448 | -2.001082 |
| C | -2.764677 | -2.263905 | -1.703537 |
| C | -4.889183 | -2.797771 | -2.727924 |
| C | -2.257130 | -3.503046 | -2.100766 |
| H | -2.129236 | -1.574342 | -1.161256 |
| C | -4.382685 | -4.024057 | -3.127734 |
| H | -5.909922 | -2.518326 | -2.964500 |
| C | -3.078504 | -4.386334 | -2.816026 |
| H | -5.012279 | -4.709699 | -3.685905 |
| H | -2.683187 | -5.348306 | -3.122839 |
| C | -0.916594 | -3.876400 | -1.773281 |
| C | 0.212580 | -4.210002 | -1.498276 |
| C | 1.528167 | -4.666307 | -1.185526 |
| C | 2.578748 | -3.761425 | -0.909909 |
| C | 1.785741 | -6.042699 | -1.152388 |
| C | 3.849681 | -4.268978 | -0.611957 |
| C | 3.049952 | -6.525005 | -0.854248 |
| H | 0.972641 | -6.727760 | -1.366974 |
| C | 4.085374 | -5.634134 | -0.583090 |
| H | 4.650239 | -3.568623 | -0.400141 |
| H | 3.228831 | -7.595195 | -0.834334 |
| H | 5.078393 | -6.004837 | -0.349746 |
| C | 2.371279 | -2.351179 | -0.934477 |
| C | 2.234871 | -1.149541 | -0.945369 |

| Atom | X | Y | Z |
|---|---|---|---|
| B (III) | | | |
| C | 4.407197 | -1.208991 | -2.287102 |
| C | 4.022437 | -2.543585 | -2.309052 |
| C | 2.666533 | -2.908464 | -2.204269 |
| C | 1.685771 | -1.884274 | -2.076470 |
| C | 2.087181 | -0.521638 | -2.062133 |
| C | 3.459799 | -0.205966 | -2.164257 |
| C | 2.241189 | -4.262744 | -2.216812 |
| C | 0.311218 | -2.223438 | -1.953633 |
| C | -0.078815 | -3.593104 | -1.976272 |
| C | 0.909760 | -4.587010 | -2.111627 |
| C | -1.466269 | -3.914951 | -1.860414 |
| H | -1.758486 | -4.960643 | -1.885755 |
| C | -2.409536 | -2.945891 | -1.706576 |
| C | -2.052586 | -1.563417 | -1.649742 |
| C | -0.657046 | -1.198424 | -1.804935 |
| C | -0.237128 | 0.146758 | -1.811960 |
| C | 1.091407 | 0.477865 | -1.934797 |
| H | 1.396010 | 1.519999 | -1.924969 |
| H | -0.987336 | 0.924720 | -1.711368 |
| H | 2.988356 | -5.044702 | -2.316785 |
| H | 5.458754 | -0.949657 | -2.359721 |
| H | 4.770199 | -3.325637 | -2.406785 |
| H | 3.761891 | 0.836672 | -2.138623 |
| H | 0.601632 | -5.628785 | -2.128700 |
| H | -3.456679 | -3.206175 | -1.600586 |
| C | -4.441073 | -1.066879 | 2.307757 |
| C | -3.462970 | -0.084634 | 2.213677 |
| C | -2.112356 | -0.430899 | 2.112523 |
| C | -1.747560 | -1.801198 | 2.094808 |
| C | -2.752162 | -2.799727 | 2.194069 |
| C | -4.091753 | -2.409274 | 2.301638 |
| C | -1.075314 | 0.556656 | 2.015023 |
| C | -0.376530 | -2.175339 | 1.964056 |
| C | 0.621720 | -1.174004 | 1.844396 |
| C | 0.225953 | 0.204305 | 1.887419 |
| C | 1.969541 | -1.566476 | 1.679122 |
| C | 2.299234 | -2.930086 | 1.666451 |
| C | 1.327216 | -3.900142 | 1.798097 |
| C | -0.021572 | -3.549761 | 1.940551 |
| C | -1.055566 | -4.535091 | 2.055718 |
| C | -2.357355 | -4.178492 | 2.174588 |
| H | -3.130874 | -4.936875 | 2.258240 |
| H | -0.769815 | -5.583166 | 2.042151 |
| H | -1.360750 | 1.604482 | 2.036031 |
| H | -5.485386 | -0.779477 | 2.379551 |
| H | -3.741457 | 0.965005 | 2.211658 |
| H | -4.859872 | -3.174058 | 2.377030 |
| H | 1.000062 | 0.960663 | 1.810192 |
| H | 3.338322 | -3.211751 | 1.535767 |
| H | 1.602944 | -4.950438 | 1.779438 |
| C | 3.003643 | -0.608054 | 1.490123 |
| C | 3.903866 | 0.173459 | 1.280276 |
| C | 5.014172 | 1.033338 | 1.045143 |
| C | 4.843383 | 2.385188 | 0.669341 |

| | | | |
|---|---|---|---|
| C | 6.314336 | 0.528051 | 1.184461 |
| C | 5.975351 | 3.182819 | 0.456369 |
| C | 7.421081 | 1.331420 | 0.965778 |
| H | 6.436642 | -0.510416 | 1.472152 |
| C | 7.251913 | 2.665386 | 0.602096 |
| H | 5.832059 | 4.219124 | 0.170114 |
| H | 8.418163 | 0.918589 | 1.081532 |
| H | 8.115033 | 3.300602 | 0.431376 |
| C | 3.549474 | 2.960840 | 0.492354 |
| C | 2.490909 | 3.519172 | 0.317739 |
| C | 1.266850 | 4.231043 | 0.118339 |
| C | 0.060562 | 3.548869 | -0.058191 |
| C | 1.275940 | 5.633421 | 0.098614 |
| C | -1.136252 | 4.252763 | -0.250399 |
| H | 0.048087 | 2.465541 | -0.038775 |
| C | 0.091556 | 6.333379 | -0.088778 |
| H | 2.214212 | 6.159729 | 0.234325 |
| C | -1.106325 | 5.658208 | -0.260642 |
| H | 0.104028 | 7.418660 | -0.100482 |
| H | -2.031824 | 6.204083 | -0.407129 |
| C | -2.370524 | 3.569726 | -0.424865 |
| C | -3.453568 | 3.037741 | -0.570163 |
| C | -4.747402 | 2.487247 | -0.693704 |
| C | -4.960010 | 1.093879 | -0.961888 |
| C | -5.866216 | 3.321395 | -0.518970 |
| C | -6.296095 | 0.611641 | -0.999848 |
| C | -7.151525 | 2.824908 | -0.578088 |
| H | -5.694175 | 4.374662 | -0.323563 |
| C | -7.364052 | 1.454136 | -0.814571 |
| H | -6.451174 | -0.444707 | -1.191416 |
| H | -7.996586 | 3.490389 | -0.435423 |
| H | -8.375200 | 1.061573 | -0.855351 |
| C | -3.911324 | 0.211423 | -1.193047 |
| C | -3.028101 | -0.616080 | -1.426341 |

| Atom | X | Y | Z |
|---|---|---|---|
| A (IV) | | | |
| C | -3.253865 | -0.463039 | 0.000000 |
| C | -4.154878 | 0.613283 | 0.000000 |
| C | -3.680051 | 1.917252 | 0.000000 |
| C | -2.317511 | 2.171821 | 0.000000 |
| C | -1.397783 | 1.109969 | 0.000000 |
| C | -1.883045 | -0.206638 | 0.000000 |
| H | -5.220402 | 0.412385 | 0.000000 |
| H | -4.382866 | 2.744857 | 0.000000 |
| H | -1.945520 | 3.188953 | 0.000000 |
| H | -1.183219 | -1.034087 | 0.000000 |
| C | 0.000000 | 1.350538 | 0.000000 |
| C | 1.204825 | 1.518576 | 0.000000 |
| C | -3.743838 | -1.805140 | 0.000000 |
| C | -4.178610 | -2.932606 | 0.000000 |
| C | 2.610485 | 1.592524 | 0.000000 |
| C | 3.323560 | 2.840832 | 0.000000 |
| C | 3.349853 | 0.394477 | 0.000000 |
| C | 4.746874 | 2.803411 | 0.000000 |
| C | 4.727056 | 0.394747 | 0.000000 |
| H | 2.800204 | -0.540985 | 0.000000 |
| C | 5.430562 | 1.615508 | 0.000000 |
| H | 5.279617 | 3.748169 | 0.000000 |
| H | 5.269714 | -0.545008 | 0.000000 |
| H | 6.515800 | 1.615845 | 0.000000 |
| C | -4.758040 | -4.235778 | 0.000000 |
| C | -6.152520 | -4.363938 | 0.000000 |
| C | -3.960104 | -5.402302 | 0.000000 |
| C | -6.754693 | -5.611546 | 0.000000 |
| H | -6.755561 | -3.462529 | 0.000000 |
| C | -4.587816 | -6.654535 | 0.000000 |
| C | -5.968923 | -6.761145 | 0.000000 |
| H | -7.837164 | -5.688472 | 0.000000 |
| H | -3.969248 | -7.545471 | 0.000000 |
| H | -6.434024 | -7.741669 | 0.000000 |
| C | 2.691198 | 4.074892 | 0.000000 |
| C | 2.228183 | 5.219245 | 0.000000 |
| C | -2.536734 | -5.330554 | 0.000000 |
| C | -1.327287 | -5.314375 | 0.000000 |
| C | 1.753100 | 6.512330 | 0.000000 |
| C | 0.333008 | 6.810074 | 0.000000 |
| C | 2.681065 | 7.600371 | 0.000000 |
| C | -0.087183 | 8.165529 | 0.000000 |
| C | -0.640155 | 5.791584 | 0.000000 |
| C | 2.258153 | 8.893962 | 0.000000 |
| H | 3.739895 | 7.366080 | 0.000000 |
| C | -1.474443 | 8.475530 | 0.000000 |
| C | 0.867694 | 9.222006 | 0.000000 |
| C | -1.982001 | 6.088534 | 0.000000 |
| H | -0.303495 | 4.759241 | 0.000000 |
| H | 2.981147 | 9.704346 | 0.000000 |
| C | -2.438432 | 7.430578 | 0.000000 |
| C | -1.904161 | 9.833554 | 0.000000 |
| C | 0.416584 | 10.558022 | 0.000000 |
| H | -2.719523 | 5.291130 | 0.000000 |

| | | | |
|---|---|---|---|
| C | -3.810908 | 7.761389 | 0.000000 |
| C | -3.282623 | 10.112257 | 0.000000 |
| C | -0.921929 | 10.860845 | 0.000000 |
| H | 1.154150 | 11.355686 | 0.000000 |
| C | -4.218550 | 9.084405 | 0.000000 |
| H | -4.544741 | 6.960543 | 0.000000 |
| H | -3.609858 | 11.147966 | 0.000000 |
| H | -1.249092 | 11.896367 | 0.000000 |
| H | -5.277737 | 9.322338 | 0.000000 |
| C | 0.097471 | -5.273392 | 0.000000 |
| C | 0.860439 | -6.462326 | 0.000000 |
| C | 0.748747 | -4.033309 | 0.000000 |
| C | 2.276484 | -6.374015 | 0.000000 |
| C | 0.252307 | -7.763213 | 0.000000 |
| C | 2.127682 | -3.951892 | 0.000000 |
| H | 0.147203 | -3.130866 | 0.000000 |
| C | 3.065623 | -7.563808 | 0.000000 |
| C | 2.915509 | -5.106850 | 0.000000 |
| C | 1.001267 | -8.889175 | 0.000000 |
| H | -0.830450 | -7.818979 | 0.000000 |
| H | 2.613175 | -2.980148 | 0.000000 |
| C | 2.436669 | -8.835117 | 0.000000 |
| C | 4.482627 | -7.479210 | 0.000000 |
| C | 4.350561 | -5.051961 | 0.000000 |
| H | 0.523786 | -9.864958 | 0.000000 |
| C | 3.226999 | -9.987497 | 0.000000 |
| C | 5.235236 | -8.656284 | 0.000000 |
| C | 5.096701 | -6.179609 | 0.000000 |
| H | 4.826271 | -4.075302 | 0.000000 |
| C | 4.612143 | -9.897053 | 0.000000 |
| H | 2.743425 | -10.960202 | 0.000000 |
| H | 6.319541 | -8.590400 | 0.000000 |
| H | 6.181523 | -6.123453 | 0.000000 |
| H | 5.211942 | -10.801785 | 0.000000 |

| Atom | X | Y | Z |
|---|---|---|---|
| | | A (V) | |
| C | 0.096693 | -1.477392 | -0.734202 |
| C | -0.908745 | -2.436603 | -0.543274 |
| C | -0.566324 | -3.765960 | -0.329828 |
| C | 0.762653 | -4.156745 | -0.296575 |
| C | 1.785846 | -3.209371 | -0.481507 |
| C | 1.436467 | -1.870609 | -0.707938 |
| H | -1.948525 | -2.129272 | -0.571005 |
| H | -1.347827 | -4.505637 | -0.187440 |
| H | 1.029151 | -5.193917 | -0.125605 |
| H | 2.214183 | -1.134614 | -0.872965 |
| C | 3.145684 | -3.611718 | -0.440617 |
| C | 4.298196 | -3.999008 | -0.403029 |
| C | -0.252721 | -0.109419 | -0.952921 |
| C | -0.582596 | 1.039304 | -1.135008 |
| C | 5.601652 | -4.531186 | -0.394457 |
| C | 6.769713 | -3.699451 | -0.287577 |
| C | 5.772534 | -5.923120 | -0.515266 |
| C | 8.048003 | -4.321971 | -0.344530 |
| C | 7.025754 | -6.494260 | -0.554153 |
| H | 4.885038 | -6.542646 | -0.588690 |
| C | 8.173596 | -5.681124 | -0.473443 |
| H | 8.926064 | -3.689173 | -0.273114 |
| H | 7.127786 | -7.569951 | -0.653364 |
| H | 9.160213 | -6.131882 | -0.509570 |
| C | -0.982138 | 2.387841 | -1.369909 |
| C | -0.048841 | 3.331752 | -1.813630 |
| C | -2.324387 | 2.785868 | -1.165282 |
| C | -0.428080 | 4.642553 | -2.059670 |
| H | 0.979160 | 3.019800 | -1.960251 |
| C | -2.688034 | 4.111883 | -1.423712 |
| C | -1.750745 | 5.032220 | -1.867593 |
| H | 0.309906 | 5.360340 | -2.402680 |
| H | -3.718754 | 4.409905 | -1.264890 |
| H | -2.052042 | 6.056647 | -2.061657 |
| C | 6.693657 | -2.326206 | -0.110709 |
| C | 6.699323 | -1.105750 | 0.071572 |
| C | -3.291633 | 1.852707 | -0.689598 |
| C | -4.097838 | 1.054740 | -0.270413 |
| C | 6.721060 | 0.256383 | 0.275351 |
| C | 5.501052 | 1.013336 | 0.489280 |
| C | 7.968703 | 0.954140 | 0.274113 |
| C | 5.583827 | 2.419206 | 0.663158 |
| C | 4.237930 | 0.390707 | 0.535304 |
| C | 8.027239 | 2.302921 | 0.448050 |
| H | 8.874611 | 0.377646 | 0.122356 |
| C | 4.398169 | 3.177434 | 0.862720 |
| C | 6.844515 | 3.081024 | 0.642307 |
| C | 3.088613 | 1.120973 | 0.728083 |
| H | 4.187227 | -0.687499 | 0.418326 |
| H | 8.986095 | 2.812895 | 0.438445 |
| C | 3.133888 | 2.528154 | 0.893417 |
| C | 4.471621 | 4.589616 | 1.032308 |
| C | 6.890596 | 4.479257 | 0.815793 |
| H | 2.123838 | 0.624073 | 0.755776 |

| | | | |
|---|---|---|---|
| C | 1.967034 | 3.300083 | 1.085753 |
| C | 3.280676 | 5.315858 | 1.221048 |
| C | 5.746617 | 5.215268 | 1.003055 |
| H | 7.857757 | 4.973902 | 0.798626 |
| C | 2.048603 | 4.673981 | 1.244461 |
| H | 1.003656 | 2.800003 | 1.104643 |
| H | 3.337545 | 6.393059 | 1.349338 |
| H | 5.803786 | 6.291968 | 1.133016 |
| H | 1.141411 | 5.252913 | 1.386162 |
| C | -5.002885 | 0.083138 | 0.250009 |
| C | -6.391012 | 0.168242 | 0.008840 |
| C | -4.495398 | -0.973829 | 1.017662 |
| C | -7.247547 | -0.823821 | 0.552518 |
| C | -6.969078 | 1.225227 | -0.773022 |
| C | -5.332980 | -1.938180 | 1.545290 |
| H | -3.426640 | -1.019389 | 1.198242 |
| C | -8.654417 | -0.755993 | 0.319589 |
| C | -6.713284 | -1.885773 | 1.327845 |
| C | -8.301924 | 1.287141 | -0.992824 |
| H | -6.303947 | 1.975369 | -1.186304 |
| H | -4.919871 | -2.747440 | 2.140324 |
| C | -9.197461 | 0.300406 | -0.455709 |
| C | -9.514838 | -1.745822 | 0.862650 |
| C | -7.608030 | -2.872656 | 1.865010 |
| H | -8.722378 | 2.093216 | -1.587454 |
| C | -10.577025 | 0.348104 | -0.672353 |
| C | -10.888417 | -1.660210 | 0.622086 |
| C | -8.940429 | -2.806563 | 1.644366 |
| H | -7.185837 | -3.679309 | 2.457446 |
| C | -11.412492 | -0.623232 | -0.137968 |
| H | -10.991199 | 1.157594 | -1.266655 |
| H | -11.546195 | -2.418022 | 1.038108 |
| H | -9.605784 | -3.559685 | 2.056813 |
| H | -12.482126 | -0.571865 | -0.315486 |

| Atom | X | Y | Z |
|---|---|---|---|
| A (VI) | | | |
| C | 0.439464 | 1.142275 | -1.330188 |
| C | 1.521188 | 2.032895 | -1.384404 |
| C | 1.299166 | 3.399932 | -1.266891 |
| C | 0.017201 | 3.896256 | -1.095290 |
| C | -1.081559 | 3.019301 | -1.038958 |
| C | -0.854785 | 1.641523 | -1.164062 |
| H | 2.525155 | 1.646847 | -1.516130 |
| H | 2.140166 | 4.084737 | -1.312364 |
| H | -0.154536 | 4.963025 | -1.002793 |
| H | -1.693593 | 0.956192 | -1.140259 |
| C | -2.393136 | 3.530737 | -0.864755 |
| C | -3.501773 | 4.012189 | -0.726543 |
| C | 0.650512 | -0.266903 | -1.447008 |
| C | 0.823234 | -1.459656 | -1.550026 |
| C | -4.753186 | 4.647463 | -0.616085 |
| C | -5.959050 | 3.921828 | -0.321002 |
| C | -4.835598 | 6.036901 | -0.826665 |
| C | -7.187562 | 4.639247 | -0.291933 |
| C | -6.040709 | 6.702670 | -0.776730 |
| H | -3.919504 | 6.576469 | -1.042290 |
| C | -7.228233 | 5.991792 | -0.512228 |
| H | -8.095591 | 4.085495 | -0.078947 |
| H | -6.075261 | 7.773572 | -0.947994 |
| H | -8.177577 | 6.516701 | -0.478901 |
| C | 0.952049 | -2.870928 | -1.717018 |
| C | -0.184625 | -3.628536 | -2.026674 |
| C | 2.199566 | -3.522627 | -1.584449 |
| C | -0.097866 | -4.998898 | -2.213272 |
| H | -1.138498 | -3.120907 | -2.116472 |
| C | 2.267108 | -4.907474 | -1.781472 |
| C | 1.132621 | -5.639440 | -2.094071 |
| H | -0.991135 | -5.567075 | -2.451120 |
| H | 3.228378 | -5.399303 | -1.680158 |
| H | 1.207397 | -6.712027 | -2.242021 |
| C | -5.963009 | 2.562805 | -0.045873 |
| C | -6.036191 | 1.362503 | 0.230952 |
| C | 3.382379 | -2.803971 | -1.243411 |
| C | 4.406747 | -2.237542 | -0.938760 |
| C | -6.133066 | 0.024168 | 0.542161 |
| C | -4.953670 | -0.805315 | 0.709247 |
| C | -7.420619 | -0.575365 | 0.703596 |
| C | -5.116757 | -2.184463 | 1.000683 |
| C | -3.651716 | -0.278042 | 0.598389 |
| C | -7.555777 | -1.900097 | 0.985989 |
| H | -8.294705 | 0.055575 | 0.585589 |
| C | -3.972727 | -3.012868 | 1.160469 |
| C | -6.416658 | -2.749152 | 1.138730 |
| C | -2.542486 | -1.076449 | 0.752037 |
| H | -3.537914 | 0.781729 | 0.391616 |
| H | -8.544321 | -2.335736 | 1.098187 |
| C | -2.669077 | -2.460067 | 1.034314 |
| C | -4.127658 | -4.399152 | 1.447934 |
| C | -6.543001 | -4.123710 | 1.424966 |
| H | -1.547487 | -0.652234 | 0.658657 |

| | | | |
|---|---|---|---|
| C | -1.545717 | -3.300993 | 1.192288 |
| C | -2.977290 | -5.196629 | 1.596462 |
| C | -5.440055 | -4.927886 | 1.573820 |
| H | -7.539495 | -4.544139 | 1.527959 |
| C | -1.706930 | -4.649037 | 1.468064 |
| H | -0.552334 | -2.875202 | 1.090230 |
| H | -3.096305 | -6.253969 | 1.815363 |
| H | -5.559083 | -5.984844 | 1.793178 |
| H | -0.832807 | -5.282374 | 1.581606 |
| C | 5.618824 | -1.576385 | -0.583743 |
| C | 5.598920 | -0.309143 | 0.038980 |
| C | 6.845715 | -2.195057 | -0.857162 |
| C | 6.828671 | 0.316528 | 0.369207 |
| C | 4.372454 | 0.369452 | 0.351898 |
| C | 8.041295 | -1.583088 | -0.532592 |
| H | 6.843306 | -3.168838 | -1.334697 |
| C | 6.829705 | 1.599458 | 0.995587 |
| C | 8.060489 | -0.326111 | 0.079964 |
| C | 4.376189 | 1.585467 | 0.945636 |
| H | 3.437706 | -0.120953 | 0.101273 |
| H | 8.981482 | -2.079152 | -0.755158 |
| C | 5.603283 | 2.248473 | 1.290142 |
| C | 8.057915 | 2.229954 | 1.325456 |
| C | 9.287555 | 0.335418 | 0.425780 |
| H | 3.438160 | 2.084716 | 1.171487 |
| C | 5.626132 | 3.503958 | 1.903338 |
| C | 8.035522 | 3.485911 | 1.937157 |
| C | 9.287053 | 1.551217 | 1.017761 |
| H | 10.223047 | -0.167659 | 0.198467 |
| C | 6.831081 | 4.114997 | 2.222510 |
| H | 4.685941 | 3.998601 | 2.130096 |
| H | 8.975775 | 3.967974 | 2.189389 |
| H | 10.222535 | 2.040391 | 1.273849 |
| H | 6.831797 | 5.090392 | 2.698865 |

| Atom | X | Y | Z |
|---|---|---|---|
| A (VII) | | | |
| C | -1.241857 | -2.379434 | 0.234512 |
| C | -1.257072 | -0.978440 | 0.155522 |
| C | -0.098998 | -0.288795 | -0.177470 |
| C | 1.080536 | -0.972021 | -0.431785 |
| C | 1.116701 | -2.374900 | -0.352660 |
| C | -0.055082 | -3.068086 | -0.020296 |
| H | -2.179923 | -0.446368 | 0.359780 |
| H | -0.117611 | 0.794666 | -0.240659 |
| H | 1.982568 | -0.435256 | -0.704983 |
| H | -0.037516 | -4.149898 | 0.042038 |
| C | 2.324448 | -3.076244 | -0.609207 |
| C | 3.366832 | -3.656207 | -0.837463 |
| C | -2.434906 | -3.087161 | 0.576139 |
| C | -3.462217 | -3.651996 | 0.868403 |
| C | 4.580693 | -4.310161 | -1.130094 |
| C | 5.827412 | -3.592581 | -1.094663 |
| C | 4.589535 | -5.667318 | -1.488475 |
| C | 7.013780 | -4.281416 | -1.464206 |
| C | 5.762721 | -6.310824 | -1.827076 |
| H | 3.645498 | -6.201492 | -1.505613 |
| C | 6.981360 | -5.606760 | -1.820179 |
| H | 7.951286 | -3.735826 | -1.446702 |
| H | 5.743592 | -7.359178 | -2.106225 |
| H | 7.900636 | -6.115031 | -2.093265 |
| C | -4.676943 | -4.307140 | 1.226027 |
| C | -4.653812 | -5.617903 | 1.714940 |
| C | -5.917290 | -3.638058 | 1.103063 |
| C | -5.826061 | -6.259725 | 2.082180 |
| H | -3.698180 | -6.122749 | 1.805247 |
| C | -7.089686 | -4.301785 | 1.481640 |
| C | -7.046550 | -5.599190 | 1.967113 |
| H | -5.788649 | -7.276160 | 2.460530 |
| H | -8.037053 | -3.782840 | 1.383590 |
| H | -7.966555 | -6.097945 | 2.254528 |
| C | 5.878784 | -2.268788 | -0.684154 |
| C | 5.904036 | -1.101695 | -0.284253 |
| C | -5.974336 | -2.309358 | 0.590652 |
| C | -6.006746 | -1.186694 | 0.141940 |
| C | 5.896300 | 0.194835 | 0.180695 |
| C | 7.090241 | 1.018699 | 0.165288 |
| C | 4.684538 | 0.749268 | 0.702212 |
| C | 7.018705 | 2.344458 | 0.663810 |
| C | 8.319374 | 0.542208 | -0.333978 |
| C | 4.636570 | 2.024465 | 1.176113 |
| H | 3.803860 | 0.116743 | 0.724602 |
| C | 8.178707 | 3.165830 | 0.656821 |
| C | 5.792422 | 2.863417 | 1.173702 |
| C | 9.442936 | 1.333052 | -0.342371 |
| H | 8.363938 | -0.472235 | -0.716129 |
| H | 3.708197 | 2.424071 | 1.573666 |
| C | 9.407942 | 2.661114 | 0.150209 |
| C | 8.114541 | 4.498317 | 1.157667 |
| C | 5.756126 | 4.185081 | 1.663645 |
| H | 10.378985 | 0.943196 | -0.731494 |

| | | | |
|---|---|---|---|
| C | 10.548043 | 3.496183 | 0.153943 |
| C | 9.275757 | 5.289540 | 1.139981 |
| C | 6.874234 | 4.980773 | 1.658945 |
| H | 4.816921 | 4.570141 | 2.050981 |
| C | 10.474830 | 4.787871 | 0.642698 |
| H | 11.485087 | 3.107152 | -0.233770 |
| H | 9.226347 | 6.305162 | 1.521943 |
| H | 6.825135 | 5.996219 | 2.040822 |
| H | 11.359431 | 5.417185 | 0.638949 |
| C | -5.990189 | 0.126415 | -0.412922 |
| C | -7.050903 | 1.031451 | -0.191877 |
| C | -4.894584 | 0.518758 | -1.194200 |
| C | -6.984233 | 2.326286 | -0.768350 |
| C | -8.197681 | 0.687942 | 0.601220 |
| C | -4.833836 | 1.780596 | -1.754058 |
| H | -4.091521 | -0.191940 | -1.358295 |
| C | -8.046032 | 3.256546 | -0.555539 |
| C | -5.865939 | 2.703510 | -1.556645 |
| C | -9.202317 | 1.570778 | 0.801793 |
| H | -8.235738 | -0.303637 | 1.038498 |
| H | -3.977455 | 2.063743 | -2.359132 |
| C | -9.167116 | 2.889119 | 0.232047 |
| C | -7.983399 | 4.552731 | -1.130990 |
| C | -5.830290 | 4.021123 | -2.126831 |
| H | -10.062473 | 1.294590 | 1.405097 |
| C | -10.195383 | 3.814679 | 0.428611 |
| C | -9.033483 | 5.447388 | -0.909505 |
| C | -6.837020 | 4.901161 | -1.924894 |
| H | -4.969101 | 4.296007 | -2.729107 |
| C | -10.127436 | 5.080466 | -0.137286 |
| H | -11.053105 | 3.531795 | 1.032207 |
| H | -8.984951 | 6.439057 | -1.350306 |
| H | -6.797287 | 5.894651 | -2.362400 |
| H | -10.934610 | 5.787899 | 0.024976 |

| Atom | X | Y | Z |
|---|---|---|---|
| A (VIII) | | | |
| C | -1.264843 | 1.974626 | -0.504057 |
| C | -1.227313 | 0.573272 | -0.560472 |
| C | -0.065256 | -0.103315 | -0.211133 |
| C | 1.066460 | 0.591903 | 0.187371 |
| C | 1.051540 | 1.996545 | 0.240451 |
| C | -0.125619 | 2.675720 | -0.105496 |
| H | -2.111223 | 0.028427 | -0.871019 |
| H | -0.043954 | -1.188259 | -0.248472 |
| H | 1.969062 | 0.059479 | 0.464890 |
| H | -0.149772 | 3.758359 | -0.062542 |
| C | 2.200127 | 2.725013 | 0.646117 |
| C | 3.165587 | 3.369708 | 1.008602 |
| C | -2.454976 | 2.684771 | -0.855328 |
| C | -3.457795 | 3.289878 | -1.154244 |
| C | 4.226415 | 4.169175 | 1.476806 |
| C | 5.563505 | 3.657933 | 1.613593 |
| C | 3.969155 | 5.499315 | 1.856165 |
| C | 6.557654 | 4.509806 | 2.169918 |
| C | 4.960718 | 6.303517 | 2.375302 |
| H | 2.959066 | 5.878089 | 1.741947 |
| C | 6.265205 | 5.797676 | 2.539275 |
| H | 7.561965 | 4.115862 | 2.282404 |
| H | 4.733523 | 7.324080 | 2.665402 |
| H | 7.042844 | 6.430577 | 2.954727 |
| C | -4.595780 | 4.059953 | -1.539028 |
| C | -4.418883 | 5.389092 | -1.942648 |
| C | -5.897779 | 3.510566 | -1.532178 |
| C | -5.497340 | 6.163746 | -2.337780 |
| H | -3.415833 | 5.801521 | -1.943949 |
| C | -6.974946 | 4.308696 | -1.937820 |
| C | -6.779686 | 5.620652 | -2.337156 |
| H | -5.338404 | 7.191330 | -2.648361 |
| H | -7.970559 | 3.878754 | -1.929574 |
| H | -7.628392 | 6.222089 | -2.646573 |
| C | 5.914272 | 2.381934 | 1.198988 |
| C | 6.289759 | 1.269426 | 0.819135 |
| C | -6.136561 | 2.169054 | -1.114431 |
| C | -6.385097 | 1.040702 | -0.756628 |
| C | 6.711024 | 0.030800 | 0.388283 |
| C | 5.839236 | -0.839530 | -0.380025 |
| C | 8.031434 | -0.421148 | 0.697285 |
| C | 6.314779 | -2.115975 | -0.776717 |
| C | 4.538071 | -0.447841 | -0.752797 |
| C | 8.469131 | -1.649752 | 0.307433 |
| H | 8.677524 | 0.240947 | 1.263198 |
| C | 5.473808 | -2.981657 | -1.527909 |
| C | 7.631197 | -2.538526 | -0.434353 |
| C | 3.722310 | -1.282596 | -1.479767 |
| H | 4.187627 | 0.536848 | -0.459049 |
| H | 9.473823 | -1.976139 | 0.559550 |
| C | 4.161912 | -2.567205 | -1.886769 |
| C | 5.942811 | -4.266431 | -1.926019 |
| C | 8.071262 | -3.814919 | -0.840235 |
| H | 2.722700 | -0.957219 | -1.753181 |

| | | | |
|---|---|---|---|
| C | 3.344095 | -3.443103 | -2.633777 |
| C | 5.089816 | -5.103566 | -2.667835 |
| C | 7.259342 | -4.656329 | -1.559663 |
| H | 9.076638 | -4.127953 | -0.572680 |
| C | 3.808245 | -4.690784 | -3.013924 |
| H | 2.343705 | -3.121424 | -2.908582 |
| H | 5.447853 | -6.083240 | -2.970877 |
| H | 7.617273 | -5.636152 | -1.861691 |
| H | 3.167335 | -5.352662 | -3.588068 |
| C | -6.686389 | -0.289729 | -0.343078 |
| C | -5.769491 | -1.035829 | 0.429551 |
| C | -7.910493 | -0.863365 | -0.711312 |
| C | -6.106945 | -2.359983 | 0.811535 |
| C | -4.504182 | -0.497885 | 0.844591 |
| C | -8.235983 | -2.152643 | -0.335997 |
| H | -8.603867 | -0.276030 | -1.303408 |
| C | -5.192054 | -3.132130 | 1.589315 |
| C | -7.350668 | -2.923253 | 0.424241 |
| C | -3.639178 | -1.231769 | 1.582407 |
| H | -4.259434 | 0.518206 | 0.553565 |
| H | -9.189603 | -2.579021 | -0.633380 |
| C | -3.947687 | -2.576544 | 1.982984 |
| C | -5.524515 | -4.458231 | 1.971437 |
| C | -7.660339 | -4.266942 | 0.826001 |
| H | -2.685486 | -0.808482 | 1.884614 |
| C | -3.066232 | -3.349017 | 2.744121 |
| C | -4.613810 | -5.196100 | 2.731846 |
| C | -6.792099 | -4.997735 | 1.561336 |
| H | -8.615788 | -4.685491 | 0.522862 |
| C | -3.397646 | -4.645494 | 3.113545 |
| H | -2.114500 | -2.921287 | 3.046285 |
| H | -4.868882 | -6.210848 | 3.023977 |
| H | -7.039032 | -6.013011 | 1.858453 |
| H | -2.701940 | -5.232260 | 3.705182 |

| Atom | X | Y | Z |
|---|---|---|---|
| A (IX) | | | |
| C | 2.184696 | -0.411432 | 0.000000 |
| C | 0.785914 | -0.520121 | 0.000000 |
| C | 0.000000 | 0.623672 | 0.000000 |
| C | 0.583578 | 1.881001 | 0.000000 |
| C | 1.982044 | 2.013682 | 0.000000 |
| C | 2.772076 | 0.854048 | 0.000000 |
| H | 0.331762 | -1.504632 | 0.000000 |
| H | -1.081922 | 0.532307 | 0.000000 |
| H | -0.028678 | 2.774201 | 0.000000 |
| H | 3.852025 | 0.943932 | 0.000000 |
| C | 2.599570 | 3.290396 | 0.000000 |
| C | 3.169220 | 4.365370 | 0.000000 |
| C | 3.003735 | -1.581823 | 0.000000 |
| C | 3.699029 | -2.570135 | 0.000000 |
| C | 3.932965 | 5.547718 | 0.000000 |
| C | 3.338456 | 6.856739 | 0.000000 |
| C | 5.337365 | 5.444469 | 0.000000 |
| C | 4.201988 | 7.988571 | 0.000000 |
| C | 6.143025 | 6.561672 | 0.000000 |
| H | 5.775791 | 4.452292 | 0.000000 |
| C | 5.565287 | 7.846743 | 0.000000 |
| H | 3.748138 | 8.973665 | 0.000000 |
| H | 7.222395 | 6.450875 | 0.000000 |
| H | 6.200600 | 8.726631 | 0.000000 |
| C | 4.573304 | -3.696513 | 0.000000 |
| C | 5.958236 | -3.489152 | 0.000000 |
| C | 4.075538 | -5.019570 | 0.000000 |
| C | 6.839647 | -4.557822 | 0.000000 |
| H | 6.329430 | -2.470145 | 0.000000 |
| C | 4.983083 | -6.086629 | 0.000000 |
| C | 6.349825 | -5.861442 | 0.000000 |
| H | 7.909364 | -4.375234 | 0.000000 |
| H | 4.594322 | -7.099178 | 0.000000 |
| H | 7.034930 | -6.703098 | 0.000000 |
| C | 1.967508 | 7.066214 | 0.000000 |
| C | 0.768416 | 7.359321 | 0.000000 |
| C | 2.675909 | -5.287610 | 0.000000 |
| C | 1.496464 | -5.556616 | 0.000000 |
| C | -0.560312 | 7.723943 | 0.000000 |
| C | -1.626318 | 6.739828 | 0.000000 |
| C | -0.908544 | 9.110779 | 0.000000 |
| C | -2.974405 | 7.183361 | 0.000000 |
| C | -1.360893 | 5.356237 | 0.000000 |
| C | -2.207831 | 9.516372 | 0.000000 |
| H | -0.103736 | 9.837641 | 0.000000 |
| C | -4.031484 | 6.232953 | 0.000000 |
| C | -3.281421 | 8.573943 | 0.000000 |
| C | -2.381010 | 4.435546 | 0.000000 |
| H | -0.324713 | 5.031479 | 0.000000 |
| H | -2.448743 | 10.575338 | 0.000000 |
| C | -3.739038 | 4.841698 | 0.000000 |
| C | -5.387153 | 6.670030 | 0.000000 |
| C | -4.631674 | 8.980943 | 0.000000 |
| H | -2.159699 | 3.372230 | 0.000000 |

| | | | |
|---|---|---|---|
| C | -4.804159 | 3.915242 | 0.000000 |
| C | -6.413456 | 5.708512 | 0.000000 |
| C | -5.654449 | 8.066029 | 0.000000 |
| H | -4.853922 | 10.044382 | 0.000000 |
| C | -6.118486 | 4.350036 | 0.000000 |
| H | -4.576891 | 2.853062 | 0.000000 |
| H | -7.447012 | 6.042476 | 0.000000 |
| H | -6.687791 | 8.400049 | 0.000000 |
| H | -6.926427 | 3.624951 | 0.000000 |
| C | 0.102074 | -5.851191 | 0.000000 |
| C | -0.361257 | -7.185746 | 0.000000 |
| C | -0.822362 | -4.798627 | 0.000000 |
| C | -1.758731 | -7.431479 | 0.000000 |
| C | 0.534822 | -8.307733 | 0.000000 |
| C | -2.182216 | -5.041499 | 0.000000 |
| H | -0.447999 | -3.780760 | 0.000000 |
| C | -2.246919 | -8.773142 | 0.000000 |
| C | -2.677094 | -6.349400 | 0.000000 |
| C | 0.070603 | -9.577867 | 0.000000 |
| H | 1.600467 | -8.108084 | 0.000000 |
| H | -2.881405 | -4.210379 | 0.000000 |
| C | -1.337497 | -9.861620 | 0.000000 |
| C | -3.644353 | -9.023007 | 0.000000 |
| C | -4.085107 | -6.632307 | 0.000000 |
| H | 0.763470 | -10.414576 | 0.000000 |
| C | -1.835720 | -11.167155 | 0.000000 |
| C | -4.100068 | -10.343712 | 0.000000 |
| C | -4.545911 | -7.903608 | 0.000000 |
| H | -4.776517 | -5.794495 | 0.000000 |
| C | -3.203489 | -11.403860 | 0.000000 |
| H | -1.137564 | -11.999376 | 0.000000 |
| H | -5.169626 | -10.533702 | 0.000000 |
| H | -5.613668 | -8.103356 | 0.000000 |
| H | -3.574500 | -12.423977 | 0.000000 |

**Time-resolved fluorescence of PyomoPy in different solvents**

Time-resolved fluorescence decay traces were collected in single photon timing (SPT) mode on a FluoTime 200 fluoromoter (PicoQuant, GmbH). The excitation source was a 405-nm pulsed diode laser (EPL405, Edinburgh Instruments, Ltd.) using a 5 MHz excitation frequency. The full width at half maximum (fwhm) of the laser pulses was around 90 ps. The fluorescence emission was collected at a 90° geometry, focused at the detector after crossing through a polarizer (set at the magic angle), 2-mm slits, and a 2-nm bandwidth monochromator. SPT was achieved by a TimeHarp200 board, set at 36 ps/channel. Fluorescence decay traces were collected for the necessary time to reach 20,000 counts at the peak channel. Time-resolved emission spectroscopy (TRES) of **PyomoPy** dissolved in different solvents was performed by collecting 51 fluorescence decay traces in the 420 - 570 nm emission range ($\Delta\lambda_{em}$ = 3 nm) during a fixed amount of time to maintain the overall intensity information.

The fluorescence decay traces were fitted to a four-exponential function, by using a Levenberg-Marquard algorithm-based nonlinear least-squares error minimization deconvolution method iterative reconvolution methods (FluoFit 4.4 package, Picoquant GmbH). For each sample, the decay traces collected at different emission wavelengths were fitted globally with the decay times linked as shared parameters, whereas the pre-exponential factors were local adjustable parameters. The quality of fittings was assessed by the value of the reduced chi-squared, $\chi^2$, parameter and random distributions of the weighted residuals and the autocorrelation functions. Figure S3 shows four decay traces of PyomoPy dissolved in ethanol (Fig. S3a) and n-hexane (Fig. S3b) at different emission wavelengths. The insets show the weighted residuals for the 4-exponential function fit.

For the TRES analysis and the estimation of the species-associated emission spectra (SAEMS), the fitting procedure described above was performed, by fitting globally the 51 decay traces. The SAEMS of each species *i* at any given emission wavelength ($SAEMS_i(\lambda_{em})$) is given by the fluorescence intensity emitted by the species *i* ($A_{i,\lambda em} \times \tau_i$), normalized by the total intensity and corrected for the different detection sensitivity using the total intensity of the steady-state spectrum ($I_{ss,\lambda em}$):

$$SAEMS_i(\lambda_{em}) = \frac{A_{i,\lambda em} \times \tau_i}{\sum_i A_{i,\lambda em} \times \tau_i} \cdot I_{ss,\lambda em} \qquad \text{(eq. S1)}$$

The approximate contribution of each species can be assessed as the area under the SAEMS. This estimation assumes equal excitation rate for all the species, as the initial amount of each form in the excited state (after the pulsd excitation) is unknown.

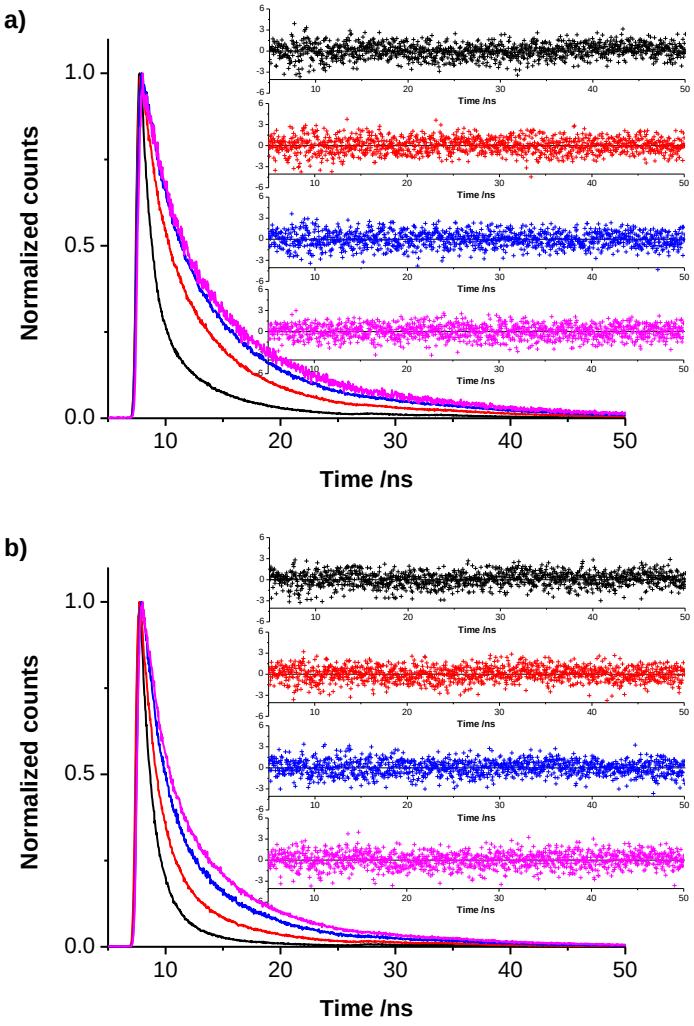
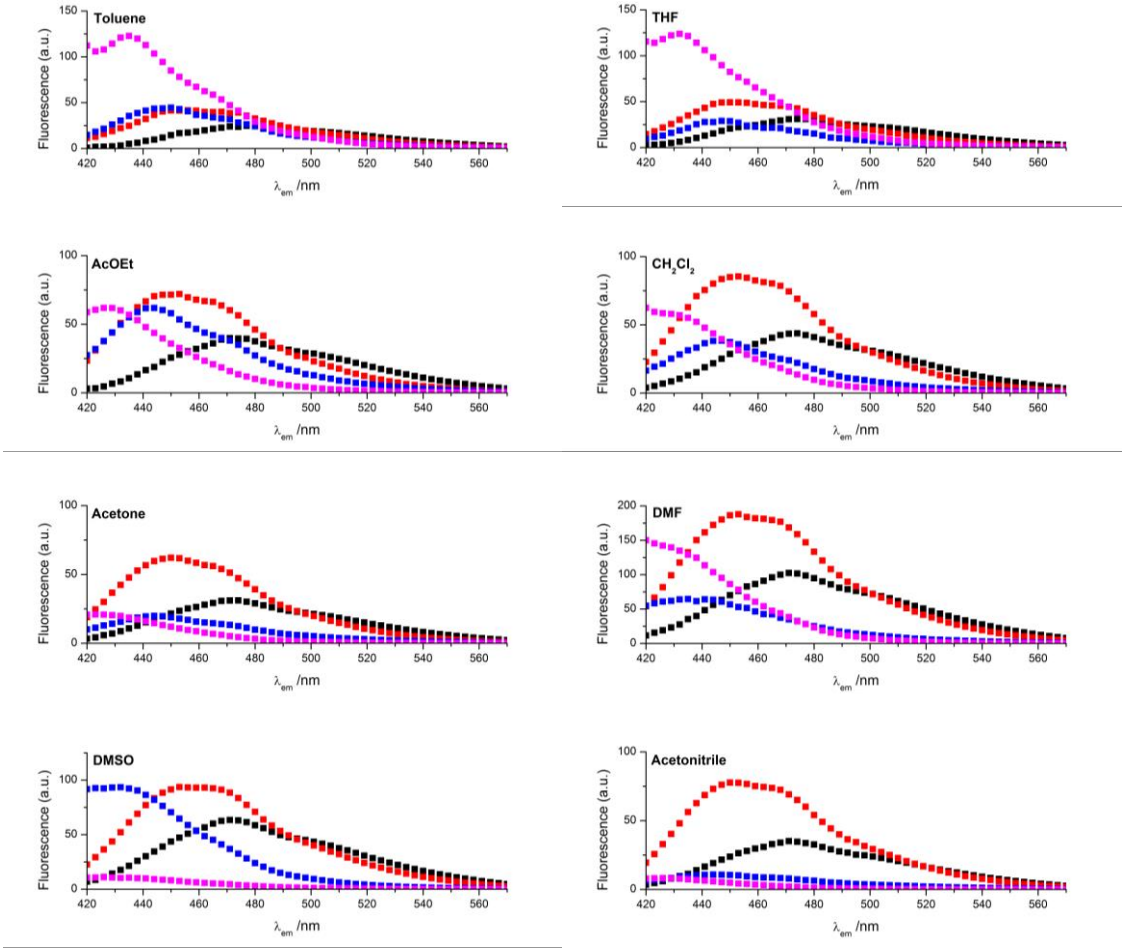



**Figure S3**. Fluorescence decay traces of **PyomoPy** dissolved in (a) ethanol and (b) n-hexane, collected at 420 (black), 460 (red), 500 (blue), and 560 nm (magenta) (extracted from the full TRES experiments). The insets show the corresponding weighted residuals from the 4-exponential function fits.

**Table S3**. Fluorescence decay times of **PyomoPy** in different solvents recovered from global analyses of 51 decay traces in the emission range 420 – 570 nm.[a]

| Solvent | $\tau_1$ /ns | $\tau_2$ /ns | $\tau_3$ /ns | $\tau_4$ /ns |
|---|---|---|---|---|
| **n-hexane** | 0.54 | 1.55 | 5.58 | 9.00 |
| **Toluene** | 0.72 | 1.94 | 5.44 | 9.17 |
| **Tetrahydrofuran** | 0.83 | 1.62 | 4.72 | 9.94 |
| **AcOEt** | 0.63 | 1.84 | 4.95 | 8.97 |
| **Dichloromethane** | 0.59 | 1.88 | 5.73 | 12.12 |
| **Acetone** | 0.40 | 1.53 | 5.31 | 9.66 |
| **Dimethylformamide** | 0.85 | 1.57 | 7.36 | 13.40 |
| **Dimethylsulfoxide** | 0.19 | 1.86 | 9.03 | 16.89 |
| **Acetonitrile** | 0.37 | 1.46 | 6.51 | 10.46 |
| **Ethanol** | 0.63 | 2.11 | 5.19 | 10.49 |
| **Methanol** | 0.32 | 1.53 | 5.28 | 10.33 |
| **1,4-dioxane** | 1.00 | 2.77 | 8.68 | 14.71 |

[a] The standard deviation from the fits were always <0.27 ns for each decay time, except for 1,4-dioxane, in which the standard deviation in $\tau_4$ was 1.34 ns.



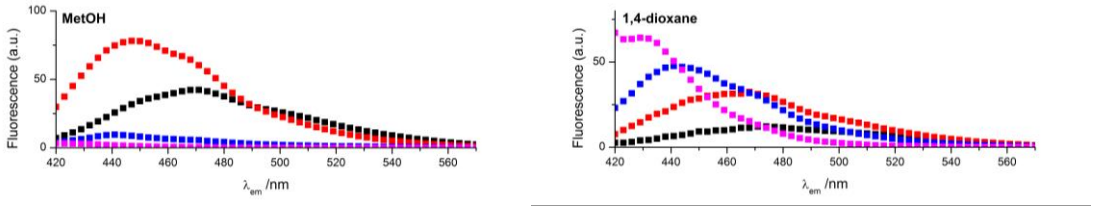



**Figure S4**. TRES deconvolution of the SAEMS associated to the shortest ($\tau_1$, magenta), short intermediate ($\tau_2$, blue), long intermediate ($\tau_3$, red), and the longest ($\tau_4$, black) decay times of PyomoPy dissolved in the different solvents tested in this work. The corresponding SAEMS on n-hexane and ethanol are displayed in Figure 2 of the main text.

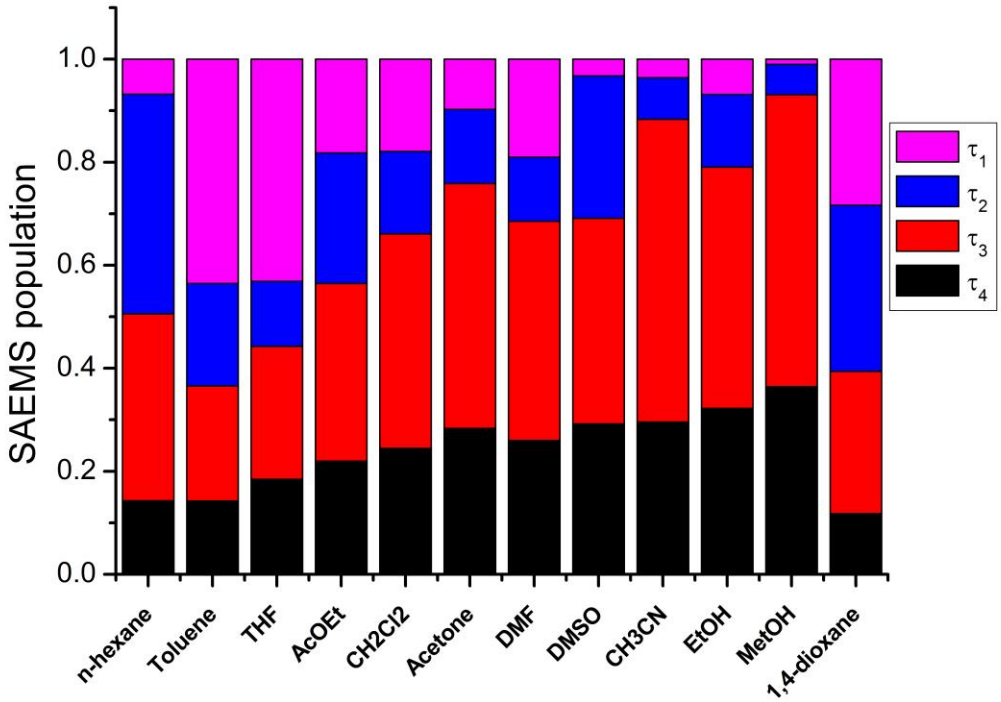



**Figure S5**. Relative population of the SAEMS associated to the shortest ($\tau_1$, magenta), short intermediate ($\tau_2$, blue), long intermediate ($\tau_3$, red), and the longest ($\tau_4$, black) decay times of PyomoPy dissolved in the different solvents tested in this work.

**Time-resolved fluorescence of PyomoPy as a function of the media viscosity**

The viscosity values of the pure solvents were taken from CRC Handbook of Chemistry and Physics.[8] Ethanol : glycerine and methanol : glycerine mixtures were prepared by mixing different proportions of each solvent within the ratio 19:1 to 1:2 for methanol : glycerine and 9:1 to 3:7 for ethanol : glycerine mixtures. The viscosity of these mixtures was measured with a falling ball viscometer (Viscoball, Fungilab). In this system the time a ball (of known size and density) requires to traverse a definite distance within the fluid is measured, and Stokes' law is used to calculate the viscosity of that fluid. Measurements were made in triplicate. The temperature of the liquid mixtures was controlled at 25 °C during the viscosity measurements.

Time-resolved fluorescence decay traces were collected and analyzed using the same instrumentation and procedures described above. Fluorescence decay traces of **PyomoPy** dissolved in ethanol:glycerine mixtures were collected in the 420-580 nm emission range ($\Delta\lambda_{em}$ = 40 nm, 5 traces). For methanol:glycerine mixtures, the same range was used but with $\Delta\lambda_{em}$ = 20 nm (9 traces).

**Table S4**. Fluorescence decay times of PyomoPy in EtOH:glycerine mixtures (between 9:1 and 3:7) of different viscosities, recovered from global analyses of 5 decay traces in the emission range 420 – 580 nm.[a]

| Viscosity /mPa·s | $\tau_1$ /ns | $\tau_2$ /ns | $\tau_3$ /ns | $\tau_4$ /ns |
|---|---|---|---|---|
| **1.667** | 0.71 | 3.58 | 8.21 | 14.18 |
| **2.969** | 0.93 | 3.86 | 8.94 | 15.77 |
| **5.616** | 1.07 | 3.87 | 9.00 | 16.58 |
| **11.677** | 0.18 | 1.73 | 6.55 | 15.77 |
| **23.665** | 0.20 | 1.77 | 6.72 | 15.96 |
| **42.652** | 0.26 | 2.22 | 7.77 | 17.09 |
| **75.646** | 0.29 | 2.38 | 8.35 | 17.50 |

[a] The standard deviation from the fits were always <1.37 ns for $\tau_4$.

**Table S5**. Fluorescence decay times of PyomoPy in MetOH:glycerine mixtures (between 19:1 and 1:2) of different viscosities, recovered from global analyses of 9 decay traces in the emission range 420 – 580 nm.[a]

| Viscosity /mPa·s | $\tau_1$ /ns | $\tau_2$ /ns | $\tau_3$ /ns | $\tau_4$ /ns |
|---|---|---|---|---|
| **0.751** | -- | 1.58 | 6.19 | 11.89 |
| **0.961** | -- | 1.57 | 6.57 | 12.76 |
| **1.244** | -- | 1.57 | 6.82 | 13.37 |
| **1.663** | -- | 1.54 | 7.14 | 14.38 |
| **2.089** | -- | 1.56 | 7.44 | 15.15 |
| **2.684** | -- | 1.57 | 7.57 | 15.50 |
| **4.067** | 0.65 | 2.04 | 7.61 | 16.11 |
| **7.940** | 0.40 | 1.86 | 7.82 | 16.91 |
| **12.660** | 0.35 | 1.99 | 8.10 | 17.19 |
| **17.250** | 0.42 | 2.17 | 8.32 | 17.34 |
| **44.320** | 0.38 | 1.79 | 8.13 | 17.10 |

[a] The standard deviation from the fits were always <0.30 ns for $\tau_4$.

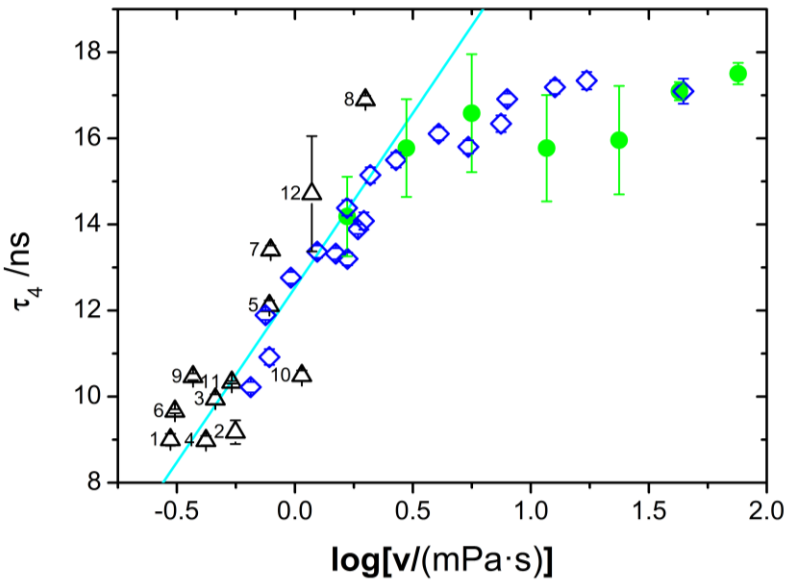



**Figure S6.** Longest decay time ($\tau_4$) of **PyomoPy** dissolved in pure solvents (black triangles), MeOH:glicerine mixtures (blue diamonds), or EtOH:glycerine mixtures (green circles) as a function of log(viscosity). Pure solvents: 1. n-hexane, 2. Toluene, 3. THF, 4. AcOEt, 5. $CH_2Cl_2$, 6. Acetone, 7. Dimethylformamide, 8. Dimethylsulfoxide, 9. $CH_3CN$, 10. Ethanol, 11. Methanol, 12. 1,4- Dioxane. MeOH:glicerine mixtures between 19:1 and 1:2. EtOH:glycerine mixtures between 9:1 and 3:7. The blue line is the linear fit of the datapoints in the linear region as detailed in the main text.

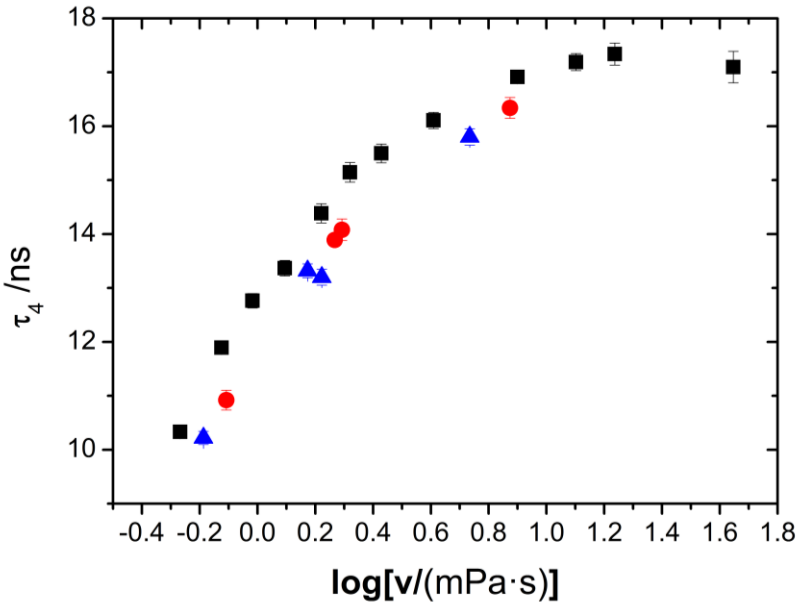



**Figure S7.** Longest decay time ($\tau_4$) of **PyomoPy** dissolved in MeOH:glicerine mixtures at 20 °C (black squares), 30 °C (red circles), and 40 °C (blue triangles), as a function of log(viscosity). At higher temperatures, the decay time is slightly smaller due to the enhancement of non-radiative deactivation processes.

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