Supporting Information

Switching between TADF and RTP: Anion-Regulated Photoluminescence in Organic Salts and Co-crystals

Zhen Xu, Duane Hean, Clàudia Climent and David Casanova* and Michael O. Wolf*

General

Solvents used were reagent grade and used without any further purification. HPLC grade solvents were used for analyses. 9-H carbazole was purchased from Sigma-Aldrich (China) and was crystallized from toluene solution before use. Other purchased chemicals were used without further purification. **Cbz-C4-Br** was synthesized following the literature procedure.¹

Spectroscopy

¹H, ¹³C{¹H}, COSY, NOESY, HSQC and HMBC NMR experiments were collected using a Bruker AV-400 spectrometer and referenced first to TMS and then to the residual protonated solvent peak. NMR solvents (Aldrich or Cambridge Isotope Laboratories) were used as received. Electrospray ionization mass spectrometry data were obtained using a Bruker Esquire LC ion trap mass spectrometer. Infrared spectroscopy was performed on an attenuated total reflection (ATR) crystal using a Perkin-Elmer Frontier FT-IR spectrometer. UV-vis absorption spectra were recorded on a Varian-Cary 5000 UV-Vis-near-IR spectrophotometer. Steady-state photoluminescence data were collected using a Photon Technology International (PTI) QuantaMaster 50 fluorimeter fitted with an integrating sphere, double excitation monochrometer and utilizing a 75 W Xe arc lamp as the source. Fluorescence and phosphorescence lifetime data were collected using a Horiba Yvon Fluorocube TCSPC apparatus with a 370 nm NanoLED (fluorescence) or a 359 nm Horiba spectral LED (phosphorescence). The photoluminescence lifetime data were fitted using the DAS6 Data Analysis software package. Time-resolved photoluminescence spectra utilizing a 1 ms delay were measured using a Photon Technology International (PTI) QuantaMaster 400 equipped with a 359 nm Horiba spectral LED. Samples for low-temperature spectroscopy and lifetime measurements were cooled using an Oxford Instruments Optistat DN. HPLC was performed using an Agilent Technologies 1260 Infinity instrument equipped with an Agilent 4.6×150 mm ZORBAX Extend-C18 column. The isocratic mobile phase was composed of 25% acetonitrile, 75% water with a flow rate of 3 mL/min. The detector wavelength was set to 292 or 360 nm.

X-Ray Diffraction

Single-crystal X-ray data were collected using a Bruker APEX DUO diffractometer with graphite monochromated Mo K α radiation ($\lambda = 0.71073$ Å) at 100 K. Raw frame data were processed using APEX2. The program SAINT+, v.7.68 was used to reduce the data and the program SADABS was used to make corrections to the empirical absorptions. Space group assignments were made using XPREP on all compounds. In all cases, the structures were solved in the Olex2 suite² of programs using Intrinsic Phasing and refined using full-matrix least-squares/difference Fourier techniques on F² using SHELXL.³ Diagrams and publication material were generated using CrystalMaker. Powder X-ray crystallography data were collected on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-K α radiation.

Powder X-Ray Diffraction (pXRD) Data





Figure S1. Powder X-ray diffraction (pXRD) patterns of **Py-Br**, **Py -Cl**, **Qui-Br** and **Qui-BF**₄ crystalline powder compared to their single crystal simulated patterns.

Photophysical Data



Figure S2. Absorption (solid lines) and photoluminescence spectra (dash lines) of all compounds in 2.5×10^{-5} M CH₂Cl₂ solution. Inset: zoomed in absorption spectra between 350-430 nm to show broad charge transfer feature of **Py-I**.

The following equations were used to determine k_{risc} :⁴

$$\frac{\phi_{DF}}{\phi_{PF}} = \frac{A_{DF}\tau_{DF}}{A_{PF}\tau_{PF}} \quad \text{eq 1.}$$

$$k_{risc} = \frac{1}{\tau_{DF}1 - \phi_{risc}\phi_{isc}} = \frac{\phi_{risc}}{\tau_{DF}}(\frac{\phi_{DF} + \phi_{PF}}{\phi_{PF}}) \approx \frac{1}{\tau_{DF}}(\frac{\phi_{DF} + \phi_{PF}}{\phi_{PF}}) \quad \text{eq 2.}$$

| Tomporatura | | Prompt | Delayed | Delayed | | |
|-------------|----------------------|-----------|---------------|-----------|------------|-----------|
| Temperature | Prompt Lifetime (ns) | Amplitude | Lifetime (ns) | Amplitude | DF/PF | Ln(Krisc) |
| 250 | 18.5 | 0.385 | 1100 | 0.615 | 94.980695 | 18.2843 |
| 260 | 16.8 | 0.382 | 992 | 0.618 | 95.5272999 | 18.3934 |
| 270 | 14.9 | 0.395 | 871 | 0.605 | 89.5344491 | 18.4594 |
| 280 | 13.4 | 0.396 | 790 | 0.604 | 89.9216041 | 18.5612 |
| 290 | 12.1 | 0.394 | 715 | 0.606 | 90.8860175 | 18.6715 |
| 300 | 11.7 | 0.379 | 685 | 0.621 | 95.9305866 | 18.7678 |

Table S1. Variable temperature lifetime data of Py-Br.

| Temperature | Prompt Lifetime (ns) | Prompt | Delayed | Delayed | DE/PE | Ln(Krisc) |
|-------------|----------------------|-----------|---------------|-----------|------------|-----------|
| remperature | rompt Licture (iis) | Amplitude | Lifetime (ns) | Amplitude | Diyii | |
| 260 | 57.1 | 0.84 | 452 | 0.16 | 1.50779751 | 15.5290 |
| 270 | 52.7 | 0.82 | 414 | 0.18 | 1.72444115 | 15.6997 |
| 280 | 48.2 | 0.78 | 392 | 0.22 | 2.29386105 | 15.9441 |
| 290 | 43.9 | 0.73 | 372 | 0.27 | 3.13414672 | 16.2237 |
| 300 | 39.7 | 0.65 | 336 | 0.35 | 4.55725635 | 16.6213 |
| 310 | 38.9 | 0.625 | 344 | 0.375 | 5.3059126 | 16.7241 |

 Table S2. Variable temperature lifetime data of Qui-Br.



Figure S3. (a) Steady-state and time-resolved photoluminescence spectra of crystalline Qui-Br at room temperature under air and at 77 K. (b) Fluorescence decay curve of crystalline Qui-Br at room temperature under air. (c) Phosphorescence decay curve of crystalline Qui-Br at room temperature under air and at 77 K. (d) Arrhenius plot of $\ln(k_{RISC})$ versus temperature to calculate ΔE_{ST} .



Figure S4. (a) Excitation power dependence of **Py-Br** delayed fluorescence. (b) Power law fitting plot of excitation power *vs.* delayed fluorescence integration (0.15 to 2 μ s).



Figure S5. (a) Excitation power dependence of **Qui-Br** delayed fluorescence. (b) Power law fitting plot of excitation power *vs.* delayed fluorescence integration (0.15 to 2 μ s).



Figure S6. Fluorescence decay curves of crystalline Py-BF₄, Py-PF₆, Py-Cl and Qui-BF₄ at room temperature under air.



Figure S7. (a) Steady-state and time-resolved photoluminescence spectra of crystalline Py-Cs-Br at room temperature under air. (b) Fluorescence decay curve of crystalline Py-Cs-Br at room temperature under air.
(c) Phosphorescence decay curve of crystalline Py-Cs-Br at room temperature under air.



Figure S8. (a) Steady-state and time-resolved photoluminescence spectra of crystalline $Py-Cs-BF_4$ at room temperature under air. (b) Fluorescence decay curve of crystalline $Py-Cs-BF_4$ at room temperature under air. (c) Phosphorescence decay curve of crystalline $Py-Cs-BF_4$ at room temperature under air.

Table S3. Chi-square values of RTP lifetime fitting.

| | RTP | Phosphorecence 77 K |
|--------------------|-------|---------------------|
| | | |
| Py-Br | 1.05 | 1.23 |
| | | |
| Py-BF ₄ | 1.41 | 1.24 |
| | | |
| Py-PF ₆ | 0.987 | 1.08 |
| | | |
| Py -Cl | 1.03 | 1.39 |

| Qui-Br | 1.41 | 1.22 |
|-----------|------|------|
| Qui-BF₄ | 1.39 | 1.17 |
| Ру-А | 1.19 | N/A |
| Py-Cs-Br | 1.16 | N/A |
| Py-Cs-BF₄ | 1.67 | N/A |

Synthesis



Py-Br



Cbz-C4-Br (0.604 g, 2.00 mmol, 1.0 equiv.) was dissolved in 5 mL pyridine. The mixture was stirred at 80 °C until all the **Cbz-C4-Br** was consumed, as monitored by TLC. Pyridine was

removed under vacuum and the product was filtered and washed with Et₂O. Dissolving the resulting solid in CH₂Cl₂ and slow evaporation of the solution afforded the pure compound as off-white crystals (0.760 g, 1.99 mmol, 100 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 9.11 (dd, *J* = 6.6, 1.4 Hz, 2H, H₁₁), 8.29 (tt, *J* = 7.8, 1.4 Hz, 1H, H₁₃), 8.09 (dt, *J* = 7.8, 1.0 Hz, 2H, H₂), 7.85 (t, *J* = 7.0 Hz, 1H, H₁₂), 7.51-7.44 (m, 4H, H₄ and H₅), 7.26 (ddd, *J* = 7.9, 6.6, 1.5 Hz, 2H, H₃), 4.79 (t, *J* = 7.0 Hz, 2H, H₁₀), 4.49 (t, *J* = 6.2 Hz, 2H, H₇), 2.10 (m, 4H, H₈ and H₉). ¹³C {¹H} NMR (101 MHz, CD₂Cl₂)) δ 144.9 (C₁₃), 144.6 (C₁₁), 140.2 (C₆), 128.1 (C₁₂), 125.9 (C₄), 122.7 (C₁), 120.3 (C₂), 119.1 (C₃), 109.0 (C₅), 61.2 (C₁₀), 42.2 (C₇), 29.4 (C₉), 25.1 (C₈). HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂: 301.1705; Found: 301.1704 [M–Br]⁺.

Py-BF₄



Py-Br (0.097 g, 0.255 mmol, 1.0 equiv.) was dissolved in a minimal amount of acetone at room temperature. An excess of saturated NH₄BF₄ aqueous solution was added and the resultant mixture was filtered. The solid was washed with deionized H₂O and then dried under vacuum. Slow evaporation of an acetone solution of the resulting solid afforded pale-yellow crystals as pure product (0.081 g, 0.209 mmol, 82 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 8.40 (d, *J*=5.5 Hz, 2H, H₁₁), 8.34 (td, *J*=8.0, 1.4 Hz, 1H, H₁₃), 8.11 (d, *J*=7.8 Hz, 2H, H₂), 7.86 (t, *J*=7.0 Hz, 1H, H₁₂), 7.50-7.44 (m, 4H, H₄ and H₅), 7.26 (ddd, *J*=7.9, 6.3, 1.8 Hz, 2H, H₃), 4.46 (t, *J*=5.8 Hz, 2H, H₇), 4.38 (t, *J*=7.4 Hz, 2H, H₁₀), 2.06 (m, 4H, H₈ and H₉). ¹³C{¹H} NMR (101 MHz, CD₂Cl₂)) δ 145.5 (C₁₃), 144.0 (C₁₁), 140.2 (C₆), 128.5 (C₁₂), 126.0 (C₄), 122.7 (C₁), 120.3 (C₂), 119.21(C₃), 108.8 (C₅), 62.0 (C₁₀), 42.0 (C₇), 29.0 (C₉), 25.0 (C₈). HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂: 301.1705; Found: 301.1703 [M-BF₄]⁺.

Py-PF₆



Py-Br (0.170 g, 0.446 mmol, 1.0 equiv.) was dissolved in minimal amount of acetone at room temperature. An excess of saturated NH₄PF₆ aqueous solution was added and the resultant mixture was filtered. The solid was washed first with deionized water and then dried under vacuum. Slow evaporation of an acetone solution of the solid afforded colorless crystals as pure product (0.199 g, 0.446 mmol, 100%). ¹H NMR (400 MHz, CD₂Cl₂) δ 8.35 (t, *J* =7.9, 1.3 Hz, 1H, H₁₃), 8.25 (d, *J* =5.9 Hz, 2H, H₁₁), 8.11 (d, *J* = 7.8 Hz, 2H, H₂), 7.86 (t, *J* = 7.0 Hz, 1H, H₁₂), 7.50-7.43 (m, H₄ and H₅), 7.26 (ddd, *J* =7.9, 6.8, 1.3 Hz, 2H, H₃), 4.46 (t, *J* = 7.2 Hz, 2H, H₇), 4.30 (t, *J* = 7.0 Hz, 2H, H₁₀), 2.05 (m, 4H, H₈ and H₉). ¹³C{¹H} NMR (101 MHz, CD₂Cl₂)) δ 145.5 (C₁₃), 143.7 (C₁₁), 140.1 (C₆), 128.6 (C₁₂), 126.0 (C₄), 122.1 (C₁), 120.4 (C₂), 119.2 (C₃), 108.7 (C₅), 62.1 (C₁₀), 42.0 (C₇), 29.0 (C₉), 24.9 (C₈). HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂: 301.1705; Found: 301.1701 [M-PF₆]⁺.

Py-Cl



Py-PF₆ (0.084 g, 0.188 mmol, 1.0 equiv.) were dissolved in a minimal amount of acetone at room temperature. Tetrabutylammonium chloride (0.105 g, 0.376 mmol, 2.0 equiv.) was then added and the resultant mixture was filtered. The collected solid was washed with cold acetone and then dried under vacuum. Slow evaporation of the crude solid in CH₂Cl₂ solution afforded white crystals as pure product (0.050 g, 0.119 mmol, 79 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 9.20 (d, *J* = 5.6 Hz, 2H, H₁₁), 8.34 (t, *J* = 7.9, 1H, H₁₃), 8.09 (d, *J* = 7.8 Hz, 2H, H₂), 7.85 (t, *J* = 6.9 Hz, 1H, H₁₂), 7.50-7.43 (m, 4H, H₄ and H₅), 7.26 (ddd, *J* = 8.0, 6.5, 1.6 Hz, 2H, H₃), 4.84 (t, *J* = 6.9 Hz, 2H, H₁₀), 4.49 (t, *J* = 6.3 Hz, 2H, H₇), 2.09 (m, 4H, H₈ and H₉). ¹³C {¹H} NMR (101 MHz, CD₂Cl₂)) δ 144.9 (C₁₁), 144.7 (C₁₃), 140.3 (C₆), 128.1 (C₁₂), 125.9 (C₄), 122.7 (C₁),

120.3 (C₂), 119.0(C₃), 108.9 (C₅), 61.2 (C₁₀), 42.2 (C₇), 29.4 (C₉), 25.1 (C₈). HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂: 301.1705; Found: 301.1705 [M–Cl]⁺.



Py-PF₆ (0.096 g, 0.215 mmol, 1.0 equiv.) was dissolved in a minimal amount of acetone at room temperature. Tetrabutylammonium iodide (0.159 g, 0.430 mmol, 2.0 equiv.) was then added and the resultant mixture was filtered. The solid was washed first with cold acetone and then dried under vacuum. Slow evaporation of a CH₂Cl₂ solution of the solid afforded white crystals as pure product (0.070 g, 0.163 mmol, 76 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 8.87 (d, J =6.0 Hz, 2H, H₁₁), 8.33 (t, J =8.0, 1H, H₁₃), 8.10 (d, J = 7.8 Hz, 2H, H₂), 7.87 (t, J = 7.3 Hz, 1H, H₁₂), 7.51-7.45 (m, 4H, H₄ and H₅), 7.26 (ddd, J =8.0, 6.2, 1.9 Hz, 2H, H₃), 4.65 (t, J = 6.9 Hz, 2H, H₁₀), 4.49 (t, J = 6.0 Hz, 2H, H₇), 2.12 (m, 4H, H₈ and H₉). ¹³C {¹H} NMR (101 MHz, CD₂Cl₂)) δ 145.1 (C₁₃), 144.3 (C₁₁), 140.2 (C₆), 128.2 (C₁₂), 126.0 (C₄), 122.7 (C₁), 120.3 (C₂), 119.1 (C₃), 109.0 (C₅), 61.4 (C₁₀), 42.1 (C₇), 29.3 (C₉), 25.0 (C₈). HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂: 301.1705; Found: 301.1703 [M–I]⁺.

Qui-Br



Cbz-C4-Br (0.604 g, 2.00 mmol, 1.0 equiv.) was dissolved in 5 mL quinoline. The mixture was stirred for 2 h at 80 °C. After cooling to room temperature, Et₂O was added and the product was filtered and washed with Et₂O. Slow evaporation of an acetone solution of the solid afforded orange crystals as pure product (0.800 g, 1.85 mmol, 93 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 10.49 (d, *J* = 5.8, 1H, H₁₁), 8.73 (d, *J* = 8.3 Hz, 1H, H₁₃), 8.11 (d, *J* = 7.9 Hz, 1H, H₁₆), 7.98 (d, *J* = 7.8 Hz, 2H, H₂), 7.93-7.79 (m, 4H, H₁₂, H₁₆, H₁₇ and H₁₈), 7.46 (d, *J* = 8.1

Hz, 2H, H₅), 7.42 (m, 2H, H₄), 7.19 (t, J=7.3 Hz, 2H, H₃), 5.25 (t, J=7.6 Hz, 2H, H₁₀), 4.46 (t, J=6.5 Hz, 2H, H₇), 2.25 (m, 2H, H₈), 2.13 (m, 2H, H₉). ¹³C{¹H} NMR (101 MHz, CD₂Cl₂) δ 150.8 (C₁₁), 147.0 (C₁₃), 140.8 (C₆), 138.0 (C₁₅), 136.2 (C₁₇), 131.2 (C₁₉), 130.5 (C₁₈), 130.2 (C₁₄), 126.4 (C₄), 123.2 (C₁), 122.5 (C₁₂), 120.8 (C₂), 119.5(C₃), 118.3 (C₁₆), 109.5 (C₅), 57.7 (C₁₀), 42.7 (C₇), 27.8 (C₉), 25.9 (C₈). HR-ESI MS: *m/z* calcd. for C₂₅H₂₃N₂: 351.1861; Found: 351.1859 [M-Br]⁺.

Qui-BF₄



Qui-Br (0.129 g, 0.300 mmol, 1.0 equiv.) was dissolved in a minimal amount of acetone at room temperature. An excess of saturated NH₄BF₄ aqueous solution was added and the resultant mixture was filtered. The solid was washed first with deionized H₂O and then dried under vacuum. Slow evaporation of a CH₂Cl₂ solution of the solid afforded yellow crystals as the pure product (0.100 g, 0.228 mmol, 77 %). ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.44 (dd, *J* = 6.2, 1.3 Hz, 1H, H₁₁), 9.22 (d, *J*=8.3 Hz, 1H, H₁₃), 8.52 (d, *J* = 9.0 Hz, 1H, H₁₆), 8.45 (dd, *J*=8.3, 1.0 Hz, 1H, H₁₉), 8.21 (ddd, *J* = 8.7 Hz, 7.0, 1.5 Hz, 1H, H₁₇), 8.12 (d, *J* = 7.5 Hz, 2H, H₂), 8.10 (m, 1H, H₁₂), 8.03 (t, *J*=7.6 Hz, 1H, H₁₈), 7.59 (d, *J* = 8.2 Hz, 2H, H₅), 7.43 (ddd, *J*=8.3, 7.1, 1.2 Hz, 2H, H₄), 7.19 (t, *J*=7.4 Hz, 2H, H₃), 5.04 (t, *J*=7.2 Hz, 2H, H₁₀), 4.43 (t, *J*=7.0 Hz, 2H, H₇), 2.06 (m, 2H, H₉), 1.92 (m, 2H, H₈). ¹³C {¹H} NMR (101 MHz, DMSO-*d*₆) δ 149.6 (C₁₁), 147.5 (C₁₃), 139.9 (C₆), 137.4 (C₁₅), 135.7 (C₁₇), 130.8 (C₁₉), 129.9 (C₁₈), 129.8 (C₁₄), 125.8 (C₄), 122.1 (C₁ and C₁₂), 120.4 (C₂), 118.9 (C₃ and C₁₆), 109.3 (C₅), 51.2 (C₁₀), 41.7 (C₇), 27.0 (C₉), 25.4 (C₈). HR-ESI MS: *m/z* calcd. for C₂₅H₂₃N₂: 351.1861; Found: 351.1859 [M-BF₄]⁺.

Cs-C4-Br

Cs-C4-Br was synthesized following literature procedure.⁵ ¹H NMR (400 MHz, CD₂Cl₂) δ 8.05 (dd, *J* = 8.0, 1.6 Hz, 2H), 8.73 (m, 2H,), 7.66 (d, *J* = 7.9 Hz, 2H), 7.40 (d, *J* = 8.6 Hz, 2H),

7.30 (m, 2H) , 4.25 (t, J = 7.0 Hz, 2H), 3.46 (t, J = 6.4 Hz, 2H), 2.03 (m, 4H). ¹³C{¹H} NMR (101 MHz, CD₂Cl₂) δ 141.5, 133.7, 125.4, 123.9, 122.5, 116.9, 47.7, 33.7, 29.9, 25.8.

Py-Cs-Br

Cs-C4-Br (0.732 g, 2.00 mmol, 1.0 equiv.) was dissolved in 5 mL pyridine. The mixture was stirred at 80 °C until all the **Cs-C4-Br** was consumed, as monitored by TLC. Pyridine was removed under vacuum and the product was filtered and washed with Et₂O. Dissolving the resultant solid in CH₂Cl₂ and slow evaporation of the solution afforded the pure compound as colourless crystals (0.800 g, 1.79 mmol, 89.8 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 9.37 (dd, *J* = 6.8, 1.5 Hz, 2H), 8.27 (tt, *J* = 7.8, 1.4 Hz, 1H), 8.09 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.86 (t, *J* = 7.0 Hz, 2H), 7.63 (m, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.29 (m, 2H), 4.87 (t, *J* = 7.6 Hz, 2H), 4.41 (t, *J* = 5.5 Hz, 2H), 2.07 (m, 4H). ¹³C{¹H} NMR (101 MHz, CD₂Cl₂)) δ 145.6, 145.3, 142.1, 133.9, 128.5, 126.2, 123.6, 122.8, 118.2, 61.2, 46.9, 28.5, 23.8. HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂O₂S: 365.1327; Found: 365.1321 [M–Br]⁺.

Py-Cs-BF₄

Py-Br (0.060 g, 0.135 mmol, 1.0 equiv.) was dissolved in a minimal amount of methanol at room temperature. An excess of saturated NH₄BF₄ aqueous solution was added and the resultant mixture was filtered. The solid was washed with deionized H₂O and then dried under vacuum. Slow evaporation of an acetone solution of the resulting solid afforded pale yellow crystals as pure product (0.050 g, 0.111 mmol, 82 %). ¹H NMR (400 MHz, CD₂Cl₂) δ 8.73 (d, *J* = 6.1 Hz, 2H), 8.34 (t, *J* = 7.8, 1H), 8.01 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.63 (ddd, *J* = 7.2, 1.6 Hz, 2H), 7.43 (d, *J* = 8.5 Hz 2H), 7.30 (ddd, *J* = 7.4, 0.9 Hz, 2H), 4.46 (t, *J* = 7.3 Hz, 2H), 4.39 (t, *J* = 5.6 Hz, 2H), 1.99 (m, 4H). ¹³C {¹H} NMR (101 MHz, CD₂Cl₂)) δ 145.6, 145.0, 142.2, 133.9, 128.9, 126.5, 123.6, 123.0, 118.1, 62.1, 46.6, 28.1, 23.8. HR-ESI MS: *m/z* calcd. for C₂₁H₂₁N₂O₂S: 365.1327; Found: 365.1322 [M–BF₄]⁺.





Figure S10. ¹³C $\{^{1}H\}$ NMR spectra of **Py-Br** in CD₂Cl₂ at 25 °C.



Figure S11. ¹H NMR spectrum of **Py-BF₄** in CD₂Cl₂ at 25 °C.



Figure S12. ¹³C $\{^{1}H\}$ NMR spectrum of Py-BF₄ in CD₂Cl₂ at 25 °C.



Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of $Py\text{-}PF_{6}$ in $CD_{2}Cl_{2}$ at 25 °C.



Figure S15. ¹H NMR spectrum of Py-Cl in CD₂Cl₂ at 25 °C.



Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of Py-Cl in CD₂Cl₂ at 25 °C.



Figure S17. ¹H NMR spectrum of Qui-Br in CD₂Cl₂ at 25 °C.



Figure S18. ${}^{13}C{}^{1}H$ NMR spectrum of Qui-Br in CD₂Cl₂ at 25 °C.



Figure S20. ¹³C{¹H} NMR spectrum of Qui-BF₄ in DMSO- d_6 at 25 °C.



Figure S21. ¹H NMR spectrum of Cs-C4-Br in CD₂Cl₂ at 25 °C.



Figure S22. ¹³C $\{^{1}H\}$ NMR spectrum of Cs-C4-Br in CD₂Cl₂ at 25 °C.



Figure S23. ¹H NMR spectrum of Py-Cs-Br in CD₂Cl₂ at 25 °C.



Figure S24. ¹³C $\{^{1}H\}$ NMR spectrum of Py-Cs-Br in CD₂Cl₂ at 25 °C.



Figure S25. ¹H NMR spectrum of Py-Cs-BF₄ in CD₂Cl₂ at 25 °C.



Figure S26. ¹³C $\{^{1}H\}$ NMR spectrum of Py-Cs-BF₄ in CD₂Cl₂ at 25 °C.

Electronic structure calculations

Electronic structure calculations were performed within the density functional theory (DFT) with the ω B97X-D exchange-correlation functional⁶ and the 6-31+G(d) basis set for all the atoms except for iodine for which 6-311G(d) and the LANL2DZ (pseudopotential) were used instead. Vertical excitations were obtained at the (linear response) time-dependent DFT (TDDFT) level with and without the Tamm-Dancoff approximation (TDA).

Unless indicated, all calculations have been done for molecules, molecular dimers, tetramers and hexamers from the crystal structure, with and without the presence of counter anions. In order to mimic the dielectric of the crystal, calculations have been performed by embedding molecules and oligomers within a dielectric continuum with the conductor-like polarizable continuum model (C-PCM) ⁷⁻⁹. Dichloromethane was used as the dielectric environment with a dielectric constant $\varepsilon = 8.93$ and optical dielectric constant of 2.03. All calculations were done with the Q-Chem package. ¹⁰

Table S4. Vertical excitation energies (in eV) to the lowest excited triplet and singlet states and oscillator strengths (in parenthesis) of **Py-Cl**, **Py-Br**, **Py-I**, **Py-BF**₄ and **Py-PF**₆ crystal dimers with two counterions computed at the ω B97X-D/6-31+G(d) level (full TDDFT linear response). CZ = carbazole. ${}^{3}\pi^{+}\pi^{+*}(Py)'$ contains ~10% CT (CZ \rightarrow Py). ΔE_{ST} indicates the singlet-triplet energy gap between ${}^{1}\pi\pi^{*}(CZ)$ and the nearest triplet state with some localization on the CZ moiety. Shading of rows to facilitate state character recognition.

| state | Py-Cl | Py-Br | Py-I | Py-BF ₄ | Py-PF ₆ |
|-------------------------------|-------------|-------------|-------------|--------------------|--------------------|
| Triplet states | , | | | | |
| $^{3}\pi\pi^{*}$ (CZ) | 3.25 | 3.23 | 3.28 | 3.13 | 3.28 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.25 | 3.23 | 3.28 | 3.13 | 3.28 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.48 | 3.48 | 3.49 | 3.42 | 3.48 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.48 | 3.48 | 3.49 | 3.42 | 3.48 |
| $^{3}\pi^{+}\pi^{+}*$ (Py)' | 3.99 | 3.98 | 3.89 | 3.80 | 4.05 |
| $^{3}\pi^{+}\pi^{+}*$ (Py)' | 4.04 | 4.01 | 3.99 | 3.89 | 4.06 |
| $^{3}\pi^{+}\pi^{+}*(Py)$ | 4.07 | 4.04 | 4.03 | 3.91 | 4.14 |
| $^{3}\pi^{+}\pi^{+}*$ (Py) | 4.12 | 4.07 | 4.12 | 4.01 | 4.14 |
| $^{3}\pi\pi^{*}$ (CZ) | 4.15 | 4.13 | 4.16 | 4.06 | 4.16 |
| $^{3}\pi\pi^{*}$ (CZ) | 4.15 | 4.13 | 4.16 | 4.06 | 4.17 |
| $^{3}\pi\pi^{*}$ (CZ)+Ry | d 4.30 | 4.25 | 4.31 | 4.14 | 4.26 |
| $^{3}\pi\pi^{*}$ (CZ)+Ry | d 4.30 | 4.25 | 4.31 | 4.14 | 4.27 |
| ${}^{3}[p(I) \rightarrow Py]$ | - | - | 4.36 | - | - |
| Singlet states | 5 | | | | |
| $^{1}\pi\pi^{*}$ (CZ) | 4.27 (0.16) | 4.27 (0.15) | 4.28 (0.17) | 4.21 (0.15) | 4.26 (0.16) |
| $^{1}\pi\pi^{*}$ (CZ) | 4.28 (0.00) | 4.27 (0.00) | 4.28 (0.00) | 4.21 (0.00) | 4.27 (0.00) |
| $p(I) \rightarrow Py$] | - | - | 4.36 (0.00) | - | - |
| $\Delta E_{\rm ST}$ | 0.124 | 0.143 | 0.114 | 0.147 | 0.095 |

Table S5. Vertical excitation energies (in eV) to the lowest excited triplet and singlet states and oscillator strengths (in parenthesis) of **Py-Cl**, **Py-Br**, **Py-I**, **Py-BF**₄ and **Py-PF**₆ crystal dimers with two counterions computed at the ω B97X-D/6-31+G(d) level within the TDA. CZ = carbazole. ${}^{3}\pi^{+}\pi^{+*}(Py)$ ' contains ~10% CT (CZ \rightarrow Py). ΔE_{ST} indicates the singlet-triplet energy gap between ${}^{1}\pi\pi^{*}$ (CZ) and the nearest triplet state with some localization on the CZ moiety. Shading of rows to facilitate state character recognition.

| state | Py-Cl | Py-Br | Py-I | Py-BF ₄ | Py-PF ₆ |
|-------------------------------|-------------|-------------|-------------|--------------------|--------------------|
| Triplet state | s | | | | |
| $^{3}\pi\pi^{*}(CZ)$ | 3.59 | 3.57 | 3.60 | 3.51 | 3.59 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.59 | 3.57 | 3.60 | 3.51 | 3.59 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.61 | 3.61 | 3.63 | 3.54 | 3.64 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.61 | 3.61 | 3.63 | 3.54 | 3.64 |
| $^{3}\pi^{+}\pi^{+}*$ (Py) | 4.15 | 4.14 | 4.07 | 3.99 | 4.22 |
| $^{3}\pi^{+}\pi^{+}*$ (Py) | 4.21 | 4.17 | 4.18 | 4.09 | 4.22 |
| $^{3}\pi\pi^{*}$ (CZ) | 4.23 | 4.21 | 4.24 | 4.14 | 4.25 |
| $^{3}\pi\pi^{*}$ (CZ) | 4.23 | 4.21 | 4.24 | 4.14 | 4.26 |
| $^{3}\pi^{+}\pi^{+}*$ (Py)' | 4.41 | 4.39 | 4.34 | 4.25 | 4.47 |
| $^{3}\pi^{+}\pi^{+}*$ (Py)' | 4.46 | 4.43 | 4.41 | 4.34 | 4.47 |
| ${}^{3}[p(I) \rightarrow Py]$ | | | 4.36 | | |
| Singlet state | S | | | | |
| $^{1}\pi\pi^{*}$ (CZ) | 4.38 (0.17) | 4.38 (0.17) | 4.38 (0.19) | 4.31 (0.17) | 4.37 (0.17) |
| $^{1}\pi\pi^{*}$ (CZ) | 4.38 (0.00) | 4.38 (0.00) | 4.38 (0.00) | 4.31 (0.00) | 4.37 (0.00) |
| $^{1}[p(I)\rightarrow Py]$ | | | 4.36 (0.00) | | |
| $\Delta E_{\rm ST}$ | 0.150 | 0.168 | 0.143 | 0.163 | 0.109 |

Table S6. Vertical excitation energies (in eV) to the lowest excited triplet and singlet states and oscillator strengths (in parenthesis) of **Py-I** crystal dimers with two counterions computed at the ω B97X-D/LANL2DZ level within the full (linear response) **TDDFT** and the **TDA**. CZ = carbazole and Py = pyridinium. ΔE_{ST} indicates the singlet-triplet energy gap between ${}^{1}\pi\pi^{*}$ (CZ) and the nearest triplet state with some localization on the CZ moiety. Shading of rows to facilitate state character recognition.

| state | TDA | TDDFT |
|-------------------------------|-------------|-------------|
| Triplet states | | |
| $^{3}\pi\pi^{*}$ (CZ) | 3.75 | 3.38 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.75 | 3.38 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.77 | 3.65 |
| $^{3}\pi\pi^{*}$ (CZ) | 3.77 | 3.65 |
| $^{3}\pi^{+}\pi^{+}*$ (Py) | 4.33 | 4.01 |
| $^{3}\pi^{+}\pi^{+}*$ (Py) | 4.46 | 4.09 |
| ${}^{3}[p(I) \rightarrow Py]$ | 4.22 | 4.22 |
| Singlet states | | |
| $^{1}\pi\pi^{*}$ (CZ) | 4.57 (0.18) | 4.47 (0.17) |
| $^{1}\pi\pi^{*}$ (CZ) | 4.57 (0.00) | 4.47 (0.00) |
| $^{1}[p(I)\rightarrow Py]$ | 4.22 (0.00) | 4.22 (0.00) |
| $\Delta E_{\rm ST}$ | 0.171 | 0.129 |



Figure S27. Molecular orbitals involved in the iodine (HOMO-3) to pyridinium (LUMO) CT transition of **Py-I** computed for the molecular dimer crystal structure.

Table S7. Vertical excitation energies (in eV) to the lowest excited triplet and singlet states and oscillator strengths (in parenthesis) of **Qui-BF**₄ crystal tetramers 1 and 2, TET-1 and TET-2, and hexamer, HEX, as indicated in Figure S18 computed at the ω B97X-D/6-31+G(d) level (full TDDFT linear response). CZ = ${}^{3}\pi\pi^{*}$ carbazole, Qui = ${}^{3}\pi^{+}\pi^{+*}$ quinolinium, CT = ${}^{3}\pi\pi^{+*}$ CZ \rightarrow Qui. ΔE_{ST} indicates the singlet-triplet energy gap between the lowest singlet and the nearest triplet state with some localization on the CZ moiety. Shading of rows to facilitate state character recognition.

| state | TET-1 | TET-2 | state | HEX |
|---------------------|--------------|--------------|----------|--------------|
| Triplet states | | | | |
| Qui & CT | 2.83 | 2.83 | Qui & CT | 2.84 |
| Qui & CT | 2.84 | 2.86 | Qui & CT | 2.84 |
| Qui | 2.88 | 2.86 | Qui & CT | 2.88 |
| Qui | 2.88 | 2.86 | Qui & CT | 2.88 |
| СТ | 3.08 | 3.07 | Qui | 2.96 |
| СТ | 3.08 | 3.07 | Qui | 2.96 |
| CZ | 3.28 | 3.29 | СТ | 3.04 |
| CZ | 3.28 | 3.29 | СТ | 3.04 |
| CZ | 3.29 | 3.29 | CT | 3.08 |
| CZ | 3.29 | 3.29 | СТ | 3.08 |
| СТ | 3.37 | 3.37 | CZ | 3.30 |
| СТ | 3.37 | 3.37 | CZ | 3.30 |
| Singlet states | | | | |
| СТ | 3.16 (0.000) | 3.15 (0.050) | CT | 3.12 (0.056) |
| СТ | 3.16 (0.047) | 3.16 (0.000) | СТ | 3.12 (0.000) |
| CT | 3.49 (0.007) | 3.48 (0.000) | CT | 3.17 (0.000) |
| CT | 3.49 (0.002) | 3.49 (0.009) | CT | 3.17 (0.047) |
| Qui & CZ & CT | 4.22 (0.020) | 4.20 (0.000) | CT | 3.46 (0.001) |
| Qui & CZ & CT | 4.22 (0.000) | 4.23 (0.010) | СТ | 3.46 (0.008) |
| $\Delta E_{\rm ST}$ | 0.085 | 0.083 | | 0.04 |



Figure S28. Representation of the crystal structure of $Qui-BF_4$ hexamer (HEX) with tetramers 1 (TET-1) and 2 (TET-2) indicated in blue and red squares, respectively. CZ = carbazole, Qui = quinolinium.



Figure S29. Example of molecular orbitals involved in the low-lying excited states of **Qui-BF**₄ computed for the crystal structure hexamer showing electron distribution delocalized over quinolinium and carbazole stacked moleties. HOMO-14 (left) and LUMO (right) exhibiting $\pi - \pi^+$ and $\pi^+ - \pi^+$ interactions, respectively.

Table S8. Vertical excitation energies (in eV) to the lowest excited singlet states and oscillator of Qui^+ molecule at the ground (GS geom.) and excited state (ES geom.) minima computed at the ω B97X-D/6-31+G(d) level in DCM solution. Character: Qui⁺ = quinolinium localized exciton, CZ = carbazole localized exciton. Molecular orbital contributions for the two states in their corresponding PES minima are shown in Figure S20.

| state | character | GS geom. | ES geom. |
|-----------------------|------------------|----------|----------|
| S ₁ | Qui ⁺ | 4.22 | 3.56 |
| S_2 | CZ | 4.28 | 4.01 |



Figure S30. Main orbital contributions to the excited singlet states of **Qui**⁺ localized on quinolinium (left) and carbazole (right) moieties at their respective potential energy minima computed at the ω B97X-D/6-31+G(d) level in DCM solution.

Table S9. Low-lying triplet state vertical excitation energies (in eV) and SOCs (in cm⁻¹) to the lowest excited singlet state (S₁) of **Py-Br** and **Py**⁺ (in parenthesis) monomers in the crystal structure computed at the TDDFT ω B97X-D/6-31+G(d) level. $\Delta E(S_1) = 4.27$ (4.28) eV.

| state | ΔE | SOC |
|----------------|-------------|---------------|
| T ₁ | 3.24 (3.23) | 2.299 (2.349) |
| T_2 | 3.49 (3.50) | 0.210 (0.192) |
| T ₃ | 4.01 (4.01) | 0.045 (0.018) |
| T_4 | 4.10 (4.12) | 0.275 (0.016) |
| T ₅ | 4.13 (4.13) | 0.462 (0.475) |
| T ₆ | 4.26 (4.26) | 0.128 (0.049) |
| T ₇ | 4.65 (4.65) | 0.079 (0.081) |
| T ₈ | 4.73 (4.78) | 2.378 (1.089) |
| T9 | 4.79 (4.92) | 1.067 (0.074) |

Table S10. Low-lying triplet state vertical excitation energies (in eV) and SOCs (in cm⁻¹) to the lowest excited singlet state (S₁) of **Qui-Br** and **Qui**⁺ (in parenthesis) monomers in the crystal structure computed at the TDA ω B97X-D/6-31+G(d) level. $\Delta E(S_1) = 4.13$ (4.19) eV.

| state | ΔE | SOC |
|----------------|-------------|----------------|
| T ₁ | 2.71 (2.74) | 1.137 (0.202) |
| T_2 | 3.25 (3.32) | 0.102 (0.159) |
| T ₃ | 3.49 (3.51) | 0.049 (0.015) |
| T_4 | 3.58 (3.58) | 3.634 (1.396) |
| T ₅ | 4.18 (4.18) | 0.086 (0.043) |
| T ₆ | 4.31 (4.31) | 23.541 (0.557) |
| T ₇ | 4.32 (4.32) | 22.267 (0.708) |



Figure S31. (a) HPLC trace of recrystallized 9-H carbazole starting materials. (b) Fluorescence spectrum of recrystallized 9-H carbazole.

| Compound | Py-BF ₄ | Py-Br | Py-Cl | Py -PF ₆ |
|-----------------------|-----------------------|----------------------|----------------------|-----------------------|
| CCDC | 2024261 | 2024263 | 20204262 | 2024264 |
| Empirical formula | $C_{21}H_{21}N_2BF_4$ | $C_{21}H_{23}N_2OBr$ | $C_{21}H_{23}N_2OCl$ | $C_{21}H_{21}N_2PF_6$ |
| Formula weight | 388.21 | 399.32 | 354.86 | 446.37 |
| Temperature/K | 100.15 | 100.15 | 100.15 | 100.15 |
| Crystal system | orthorhombic | orthorhombic | orthorhombic | orthorhombic |
| Space group | Pbca | Pbca | Pbca | Pbca |
| a/Å | 15.42(7) | 15.2783(11) | 15.316(19) | 16.349(7) |
| b/Å | 9.79(5) | 9.6864(7) | 9.637(14) | 9.779(4) |
| c/Å | 25.07(11) | 25.9263(19) | 25.52(4) | 24.784(10) |
| a/° | 90 | 90 | 90 | 90 |
| β/° | 90 | 90 | 90 | 90 |
| γ/° | 90 | 90 | 90 | 90 |
| Volume/Å ³ | 3786(30) | 3836.9(5) | 3767(9) | 3962(3) |
| Z | 8 | 8 | 8 | 8 |
| $\rho_{calc}g/cm^3$ | 1.362 | 1.383 | 1.251 | 1.496 |

Table S11. Summary of crystallographic data

| μ/mm^{-1} | 0.107 | 2.153 | 0.214 | 0.204 |
|------------------------------------|-----------------------------|-----------------------|---------------------------------|-------------------------|
| F(000) | 1616.0 | 1648.0 | 1504.0 | 1840.0 |
| Crystal size/mm ³ | $0.367 \times 0.111 \times$ | 0.33 	imes 0.17 	imes | $0.333 \times 0.09 \times 0.05$ | 0.455 	imes 0.111 	imes |
| | 0.08 | 0.025 | | 0.09 |
| Radiation/Å | 0.71073 | 0.71073 | 0.71073 | 0.71073 |
| $2\theta_{max}$ /° | 52.888 | 56.564 | 53.074 | 61.284 |
| Reflections collected | 15716 | 27795 | 62541 | 56137 |
| Unique reflections | 3810 | 4743 | 3899 | 6096 |
| Goodness-of-fit on F ² | 1.004 | 1.040 | 1.202 | 1.025 |
| Final R ₁ indexes | 0.0915 | 0.0684 | 0.0914 | 0.0495 |
| Final wR (F ²) indexes | 0.1088 | 0.1391 | 0.2063 | 0.0902 |

| Compound | Py-I | Qui-BF ₄ | Qui-Br |
|-----------------------|--------------------|----------------------|--------------------------------|
| CCDC | 2024266 | 2024268 | 2024267 |
| Empirical formula | $C_{21}H_{21}N_2I$ | $C_{25}H_{23}N_2BF4$ | $C_{25}H_{24,22}N_2O_{0.61}Br$ |
| Formula weight | 428.30 | 438.26 | 442.20 |
| Temperature/K | 100.15 | 100.15 | 100.15 |
| Crystal system | orthorhombic | monoclinic | monoclinic |
| Space group | Pbca | $P2_1/n$ | $P2_1/n$ |
| a/Å | 15.18(3) | 10.349(13) | 10.1665(7) |
| b/Å | 9.822(16) | 16.85(2) | 16.1182(13) |
| c/Å | 24.70(4) | 12.139(18) | 13.0048(11) |
| $\alpha/^{\circ}$ | 90 | 90 | 90 |
| β/° | 90 | 101.03(3) | 99.468(4) |
| γ/° | 90 | 90 | 90 |
| Volume/Å ³ | 3683(11) | 2077(5) | 2102.0(3) |

| Z | 8 | 4 | 4 |
|------------------------------------|--------------------------------|---------------------------------|---------------------------|
| $\rho_{calc}g/cm^3$ | 1.545 | 1.401 | 1.397 |
| μ/mm^{-1} | 1.743 | 0.107 | 1.972 |
| F(000) | 1712.0 | 912.0 | 912.0 |
| Crystal size/mm ³ | $0.387 \times 0.1 \times 0.05$ | $0.333 \times 0.09 \times 0.05$ | $0.3\times0.08\times0.07$ |
| Radiation/Å | 0.71073 | 0.71073 | 0.71073) |
| $2\theta_{max}$ /° | 61.176 | 53.084 | 52.79 |
| Reflections collected | 23735 | 24421 | 17071 |
| Unique reflections | 5619 | 4279 | 4277 |
| Goodness-of-fit on F ² | 1.023 | 1.022 | 1.059 |
| Final R ₁ indexes | 0.0643 | 0.1220 | 0.0949 |
| Final wR (F ²) indexes | 0.1138 | 0.1748 | 0.1666 |

| Compound | Ру-А | Py-Cs-BF ₄ | Py-Cs-Br |
|-------------------|--|---------------------------|---|
| CCDC | 2024265 | 2024270 | 2024267 |
| Empirical formula | $C_{21}H_{22.25}B_{0.38}Br_{0.6}F_{1.51}N$ | | C _{21.5} H ₂₃ BrClN ₂ O _{2.5} S |
| | ₂ O _{0.28} | $C_{21}H_{21}BN_2O_2F_4S$ | |
| Formula weight | 388.21 | 452.27 | 497.01 |
| Temperature/K | 100.15 | 100.15 | 120 |
| Crystal system | orthorhombic | monoclinic | triclinic |
| Space group | Pbca | $P2_1/c$ | P-1 |
| a/Å | 15.183(8) | 13.094(2) | 8.1050(6) |
| b/Å | 9.740(5) | 8.1898(14) | 12.2348(9) |
| c/Å | 25.145(15) | 18.731(3) | 23.4041(16) |
| $\alpha/^{\circ}$ | 90 | 90 | 95.281(2) |
| β/° | 90 | 98.965(4) | 95.216(2) |
| γ/° | 90 | 90 | 106.432(2) |

| Volume/Å ³ | 3719(4) | 1984.1(6) | 2199.9(3) |
|------------------------------------|----------------------------------|-------------------------------|---------------------------------|
| Z | 8 | 4 | 4 |
| $\rho_{calc}g/cm^3$ | 1.387 | 1.514 | 1.501 |
| μ/mm ⁻¹ | 1.384 | 0.222 | 2.108 |
| F(000) | 1609.0 | 936.0 | 1016.0 |
| Crystal size/mm ³ | $0.356 \times 0.201 \times 0.09$ | $0.354\times0.157\times0.112$ | $0.354 \times 0.278 \times 0.1$ |
| Radiation/Å | 0.71073 | 0.71073 | 0.71073 |
| $2\theta_{max}$ /° | 61.322 | 61.068 | 61.322 |
| Reflections collected | 24415 | 47914 | 85969 |
| Unique reflections | 5700 | 6051 | 13535 |
| Goodness-of-fit on F ² | 1.066 | 1.008 | 1.010 |
| Final R ₁ indexes | 0.1082 | 0.0350 | 0.0427 |
| Final wR (F ²) indexes | 0.1947 | 0.0891 | 0.0813 |

References

- Foster, E. L.; Tria, M. C. R.; Pernites, R. B.; Addison, S. J.; Advincula, R. C. Soft Matter 2012, 8, 353–359.
- Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. J. Appl. Crystallogr. 2009, 42, 339–341.
- 3. Sheldrick, G. M. Acta Cryst. 2015, A71, 3–8.
- 4. Dias, F. B.; Penfold, T. J.; Monkman, A. P. Methods Appl. Fluoresc. 2017, 5, 012001.
- Yang, J.; Gao, H.; Wang, Y.; Yu, Y.; Gong, Y.; Fang, M.; Ding, D.; Hu, W.; Tang, B.
 Z.; Li, Z. Mater. Chem. Front. 2019, 3, 1391–1397.
- 6. Chai, J.-D.; Head-Gordon, M. Phys. Chem. Chem. Phys. 2008, 10, 6615–6620.
- 7. and, V. B.; Cossi, M. J. Phys. Chem. A. 1998, 102, 1995–2001.
- 8. Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. J. Comput. Chem. 2003, 24, 669-681.
- 9. Truong, T. N.; Stefanovich, E. V. Chem. Phys. Lett. 1995, 240, 253-260.
- 10. Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S.-P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; O'Neill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.; Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt, A.; Stein, T.; Stueck, D.; Su, Y.-C.; Thom, A. J. W.; Tsuchimochi, T.; Vanovschi, V.; Vogt, L.; Vydrov, O.; Wang, T.; Watson, M. A.; Wenzel, J.; White, A.; Williams, C. F.; Yang, J.; Yeganeh, S.; Yost, S. R.; You, Z.-Q.; Zhang, I. Y.; Zhang, X.; Zhao, Y.; Brooks, B. R.; Chan, G. K. L.; Chipman, D. M.; Cramer, C. J.; Goddard, W. A.; Gordon, M. S.; Hehre, W. J.; Klamt, A.; Schaefer, H. F.; Schmidt, M. W.; Sherrill, C. D.; Truhlar, D. G.; Warshel, A.; Xu, X.; Aspuru-Guzik, A.; Baer, R.; Bell, A. T.; Besley, N. A.; Chai, J.-D.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Gwaltney, S. R.; Hsu, C.-P.; Jung, Y.; Kong, J.; Lambrecht, D. S.; Liang, W.; Ochsenfeld, C.; Rassolov, V. A.; Slipchenko, L. V.; Subotnik, J. E.; Van Voorhis, T.; Herbert, J. M.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M.; Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Kus, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L.;

Zimmerman, P. M.; Zuev, D.; Ben Albrecht; Alguire, E.; Austin, B.; Beran, G. J. O.;
Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova,
D.; Chang, C.-M.; Chen, Y.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.;
Diedenhofen, M.; Distasio, R. A.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.; Hanson-Heine, M.
W. D.; Harbach, P. H. P.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T.-C.; Ji, H.; Kaduk, B.; Khistyaev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.;
Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K.

V.; Levchenko, S. V.; Lin, C. Y. Mol. Phys. 2015, 113, 184-215.