Supporting Information

Purely organic room-temperature phosphorescence endowing fast intersystem crossing from through-space spin-orbit coupling

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S1 – General experimental details

All reactions were carried out under nitrogen atmosphere. Starting materials and solvent were used without treatment. 10-(5-iodo-9,9-dimethyl-9H-xanthen-4-yl)-10H-phenothiazine (XPI) and 9-(5-iodo-9,9-dimethyl-9H-xanthen-4-yl)-9H-carbazole (XCI) were prepared according to a previous report. Furthermore, it should be noted that carbazole used in our experiment was made by ourself, according to a previous report. 2-methyltetrahydrofuran was washed with 10% aqueous NaOH, dried, distilled from sodium metal.

1H and 13C spectra were carried out on QOne Instruments Quantum-I 400 M and all NMR data was processed in MestReNova. UV-visible spectra were collected on Shimadzu UV-2600. High resolution mass spectroscopy was carried out on Bruker FTMS. Single crystal XRD of XPF, XPC were carried out on Bruker D8 Venture and XPT was carried out on Rigaku XtaLAB Synergy. DSC-TGA was carried out on PE STA 8000. Cyclic Voltammetry was conducted on CHI760E with 0.1 M tetrabutylammonium hexafluorophosphate in dichloromethane as electrolyte at a scan rate of 100 mV s⁻¹ while Pt plate, glassy carbon and Ag/AgCl electrode were employed as counter electrode, working electrode and reference electrode, respectively.

Phenothiazine (PTZ), dibenzofuran (DBF) and dibenzothiophene (DBT) in spectra characterization were purified through silica gel column chromatography and recrystallization.

S2 – Synthesis and characterization

Abbreviation
Scheme S1. Synthetic routes for XPT, XPF, and XPC, together with abbreviation for segments.

10-(5-(dibenzo[b,d]thiophen-2-yl)-9,9-dimethyl-9H-xanthen-4-yl)-10H-phenothiazine (XPT)

Into a 50 mL two-necked round-bottom flask was added XPI (267 mg, 0.5 mmol), dibenzothiophene-2-boronic acid (148 mg, 0.65 mmol), K₂CO₃ (207 mg, 1.5 mmol), Pd(PPh₃)₄ (17 mg, 0.015 mmol) under nitrogen atmosphere. 15 mL of toluene, 3 mL ethanol and 3 mL H₂O was purged with nitrogen for 30 min, which was transferred into the flask through syringe. The mixture was stirred and refluxed overnight. After cooled to room temperature, saturated solution of NaCl was added and the mixture was extracted with DCM three times. The combined organic layer was dried over sodium sulfate. The solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography using PE/DCM = 6/1 as eluent. Colorless crystal was obtained after recrystallization in DCM and PE in 83% yield (245 mg).

¹H-NMR (400 MHz, CDCl₃) δ 7.19-7.36 (m, 12H), 6.91 (d, 2H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) = 156.43, 155.19, 147.32, 132.70, 131.56, 131.02, 130.89, 129.12
128.75, 126.77, 126.58, 126.20, 125.06, 124.76, 124.59, 123.62, 123.54, 122.34, 121.27, 120.96, 114.62, 111.43, 110.79, 35.10, 31.50.

HRMS (ESI) Calcd. for C_{39}H_{28}NO_{2}S 590.1612, Found 590.1608 [M+H]^+.

10-(5-(dibenzo[b,d]furan-2-yl)-9,9-dimethyl-9H-xanthen-4-yl)-10H-phenothiazone (XPF)
Into a 50 mL two-necked round-bottom flask was added XPI (267 mg, 0.5 mmol), dibenzo[b,d]furan-2-ylboronic acid (138 mg, 0.65 mmol), K_{2}CO_{3} (207 mg, 1.5 mmol), Pd(PPh_{3})_{4} (17 mg, 0.015 mmol) under nitrogen atmosphere. 15 mL of toluene, 3mL ethanol and 3 mL H_{2}O was purged with nitrogen for 30 min, which was transferred into the flask through syringe. The mixture was stirred and refluxed overnight. After cooled to room temperature, saturated solution of NaCl was added and the mixture was extracted with DCM three times. The combined organic layer was dried over sodium sulfate. The solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography using PE/DCM = 6/1 as eluent. Colorless crystal was obtained after recrystallization in DCM and petroleum ether in 61% yield (174 mg).

^{1}H-NMR (400 MHz, CDCl_{3}) δ 7.19-7.36 (m, 12H), 6.91 (d, 2H). ^{13}C NMR (100 MHz, CDCl_{3}) δ (ppm) = 147.37, 139.80, 138.15, 136.00, 135.12, 133.24, 132.78, 131.01, 130.96, 128.64, 126.48, 126.26, 126.15, 125.10, 124.70, 124.09, 123.58, 122.65, 121.90, 121.84, 121.77, 114.48, 35.13, 31.41. HRMS (ESI) Calcd. for C_{39}H_{28}NO_{2}S 574.1841, Found 574.1834 [M+H]^+.

10-(5-(9H-carbazol-9-yl)-9,9-dimethyl-9H-xanthen-4-yl)-10H-phenothiazone (XPC)
Into a 100 mL two-necked round-bottom flask was added XCI (338 mg, 0.67 mmol), phenothiazine (279 mg, 1.4 mmol), K_{2}CO_{3} (793 mg, 5.74 mmol), copper powder (311 mg, 4.9 mmol), 18-Crown-6 (37 mg, 0.14 mmol) under nitrogen atmosphere. 24 mL of dry 1,2-dichlorobenzene was added into the flask through a syringe. The mixture was stirred and refluxed for 72 h. After cooling to room temperature, DCM was added to the solution, which was then filtered to get rid of excess copper powder. The solvent of the filtrate was removed under reduced pressure. The residue was extracted with water
and DCM. The organic layer was dried over Na₂SO₄ and the solvent was evaporated to dryness. The crude product was purified with column chromatography on silica gel using gradient of 10%-17% of DCM in PE. GPC was employed to further purify the compound. Colorless crystal was obtained after recrystallization in DCM and petroleum ether in 56.0% yield (215 mg).

¹H-NMR (400 MHz, CDCl₃) δ 7.19-7.36 (m, 12H), 6.91 (d, 2H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) = 145.96, 140.30, 132.75, 127.44, 125.94, 125.65, 125.18, 124.69, 123.86, 123.21, 119.78, 119.34, 110.07, 35.14, 31.51. HRMS (ESI) Calcd. for C₃₀H₂₉N₂O₅ 573.2001, Found 573.1999 [M+H]⁺.

**S3 – ¹H and ¹³C spectra of new compounds**

![Chart S1. ¹H-NMR spectrum of XPT in CDCl₃.](image-url)
**Chart S2.** $^{13}$C-NMR spectrum of XPT in CDCl$_3$.

**Chart S3.** $^1$H-NMR spectrum of XPF in CDCl$_3$.
Chart S4. $^{13}$C-NMR spectrum of XPF in CDCl$_3$.

Chart S5. $^1$H-NMR spectrum of XPC in CDCl$_3$. 
S4 – High-resolution mass spectra (HRMS)

Chart S6. $^{13}$C-NMR spectrum of XPC in CDCl$_3$.

Chart S7. High-resolution mass spectrum of XPT.
Chart S8. High-resolution mass spectrum of XPF.
**Chart S9.** High-resolution mass spectrum of XPC.

**S5 – TGA and DSC curves**
Chart S10. TGA and DSC curves of XPT in the range from 100 to 400 °C under N\textsubscript{2} atmosphere, the heating rate is 10 °C/min.

Chart S11. TGA and DSC curves of XPF in the range from 100 to 400 °C under N\textsubscript{2} atmosphere, the heating rate is 10 °C/min.

Chart S12. TGA and DSC curves of XPC in the range from 100 to 400 °C under N\textsubscript{2} atmosphere, the heating rate is 10 °C/min.
**S6 – Crystal data and structure refinement**

**Table S1.** Crystal Data and Structure Refinement for XPT.

| Parameter                              | Value                                      |
|----------------------------------------|--------------------------------------------|
| Empirical formula                      | C78 H54 N2 O2 S4                           |
| Formula weight                         | 1179.47                                    |
| Temperature                            | 293(2) K                                   |
| Wavelength                             | 1.54184 Å                                  |
| Crystal system                         | monoclinic                                 |
| Space group                            | P 2\(_{1}/c\)                              |
| Unit cell dimensions                   | a = 7.709 Å alpha = 90 deg.                |
|                                       | b = 36.155(3) Å beta = 91.2600(10) deg.   |
|                                       | c = 20.74770(10) Å gamma = 90 deg.        |
| Volume                                 | 5781.15(6) Å\(^3\)                        |
| Z                                      | 4                                          |
| Density (calculated)                   | 1.355 Mg/m\(^3\)                          |
| Absorption coefficient                 | 1.929 mm\(^{-1}\)                         |
| F(000)                                 | 2464                                       |
| Crystal size                           | 0.11 x 0.09 x 0.06 mm\(^3\)               |
| Theta range for data collection        | 2.456 to 76.522                            |
| Index ranges                           | -9<=h<=9, -45<=k<=44, -18<=l<=26           |
| Reflections collected                  | 39434                                      |
| Independent reflections               | 11689 [R(int) = 0.0490]                    |
| Absorption correction                  | Multi-scan                                 |
| Max. and min. transmission            | 0.7538 and 0.5062                          |
| Refinement method                     | Full-matrix least-squares on F2            |
| Data / restraints / parameters         | 11689 / 0 / 780                            |
| Goodness-of-fit on F2                  | 1.078                                      |
| Final R indices [I>2sigma(I)]          | R1 = 0.0433, wR2 = 0.1244                  |
| R indices (all data)                   | R1 = 0.0489, wR2 = 0.1127                  |
| Largest diff. peak and hole            | 0.504 and -0.577 e.Å\(^{-3}\)             |

**Table S2.** Crystal Data and Structure Refinement for XPF.

| Parameter                              | Value                                      |
|----------------------------------------|--------------------------------------------|
| Empirical formula                      | C39 H27 N O2 S                            |
| Formula weight                         | 573.67                                     |
| Temperature                            | 150.0 K                                    |
| Wavelength                             | 1.54178 Å                                  |
| Crystal system                         | monoclinic                                 |
| Space group                            | C 1 c 1                                    |
| Unit cell dimensions                   | a = 17.1409(9) Å alpha = 90 deg.          |
|                                       | b = 18.2898(11) Å beta = 98.599(4) deg.   |
|                                       | c = 9.1601(5) Å gamma = 90 deg.           |
| Volume                                 | 2839.4(3) Å\(^3\)                        |
### Table S3. Crystal Data and Structure Refinement for XPC.

| Property                                      | Value                                      |
|------------------------------------------------|--------------------------------------------|
| Empirical formula                             | C39 H28 N2 O S                             |
| Formula weight                                 | 572.69                                     |
| Temperature                                   | 150.0 K                                    |
| Wavelength                                    | 1.54178 Å                                  |
| Crystal system                                | monoclinic                                 |
| Space group                                    | P 1 21/n 1                                 |
| Unit cell dimensions                          |                                           |
| a                                             | 12.2936(5) Å                               |
| alpha                                         | 90 deg.                                    |
| b                                             | 18.5682(8) Å                               |
| beta                                          | 114.617(2) deg.                            |
| c                                             | 13.7403(6) Å                               |
| gamma                                         | 90 deg.                                    |
| Volume                                        | 2851.4(2) Å                                |
| Z                                             | 4                                          |
| Density (calculated)                          | 1.334 Mg/m³                                |
| Absorption coefficient                        | 1.283 mm⁻¹                                 |
| F(000)                                        | 1200                                       |
| Crystal size                                  | 0.35 x 0.25 x 0.2 mm³                      |
| Theta range for data collection               | 4.266 to 74.632                            |
| Index ranges                                  | -15<=h<=13, -23<=k<=23, -16<=l<=17         |
| Reflections collected                         | 33955                                      |
| Independent reflections                       | 5763 [R(int) = 0.0284]                     |
| Absorption correction                         | Multi-scan                                 |
| Max. and min. transmission                    | 0.7538 and 0.5885                          |
| Refinement method                             | Full-matrix least-squares on F2            |
| Data / restraints / parameters                | 5763 / 0 / 390                             |
| Goodness-of-fit on F2                         | 1.033                                      |
S7 – Supplementary photophysical data

As the importance of $k_{ISC}$ value discussed in the manuscript, details and calculation equations is expressed here. As we known,

$$\Phi_{ISC} = \frac{k_{ISC}}{k_{ISC} + k_F + k_{IC}} \quad \Phi_F = \frac{k_F}{k_{ISC} + k_F + k_{IC}}$$

considering the non-emissive solution at room temperature and the overwhelming effect of the intersystem crossing decay of singlet excitons, we assume that $\Phi_{ISC} + \Phi_F = 1$.

So, $\Phi_{ISC} = \frac{k_{ISC}}{k_{ISC} + k_F} = k_{ISC} \cdot \tau_F \quad \Phi_F = \frac{k_F}{k_{ISC} + k_F}$

Therefore,

$$k_{ISC} = \frac{1 - \Phi_F}{\tau_F}$$

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**Figure S1.** (Upper) Two different molecular conformations of XPT in single crystal. (Down) Molecular packing of XPT, XPF and XPC.
Figure S2. (a) Delayed PL spectra of XPT crystal at 77 K. The excitation wavelength 380 nm. (b) PL spectra of XPT solution in THF at room temperature. The excitation wavelength is 320 nm. (c) PL spectra of XPT amorphous powder at room temperature. The excitation wavelength is 320 nm.

Figure S3. Decay curve of XPT crystal at 77 K at 495 nm. The excitation wavelength 380 nm.

Figure S4. The prompt time dependent PL spectra of XPT crystal. The excitation wavelength 380 nm.
Figure S5. Delayed PL spectra of XPT crystal (delayed 2 ms) at different temperature. The excitation wavelength 380 nm.

Figure S6. Time dependent decay curves of XPT crystal at 448 nm. The excitation wavelength 377.2 nm.

Figure S7. PL spectra of XPT and DBT in crystal state at 77 K. The delayed spectra delayed 1 ms. The excitation wavelength: XPT, 380 nm; DBT 320 nm.
Figure S8. PL spectra of XPT and DBT in 2-Me-THF solution (Concentration: $10^{-5}$ M) at 77 K. The delayed spectra delayed 1 ms. The excitation wavelength: XPT, 320 nm; DBT, 280 nm.

Figure S9. PL spectra of DBT in crystal. The excitation wavelength is 320 nm.

Figure S10. PL spectra of DBT in 2-Me-THF solution (Concentration: $10^{-5}$ M). The excitation wavelength is 280 nm.
Figure S11. Lifetime of DBT solution in 2-Me-THF at 77 K at 426 nm. The excitation wavelength is 280 nm.

Figure S12. PL spectra of X in THF solution (Concentration: 10^{-5} M) at room temperature. The excitation wavelength is 260 nm.

Figure S13. PL of XPF in crystal state at room temperature. The excitation wavelength is 320 nm.
Figure S14. Lifetime of XPF in crystal state at room temperature at 525 nm. The excitation wavelength is 320 nm.

Figure S15. PL spectra of XPF in 2-Me-THF solution (10^{-5} M) at 77 K. The excitation wavelength is 320 nm.

Figure S16. Lifetime of XPF 2-Me-THF solution (10^{-5} M) at 77 K at 487 nm. The excitation wavelength is 320 nm.
Figure S17. PL spectra of XPF in crystal state at 77 K. The excitation wavelength is 320 nm.

Figure S18. Lifetime of XPF in crystal state at 77 K at 525 nm. The excitation wavelength is 320 nm.

Figure S19. PL spectra of XPC in solution (10^{-5} M). The excitation wavelength is 320 nm. The solvent: RT, THF; 77 K, 2-Me-THF.
Figure S20. Lifetime of XPC in 2-Me-THF solution (10^{-5} M) at 77 K at 495 nm. The excitation wavelength is 320 nm.

Figure S21. PL spectra of XPC in crystal state at room temperature. The excitation wavelength is 400 nm.

Figure S22. Lifetime of XPC in crystal state at room temperature at 515 nm. The excitation wavelength is 400 nm.
**Figure S23.** PL spectra of XPC in crystal state at 77 K. The excitation wavelength is 400 nm.

**Figure S24.** Lifetime of XPC in crystal state at 77 K at 503 nm. The excitation wavelength is 400 nm.

**Figure S25.** PL spectra of XPF, XPT and XPC in crystal state at 77 K. The excitation wavelength is 320 nm for XPF, 380 nm for XPT, 400 nm for XPC.
Figure S26. Delayed PL spectra of XPF, XPT and XPC in crystal state at 77 K (delayed 1 ms). The excitation wavelength is 320 nm for XPF, 380 nm for XPT, 400 nm for XPC.

Figure S27. PL spectra of XPF, XPT and XPC in 2-Me-THF solution at 77 K. The excitation wavelength is 320 nm.

Figure S28. Delayed PL spectra of XPF, XPT and XPC in 2-Me-THF solution at 77 K (delayed 1 ms). The excitation wavelength is 320 nm.
Figure 29. PL spectra of XPF, XPT and XPC crystal at room temperature. The excitation wavelength is 320 nm for XPF, 380 nm for XPT, 400 nm for XPC.

Figure S30. Fluorescence and phosphorescence contribution to PL spectra of XPT crystal at room temperature. The excitation wavelength is 380 nm.

Figure S31. Fluorescence and phosphorescence contribution to PL spectra of XPF crystal at room temperature. The excitation wavelength is 320 nm.
Figure S32. Fluorescence and phosphorescence contribution to PL spectra of XPC crystal at room temperature. The excitation wavelength is 400 nm.

Figure S33. PL spectra of DBF in 2-Me-THF solution (Concentration: $10^{-5}$ M). The excitation wavelength is 280 nm.

Figure S34. PL spectra of DBF in crystal. The excitation wavelength is 290 nm at room temperature and 295 nm at 77 K.
Figure S35. PL spectra of Cz in 2-Me-THF solution (Concentration: $10^{-5} \text{ M}$). The excitation wavelength is 280 nm.

Figure S36. PL spectra of Cz in crystal state at 77 K. The excitation wavelength is 280 nm.

Figure S37. Lifetime of DBF solution in 2-Me-THF at 77 K at 408 nm. The excitation wavelength is 280 nm.
Figure S38. Lifetime of Cz solution in 2-Me-THF at 77 K at 408 nm. The excitation wavelength is 280 nm.

S8 – Cyclic voltammetry

Figure S39. Cyclic voltammetry curve of XPC.

Figure S40 Cyclic voltammetry curve of XPF.
Figure S41. Cyclic voltammetry curve of XPT.

| Compound | XPT   | XPF   | XPC   |
|----------|-------|-------|-------|
| HOMO     | -5.02 eV | -5.03 eV | -4.95 eV |

HOMOs from DFT calculation are \(-5.00, -5.02,\) and \(-4.95\) eV, respectively. HOMO calculated from cyclic voltammetry are \(-5.02, -5.03,\) and \(-4.95\) eV, respectively. For XPC, the values of HOMO from cyclic voltammetry and DFT are the same. As for a reversible oxidation profile, the value of HOMO is calculated as follows. First, the average of oxidation peak and reduction peak of phosphors was calculated. The average of oxidation peak and reduction peak of ferrocene was also calculated. Then, the difference between the two averages was calculated and denoted by \(E_{\text{OX}}\). The oxidation value of ferrocene is \(-4.8\) eV. Finally, HOMO of the phosphors was calculated according to the following equation: \(HOMO = -(4.8 + E_{\text{OX}})\) eV.

S9 – Density functional theory calculation

Based on the optimized geometry of ground (S\(_0\)) state, the excited-state electronic structures of compounds XPT, XPF and XPC were evaluated at the (TD)B3LYP/6-31G* level using the Gaussian 09 package\(^3\), including the excitation energies and natural transition orbitals (NTOs). At the same level, the spin-orbit coupling matrix elements (\(\zeta\)) between singlet and triplet excited states were calculated by the Beijing Density Function (BDF) program\(^4,5\).
Figure S42. Calculated energy diagram, spin-orbit coupling (SOC) matrix element values of XPF and XPC.

Table S4. Computed Cartesian coordinates of XPT

|     | X        | Y        | Z        |
|-----|----------|----------|----------|
| S   | -2.07509451 | -3.20436200 | 1.39295968 |
| S   | -4.44357426 | 2.28788827  | 0.90092568 |
| O   | 1.80242207  | 0.30859139  | -0.39714593 |
| N   | 0.61940320  | -2.02665841 | 0.59529416 |
| C   | -0.22215225 | -2.37403848 | -0.48967485 |
| C   | -2.17362782 | 1.81011290  | -0.37514313 |
| C   | 2.02930766  | -1.92952012 | 0.35605555 |
| C   | -0.79372941 | 1.84269853  | -0.60612097 |
| H   | -0.38759462 | 1.38755332  | -1.50062299 |
| C   | -1.16540453 | -1.95386433 | 2.27616801 |
| C   | -3.22615718 | 1.24818772  | -1.20727245 |
| C   | 3.99778057  | -0.69851658 | -0.41522736 |
| C   | 0.06028344  | 2.47814893  | 0.29516529 |
| C   | 0.10621261  | -1.55532185 | 1.82967877 |
| C   | 0.21841748  | -2.27325081 | -1.81626018 |
| H   | 1.21907181  | -1.91974289 | -2.0267456 |
| C   | 2.62482917  | -0.76450442 | -0.15168553 |
| C   | -1.52253238 | -2.85944105 | -0.26363590 |
| C   | 2.83439872  | -3.03176292 | 0.63175070 |
| H   | 2.36375047  | -3.92423937 | 1.02578161 |
| C   | 4.77607266  | -1.81712716 | -0.10840371 |
| H   | 5.84276015  | -1.79432889 | -0.28850620 |
| C   | 1.51459819  | 2.63622353  | 0.02278676 |
| C   | 4.20575729  | -2.97449085 | 0.41302003 |
| H   | 4.82862487  | -3.83183461 | 0.63842814 |
| C   | 2.36318820  | 1.57456701  | -0.3342398 |
| C   | 3.72490804  | 1.75426105  | -0.60476513 |
| C   | -0.48544152 | 3.05989264  | 1.45754018 |
|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| S   | 1.03740115| -3.98767011| 0.5656688 |
| O   | -1.81712269| 0.56011145| -0.35801933|
| O   | 4.30606178| -0.09838444| -1.46182202|
| N   | -1.24922814| -1.98135033| 0.60123435|
| C   | -4.32829504| 1.89395340| -0.08706267|
| C   | -1.01733445| -2.59265806| -0.65560294|
| C   | -3.00638664| 2.65836413| -0.23346976|
| C   | -2.51723658| -1.35298065| 0.83460886|
| C   | 3.05212827| 0.45496589| -1.35464558|
| C   | -4.04214548| 0.54704323| 0.58437733|
| C   | 0.73421603| 0.69638920| -1.76747561|
| C   | -0.16894147| 0.36826603| -2.26309794|
| C   | -2.80490724| -0.06370960| 0.35722363|
| C   | 0.67798398| 1.80431859| -0.89553063|
| C   | -4.71303333| -1.43257255| 1.83069024|
| H   | -5.46214529| -1.96002405| 2.40893208|
| C   | -1.82116150| 1.94136002| -0.42751489|
| C   | -0.58565087| 2.56233633| -0.68823055|
| C   | -0.18657323| -1.68782553| 1.49617957|
| C   | 1.84416294| 2.22640946| -0.24732663|
| H   | 1.80777050| 3.05962357| 0.44457490|
| C   | -1.72963502| 4.70188375| -0.51608067|
| H   | -1.69563928| 5.78441481| -0.55529721|
| C   | 0.06354430| -3.47515755| -0.83302313|
| C   | -4.98251371| -0.15843781| 1.34094457|
| H   | -5.94865492| 0.28471747| 1.54363102|
| C   | -0.57452556| 3.96141347| -0.73326527|
| H   | 0.35834608| 4.46563654| -0.95582918|
| C   | 1.91719899| 0.00728542| -2.00997822|
| H   | 1.94952372| -0.84673951| -2.67366635|
| C   | 3.04241706| 1.55004976| -0.47675999|
| C   | 0.96602986| -2.49097759| 1.52761843|
| C   | 2.02305322| -2.18686787| 2.38181679|
| H   | 2.90912779| -2.81099684| 2.36303020|
| C   | -1.85804700| -2.35993437| -1.75240412|
| H   | -2.71258938| -1.70786308| -1.64147156|
| C   | 5.08815249| 2.52852352| 0.87161103|
| H   | 4.56759126| 3.33182002| 1.38036055|
| C   | -5.37419153| 2.70625833| 0.69748845|
| H   | -5.03020872| 2.93378727| 1.70903171|
|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| S | 3.14888662    | -2.97535700   | -0.98152744   |
| O | -1.38508134   | -0.03406511   | 0.21557159    |
| N | 0.13744163    | 2.23043626    | 0.69351831    |
| N | 0.24967076    | -2.05286987   | -0.81633772   |
| C | -1.16898610   | -2.04625291   | -1.01572308   |
| C | 1.03175694    | 2.93089823    | -0.12305358   |
| C | 2.34437378    | 2.75602665    | 0.37761000    |
| C | -2.00034433   | -1.04707229   | -0.48300228   |
| C | -2.05433173   | 1.16040375    | 0.34974375    |
| C | 0.75740491    | -2.63581640   | 0.37178400    |

Table S6. Computed Cartesian coordinates of XPC
C  0.86164714  1.6333206  1.73075732
C  2.10441145 -3.02869787  0.45930074
C -1.25722387  2.30381001  0.59545583
C -1.74544192 -3.0772273  -1.75221341
H  -1.09387144 -3.83917313 -2.16072073
C  1.06489536 -1.29859054 -1.69745865
C  -3.9042317 -1.08750697 -0.63998484
C  -3.44880089  1.23314616  0.24991704
C  2.23524828  1.92984887  1.56113170
C  0.52731995 -0.28145307 -2.49530653
H  -0.52988380 -0.06263120 -2.44194017
C  2.44009403 -1.56591286 -1.80782055
C  0.40267424  0.88691829  2.81455607
H  -0.65019797  0.67130272  2.94278745
C  -1.91256734  3.53800790  0.72437922
H  -1.30793903  4.41418986  0.92337807
C  -3.92843488 -2.13076323 -1.39880217
H  -4.99840853 -2.18764750 -1.54859460
C  -4.04745287  2.49072214  0.35968361
H  -5.12208663  2.58243154  0.27728743
C  3.41780436  3.35628048 -0.28555984
H  4.42997854  3.22862820  0.08179407
C  -0.06416468 -2.86090247  1.48357806
H  -1.10821398 -2.58499714  1.44043420
C  0.77967500  3.69118347 -1.26474985
H  -0.22613910  3.81644736 -1.64586425
C  -3.11966889 -3.11500484 -1.95661785
H  -3.56185004 -3.91523125 -2.53784718
C  -4.24912549 -0.06578027  0.11231751
C  2.61091099 -3.57437780  1.63616640
C  3.66005198 -3.84393034  1.67933745
C  3.16236766  1.44611421  2.48826801
H  4.21894664  1.65968489  2.37057847
C  3.24669492 -0.80490500 -2.65013594
H  4.30842256 -1.01953613 -2.69419693
C  1.33132899  0.44633411 -3.36774005
H  0.88314001  1.22482715 -3.97346542
C  1.34486810  0.42174303  3.72453007
H  1.01459076 -0.16875955  4.57130189
C  2.71183842  0.69296283  3.56486208
H  3.42051190  0.30890095  4.28924964
C  -3.29135495  3.63507572  0.59100658
H  -3.77934013  4.59779625  0.68493097
C  0.43729586 -3.45112009  2.64027096
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