Supporting Information for

D-A type luminophores with twisted molecular conformation constructed by phenoxazine and diphenylsulfone showing high contrast mechanofluorochromism

Hongke Zhou,a Zhan Zhang,a Xingliang Liu,a Defang Xu,b* Weidong Zhang,a Shengjie Fu,a Xiucun Fenga and Qian Huanga

aSchool of Chemical Engineering, Qinghai University, Xining 810016, China
bState Key Laboratory of Plateau Ecology and Agriculture, Qinghai University, Xining 810016, China

E-mail address: xudefang123@163.com.
Table S1. Crystallographic experimental details for PTZ-DPS (CCDC 1969955) and BPTZ-DPS (CCDC 1969954).

<table>
<thead>
<tr>
<th>Compound</th>
<th>PTZ-DPS</th>
<th>BPTZ-DPS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C_{28}H_{22}BrNO_{3}S</td>
<td>C_{44}H_{36}N_{2}O_{4}S</td>
</tr>
<tr>
<td>Formula weight</td>
<td>532.43</td>
<td>688.81</td>
</tr>
<tr>
<td>Temperature/K</td>
<td>293.51(10)</td>
<td>293.50(10)</td>
</tr>
<tr>
<td>Crystal system</td>
<td>triclinic</td>
<td>monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>P-1</td>
<td>P2/c</td>
</tr>
<tr>
<td>a/Å</td>
<td>9.9624(5)</td>
<td>13.9869(6)</td>
</tr>
<tr>
<td>b/Å</td>
<td>13.4464(7)</td>
<td>5.09616(15)</td>
</tr>
<tr>
<td>c/Å</td>
<td>19.3712(10)</td>
<td>24.4610(8)</td>
</tr>
<tr>
<td>α/°</td>
<td>87.677(4)</td>
<td>90</td>
</tr>
<tr>
<td>β/°</td>
<td>76.294(5)</td>
<td>104.972(4)</td>
</tr>
<tr>
<td>γ/°</td>
<td>73.020(5)</td>
<td>90</td>
</tr>
<tr>
<td>Volume/Å³</td>
<td>2410.0(2)</td>
<td>1684.38(11)</td>
</tr>
<tr>
<td>Z</td>
<td>43.384</td>
<td>2</td>
</tr>
<tr>
<td>ρ_{calc} g/cm³</td>
<td>1.467</td>
<td>1.358</td>
</tr>
<tr>
<td>μ/mm⁻¹</td>
<td>3.384</td>
<td>1.248</td>
</tr>
<tr>
<td>F(000)</td>
<td>1088.0</td>
<td>724.0</td>
</tr>
<tr>
<td>Crystal size/mm³</td>
<td>0.13 × 0.11 × 0.07</td>
<td>0.19 × 0.15 × 0.12</td>
</tr>
<tr>
<td>Radiation</td>
<td>CuKα (λ = 1.54184)</td>
<td>CuKα (λ = 1.54184)</td>
</tr>
<tr>
<td>2Θ range for data collection/°</td>
<td>20.088 to 133.198</td>
<td>7.482 to 133.188</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-11 ≤ h ≤ 9, -15 ≤ k ≤ 14, -23 ≤ l ≤ 20</td>
<td>-16 ≤ h ≤ 16, -6 ≤ k ≤ 3, -29 ≤ l ≤ 28</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>15163</td>
<td>5537</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>8403 [R_{int} = 0.0284, R_{sigma} = 0.0399]</td>
<td>2963 [R_{int} = 0.0163, R_{sigma} = 0.0221]</td>
</tr>
<tr>
<td>Data/restraints/parameters</td>
<td>8403/0/615</td>
<td>2963/0/232</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.021</td>
<td>1.059</td>
</tr>
<tr>
<td>Final R indexes [I&gt;=2σ (I)]</td>
<td>R₁ = 0.0472, wR₂ = 0.1251</td>
<td>R₁ = 0.0405, wR₂ = 0.1054</td>
</tr>
<tr>
<td>Final R indexes [all data]</td>
<td>R₁ = 0.0629, wR₂ = 0.1391</td>
<td>R₁ = 0.0500, wR₂ = 0.1140</td>
</tr>
<tr>
<td>Largest diff. peak/hole / e Å⁻³</td>
<td>0.33/-0.65</td>
<td>0.17/-0.29</td>
</tr>
</tbody>
</table>
Fig. S1 Maximum emission wavelengths of PXZ-DPS (a) and BPXZ-DPS (b) upon repeating treated by grinding and fuming with DCM.

Fig. S2 $^1$H NMR (400 MHz) spectrum of PXZ-DPS.
Fig. S3 $^1$H NMR (400 MHz) spectrum of PXZ-DPS.

Fig. S4 $^{13}$C NMR (100 MHz) spectrum of PXZ-DPS.
Fig. S5 MALDI/TOF MS spectrum of PXZ-DPS.

Fig. S6 $^1$H NMR (400 MHz) spectrum of BPXZ-DPS.
Fig. S7 $^1$H NMR (400 MHz) spectrum of BPXZ-DPS.

Fig. S8 $^{13}$C NMR (100 MHz) spectrum of BPXZ-DPS.
Fig. S9 MALDI/TOF MS spectrum of BPXZ-DPS.