Supporting Information

A dual fluorescent/phosphorescent zincophosphite with interesting water adsorption and structural transformation properties

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Fig. S1 X-ray powder pattern of NTOU-6 (top). Powder pattern simulated on the basis of the atomic coordinates derived by single-crystal X-ray diffraction (bottom).

Fig. S2 TGA curve for NTOU-6 in N2 at 5 °C min⁻¹ from 40 to 550°C.
Fig. S3 X-ray powder patterns of NTOU-6 for thermal-stability testing: simulated, as-synthesized, holding for 1 h at 100°C, 200°C, and 250°C.

Fig. S4 X-ray powder patterns of NTOU-6 for chemical-stability studies conducted by suspending the powder samples in organic solvents for several days: (a) hexane, (b) ethanol, (c) methanol, and (d) DMF.
Fig. S5 The X-ray powder patterns of NTOU-6 for the water-stability testing.

Fig. S6 NTOU-6 with 4-, and 8- member rings alone b axis.
**Fig. S7** The 12-membered rings in compound NTOU-6b made up of two [ZnO$_2$(H$_2$O)$_4$]$^{2-}$ groups, four ZnO$_4$ units, and six HPO$_3$ tetrahedra.

**Fig. S8** Comparison of the emission and excitation spectra for the title compound and triazole molecules.
Fig. S9 Emission spectra of repeated excitation showing the photostability of NTOU-6.

Fig. S10 Reproducibility test for NTOU-6 at different excitation wavelengths by using different batches.
**Fig. S11** Thermostability test on NTOU-6 by comparing the emission spectra before and after heating. Experimental conditions: the compound was heated to 100°C and held for 1 hour, then cooled to room temperature before recording the fluorescence spectra.

**Table S1.** The lifetime for NTOU-6 and triazole ligands in the solid state.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Ex: 350 nm/Em: 420 nm</th>
<th>Ex: 350 nm/Em: 520 nm</th>
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<tbody>
<tr>
<td>NTOU-6</td>
<td>1.75 ns</td>
<td>0.9 μs</td>
</tr>
<tr>
<td></td>
<td>$\chi^2$: 1.29</td>
<td>$\chi^2$: 1.20</td>
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<tr>
<td>Triazole</td>
<td>2.79 ns</td>
<td>3.58 ns</td>
</tr>
<tr>
<td></td>
<td>$\chi^2$: 1.25</td>
<td>$\chi^2$: 1.33</td>
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