A new layered aluminoborate \([\text{Zn(dien)}_2]_2[\text{Al(OH)}_2\text{B}_5\text{O}_9\text{F}]\) templated by transition metal complex

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### Table S1. Hydrogen bonds for 1 [Å and °].

<table>
<thead>
<tr>
<th>D-H···A</th>
<th>d(D-H)</th>
<th>d(H···A)</th>
<th>d(D···A)</th>
<th>&lt;(DHA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1-H1E···F1#1</td>
<td>0.84</td>
<td>2.13</td>
<td>2.596(9)</td>
<td>115</td>
</tr>
<tr>
<td>N1-H1A···F1#2</td>
<td>0.92</td>
<td>2.01</td>
<td>2.926(9)</td>
<td>176</td>
</tr>
<tr>
<td>N1-H1B···O7#3</td>
<td>0.92</td>
<td>2.11</td>
<td>3.017(10)</td>
<td>169</td>
</tr>
<tr>
<td>N2-H2C···O1#3</td>
<td>0.93</td>
<td>2.19</td>
<td>3.077(10)</td>
<td>159</td>
</tr>
<tr>
<td>N3-H3B···O8#4</td>
<td>0.92</td>
<td>2.17</td>
<td>3.026(9)</td>
<td>154</td>
</tr>
<tr>
<td>N3-H3A···O9</td>
<td>0.92</td>
<td>2.01</td>
<td>2.921(10)</td>
<td>171</td>
</tr>
<tr>
<td>N4-H4A···O10#4</td>
<td>0.92</td>
<td>2.28</td>
<td>3.152(9)</td>
<td>158</td>
</tr>
<tr>
<td>N4-H4A···O8#4</td>
<td>0.92</td>
<td>2.29</td>
<td>3.049(9)</td>
<td>140</td>
</tr>
<tr>
<td>N4-H4B···O3#3</td>
<td>0.92</td>
<td>2.04</td>
<td>2.952(9)</td>
<td>169</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms: (#1) x-1, -y+1, z-1/2; (#2) x+1, -y+1, z+1/2; (#3) x+1, y, z+1; (#4) x, -y+2, z+1/2.

Fig. S1 View of the linkages of B5O9F cluster (a) and AlO3(OH) unit (b).

Fig. S2 (a) Elliptical 11-MR opening (H atoms of OH groups are omitted for clarity). (b) The mer-[Zn(dien)]^{2+} cation in 1 (H atoms bonded to C and N atoms have been omitted for clarity).
Fig. S3 Viewed along the [10-1] direction, showing parallel stacking.

Fig. S4 [Zn(dien)$_2$]$^{2+}$ cations located in the channels, showing same chiral configuration.
Fig. S5 (a) UV-vis optical diffuse reflectance spectra for 1. (b) The solid-state emission spectra of 1 at room temperature.

Fig. S6 Contour plots and orbital gaps of frontier orbital for (a) [Zn(dien)$_2$]$^{2+}$ cation and (b) [{Al(OH)}${B_5O_9F}$]$^{2-}$ species, respectively.

Fig. S7 TG curve of 1.
The symmetric stretching vibrations of N-H are observed in the range of 3322-3185 cm\(^{-1}\). The absorption peak at 1601 cm\(^{-1}\) is related to the asymmetric stretching vibrations and symmetric bond-bending vibrations of N-H and C-H bonds. The vibration absorption region of 1422-1207 cm\(^{-1}\) is due to B-O bond asymmetric stretching of BO\(_3\) units, while that of BO\(_4\) units appears in the range 1145-1028 cm\(^{-1}\). The presence of an absorption peak at 852 cm\(^{-1}\) originates from vibration of AlO\(_4\) units.\(^1\)

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Fig. S10 EDS spectrum of 1.