Electronic Supplementary Material for CrystEngComm
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Supporting Information:

A new layered aluminoborate $[Zn(dien)_2][\{Al(OH)\}\{B_5O_9F\}]$ templated by transition metal complex

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

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

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.

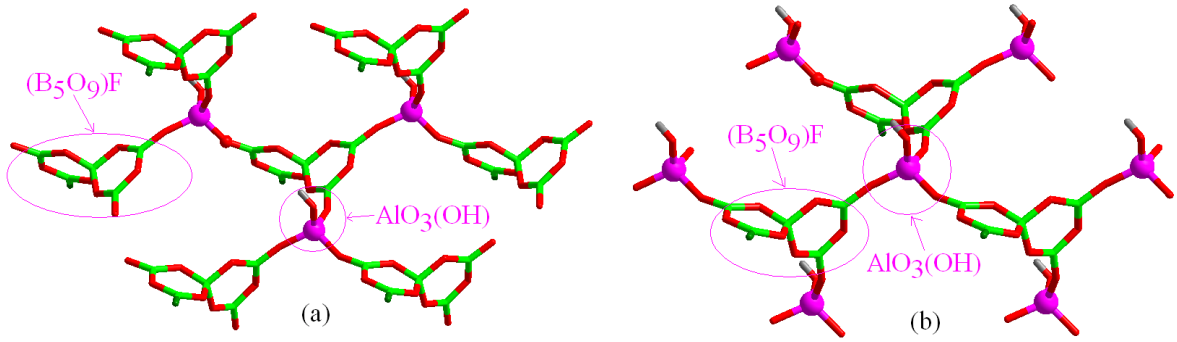


Fig. S1 View of the linkages of B_5O_9F cluster (a) and $AlO_3(OH)$ unit (b).

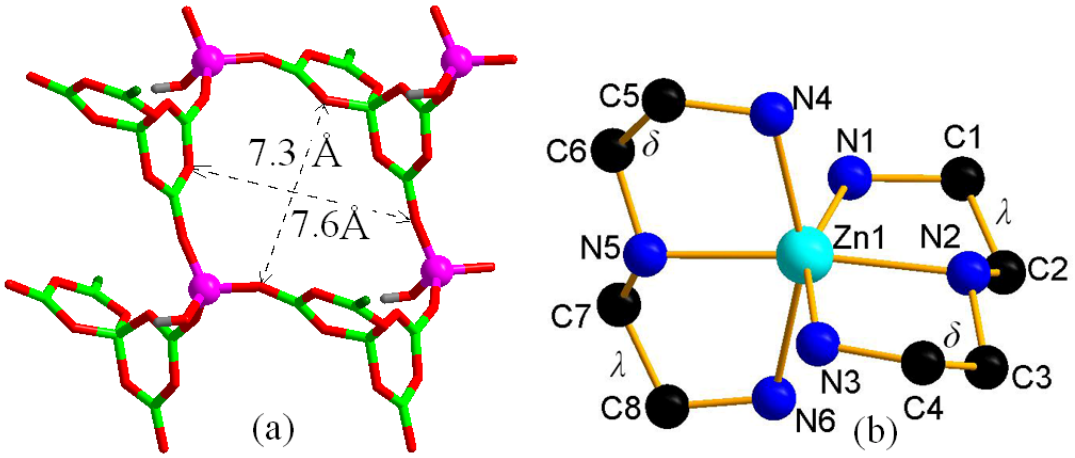


Fig. S2 (a) Elliptical 11-MR opening (H atoms of OH groups are omitted for clarity). (b) The *mer*-$[Zn(dien)_2]^{2+}$ cation in **1** (H atoms bonded to C and N atoms have been omitted for clarity).

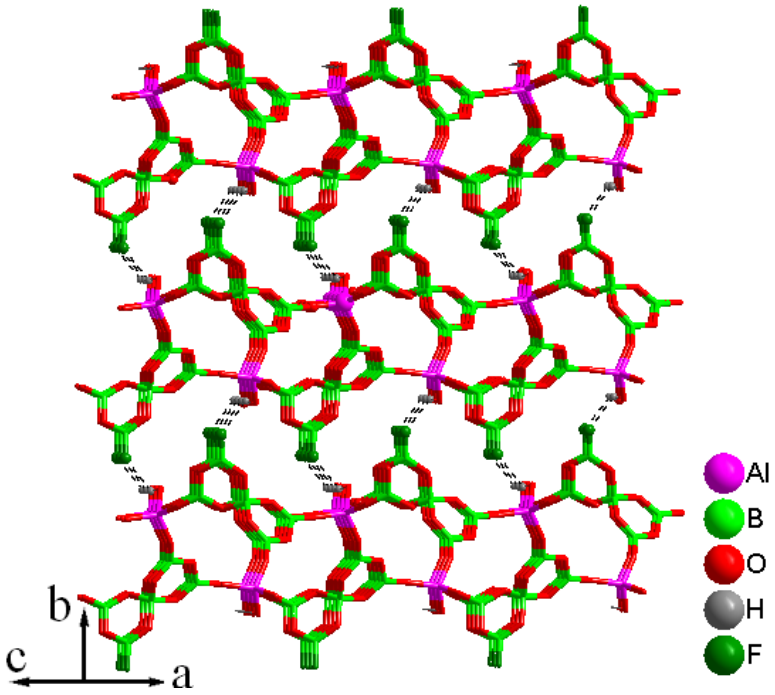


Fig. S3 Viewed along the [10-1] direction, showing parallel stacking.

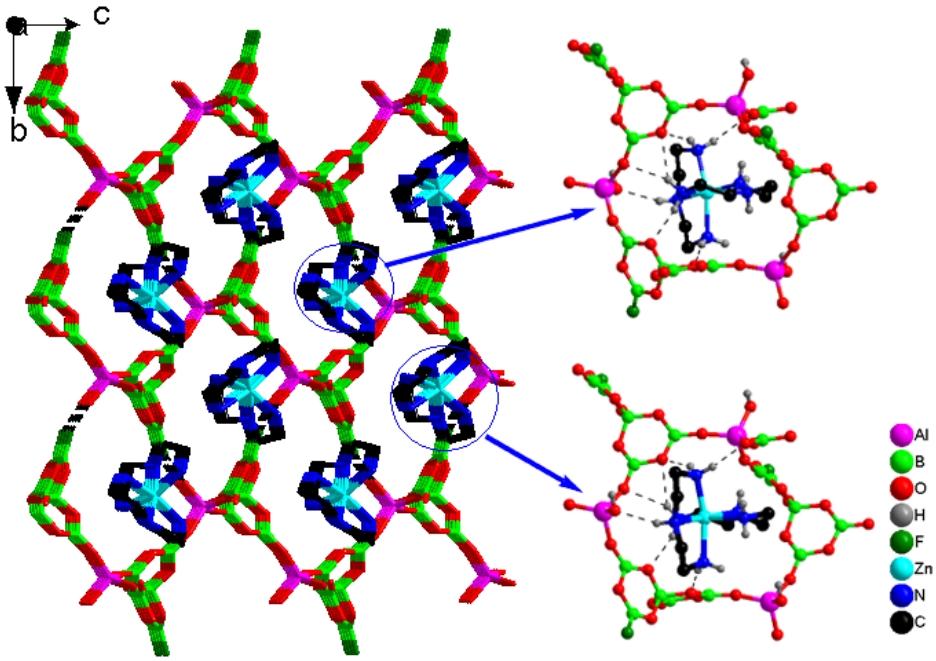
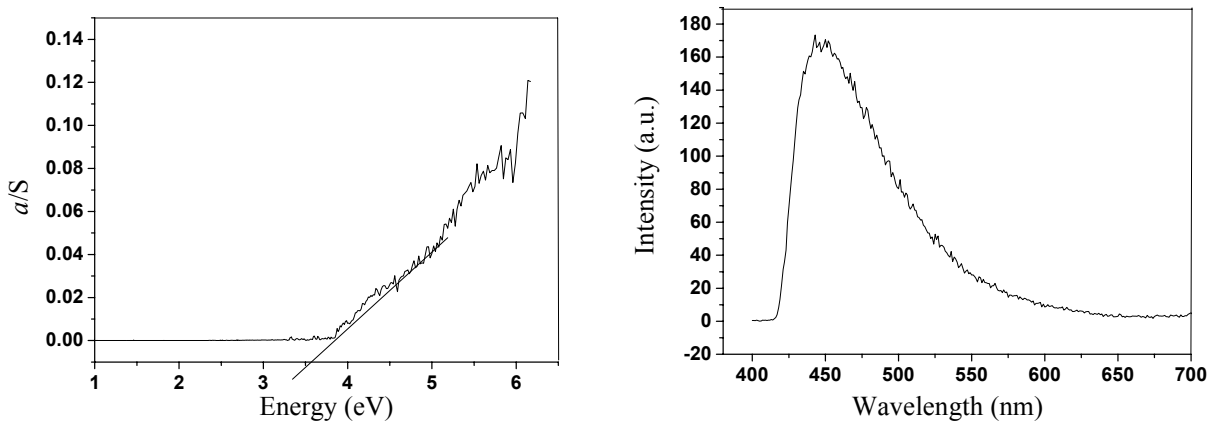
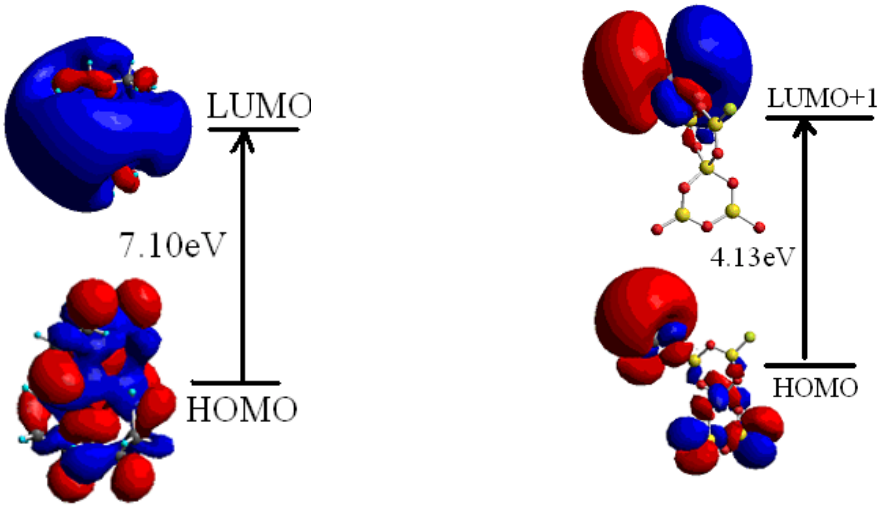


Fig. S4 $[Zn(dien)_2]^{2+}$ cations located in the channels, showing same chiral configuration.



(a) (b)

Fig. S5 (a) UV-vis optical diffuse reflectance spectra for **1**. (b)The solid-state emission spectra of **1** at room temperature.



(a) (b)

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.

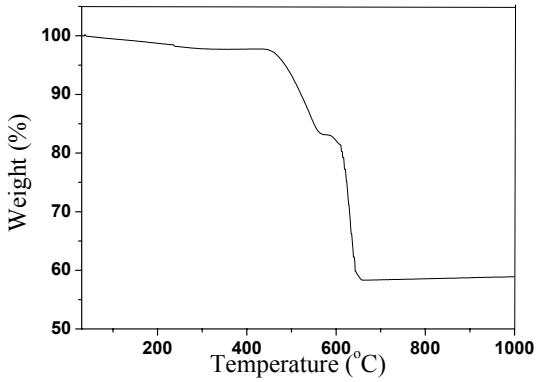


Fig. S7 TG curve of **1**.

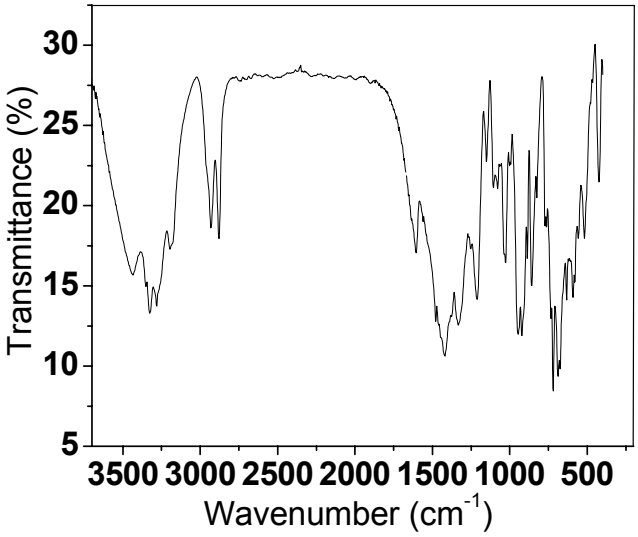


Fig. S8 IR spectrum of **1**.

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 1422-1207cm^{-1} is due to B-O bond asymmetric stretching of BO_3 units, while that of BO_4 units appears in the range 1145-1028cm^{-1}. The presence of an absorption peak at 852 cm^{-1} originates from vibration of AlO_4 units.[1]

1. H. S. Song, J. Zhang, J. Lin, S. J. Liu, J. J. Luo, Y. Huang, E. M. Elssfah, A. Elsanousi, X. X. Ding, J. M. Gao, and C. Tang, *J. Phys. Chem. C,* **2007**, 111, 1136.

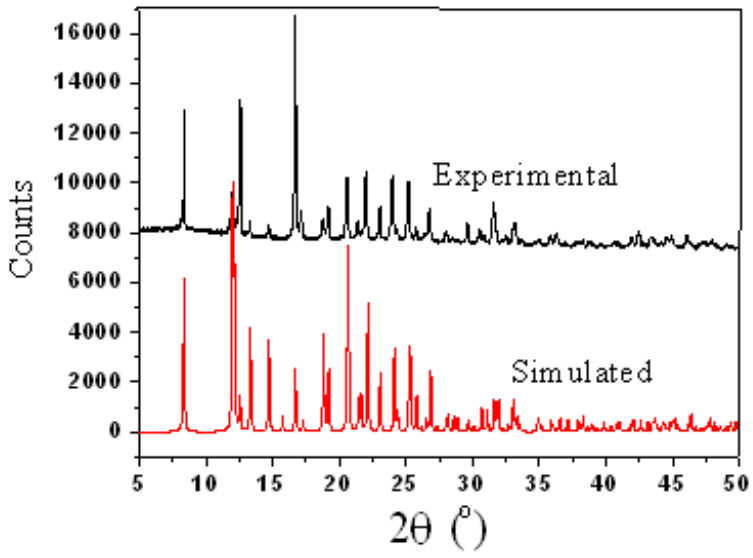


Fig. S9 Simulated and experimental powder XRD patterns of **1**.

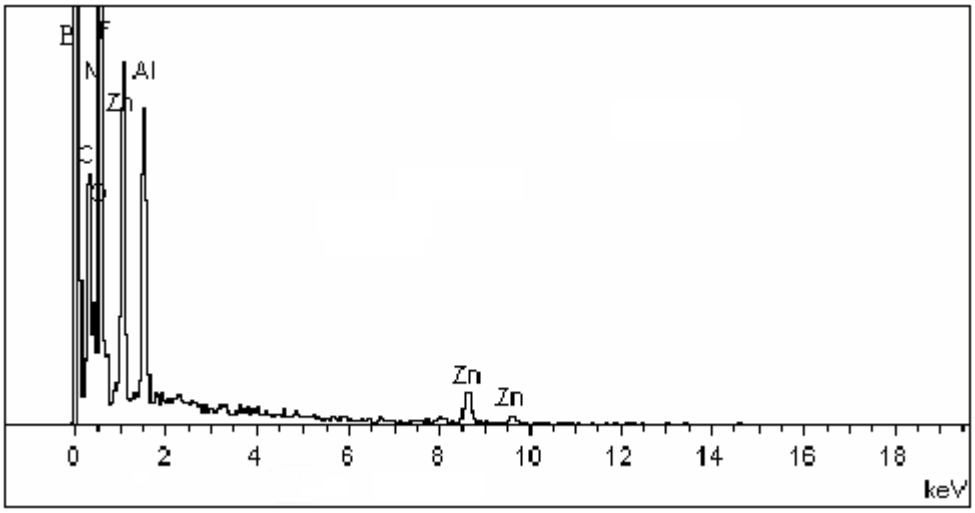


Fig. S10 EDS spectrum of **1**.