

Supporting Information for

New 3-D polyoxovanadoborate architectures based on $[V_{12}B_{18}O_{60}]^{16-}$ clusters

Jian Zhou,* Xing Liu, Rong Chen, Hong-Ping Xiao, Feilong Hu, Huahong Zou, Yun Zhou, Chun

Liu, and Ligang Zhu

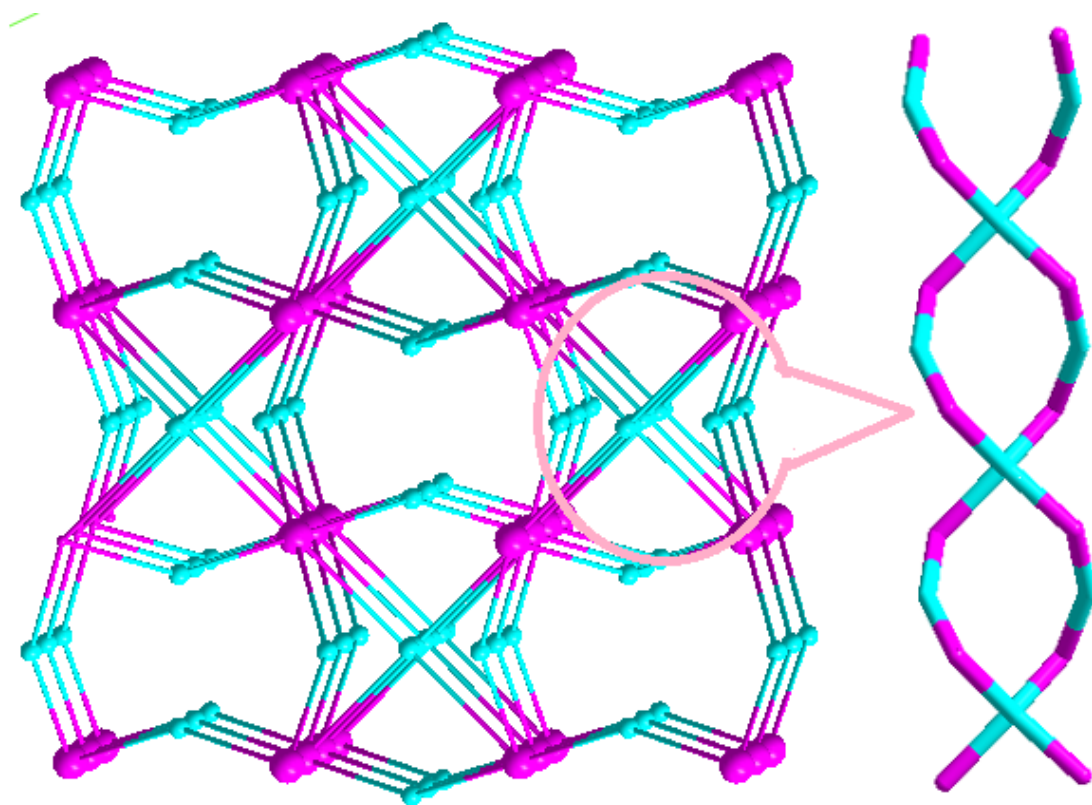


Fig. S1 View of the 3-D simplified framework of **2**, showing the helical channels.

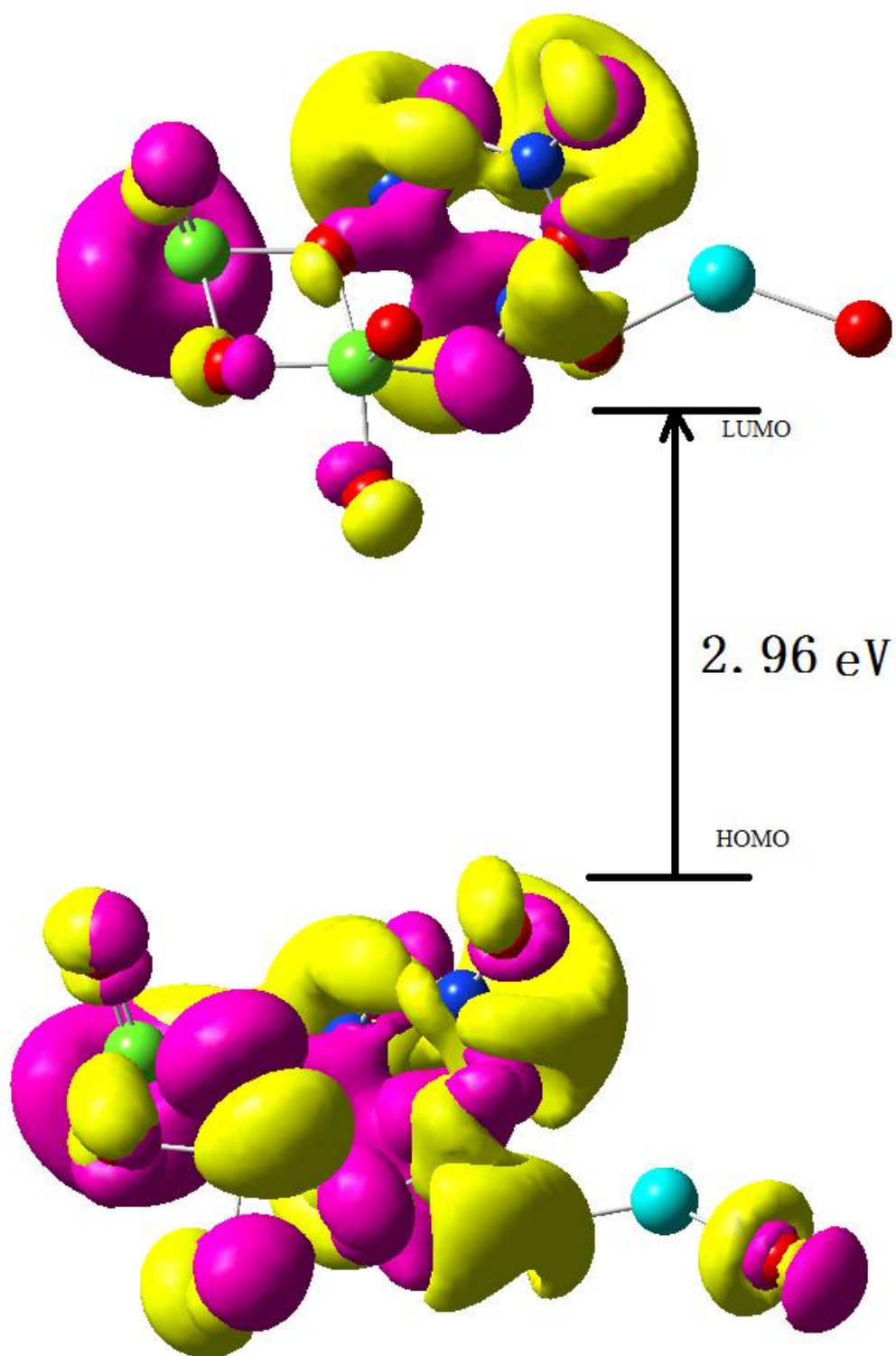
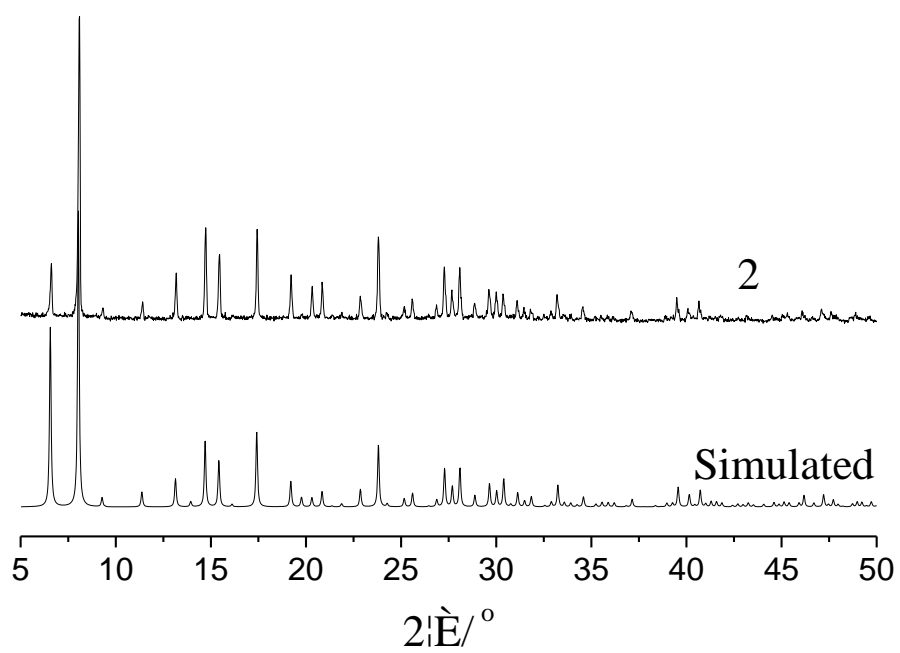
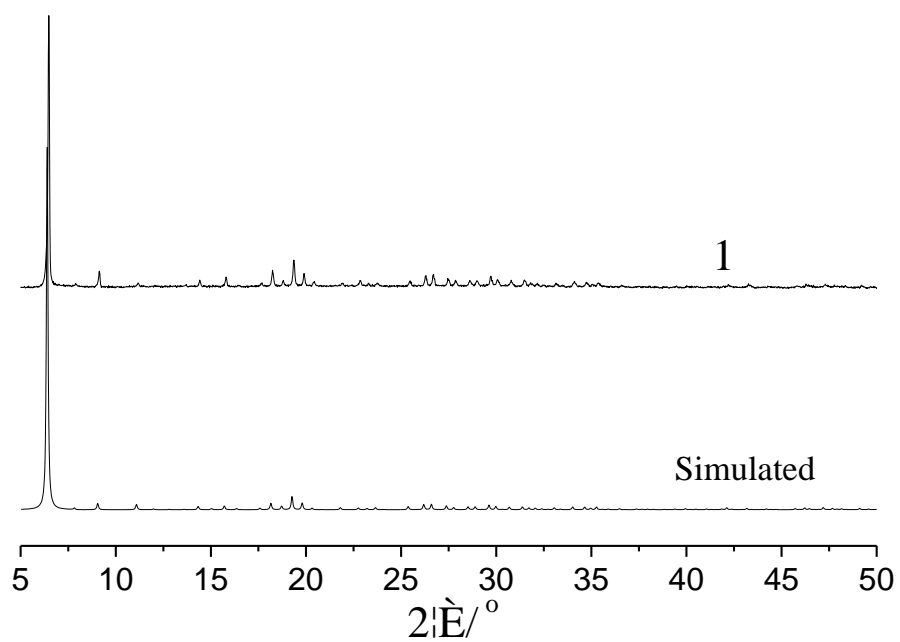


Fig. S4 Contour plots and orbital gaps of frontier orbital for [CdB₃V₂O₁₁]
species.



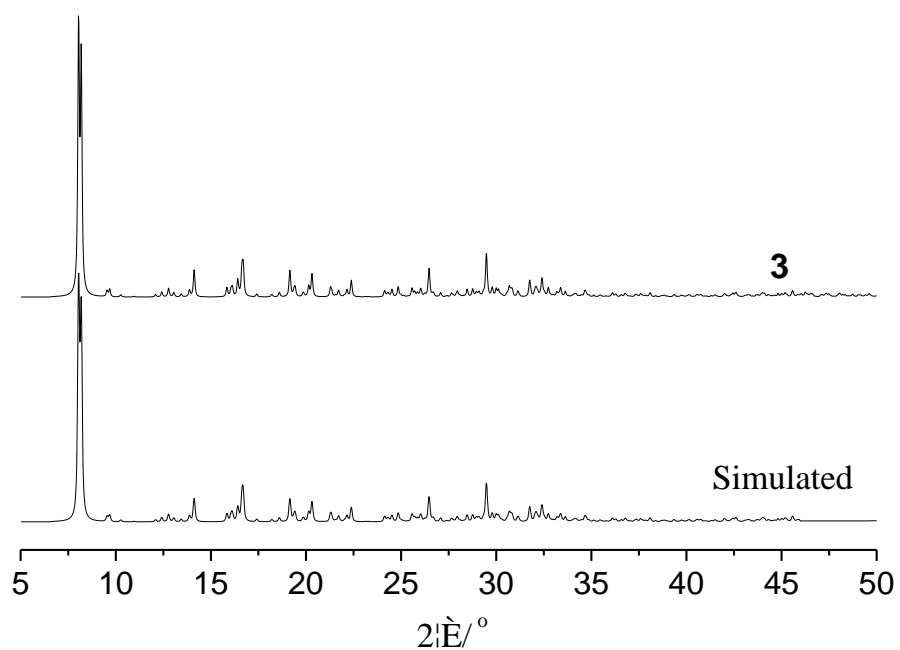


Fig. S4 Simulated and experimental powder XRD patterns of **1 - 3**.

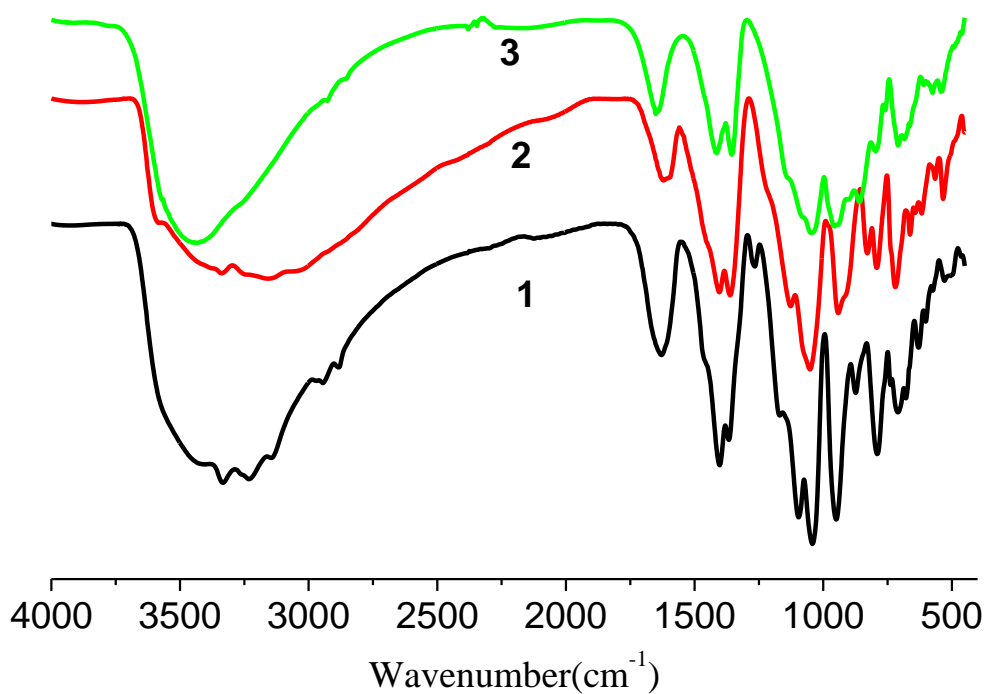


Fig. S5 IR spectra of **1-2**.

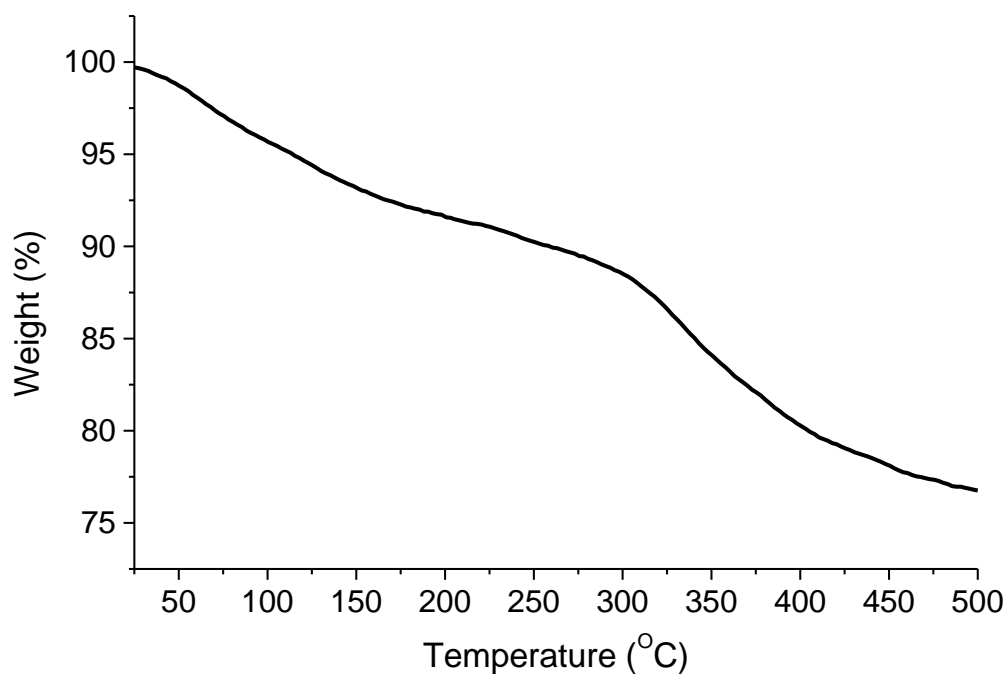


Fig. S6 TG curve of **1**.

As shown in Fig. S6, a two-step weight loss occurs in the range of 25-475 °C which is related to the removal of H₂O molecules, -OH groups and the dien ligands (found, 23.6 %; calcd, 24.2 %).