

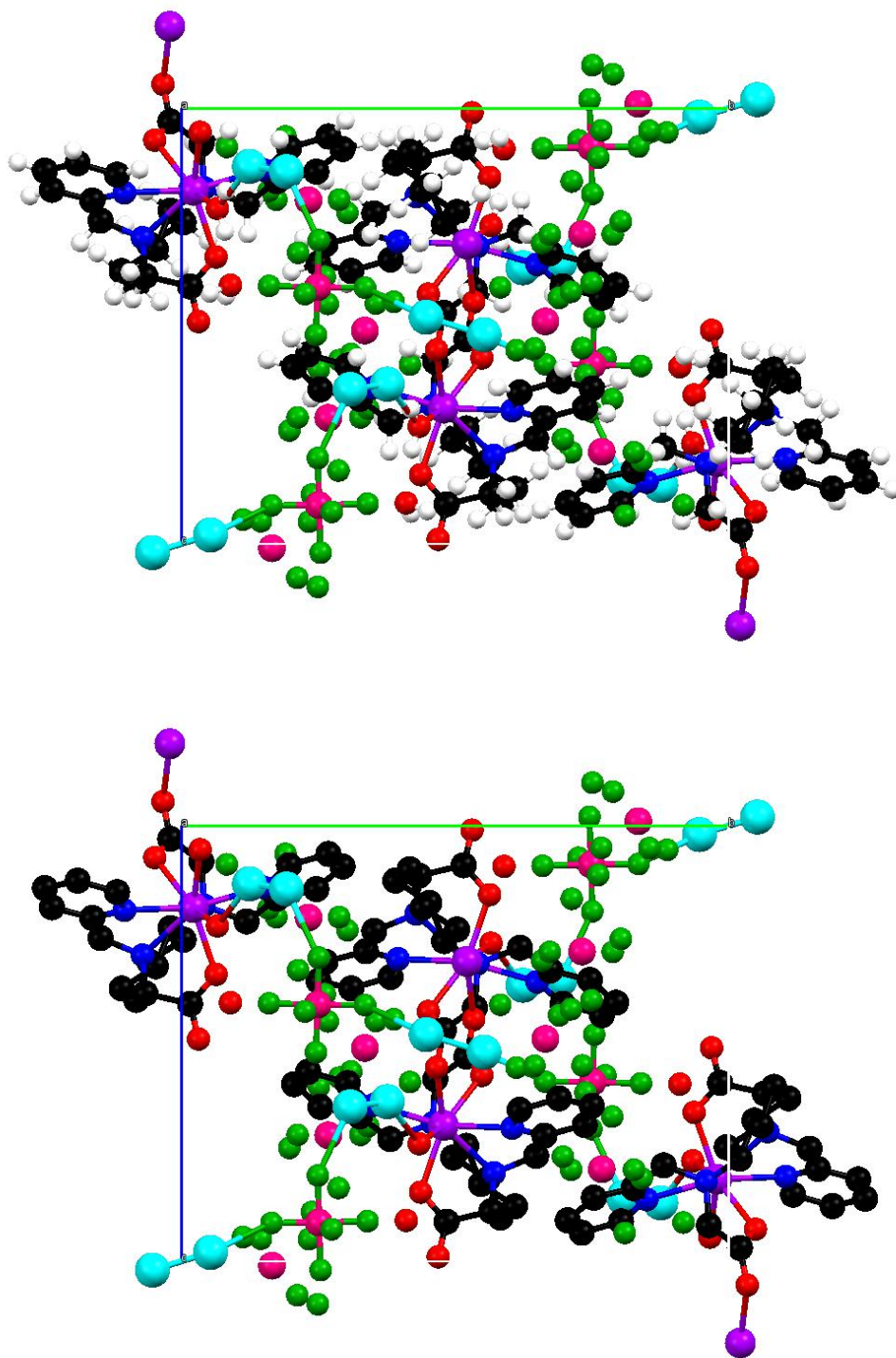
## SUPPORTING INFORMATION

### **Metal Ion Complexes of *N,N'*-Bis(2-Pyridylmethyl)-*trans*-1,2-Di-aminocyclohexane-*N,N'*-Diacetic Acid, H<sub>2</sub>bpcd: Lanthanide(III)- bpcd<sup>2-</sup> Cationic Complexes**

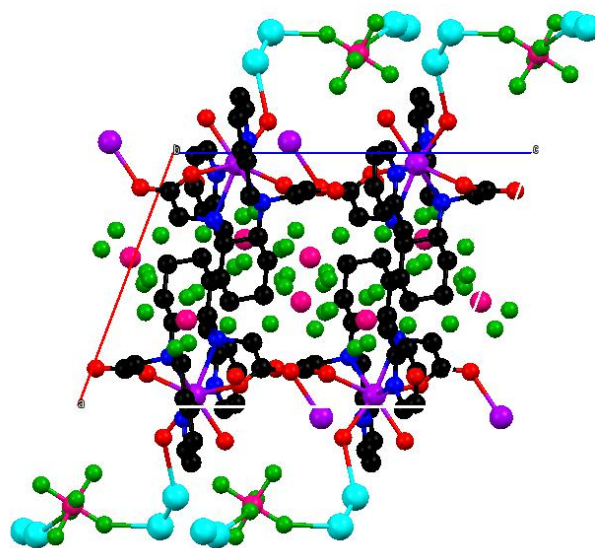
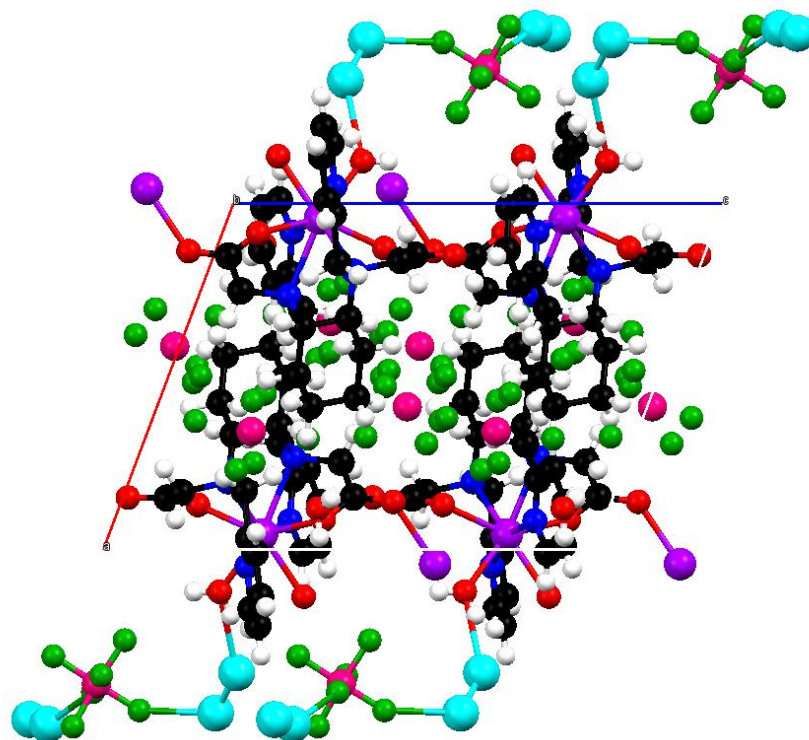
Craig C. McLauchlan,<sup>#</sup> Jan Florián,<sup>±</sup> Daniel S. Kissel,<sup>±</sup> and Albert W. Herlinger\*<sup>±</sup>

<sup>#</sup>Department of Chemistry, Illinois State University, Campus Box 4160, Normal, IL 61790-4160  
USA

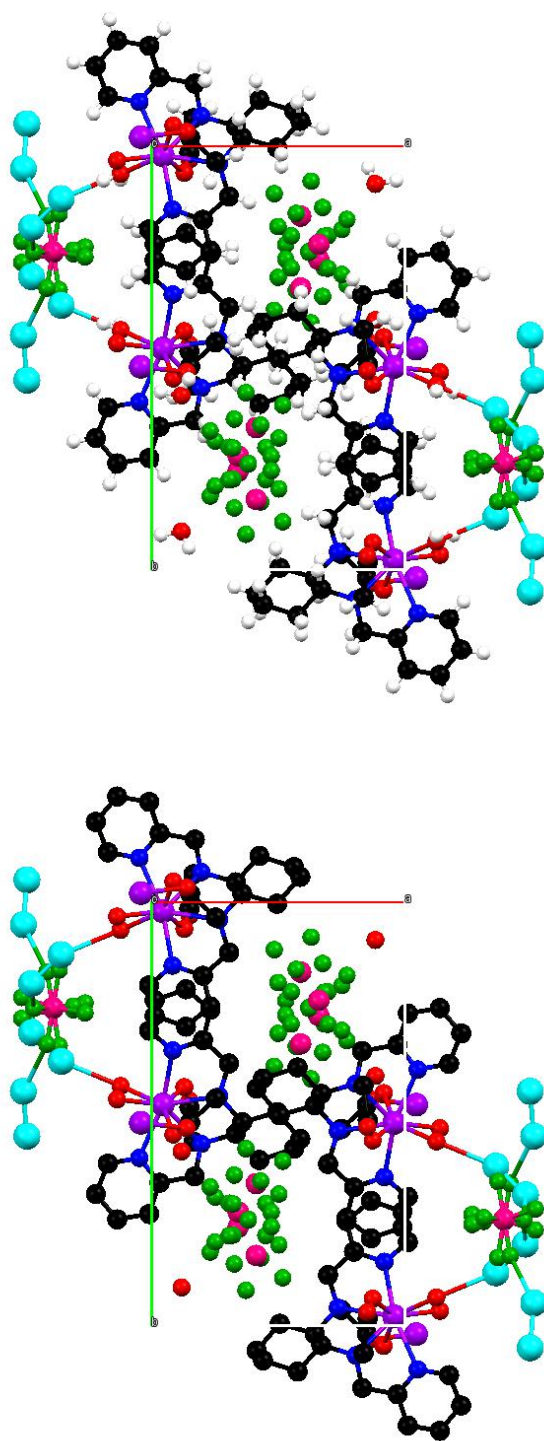
<sup>±</sup>Department of Chemistry and Biochemistry, Loyola University Chicago, 1032 W Sheridan Rd.,  
Chicago, IL 60660 USA



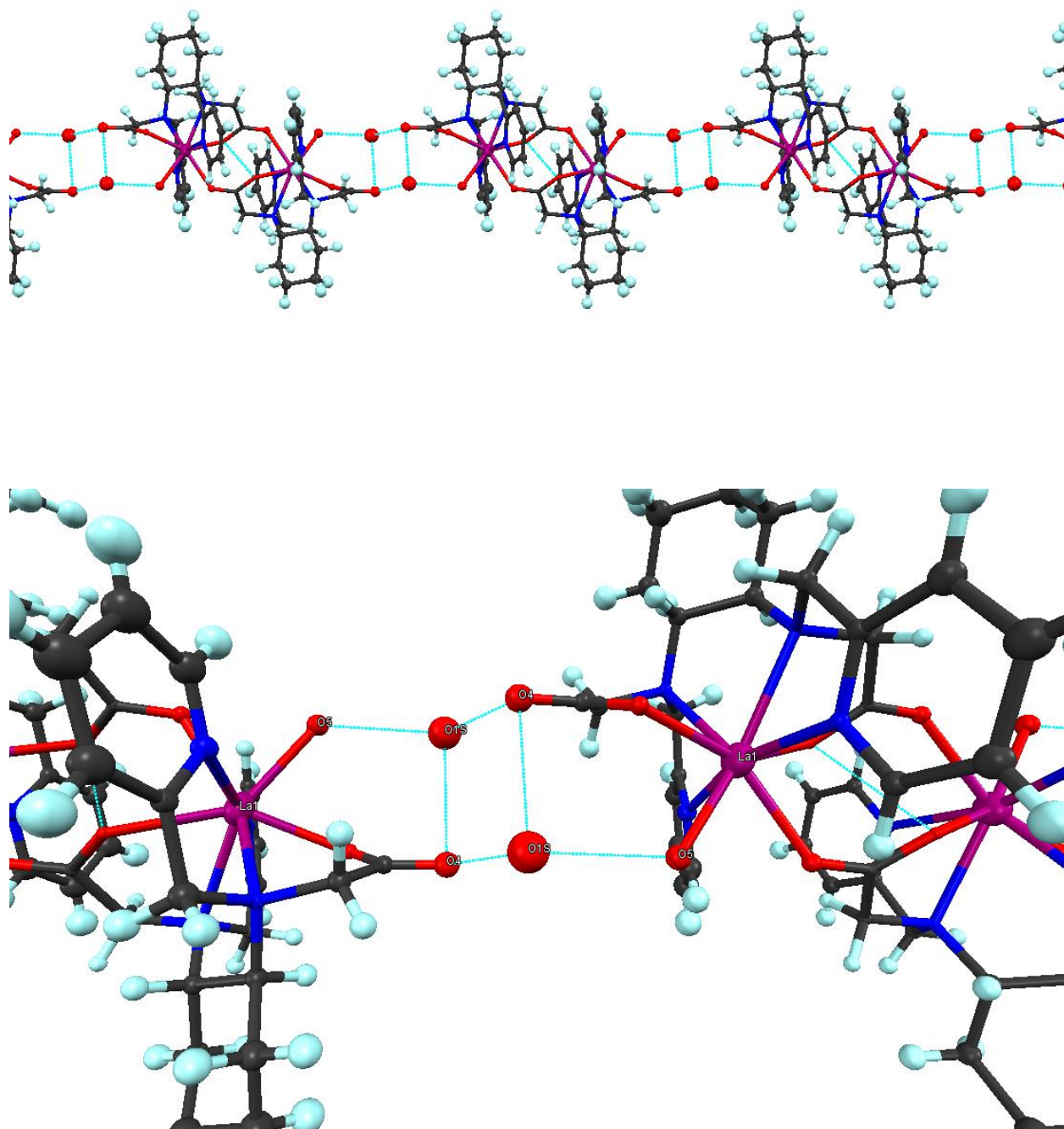
**Figure S1.** Packing diagram for  $\text{Na}_{2.34}[\text{La}_{1.22}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O}_4)_2(\text{H}_2\text{O})_2][\text{PF}_6]_2 \cdot 2\text{H}_2\text{O}$  along  $a$  with and without H atoms.



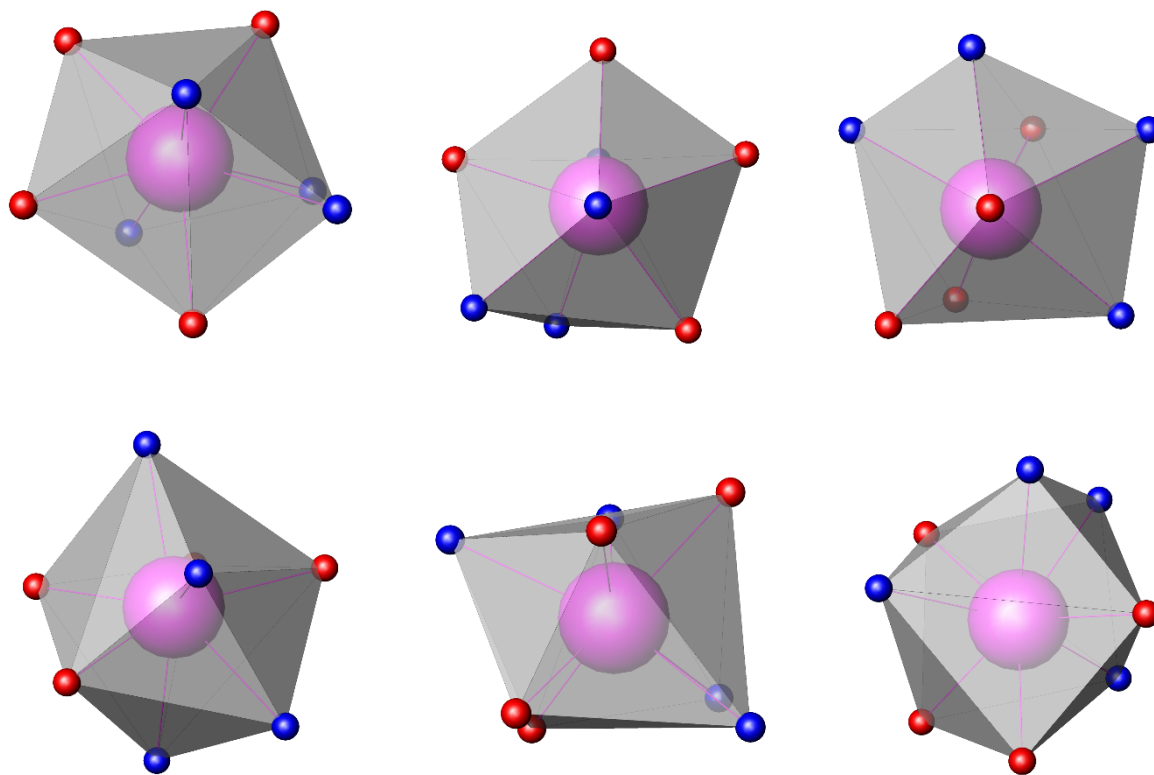
**Figure S2.** Packing diagram for Na<sub>2.34</sub>[La<sub>1.22</sub>(C<sub>22</sub>H<sub>26</sub>N<sub>4</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>][PF<sub>6</sub>]<sub>2</sub>·2H<sub>2</sub>O along *b* with and without H atoms.



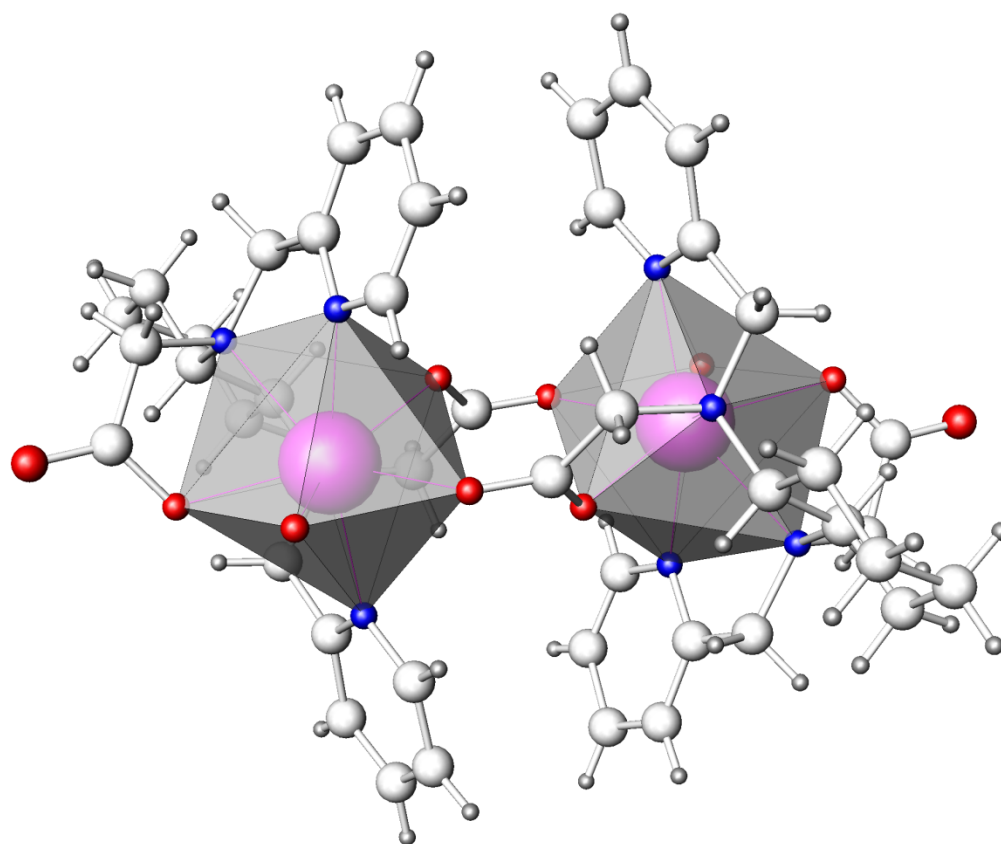
**Figure S3.** Packing diagram for  $\text{Na}_{2.34}[\text{La}_{1.22}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O}_4)_2(\text{H}_2\text{O})_2][\text{PF}_6]_2 \cdot 2\text{H}_2\text{O}$  along  $c$  with and without H atoms.



**Figure S4.**  
Chain description of the La dimers for  $\text{Na}_{2.34}[\text{La}_{1.22}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O}_4)_2(\text{H}_2\text{O})_2][\text{PF}_6]_2 \cdot 2\text{H}_2\text{O}$ .



**Figure S5.** Six views of coordination polyhedron for La in  $\text{Na}_{2.34}[\text{La}_{1.22}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O}_4)_2(\text{H}_2\text{O})_2][\text{PF}_6]_2 \cdot 2\text{H}_2\text{O}$  with a  $\text{N}_4\text{O}_4$  donor atom set and  $C_2$  symmetry to determine polyhedral geometry.. The top set are portrayed in an attempt to highlight a dodecahedral geometry (DD-8), whereas the bottom set are an attempt to highlight a square anti-prismatic geometry (SAPR-8). The geometry appears more consistent with the DD-8 description.



**Figure S6.** Coordination polyhedron depiction for the dimeric  $[\text{La}_2(\text{bpcd})_2(\text{H}_2\text{O})_2]^{2+}$  cation in  $\text{Na}_{2.34}[\text{La}_{1.22}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O}_4)_2(\text{H}_2\text{O})_2][\text{PF}_6]_2 \cdot 2\text{H}_2\text{O}$ .