

Supporting Materials

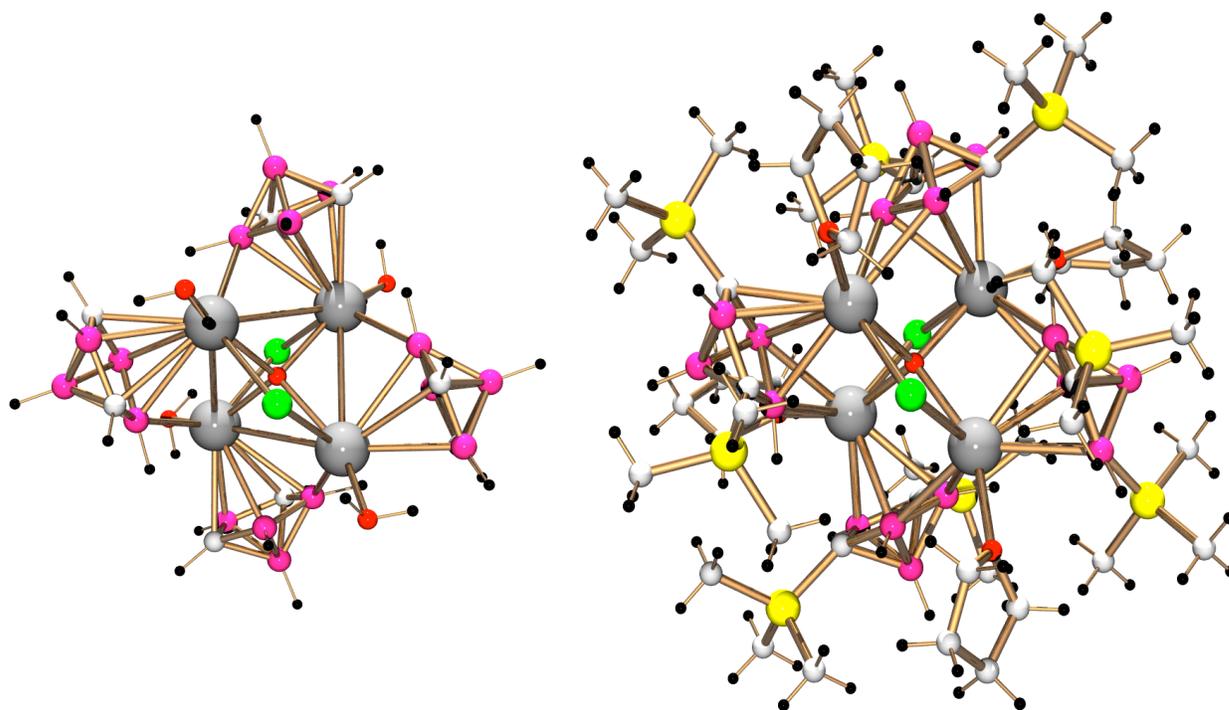


Figure 1. Calculated structure of model system $\text{La}_4\text{OCl}_2(\text{C}_2\text{B}_4\text{H}_6)_4(\text{OH}_2)_4$ (left) as compared with crystallographically determined structure of $\text{Nd}_4\text{OCl}_2(\text{C}_2\text{B}_4\text{H}_4[\text{SiMe}_3]_2)_4(\text{THF})_4$ (right), in the same orientation. Color scheme: B, pink; C, light grey; M, grey; O, red; Si, yellow; H, black.

Table 1. Selected interatomic distances (Å) for calculated structure of $\text{La}_4\text{OCl}_2(\text{C}_2\text{B}_4\text{H}_6)_4(\text{OH}_2)_4$ and crystallographically determined structure of $\text{Nd}_4\text{OCl}_2(\text{C}_2\text{B}_4\text{H}_4[\text{SiMe}_3]_2)_4(\text{THF})_4$.

| | $\text{La}_4\text{OCl}_2(\text{C}_2\text{B}_4\text{H}_6)_4(\text{OH}_2)_4$ | $\text{Nd}_4\text{OCl}_2(\text{C}_2\text{B}_4\text{H}_4[\text{SiMe}_3]_2)_4(\text{THF})_4$ |
|-----------------------|--|--|
| M-M | 3.957, 4.092, 3.898, 3.957, 4.088 | 3.828, 3.966, 3.825, 3.979, 3.828 |
| M-O | 2.421, 2.457 | 2.378, 2.369 |
| M-O _{THF} | 2.575, 2.451 | 2.484, 2.499 |
| M-Cl | 2.951, 2.969 | 2.780, 2.797 |
| M-C | 2.840, 2.753 | 2.778, 2.795 |
| M-B | 2.780, 2.891, 2.850 | 2.766, 2.786, 2.766 |
| M-B _{BRIDGE} | 2.863, 2.968 | 2.770, 2.877 |