Tetrametallic lanthanide(III) phosphonate cages: synthetic, structural and magnetic studies

Karzan H. Zangana, Eufemio Moreno Pineda and Richard E. P. Winpenny*

School of Chemistry and Photon Science Institute, The University of Manchester, Oxford Road, Manchester M13 9PL, UK.

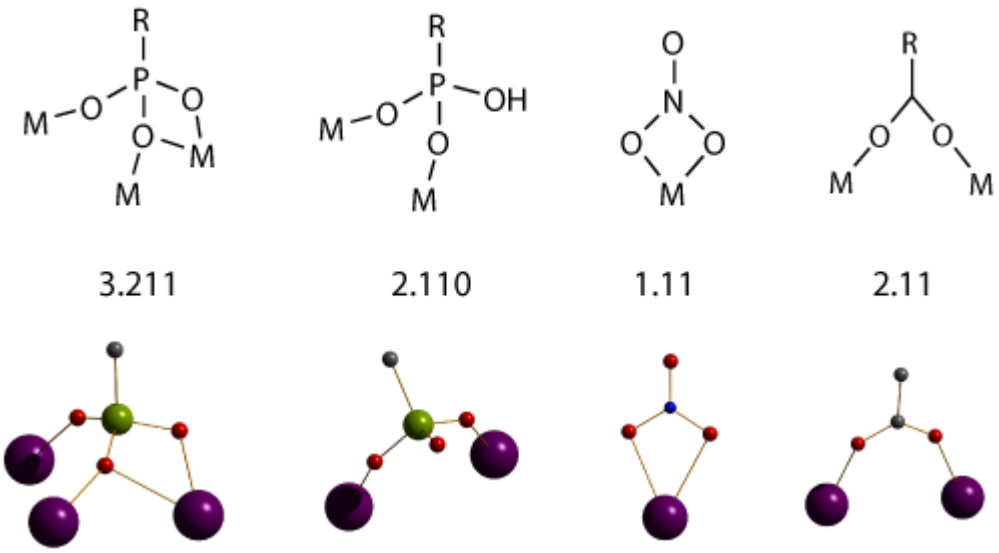

Figure S1. Scheme for binding modes by Harris notation of the phosphonates, nitrates and acetates in the clusters **1**−**5**. Scheme: La, purple; P, light green; O, red; C, grey; N, cyan; H omitted for clarity.

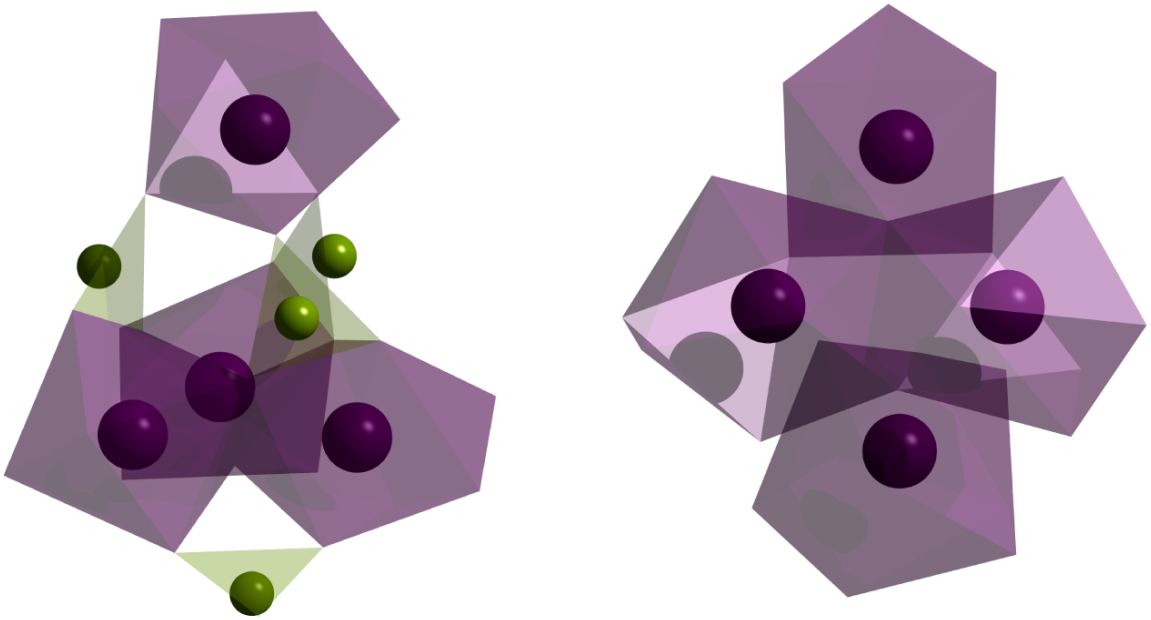

Figure S2. Left**;** Polyhedral view of $\{Ln_4P_4\}$ core. Right; Polyhedral view of metal core of the clusters **1**−**5**.

Table S3. Selected bond distances and angles of **1**−**5**.

	1	**2**	**3**	**4**	**5**
Ln1…Ln2	3.8642(6)	3.86034(6)	3.83996(9)	3.81835(2)	3.79389(5)
Ln2…Ln3	3.8104(6)	3.81040(5)	3.78803(8)	3.77887(3)	3.74962(5)
Ln1…Ln3	3.8151(8)	3.81543(7)	3.79302(10)	3.77498(4)	3.75378(7)
Ln1…O1…Ln2/°	109.1(2)	108.9690(1)	109.1750(15)	109.0140(3)	109.4290(1)
Ln2…O1…Ln3/°	108.8(3)	108.3313(5)	107.9582(8)	108.6251(2)	108.6518(6)
Ln1…O1…Ln3/°	108.9(2)	108.8080(1)	108.700(2)	108.1132(4)	108.9010(13)

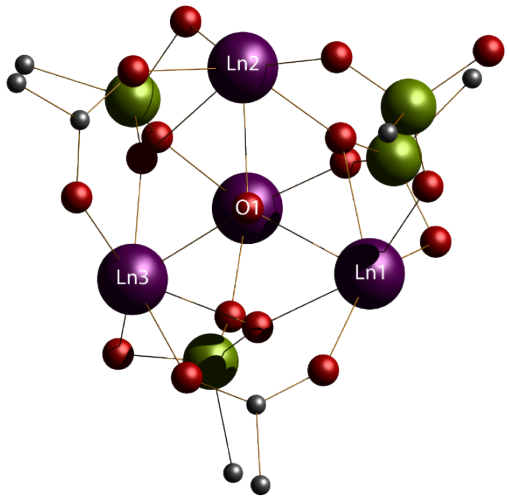

Figure S3. {Ln_3} moiety for Ln_4P_4 clusters. Scheme: La, purple; P, light green; O, red; C, grey; H omitted for clarity.