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Supplementary Material

Hydrated lanthanoid complexes of 5-(2'-pyridyl)tetrazole formed in the presence of dimethyl sulfoxide

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Supplementary Material, comprising of structural data for $[\text{Y}(\text{pytz})_2(\text{H}_2\text{O})_4](\text{pytz})\cdot(\text{Hpytz})\cdot 4\text{H}_2\text{O}$ (selected bond lengths and angles, and hydrogen bond information), and synthesis of $[\text{Eu}(\text{pytz})_3(\text{H}_2\text{O})_3]\cdot 3\text{H}_2\text{O}$.

Table S1. Selected bond lengths [Å] and angles [°] for [Y(pytz)₂(H₂O)₄](pytz).(Hpytz).4H₂O.

Y(1)-O(3)	2.2907(14)
Y(1)-O(4)	2.3009(14)
Y(1)-O(1)	2.3350(14)
Y(1)-O(2)	2.3637(15)
Y(1)-N(14)	2.4392(16)
Y(1)-N(24)	2.4666(16)
Y(1)-N(252)	2.5665(16)
Y(1)-N(152)	2.5853(17)
O(3)-Y(1)-O(4)	74.96(5)
O(3)-Y(1)-O(1)	111.98(5)
O(4)-Y(1)-O(1)	73.20(5)
O(3)-Y(1)-O(2)	74.97(5)
O(4)-Y(1)-O(2)	123.52(5)
O(1)-Y(1)-O(2)	75.48(5)
O(3)-Y(1)-N(14)	141.07(6)
O(4)-Y(1)-N(14)	142.84(6)
O(1)-Y(1)-N(14)	81.50(5)
O(2)-Y(1)-N(14)	73.58(5)
O(3)-Y(1)-N(24)	83.97(5)
O(4)-Y(1)-N(24)	78.62(5)
O(1)-Y(1)-N(24)	141.99(5)
O(2)-Y(1)-N(24)	142.41(5)
N(14)-Y(1)-N(24)	108.11(5)
O(3)-Y(1)-N(252)	76.85(5)
O(4)-Y(1)-N(252)	136.04(5)
O(1)-Y(1)-N(252)	149.79(5)
O(2)-Y(1)-N(252)	79.50(5)
N(14)-Y(1)-N(252)	75.36(5)
N(24)-Y(1)-N(252)	65.41(5)
O(3)-Y(1)-N(152)	151.58(5)
O(4)-Y(1)-N(152)	82.36(5)
O(1)-Y(1)-N(152)	76.56(5)
O(2)-Y(1)-N(152)	132.88(5)
N(14)-Y(1)-N(152)	65.33(5)
N(24)-Y(1)-N(152)	74.84(5)
N(252)-Y(1)-N(152)	109.95(5)

Table S2. Hydrogen bonds for [Y(pytz)₂(H₂O)₄](pytz)·(Hpytz)·4H₂O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(31)	0.799(16)	2.010(17)	2.806(2)	174(3)
O(1)-H(1B)...N(12) ¹	0.812(15)	1.918(15)	2.722(2)	170(2)
O(2)-H(2A)...N(11) ¹	0.779(15)	2.236(16)	2.994(2)	165(3)
O(2)-H(2B)...O(5)	0.785(16)	1.882(18)	2.650(2)	166(3)
O(3)-H(3A)...N(21) ²	0.768(15)	1.984(16)	2.750(2)	174(3)
O(3)-H(3B)...N(34) ³	0.833(16)	1.88(2)	2.668(2)	159(3)
O(4)-H(4A)...N(352) ³	0.830(16)	2.02(2)	2.801(2)	157(3)
O(4)-H(4B)...O(6)	0.760(14)	1.906(15)	2.665(2)	177(3)
O(5)-H(5A)...N(33) ³	0.783(15)	2.032(15)	2.803(2)	168(2)
O(5)-H(5B)...O(7) ⁴	0.847(15)	1.845(15)	2.691(2)	177(2)
O(6)-H(6A)...N(32)	0.826(16)	2.005(17)	2.794(2)	159(2)
O(6)-H(6B)...O(5) ⁵	0.806(15)	1.985(16)	2.767(2)	163(3)
O(7)-H(7A)...N(23)	0.810(16)	2.126(17)	2.936(2)	178(3)
O(7)-H(7B)...N(22) ⁶	0.845(16)	2.052(16)	2.878(2)	165(3)

Symmetry transformations used to generate equivalent atoms:

¹ 1-x,1-y,1-z ; ² 1-x,-y,2-z; ³ 1-x,-y,1-z ; ⁴ x+1,y,z; ⁵ x-1,y,z; ⁶ -x,-y,2-z

Synthesis of [Eu(**pytz**)₃(H₂O)₃].3H₂O

Triethylamine (86 μ L, 0.61 mmol) was added to a solution of H**pytz** (0.09 g, 0.61 mmol) in methanol (20 ml). This was then added to a solution of Eu(NO₃)₃(DMSO)₃¹ (0.10 g, 0.22 mmol) in methanol (10 mL), and the reaction stirred (72 hrs). The resulting opaque solution was concentrated under reduced pressure, yielding an oily residue, which deposited colourless crystals after 48 hrs. A single crystal structure determination revealed that the crystals were the previously reported [Eu(**pytz**)₃(H₂O)₃].3H₂O.²

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2. Y.-S. Zhou, D.-H. Xu and L.-J. Zhang, *Chem. Res. Chin. Univ.*, 2010, **26**, 866.