Supporting Information

A series of lanthanide complexes with Keggin-type monolacunary phosphotungstate: synthesis and structural characterization

Vladimir S. Korenev*, Taisiya S. Sukhikh, Maxim N. Sokolov

Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Lavrentieva St. 3, 630090 Novosibirsk, Russia

* Correspondence: wkorenev@niic.nsc.ru

Content

1. IR spectroscopy

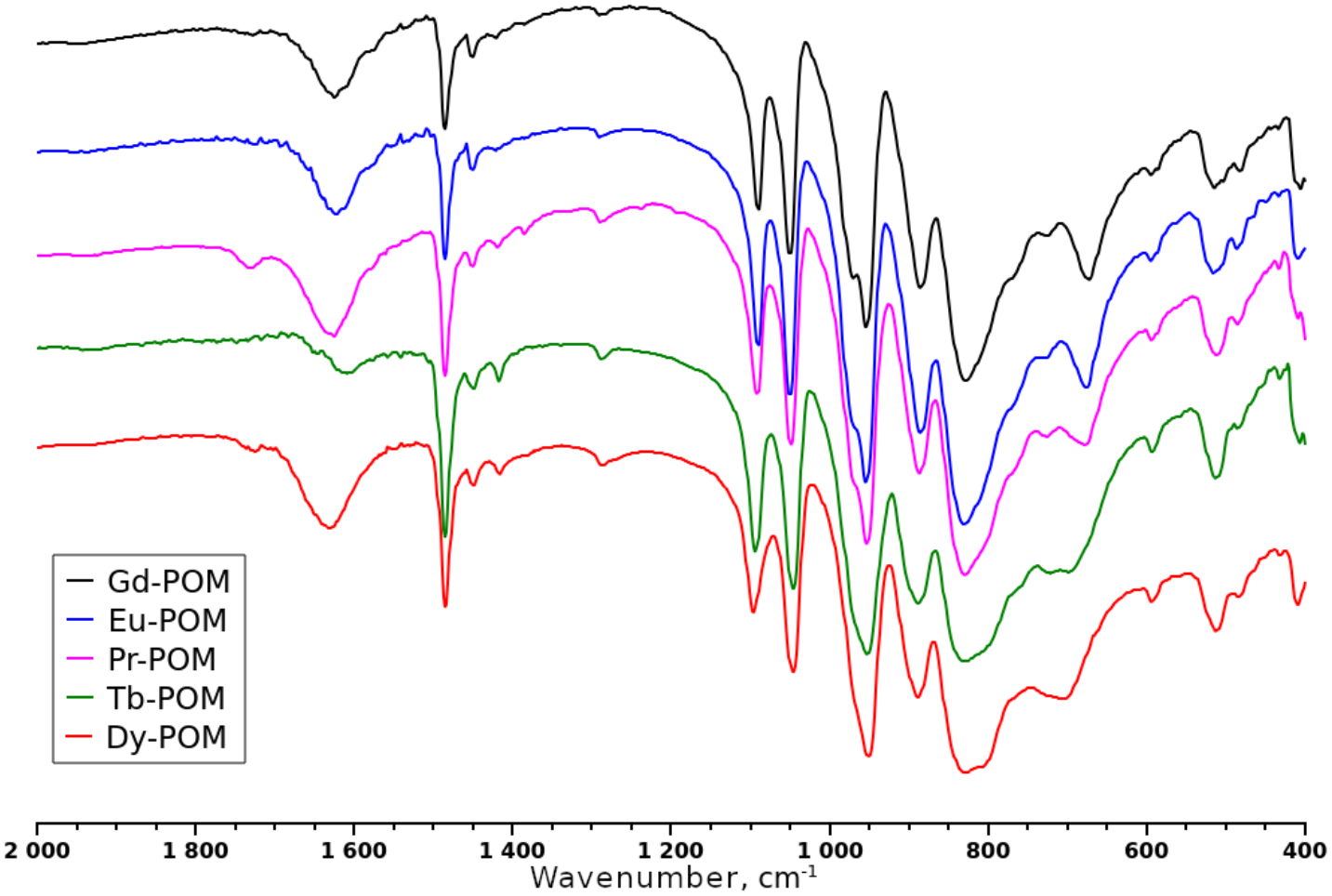

Figure S1. IR spectra of $Cat_4Ln(PW_{11}O_{39})\cdot xH_2O$ complexes (Ln from the top to the bottom): Gd, Eu, Pr, Tb and Dy.

2. Crystal data and structure refinement

Table S1. Crystal data and structure refinement for **1–3Gd**

Identification code	**1Gd**	**2Gd**	**3Gd**
Empirical formula	$C_8H_{32}GdK_2N_2O_{46}PW_{11}$	$C_{24}H_{72}Gd_2K_2N_6O_{104}P_2W_{22}$	$C_{27.7}H_{83.09}Gd_2K_{1.07}N_{6.92}O_{96.15}P_2W_{22}$
Formula weight	3181.12	6648.21	6539.25
Temperature/K	150(2)	150(2)	150(2)
Space group	*P*–1	*P*–1	$P2_1/c$
a/Å	11.7135(17)	12.7931(18)	12.9425(9)
b/Å	11.9150(18)	13.0106(18)	22.1257(14)
c/Å	19.417(3)	23.291(4)	20.5429(14)
α/°	95.738(6)	73.941(4)	90
β/°	92.399(6)	80.599(6)	99.701(2)
γ/°	117.621(6)	61.754(4)	90
Volume/Å^3	2377.1(7)	3279.4(8)	5798.6(7)
Z	2	1	2
ρ_{calc}g/cm^3	4.444	3.346	3.731
μ/mm^{-1}	28.190	20.386	23.019
F(000)	2786.0	2914.0	5747.0
Crystal size/mm^3	0.06 × 0.05 × 0.01	0.15 × 0.1 × 0.06	0.1 × 0.09 × 0.05
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.032 to 48.814	3.642 to 56.546	3.192 to 54.706
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -22 ≤ l ≤ 22	-16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -30 ≤ l ≤ 30	-16 ≤ h ≤ 15, -28 ≤ k ≤ 28, -26 ≤ l ≤ 26
Reflections collected	12845	28316	68148
Independent reflections	12845 [R_{int} = 0.0869, R_{sigma} = 0.1094]	28316 [R_{int} = 0.0860, R_{sigma} = 0.0849]	12879 [R_{int} = 0.0539, R_{sigma} = 0.0422]
Data/restraints/parameters	12845/111/581	28316/888/637	12879/888/614
Goodness-of-fit on F^2	1.032	1.172	1.197
Final R indexes [I>=2σ (I)]	R_1 = 0.0644, wR_2 = 0.1526	R_1 = 0.1085, wR_2 = 0.2447	R_1 = 0.0548, wR_2 = 0.1117
Final R indexes [all data]	R_1 = 0.0918, wR_2 = 0.1706	R_1 = 0.1244, wR_2 = 0.2527	R_1 = 0.0698, wR_2 = 0.1191
Largest diff. peak/hole / e Å^{-3}	4.29/-2.65	5.20/-5.82	1.95/-2.07