ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

2022. Том 63, № 10 *Октябрь* *DOI: 10.26902/JSC_id99148*

SUPPLEMENTARY MATERIALS TO: A NEW MONOMER Ce(III) COMPLEX BASED ON BIS[(2-PYRIDYL)METHYLENE]PYRIDINE-2,6-DICARBOHYDRAZONE: SYNTHESIS, DNA BINDING, APOPTOSIS, AND MOLECULAR DOCKING

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Table 1. Crystal data and refinement results for complex

Parameter	**$C_{44}H_{41}Ce_3N_{21}O_{21}$**
Formula weight	1620.34
Crystal system, space group	triclinic, P-1
a, [Å]	13.4703(6)
b, [Å]	15.4973(7)
c ,[Å]	17.1092(7)
α,(deg)	107.643(2)
β,(deg)	112.104(2)
γ,(deg)	95.845(2)
V, [Å^3]	3057.7(2)
Z	2
ρ_{calcd}, mg/cm^{-3}	1.760
Absorption coefficient, mm^{-1}	2.284
Crystal size, mm	0.19x 0.16x 0.13
θ Range for data collection, deg	4.496 to 52.778
F(000)	1588.0
Limiting indices	$-16 \le h \le 16$, $-19 \le k \le 19$, $-21 \le l \le 21$
Reflections collected / unique	61343/12503 [Rint = 0.0643, Rsigma = 0.0452]
Data / restraints / parameters	12503 / 1123 / 806
Goodness-of-fit on F^2	1.024
Final R indices ($I > 2\sigma(I)$)	$R_1 = 0.0370$, $wR_2 = 0.0800$
R indices (all data)	$R_1 = 0.0562$, $wR_2 = 0.0885$
Largest diff. peak and hole, e.Å^{-3}	0.77 / -1.11
CCDC	2122027

Table 2. Selected bond lengths and angles of the crystal structures

Bond length	**d, Å**	**Bond length**	**d, Å**
Ce3-O1	2.460(3)	Ce2-O2	2.556(3)
Ce3-O3	2.466(3)	Ce2-O4	2.558(3)

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Ce3-O5	2.594(3)	Ce2-O11	2.454(4)
Ce3-O6	2.616(3)	Ce2-O18	2.472(4)
Ce3-O12	2.639(3)	Ce2-O19	2.610(4)
Ce3-O14	2.594(3)	Ce2-O21	2.662(4)
Ce3-N1	2.695(4)	Ce2-N6	2.614(4)
Ce3-N2	2.591(4)	Ce2-N7	2.858(5)
Ce3-N8	2.740(4)	Ce2-N13	2.601(4)
Ce3-N9	2.615(4)	Ce2-N14	2.814(4)
Ce1-O1	2.563(3)	Ce1-O9	2.638(3)
Ce1-O2	2.529(3)	Ce1-O15	2.565(3)
Ce1-O3	2.578(3)	Ce1-O17	2.548(3)
Ce1-O4	2.574(3)	Ce1-N4	2.705(4)
Ce1-O8	2.576(3)	Ce1-N11	2.703(4)

Bond angle	**ω, deg**	**Bond angle**	**ω, deg**
O1-Ce3-O3	66.37(10)	O11-Ce2-O2	80.97(11)
O1-Ce3-N2	61.24(12)	O11-Ce2-O4	72.78(11)
O3-Ce3-N9	61.43(12)	O11-Ce2-N6	74.99(13)
O5-Ce3-O6	48.77(11)	O11-Ce2-N7	63.81(12)
O14-Ce3-O12	48.72(11)	O18-Ce2-O19	77.61(13)
N1-Ce3-N8	69.91(13)	O18-Ce2-O21	67.83(12)
N2-Ce3-N1	60.46(13)	O18-Ce2-N6	139.28(13)
N9-Ce3-N8	59.87(12)	O18-Ce2-N7	137.82(13)
O1-Ce1-O3	63.26(10)	O19-Ce2-O21	48.08(12)
O1-Ce1-N4	59.53(11)	N6-Ce2-O21	71.45(13)
O2-Ce1-O1	119.88(10)	N6-Ce2-N7	59.59(13)
O2-Ce1-O4	61.88(10)	N14-Ce2-N7	68.10(13)
O3-Ce1-N4	119.48(11)	Ce3-O1-Ce1	115.51(12)
O4-Ce1-O3	119.95(10)	Ce1-O2-Ce2	117.79(12)
O4-Ce1-N11	60.63(11)	Ce3-O3-Ce1	114.75(12)
O8-Ce1-O9	48.60(11)	Ce2-O4-Ce1	116.04(12)
O17-Ce1-O15	49.92(11)	N5-N6-Ce2	118.2(3)
O2-Ce2-O4	61.73(10)	N10-N9-Ce3	118.8(3)
O2-Ce2-N6	59.66(12)	N12-N13-Ce2	119.5(3)
O4-Ce2-N13	61.05(11)		

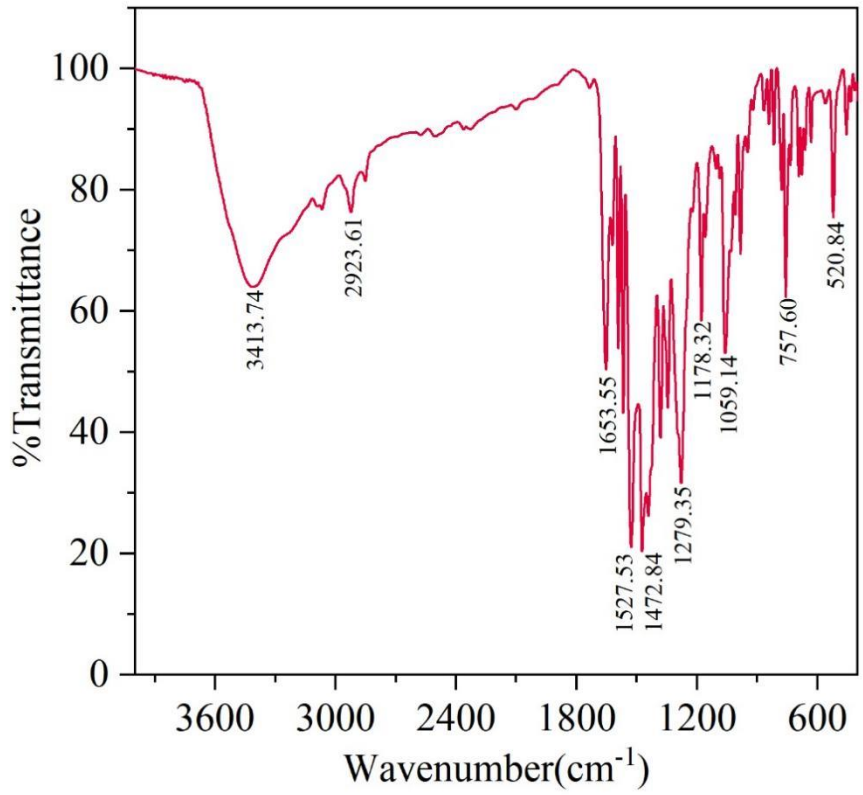

Fig.S1 IR spectrum of Ce(III) complex

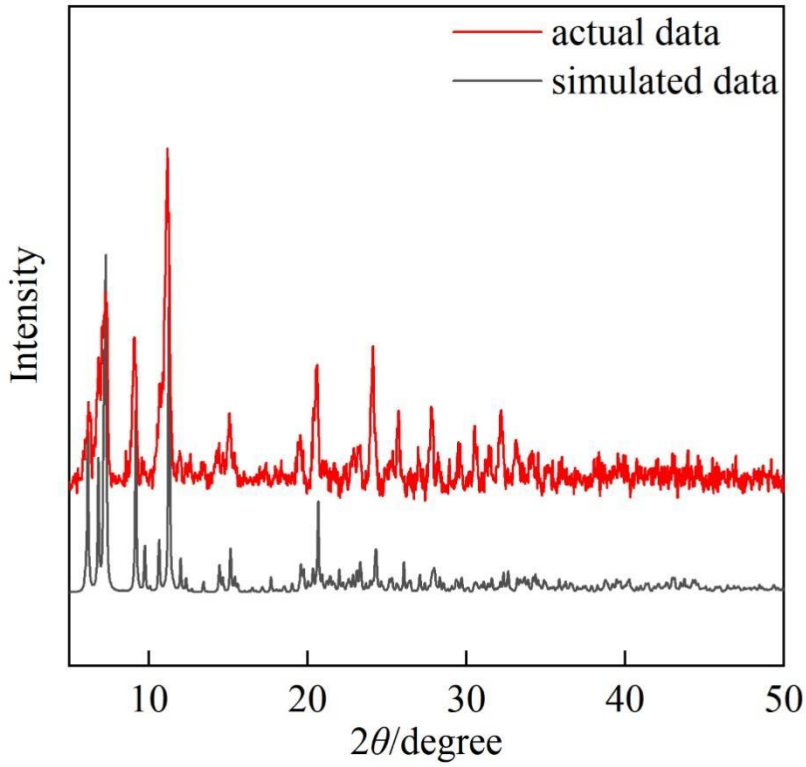

Fig.S2 The PXRD pattern of the complex