

Synthetic approach to heteroleptic Zn₂Ln₂ complexes featuring photoluminescence, antibacterial and anticancer properties

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Table S1. Crystal Data, Data Collection and Structure Refinement Parameters for **1-3**

Identification code	1	2	3
CCDC	2404150	2404151	2404152
formula	C ₁₆ H ₈ F ₆ N ₂ O ₄ Zn	C ₆₈ H ₄₄ F ₆ Gd ₂ N ₄ O ₃₀ Zn ₂	C ₆₈ H ₉₉ Eu ₂ F ₆ N ₅ O ₂₆ S ₂ Zn ₂
molecular wt	471.61	1956.31	2015.30
temperature (K)	150(2)	150(2)	150(2)
crystal syst	monoclinic	triclinic	triclinic
space group	<i>C2/c</i>	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	19.1538(16)	11.020(2)	11.593(4)
<i>b</i> (Å)	11.4080(9)	11.076(3)	12.012(5)
<i>c</i> (Å)	7.4290(6)	14.419(4)	16.849(6)
<i>α</i> (deg)	90	88.514(10)	88.419(6)
<i>β</i> (deg)	101.402(3)	82.489(10)	70.048(6)
<i>γ</i> (deg)	90	79.479(8)	80.180(6)
<i>V</i> (Å ³)	1591.2(2)	1715.5(7)	2172.0(14)
<i>Z</i>	4	1	1
<i>D</i> _{calcd} (g·cm ⁻³)	1.969	1.894	1.541
linear absorption (<i>μ</i>) (cm ⁻¹)	16.41	27.10	21.03

$2\theta_{\max}$ (deg)	60	50	54
no. of unique reflns, R_{int}	2331, 0.0495	6026, 0.0520	9457, 0.0257
no. of obsd reflns ($I > 2\sigma(I)$)	1816	4735	7899
no. of params	132	557	567
R_I (on F for obsd reflns)	0.0418	0.0420	0.0321
wR_2 (on F^2 for all reflns)	0.1016	0.0930	0.0840
$GOOF$	1.062	1.040	1.019
diff. peak/hole ($\text{e } \text{\AA}^{-3}$)	0.956/-0.846	0.828/-0.809	0.832/-0.484

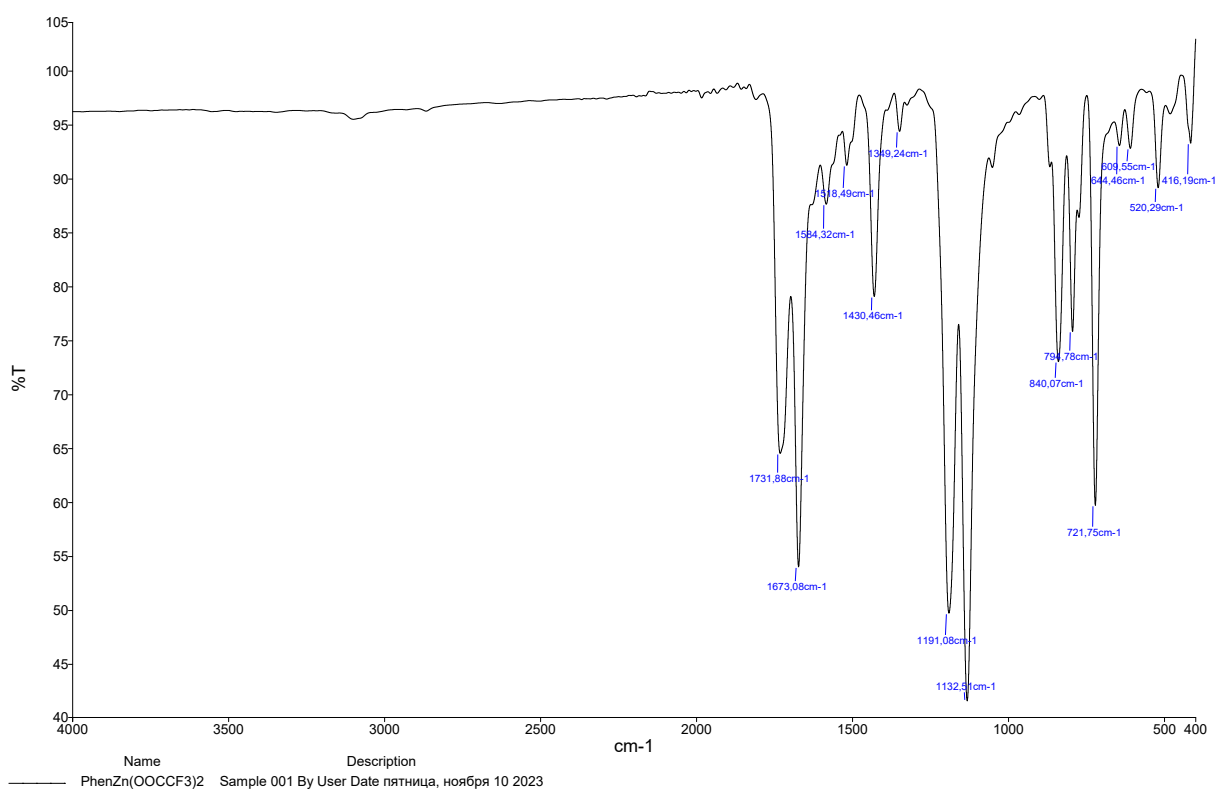


Fig. S1. IR-spectrum of 1

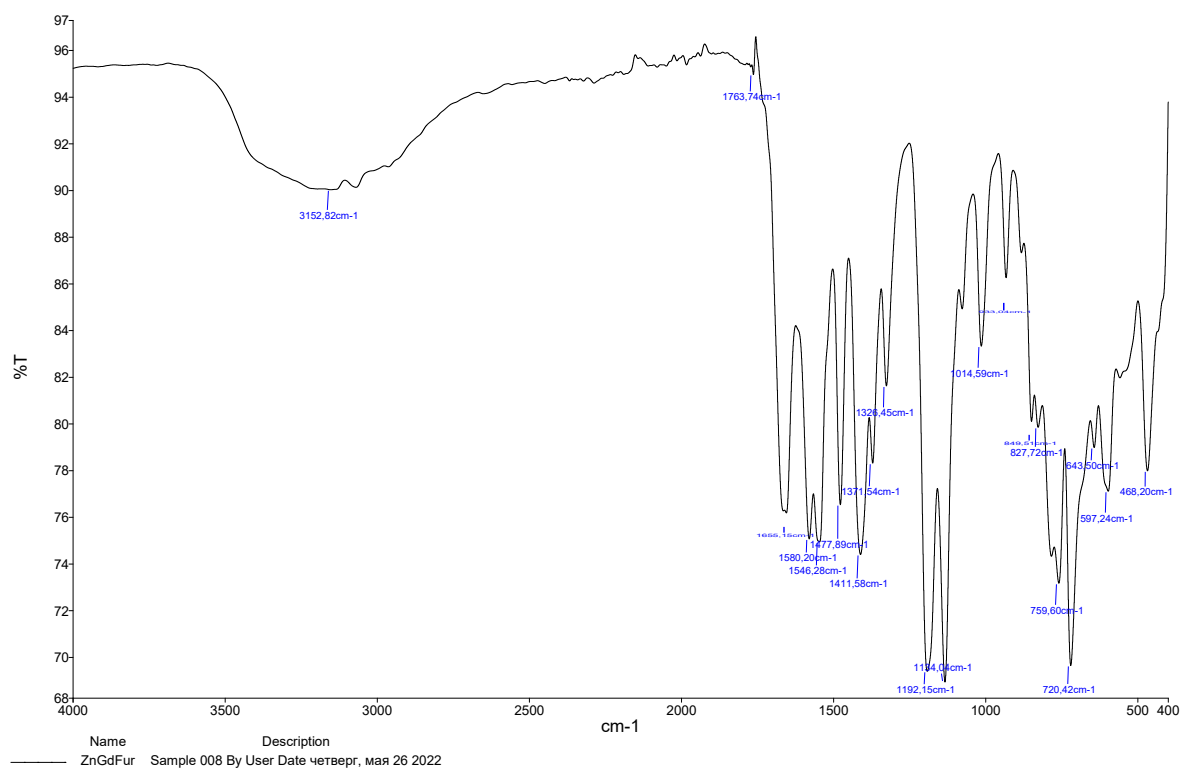


Fig. S2. IR-spectrum of 2

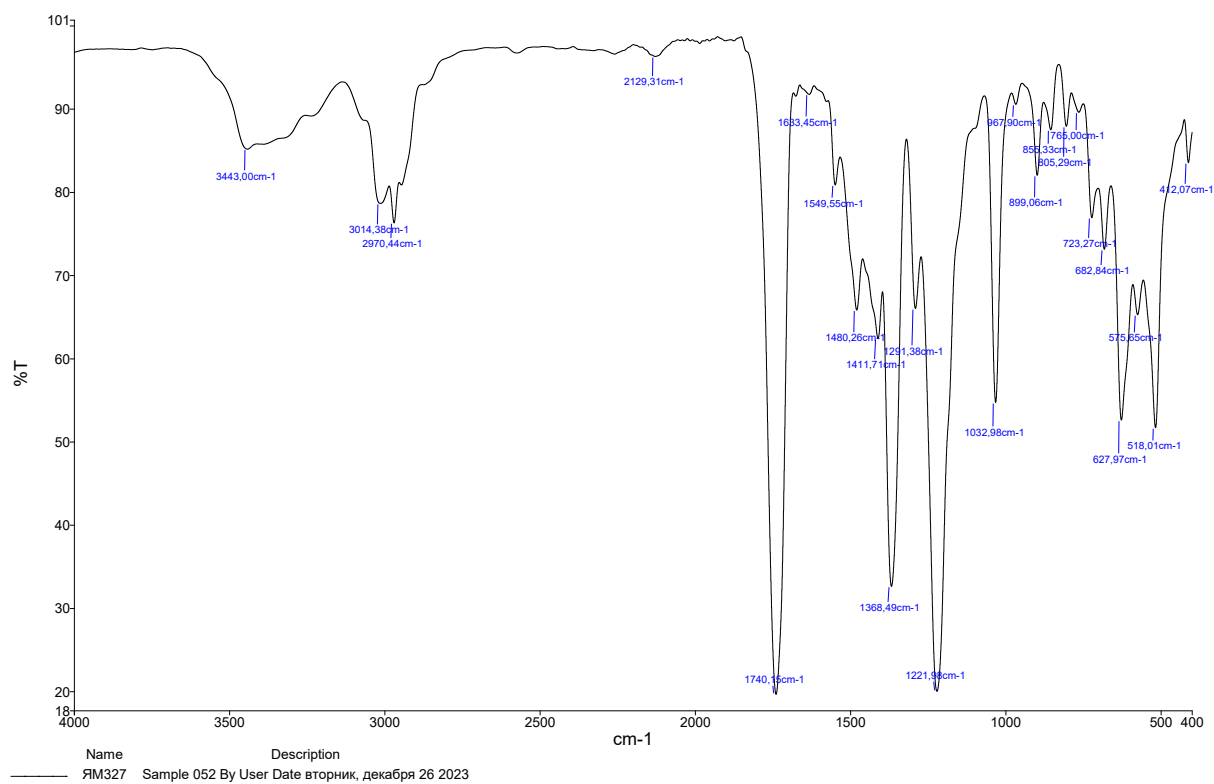


Fig. S3. IR-spectrum of 3