Supplementary information

Synthesis, crystal structure and spin-orbit coupling analysis for mono-scorpionate Eu(III) complexes

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Table S1. Crystal data and structure refinement for the compounds.

Identification code	(1)	(1a)	(2)	(3)
Empirical formula	$C_{14}H_{18}EuN_{11}O_{10}$	$C_{10}H_{12}EuN_9O_{10}$	$C_{18}H_{25}EuN_{10}O_9$	$C_{32.9}H_{37.24}Eu_2F_{18}N_{14}O_{20.73}S_6$
Formula weight	652.35	570.25	677.44	1798.66
Temperature/K	150(2)	150(2)	150(2)	150(2)
Space group	*P*–1	*I*2/*c*	$P2_1/n$	$P2_1/c$
a/Å	9.4083(2)	14.9027(3)	10.8259(6)	21.596(3)
b/Å	11.0349(3)	15.6143(3)	14.9846(7)	17.912(2)
c/Å	11.7157(3)	16.1279(4)	16.4034(8)	18.668(2)
α/°	99.6960(10)	90	90	90
β/°	93.4410(10)	108.4710(10)	95.786(2)	115.419(4)
γ/°	102.6850(10)	90	90	90
Volume/Å^3	1163.71(5)	3559.55(13)	2647.4(2)	6522.3(14)
Z	2	8	4	4
ρ_{calc}g/cm^3	1.862	2.128	1.700	1.832
μ/mm^{-1}	2.769	3.601	2.434	2.224
F(000)	644.0	2224.0	1352.0	3530.0
Crystal size/mm^3	0.16 × 0.15 × 0.10	0.20 × 0.16 × 0.08	0.10 × 0.10 × 0.08	0.12 × 0.10 × 0.03
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.168 to 59.232	3.886 to 61.058	4.316 to 61.048	3.086 to 51.484
Index ranges	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16	-21 ≤ h ≤21, -22 ≤ k ≤ 22 -22 ≤ l ≤ 22	-13 ≤ h ≤15, -21 ≤k ≤ 21 -23 ≤ l ≤ 22	
Reflections collected	26611	44683	36783	
Independent reflections	6515 [R_{int}=0.0256, R_{sigma}=0.0220]	5332 [R_{int}=0.0308, R_{sigma}=0.0207]	8022 [R_{int}=0.0473, R_{sigma}=0.0393]	5332 [R_{int}=0.0308, R_{sigma}=0.0207]
Data/restraints/parameters	6515/3/333	5332/2/277	8022/0/350	5332/2/277
Goodness-of-fit on F^2	1.062	1.091	1.072	1.091
Final R indexes [I>=2σ (I)]	R_1=0.0151, wR_2=0.0357	R_1=0.0184, wR_2=0.0370	R_1=0.0276, wR_2=0.0525	R_1=0.0184, wR_2=0.0370
Final R indexes [all data]	R_1=0.0156, wR_2=0.0360	R_1=0.0281, wR_2=0.0414	R_1=0.0354, wR_2=0.0581	R_1=0.0281, wR_2=0.0414
Largest diff. peak/hole/e Å^{-3}	0.42/-0.55	0.55/-0.84	0.52/-0.62	0.55/-0.84

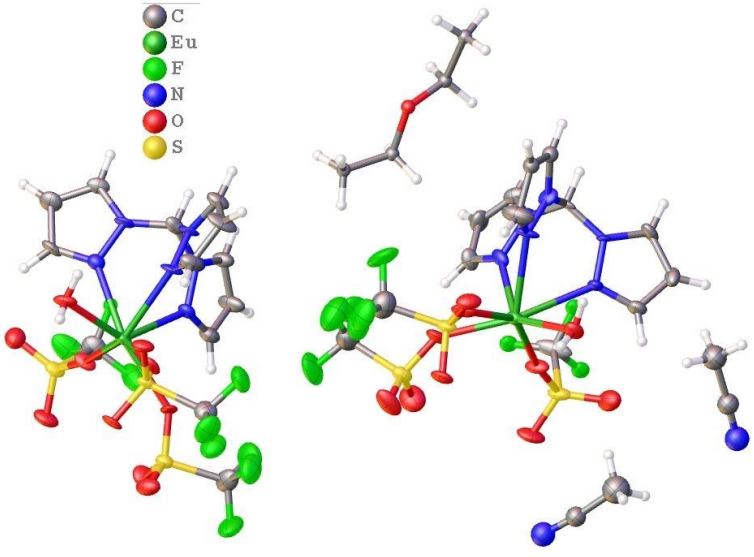

Figure S1. The asymmetric unit in the crystal structure of $[Eu(HCPz_3)H_2O(CF_3SO_3)_3]_2$ (**3**).

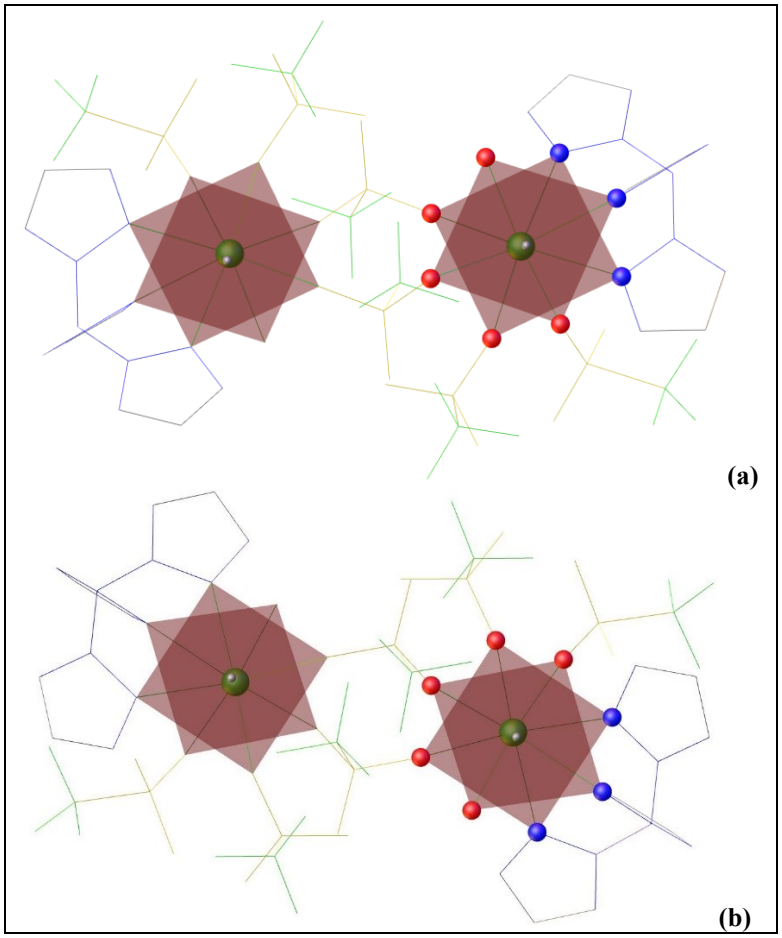

Figure S2. Square antiprism coordination environment - of Eu^{3+} sites in $[Eu(HCPz_3)H_2O(CF_3SO_3)_3]_2$ (**3**) for: (**a**) around Eu1 central atom; (**b**) around Eu2 central atom.

Table S2. Geometry analysis of the complexes by SHAPE software.

Compound	CN	Polyhedron geometry		
$[Eu(HCPz_3)(NO_3)_3H_2O]$ **1**	$[ML_{10}]$	Sphenocorona C_{2v}	Bicapped square antiprism D_{4d}	
		3.534	6.356	
$[Eu(HCPz_3)(NO_3)_3H_2O]$ **1a**	$[ML_{10}]$	Sphenocorona C_{2v}	Bicapped square antiprism D_{4d}	
		3.225	4.793	
$[Eu(HC(Pz^{Me_2})_3)(NO_3)_3]$ **2**	$[ML_9]$	Spherical tricapped trigonal prism D_{3h}	Spherical capped square antiprism C_{4v}	Muffin C_s
		2.05	2.910	3.027
$[Dy(Rad)(NO_3)_3]$	$[ML_9]$	**2.220**	3.025	3.256
$[Eu(HCPz_3)H_2O(OTf)_3]_2$ **3**				
Eu01	$[ML_8]$	Square antiprism D_{4d}	Triangular dodecahedron D_{2d}	Biaugmented trigonal prism C_{2v}
		0.354	2.184	1.543
Eu02	$[ML_8]$	Square antiprism D_{4d}	Triangular dodecahedron D_{2d}	Biaugmented trigonal prism C_{2v}
		0.426	1.919	1.368

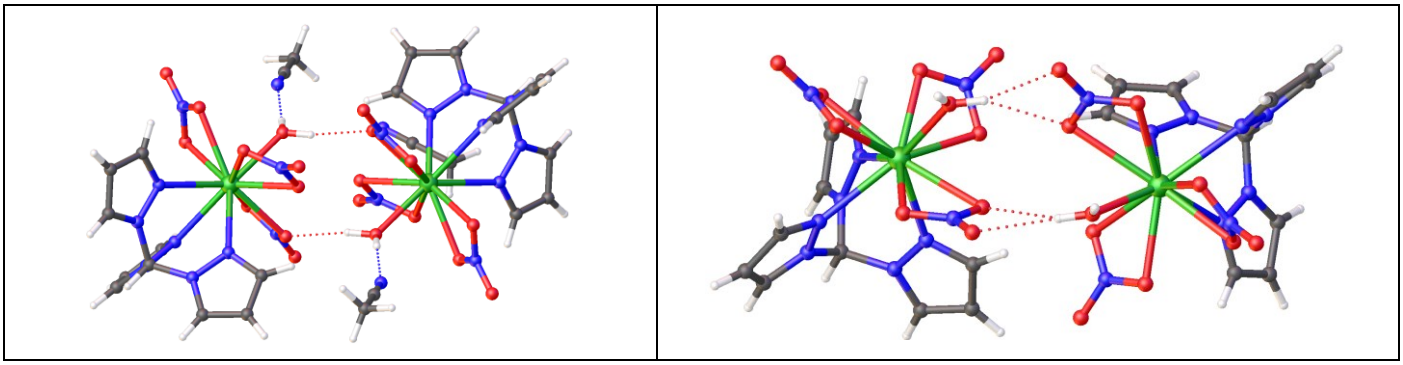

Figure S3. Dimerized species in **1** (left) and **1a** (right).

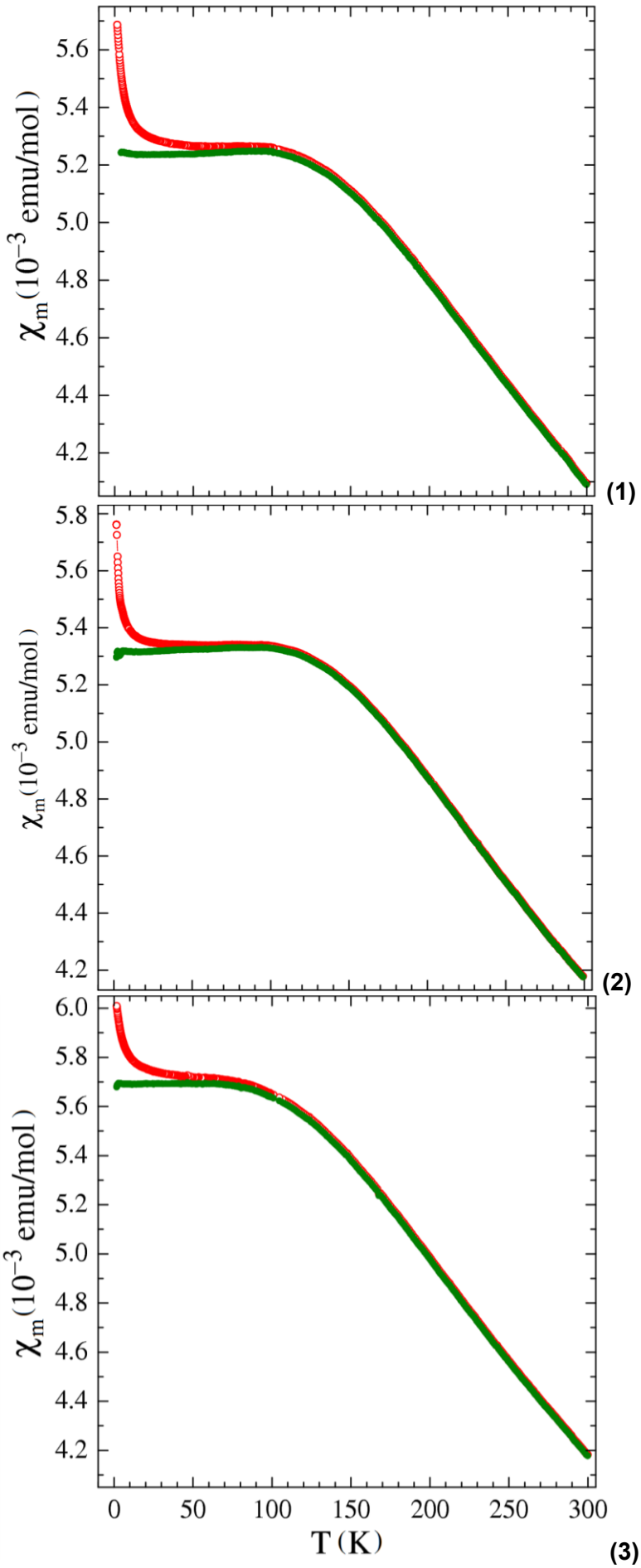

Figure S4. The temperature-dependent molar magnetic susceptibility χ_M of **1–3** at a field of 1 kOe (open red circles). Solid green circles show the χ_M data after subtraction of the contribution from Eu(II) impurities (0.01-0.017 %).