

Supporting Information on

Tripodal oxazolidine-N-oxyl biradical complexes of Dy³⁺ and Eu³⁺

by Philippe Rey¹, Andrea Caneschi², Taisiya S. Sukhikh¹ and Kira E. Vostrikova¹

¹ Nikolaev Institute of Inorganic Chemistry, Siberian Branch, Russian Academy of Sciences;

² Dipartimento di Ingegneria Industriale - DIEF, Università degli Studi di Firenze, INSTM Research Unit of Firenze, Italy

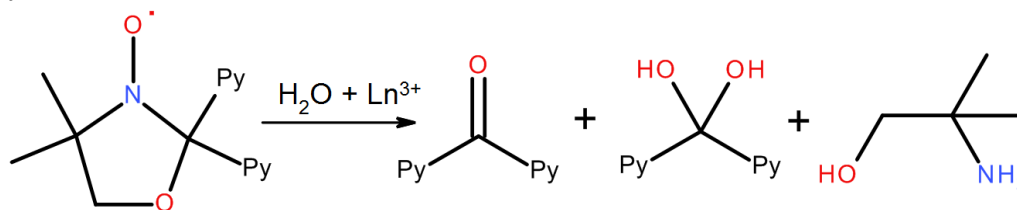


Figure S1. Catalytic hydrolysis transformation of the paramagnetic ligand. In addition, both intermediate hydrolysates and the products of their condensation with the initial radical can be also formed.

Table S1. Geometry analysis of the complexes by SHAPE software

compound	C _{4v} (Spherical capped square antiprism)	D _{3h} (Spherical tricapped trigonal prism)	C _s (Muffin)
[1]·0.5CH ₂ Cl ₂ ·0.5Et ₂ O	0.414	1.300	1.118
[2]·CH ₂ Cl ₂	0.457	1.104	1.217

*SHAPE 2.1 program for the stereochemical analysis of molecular fragments by means of continuous shape measures and associated tools.

<http://www.ee.ub.edu/>

Table S2. Crystal data and structure refinement for compounds 1–3.

Identification code	1·0.5CH ₂ Cl ₂ ·0.5Et ₂ O	2·CH ₂ Cl ₂	3
Empirical formula	C _{35.5} H ₃₈ Cl ₂ DyF ₉ N ₆ O _{13.5} S ₃	C ₃₄ H ₃₄ Cl ₂ EuF ₉ N ₆ O ₁₃ S ₃	C ₄₈ H ₃₄ Eu ₂ F ₁₂ N ₈ O ₁₈ S ₄
Formula weight	1229.85	1224.71	1670.99
Temperature/K	150(2)	150(2)	150(2)
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> /Å	17.5302(5)	17.6466(4)	13.395(13)
<i>b</i> /Å	13.8515(4)	13.9526(4)	11.949(10)
<i>c</i> /Å	19.7023(5)	19.5398(5)	18.053(17)
β/°	90.8890(10)	91.9500(10)	96.106(16)
Volume/Å ³	4783.5(2)	4808.2(2)	2873(5)
<i>Z</i>	4	4	2
ρ _{calc} /g/cm ³	1.708	1.692	1.931
μ/mm ⁻¹	1.850	1.645	2.427
<i>F</i> (000)	2452.0	2440.0	1640.0
Crystal size/mm ³	0.14 × 0.1 × 0.1	0.12 × 0.11 × 0.1	? × ? × ?
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.594 to 51.362	3.588 to 55.794	3.998 to 37.792
Index ranges	-21 ≤ <i>h</i> ≤ 21, -16 ≤ <i>k</i> ≤ 16, -24 ≤ <i>l</i> ≤ 23	-23 ≤ <i>h</i> ≤ 23, -18 ≤ <i>k</i> ≤ 18, -25 ≤ <i>l</i> ≤ 25	-12 ≤ <i>h</i> ≤ 11, -9 ≤ <i>k</i> ≤ 9, -16 ≤ <i>l</i> ≤ 16
Reflections collected	49043	71764	5053
Independent reflections	9073 [R _{int} = 0.0594, R _{sigma} = 0.0409]	11480 [R _{int} = 0.0596, R _{sigma} = 0.0392]	1988 [R _{int} = 0.1388, R _{sigma} = 0.1710]
Data/restraints/parameters	9073/64/653	11480/67/661	1988/18/285
Goodness-of-fit on <i>F</i> ²	1.045	1.020	1.009
Final <i>R</i> indexes [I ≥ 2σ (<i>I</i>)]	R ₁ = 0.0476, wR ₂ = 0.1270	R ₁ = 0.0514, wR ₂ = 0.1311	R ₁ = 0.0762, wR ₂ = 0.1578
Final <i>R</i> indexes [all data]	R ₁ = 0.0568, wR ₂ = 0.1362	R ₁ = 0.0661, wR ₂ = 0.1428	R ₁ = 0.1507, wR ₂ = 0.1943
Largest diff. peak/hole / e Å ⁻³	2.06/-1.27	2.02/-0.89	0.92/-0.77

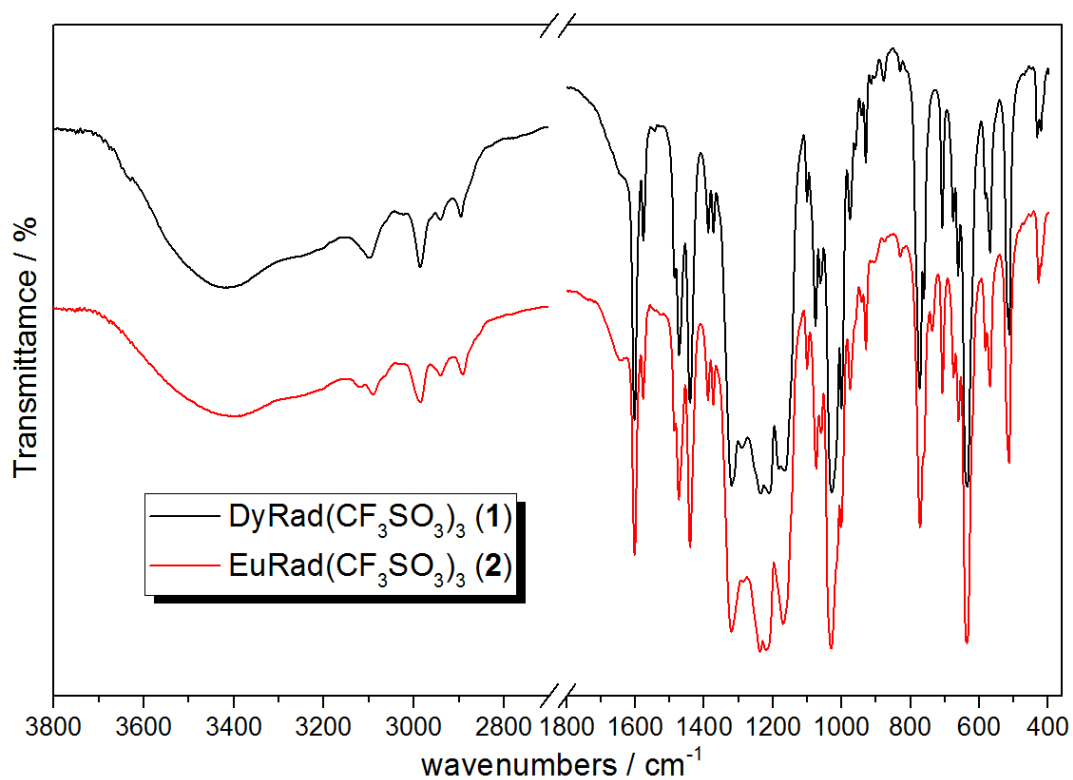


Figure S2. FTIR spectra of **1** and **2**.

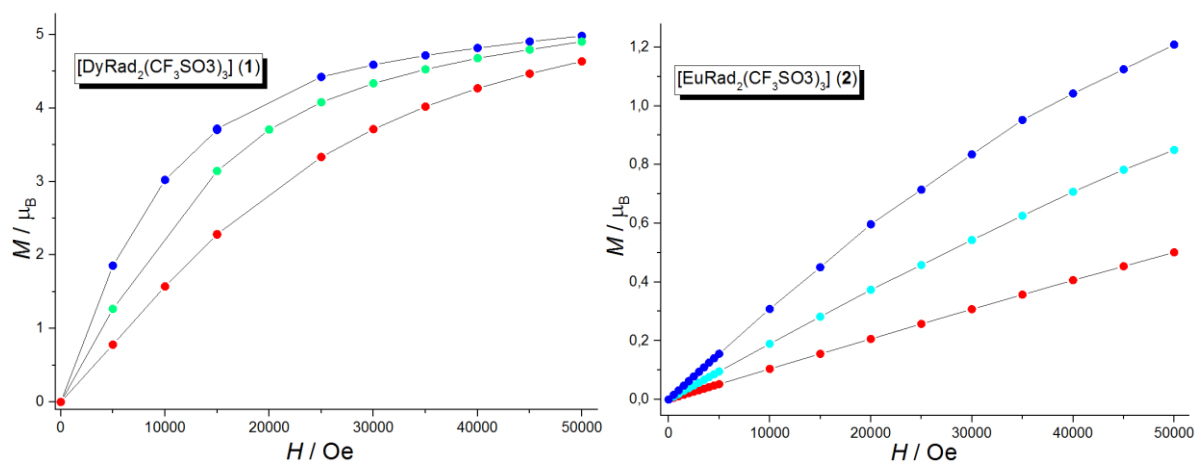


Figure S3. M/H plots for **1** and **2** at the 2, 5 and 10 K.

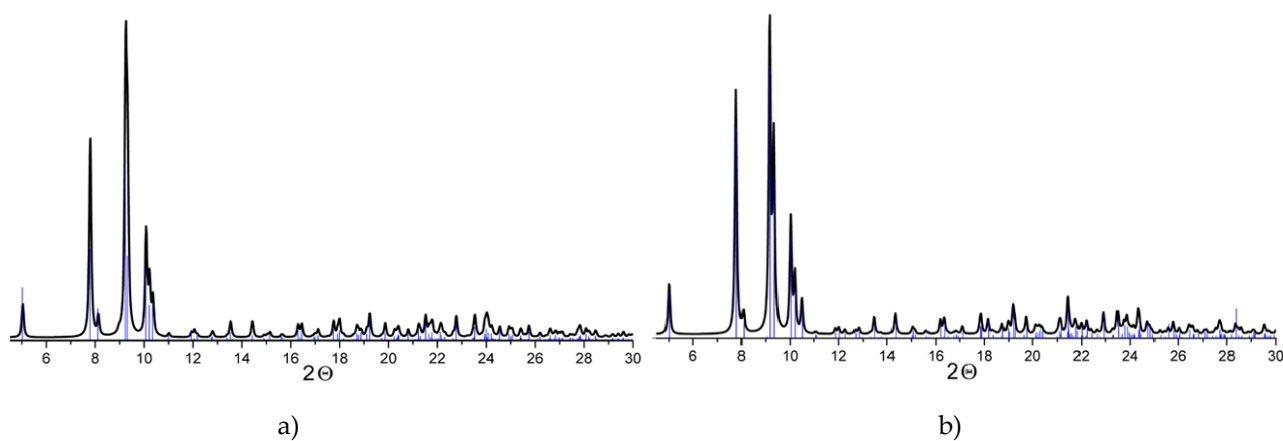


Figure S4. PRX patterns (plots) and theoretical simulations (blue lines) for **1** (Dy) (a) and **2** (Eu) (b).