

Electronic Supporting Information for:

Complexation of Am(III) and Eu(III) with DRAPA (N,N-dialkyl-6-amide-pyridine-2-carboxylic acid)

Chao Xu,^a Tingting Liu,^{a,b} Qian Liu,^b Suliang Yang,^b Dingming Li^a and Guoxin Tian^{*a,b}

a. College of Nuclear Science and Technology, Harbin Engineering University, Harbin, Heilongjiang, 150001, China.

b. Department of Radiochemistry, China Institute of Atomic Energy, Beijing, 102413, China.



202209
Am-DMAPA1-3.cif



Eu-DMAPA1-3.cif

Cif file of AmL₃, CCDC 2278529 and EuL₃, CCDC 2278528

Table 1. Crystal data and structure refinement for AmL₃ and EuL₃ complexes

Complex	AmL ₃	EuL ₃
Empirical formula	C ₂₇ H ₂₇ N ₆ O ₉ Am	C ₂₇ H ₂₇ N ₆ O ₉ Eu
Formula weight	821.54	731.58
Temperature, K	100.00(10)	100.01(10)
Crystal system	monocline, P2 ₁ /c	monocline, P2 ₁ /c
Unit cell dimensions	a = 1.471 nm b = 1.940 nm c = 1.227 nm	a = 1.470 nm b = 2.072 nm c = 1.222 nm
Volume, nm ³	3.297	3.547
Z	4	4
Density (calculated), g/cm ³	1.655	1.594
Absorption coefficient, μ/mm ⁻¹	2.054	1.703
F(000)	1588.0	2004
Crystal size/mm	0.15 × 0.15 × 0.15	0.2 × 0.2 × 0.2
Radiation parameter	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
Theta range for data collection Θ, (°)	6.664 ~ 61.786	6.502 ~ 59.528
Index ranges	-18 ≤ h ≤ 20, -22 ≤ k ≤ 26, -17 ≤ l ≤ 14	-19 ≤ h ≤ 19, -21 ≤ k ≤ 20, -28 ≤ l ≤ 27
Reflections collected	34461	19746
Independent reflections	8262 [R _{int} = 0.0825]	9946 [R _{int} = 0.0414]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data/restraints/parameters	8262/12/394	9946/26/394
Goodness-of-fit on F ²	1.047	1.026
Final R indices [I > 2σ(I)]	R ₁ = 0.0497, wR ₂ = 0.1174	R ₁ = 0.0370, wR ₂ = 0.0782
R indices (all data)	R ₁ = 0.0838, wR ₂ = 0.1314	R ₁ = 0.0478, wR ₂ = 0.0833
Largest diff. peak and hole	3750, -2230 e · nm ⁻³	1430, -970 e · nm ⁻³