

Supplementary Information

Calix[6]arene-picolinamide extractants for radioactive waste treatment: effect of modification of the basicity of the pyridine N atom on the extraction efficiency and An/Ln separation

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Table SI-1. Conformational Parameters ϕ and χ ($^{\circ}$) of the calix[6]arene derivative **5** in the **5**:2DMSO complex (the *Symbolic Representation* of the molecular conformation is C_i ++,-+,-+), and dihedral angles δ ($^{\circ}$) between the reference plane **R** (the weighted least squares plane through the CH₂ bridging groups) and the planes of the aromatic rings (**A,B,C,A',B',C'**) in the host according to standard rules for calixarenes.

	Conformational Parameters ($^{\circ}$)		Dihedral Angles ($^{\circ}$)	
	ϕ	χ		δ
A-B	91.6 (3)	89.8(4)	A-R	71.0(6)
B-C	-33.6(5)	101.0(5)	B-R	283.8(8)
C-A'	-94.7(5)	22.3(7)	C-R	217.7(8)
A'-B'	-91.6(6)	-89.8(4)	A'-R	289.0(6)
B'-C'	33.6(5)	-101.0(5)	B'-R	76.2(8)
C'-A	94.7(5)	-22.3(7)	C'-R	142.3(8)

Figure SI-1. Distribution coefficients for Eu(III) (D_{Eu}) vs. acid concentration of the aqueous phase in the extraction to a mixture of NPHE/DCE = 70:30 v/v solutions of ligands **1-5** ($1 \cdot 10^{-3} \text{ mol} \cdot \text{L}^{-1}$) and BrCosan ($2 \cdot 10^{-3} \text{ mol} \cdot \text{L}^{-1}$).

