Remarkable enhancement in Am^{3+}/Eu^{3+}selectivity by an ionic liquid based solvent containing bis-1,2,4-triazinyl pyridine derivatives: DFT validation of experimental results

A. Bhattacharyya[1,*], S.A. Ansari[1], T.Gadly[2], S.K. Ghosh[2], M. Mohapatra[1] and P.K. Mohapatra[1,*]

1. Radiochemistry Division; 2. Bioorganic Division,

Bhabha Atomic Research Centre, Trombay, Mumbai-400085, India

Supporting Information

Distribution Studies

Figure S1: Effect of aqueous phase acidity on the extraction of Am^{3+} and Eu^{3+} by 0.01 M MeBTP in different $C_nmim.NTf_2$

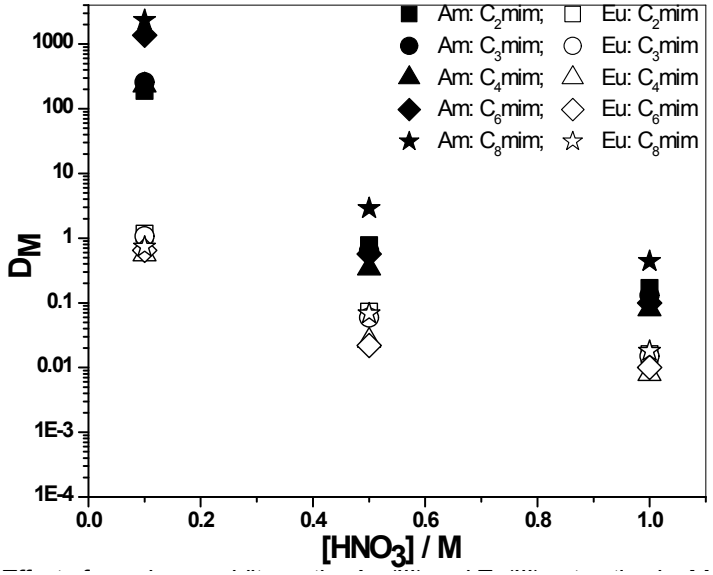


Figure S2: Effect of aqueous phase acidity on the selectivity of Am^{3+} over Eu^{3+} by 0.01 M MeBTP in different $C_nmim.NTf_2$

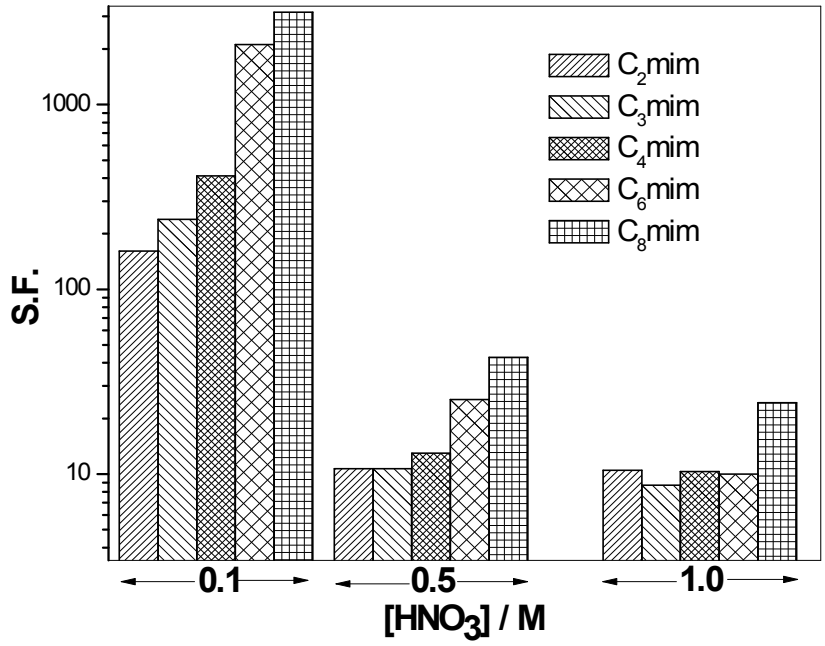


Figure S3: Effect of aqueous phase acidity on the extraction of Am^{3+} and Eu^{3+} by 0.01 M EtBTP in different $C_nmim.NTf_2$

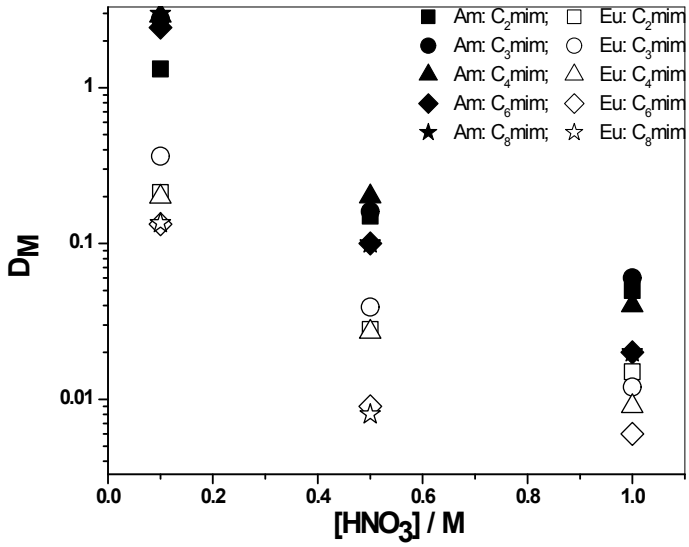


Figure S4: Effect of aqueous phase acidity on the selectivity of Am^{3+} over Eu^{3+} by 0.01 M EtBTP in different $C_nmim.NTf_2$

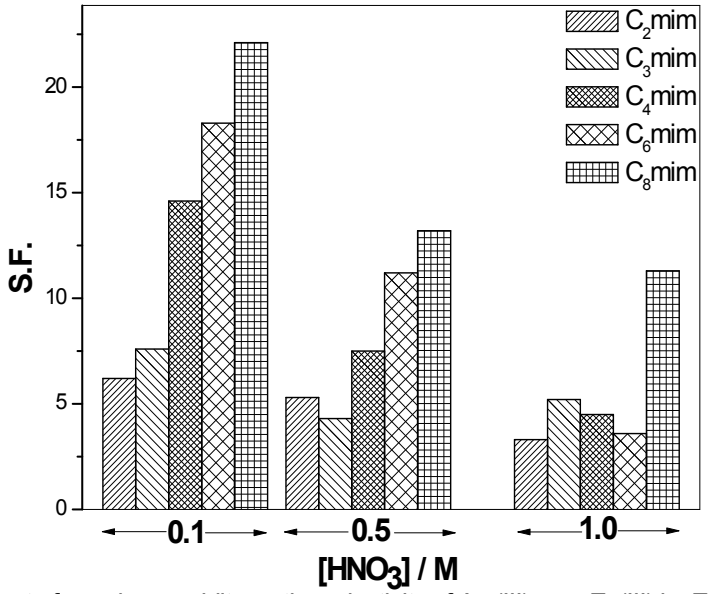


Figure S5: Effect of aqueous phase acidity on the extraction of Am^{3+} and Eu^{3+} by 0.01 M *n*-PrBTP in different $C_nmim.NTf_2$

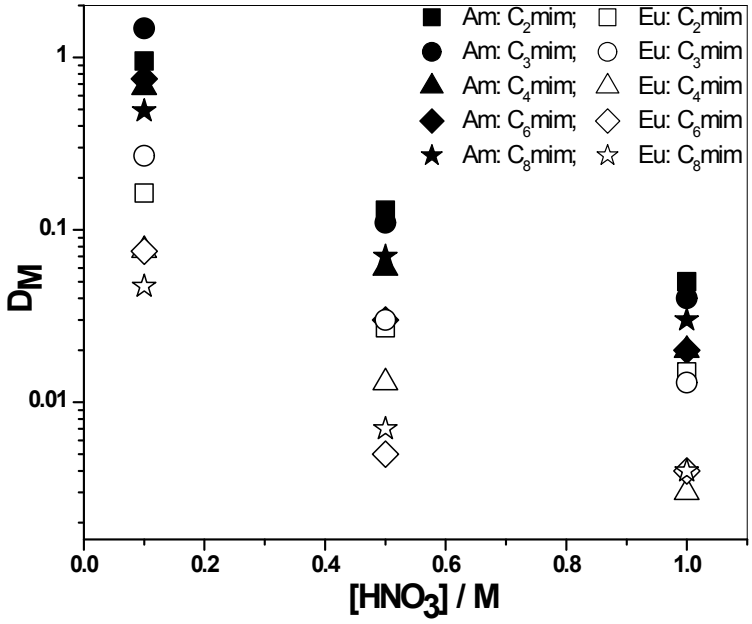


Figure S6: Effect of aqueous phase acidity on the selectivity of Am^{3+} over Eu^{3+} by 0.01 M *n*-PrBTP in different $C_nmim.NTf_2$

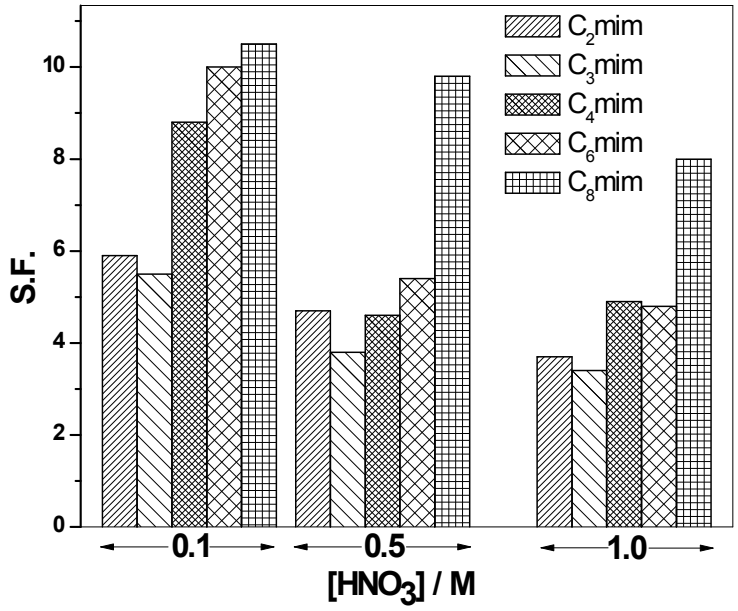


Figure S7: Effect of MeBTP concentration on the Am^{3+} and Eu^{3+} extraction; Org. phase: 0.004-0.02 M MeBTP in C_4mim.NTf_2; Aq. Phase: 0.1 M HNO_3

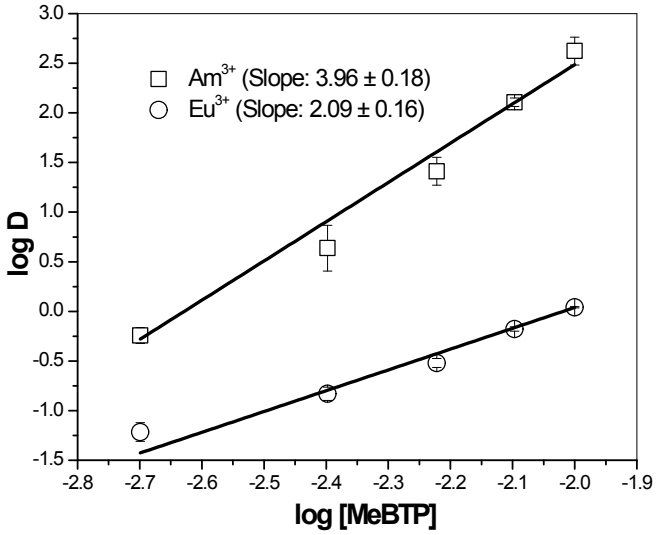


Figure S8: Effect of EtBTP concentration on the Am^{3+} and Eu^{3+} extraction; Org. phase: 0.004-0.02 M EtBTP in $C_4mim.NTf_2$; Aq. Phase: 0.1 M HNO_3

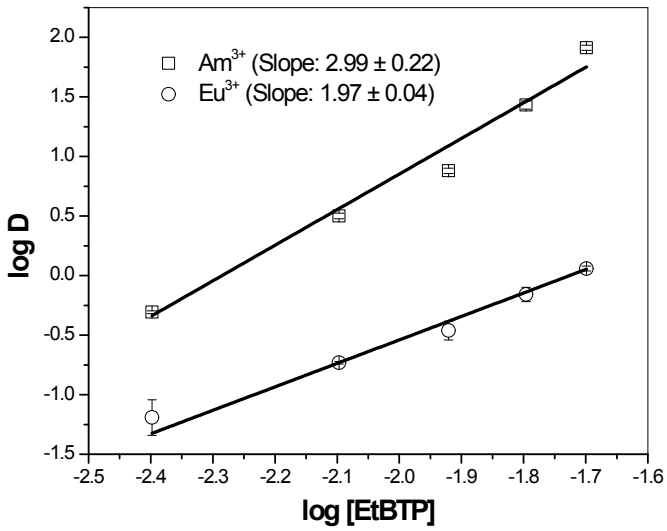
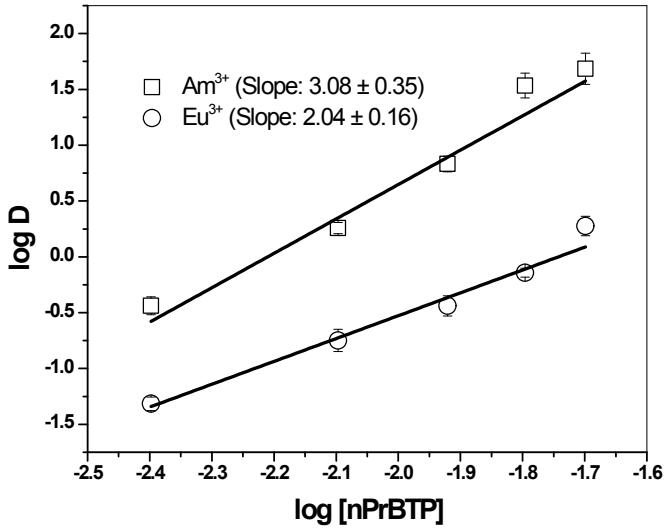


Figure S9: Effect of nPrBTP concentration on the Am^{3+} and Eu^{3+} extraction; Org. phase: 0.004-0.02 M nPrBTP in C_4mim.NTf_2; Aq. Phase: 0.1 M HNO_3



Luminescence Studies

Figure S10: Decay of Eu^{3+} complexes in the organic extract (λ_{ex} = 327 nm (for Eu-MeBTP), 359 nm (for Eu-EtBTP) and 358 nm (for Eu-nPrBTP) and λ_{em} = 616 nm): Org. Phase: 0.01 M RBTP + 1 M 2-bromooctanoic acid in *n*-dodecane; Aq. Phase : 0.1 M HNO_3

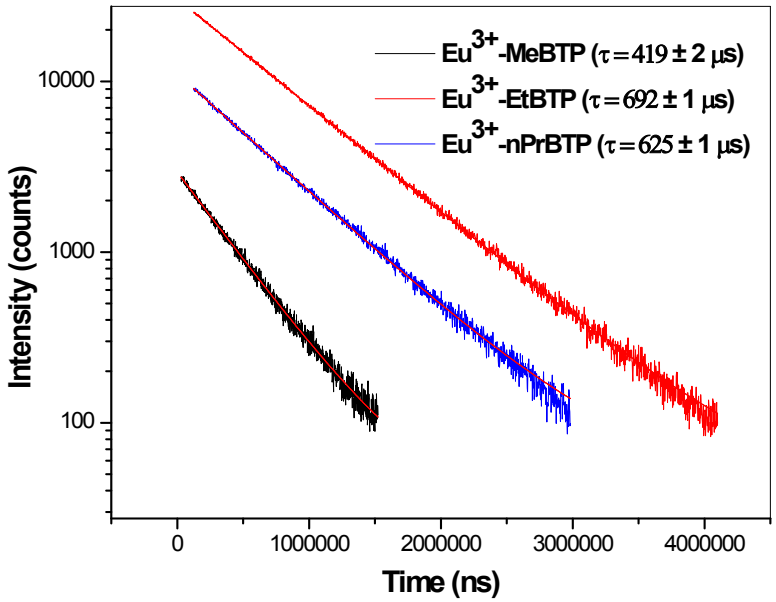


Figure S11: Decay of Eu^{3+} complexes in the organic extract (λ_{ex} = 247 nm and λ_{em} = 616 nm): Org. Phase: 0.01 M RBTP in C_4mim.NTf_2; Aq. Phase : 0.1 M HNO_3

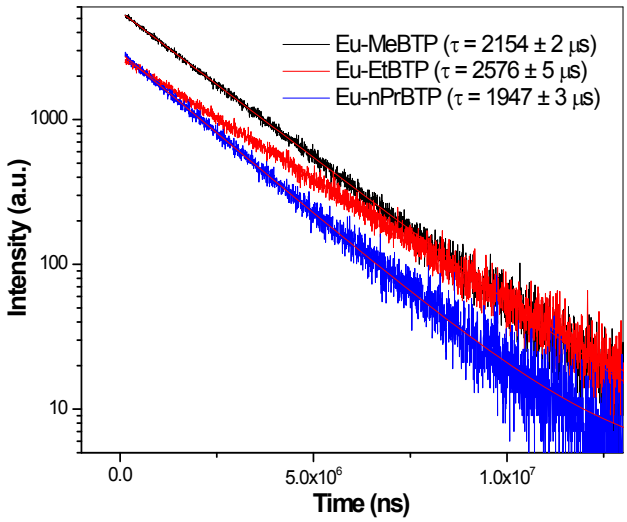


Table S12: Two center Mayer's bond orders in the 'M-N' bonds in different Am^{3+} and Eu^{3+} complexes of MeBTP (L: Me-BTP; BOA: 2-bromo octanoic acid)

M^{3+}	$M(L)(BOA)_3$	$[M(L)_2(NO_3)_2]^+$	$[M(L)_3]^{3+}$
Am^{3+}	$Am\text{-}N_c = 0.297$	$Am\text{-}N_c = 0.311(2)$	$Am\text{-}N_c = 0.359(5)$
	$Am\text{-}N_l = 0.28(4)$	$Am\text{-}N_l = 0.30(1)$	$Am\text{-}N_l = 0.346(9)$
Eu^{3+}	$Eu\text{-}N_c = 0.213$	$Eu\text{-}N_c = 0.253(3)$	$Eu\text{-}N_c = 0.305(2)$
	$Eu\text{-}N_l = 0.211(6)$	$Eu\text{-}N_l = 0.253(4)$	$Eu\text{-}N_l = 0.299(6)$