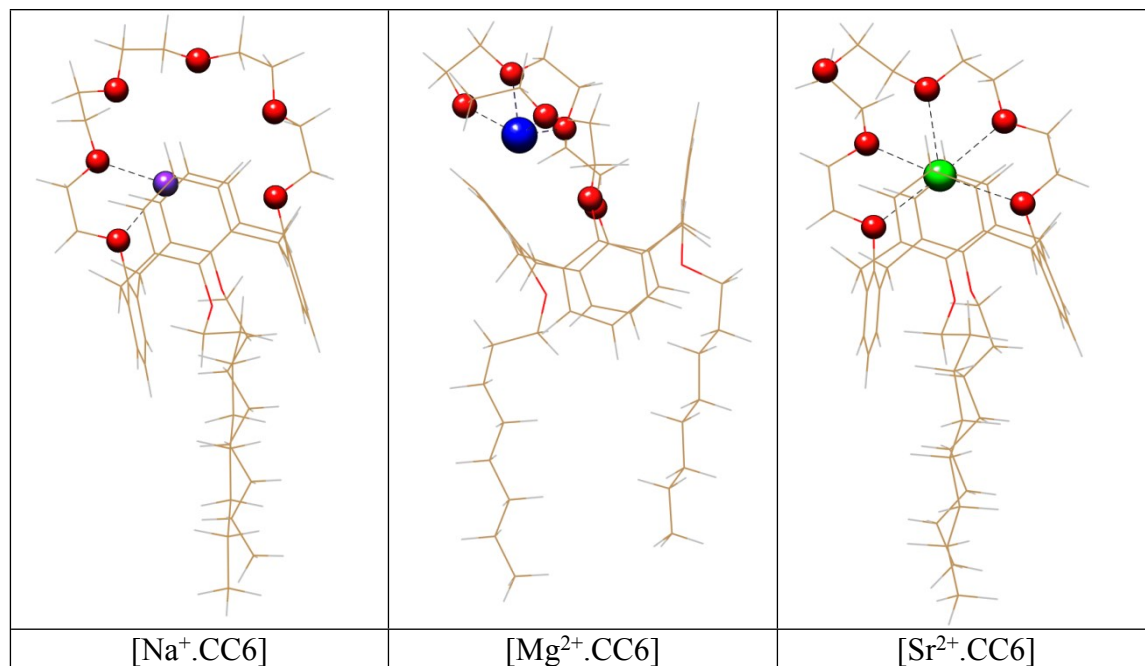


## Supporting information

*Achieving Highly Efficient and Selective Cesium Extraction using 1,3 di-octyloxy-calix [4]arene-crown-6 in n-octanol based Solvent System:  
Experimental And DFT Investigation*



**Fig.S1:** Optimized structures of M.CC6 complexes. (M= Na<sup>+</sup>, Mg<sup>2+</sup> and Sr<sup>2+</sup>)

**Table S1:** Mulliken charges, HOMO-LUMO gap of M.CC6 complexes. (M= Na<sup>+</sup>, Mg<sup>2+</sup>, Sr<sup>2+</sup> and Cs<sup>+</sup>)

Complex	Charge	HOMO-LUMO ( $\Delta E$ , eV)
	M	
Na <sup>+</sup> .CC6	0.653	-5.46
Mg <sup>2+</sup> .CC6	1.468	-4.81
Sr <sup>2+</sup> .CC6	1.329	-5.29
Cs <sup>+</sup> .CC6	0.946	-5.54

**Table S2:** Reorganization energies of CC6 ligand upon complexation with M. (M= Na<sup>+</sup>, Mg<sup>2+</sup>, Sr<sup>2+</sup> and Cs<sup>+</sup>)

M. CC6	Reorganization energy
Na <sup>+</sup> .CC6	+6.00
Mg <sup>2+</sup> .CC6	+34.41
Sr <sup>2+</sup> .CC6	+22.27
Cs <sup>+</sup> .CC6	+3.49