*Desalination and Water Treatment*
www.deswater.com

38 (2012) 1–7
January


doi: 10/5004/dwt.2012.2279

Taylor & Francis
Taylor & Francis Group

# Designing of ligands for solvent extraction of $Cs^+$ using molecular modeling approach

Shobha K. Nagappayya[a], Vilas G. Gaikar[a,*], Sk. Musharaf Ali[b]

[a]*Department of Chemical Engineering, Institute of Chemical Technology, Matunga, Mumbai 400019, India*
*Fax: +91 22 33611020; email: vg.gaikar@ictmumbai.edu.in*
[b]*Chemical Engineering Division, Bhabha Atomic Research Centre, Mumbai 400085, India*

Received 9 December 2010; Accepted 13 June 2011

**ABSTRACT**

A molecular modelling (MM) approach has been adopted for designing new ligands for the extraction of $Cs^+$. The structures of the metal ion-ligand complexes were initially optimized using FORCITE molecular mechanics module of Materials Studio 3.2. The ab initio DMol$^3$ DFT calculations were further conducted on the MM optimized structures. The selectivity of designed ligands for $Cs^+$ was ascertained by interaction, strain and hydration energies.

*Keywords:* Molecular modeling; Extraction; DFT calculations; Crown ethers; Complexation; $Cs^+$ ion

*Corresponding author.

*Proceedings of DAE-BRNS Biennial Symposium on Emerging Trends in Separation Science and Technology, Kalpakkam, India, March 1–4, 2010*