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Solubility of dialkylalkyl phosphonates in supercritical carbon dioxide: Experimental and modeling approach

K.C. Pitchaiah, C.V.S. Brahmananda Rao, N. Sivaraman, M. Joseph, Giridhar Madras, Ilia Brondz

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K.C. Pitchaiah¹, C.V.S. Brahmananda Rao¹, N. Sivaraman^{1,*}, M. Joseph¹, Giridhar Madras² and Ilia Brondz³

¹Chemistry Group, Indira Gandhi Centre for Atomic Research, HBNI, Kalpakkam-603 102, India ² Indian Institute of Science, Bangalore-560012, India ³Norwegian Drug Control and Drug Discovery Institute AS, Ski, Norway

*Corresponding author: email: <u>sivaram@igcar.gov.in</u>

Abstract

Dialkylalkyl phosphonates have found renewed interest in the selective extraction of actinides from different matrices. In this context, two dialkylalkyl phosphonates, dibutylbutyl phosphonate (DBBP) and diamylamyl phosphonate (DAAP) were synthesised and their solubilities in supercritical carbon dioxide (SCCO₂) medium were determined in the pressure range of 10 to 25 MPa at 313 to 333 K. Solubility studies were carried out to examine their utility as ligands during supercritical fluid extraction of actinides. Solubilities of dialkylalkyl phosphonates ranged from 0.06 to 0.12 mole fraction. Experimental solubilities were correlated using Mendez-Santiago, Chrastil, solution theory with Wilson activity coefficient model and association model based on van Laar activity coefficient model. Comparison among these models revealed that the association model with van Laar activity coefficient model provides better solubility predictions. SCCO₂ containing DAAP was employed for the (i) selective extraction of uranium in the presence of simulated fission products and (ii) extraction of uranyl nitrate from acidic medium.

Keywords: Solubility, Phosphonates, Supercritical Carbon Dioxide, Semi-empirical Models, Selective Extraction.

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