Synthesis and Crystal Structure Analysis of C_{60} Fulleride Dianions in Solvates of $[A([2.2.2]crypt)]_2[C_{60}]$ (A = K, Rb, Cs)

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

Reduction of C_{60} with the alkali metals A = K, Rb and Cs in tetrahydrofuran as a solvent and addition of [2.2.2]crypt [1], dimethylformamide and cyclohexane lead to the formation of crystalline samples of $[A([2.2.2]crypt)]_2[C_{60}](C_6H_{12})_2(C_3H_7NO)_2(C_4H_8O)_2$ (A = K, Rb, Cs) **1a**, **1b** and **1c** as major fractions. As a by-product of compound **1a**, a second minor fraction containing $[K([2.2.2]crypt)]_2[C_{60}](C_3H_7NO)_4$ **2** was obtained. The structures of the four compounds have been determined by single-crystal X-ray analyses. The $[C_{60}]^{2-}$ dianions are predominantly ordered. As the main structural motif the structures of compounds **1a**, **1b** and **1c** contain pseudo-hexagonal layers of $[C_{60}]^{2-}$ dianions. Compound **1c** contains a rare example of a Cs^+ sequestering [2.2.2]crypt molecule. The packing of the ionic units in compound **2** also shows layers of distorted hexagons formed by $[C_{60}]^{2-}$ dianions which arranged in pairs with short contacts of 10.3 Å between their centers of gravity.

Key words: Fullerides, Crystal Structure, Dianion, Hexagonal Packing