

# Quantum-Chemical Estimation of Outersphere Cations Influence on Charge Transfer at the $\text{NbF}_7^{2-}$ Reduction. I. Electronic Structure of Complexes

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Quantum-chemical calculations of the parameters of the  $n\text{M}^+ \cdot \text{NbF}_7^{q-}$  type particles, where M stands for Na, K, Cs;  $q = 2, 3$  and  $n = 0-7$  have been performed. Within the framework of this approximation, compositions for the most stable particles in molten salts were obtained. It is shown that electron transfer onto the particle results in a different redistribution of the electron density with the Na and K-particles on one hand and Cs-containing particles on the other hand. Energies and some other characteristics of the electron structure and particle geometry were determined depending on the  $n$  and M values.

*Key words:* *ab initio*; Outersphere Cations; Electron Transfer; Electrode Reaction;  
Niobium Fluoride Complex.