Ab Initio Estimation of NbF_6^-, $NbClF_6^{2-}$, and NbF_7^{2-} Complexes Stability in Alkali Chloride Melts

Vyacheslav G. Kremenetsky[a], Sergey A. Kuznetsov[a], Olga V. Kremenetskaya[b], Veniamin V. Soloviev[c], Lyudmila A. Chernenko[c], and Anatoliy D. Fofanov[b]

[a] Institute of Chemistry, Kola Science Center RAS, 26a Akademgorodok, 184209 Apatity, Russia
[b] Petrozavodsk State University, Lenin avenue 33, 185910 Petrozavodsk, Russia
[c] Poltava National Technical University, Pershotravnevyi prospekt 24, 36011 Poltava Ukraine

Reprint requests to Dr. V. G. K.; E-mail: kreme_vg@chemy.kolasc.net.ru

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Quantum-chemical calculations of the parameters of the $n\mathrm{M}^+ \cdot \mathrm{NbClF}_6^{2-}$ type particles have been performed, where M stands for Na, K, Cs and $n = 0 - 6$. Under certain conditions such particles may exist in melts of alkali metal chlorides. Within the framework of this approximation, compositions for the most stable particles in molten salts were obtained. Relative stability of the particles containing the NbF_6^-, $NbClF_6^{2-}$, and NbF_7^{2-} complexes has been calculated. Energies and some other characteristics of the electron structure and the particle geometry structure were determined depending on the n and M values. For estimation of the third sphere's influence, the systems ($M_2NbF_7 + 8MCl$) and ($M_2NbF_7 + 15MCl$) are surveyed. The chlorine anion enters the first coordination sphere in the Na-system only, i. e. in this system the true complex $NbClF_7^{3-}$ is formed.

Key words: Ab Initio Calculations; Chloride-Fluoride Niobium Complex; Outersphere Cations; Structure Parameters.