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CONTINUOUS INDICATOR FIELDS IN MODELLING OF Am³⁺/Eu³⁺ SEPARATION FACTORS

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In the framework of the Continuous Molecular Fields (CMF) approach [1] for building 3D-QSAR models continuous functions are used for the description of molecular fields instead of finite sets of molecular descriptors (such as interaction energies computed at grid nodes) commonly applied for this purpose (in CoMFA, CoMSIA, GRID, etc.). In this work, a novel type of molecular fields, Continuous Indicator Fields (CIFs) [2], is suggested to provide 3D structural description of molecules. The values of CIFs are calculated as the degree to which a point with 3D coordinates belongs to an atom of a certain type. CIFs can be considered as a 3D analog of atom-centered fragment descriptors.

This approach is applied to building 3D-QSAR models of separation factors of Am³⁺/Eu³⁺ for the datasets of 47 polyazaheterocyclic ligands. It is shown that even in the simplest form this method provides either comparable or enhanced predictive performance of models in comparison with state-of-the-art 3D-QSAR methods based on interaction molecular fields of physico-chemical nature.

Graphical analysis of 3D-QSAR models based on the use of CIFs shows the preferable positions (in physical 3D space) of structural features important for strong binding of ligands to proteins. This allows for a clear interpretation of 3D-QSAR models by visualizing the overlap between the fields of regression coefficients specifying the preferable positions of atoms with CIFs describing their actual position for a given molecule. This directs the process of lead optimization towards the better overlap between them.

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AB-INITIO INVESTIGATION OF RARE-EARTH FLUORITES GDLIF₄ AND LULIF₄ UNDER HYDROSTATIC PRESSURE

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The interest in fluorite rare-earth compounds (with the scheelite $CaWO_4$ structure) increases significantly due to their possible application in laser technologies and microelectronics [1,2]. When a stress is applied the present materials undergo to the phase transitions.

That to investigate the phase transitions in $LuLiF_4$ and $GdLiF_4$ compounds we performed ab-initio calculations by means of DFT [3, 4] with using VASP 5.2 [5] (Vienna Ab-Initio Simulation Package) program, the part of the MedeA[1] interface. The ferroelastic phase transition of the $LuLiF_4$ scheelite ($I4_1/a$, Z=4) from the tetragonal structure to the fergusonite one (C12/c1, Z=4) has been found at 10.5 GPa [6]. It has been identified as the second-order transition from the pressure dependence of the structural parameters, order parameter and cell volume. The absence of the phase transitions to the $P2_1/c$ and P12/c1 structure symmetries has been shown. In order to find the similar phase transitions in $GdLiF_4$, the behavior of the order parameter for the C12/c1 symmetry, as well as the enthalpy difference between two symmetries $I4_1/a$ and P12/c1 versus the pressure have been investigated. One can conclude that the order parameter of $GdLiF_4$ structure is changed at a pressure close to 16 GPa. The coincidence of enthalpy of the $I4_1/a$ and P12/c1 symmetries is observed near 18 GPa. Thus, the transitions to the C12/c1 and P12/c1 symmetries compete with each other. The fact that the $GdLiF_4$ compound undergoes a structural decomposition can be explained based on this assumption.

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