METAL ORGANIC FRAMEWORKS – NEW MATERIALS, NEW CHEMISTRY

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The critical part of metal organic frameworks constitute octahedral nodes based on six-coordinate cations (III) of the first row transition metals or Group13 elements. Despite structural similarities (d2sp3 hybridization of atomic orbitals of metals) there exist fundamental differences in nature of chemical Me3+-O bonds formed by transition or main group metals.. Such complexes are discussed in this work on the base of structural, thermodynamic, and electronic properties of complexes representing selected fragments of MIL-53 MOFs. The presented findings were determined within the advanced theoretical studies.