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Electronic structure, aromaticity and spectra of hetero[8]circulenes 455

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The present review illustrates progress in experimental and theoretical chemistry in investigation of electronic structures and physicochemical properties of hetero[8]circulenes, which are the only representatives of planar heteroannulated cyclooctatetraenes. It is shown, that high molecular symmetry and specific π -extended structure of hetero[8]circulenes are the main factors responsible for high stability of their crystal packing, optical and magnetic properties. The symmetry effects determine also numerous prohibitions of electronic and vibrational transitions in UV-visible, IR and Raman spectra. The special attention is devoted to the aromaticity of hetero[8]circulenes containing the internal eight-membered cyclooctatetraene antiaromatic ring. The planar structure of the cyclooctatetraene core is stabilized by the external polyaromatic system composed of the condensed five- and six-membered aromatic rings. Due to high thermal and chemical stability of hetero[8]circulenes together with their semiconducting properties these compounds can be considered as promising materials for molecular electronics and nanophotonics. Hetero[8]circulenes are already used in organic light-emitting diodes and field-effect transistor technology. Bibliography — 154 references.

Electrochemical synthesis of cyclopropanes 485

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Data on the use of electrochemical methods for the synthesis of cyclopropanes are considered and generalized. The main attention is given to the most efficient methods of cyclopropane synthesis — electrocatalytic cascade and multicomponent transformations of C–H acids and also combined electrolysis of C–H acids and activated alkenes or carbonyl compounds in the presence of alkali metal halides as mediators. Bibliography — 62 references.

Stability and thermal evolution of transition metal and silicon clusters 498

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The results of computer simulation studies of transition metal and silicon clusters published in the last decade are summarized. Comparative analysis of the stability and thermal evolution of nanoclusters is performed depending on the preparation method, type of bonds, atom packing, coherence of the constituent nanofragments, surface morphology, and change in the relationship between the short- and long-range ordering with increasing size. Taking account of the substrate nature and dimensionality of the cluster disperse systems being simulated, most important structure-dependent kinetic and mechanical characteristics are discussed, including specific temperature ranges of disordering corresponding to isomerization and quasi-melting. Bibliography — 263 references.

Nanostructured diborides of titanium, zirconium and hafnium: synthesis, properties, size effects and stability 540

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Methods for the synthesis of nanopowders, nanowhiskers and films based on titanium, zirconium and hafnium diborides are considered. The consolidation approaches to the preparation of bulk nanomaterials are analyzed. Information on physicochemical and physicomaterial properties is generalized with the analysis of size effects. Data on the thermal stability and effects of radiation, deformation and corrosion exposures on TiB₂, ZrB₂ and HfB₂ nanostructures are given. Some less investigated issues of the discussed area of research are noted. Bibliography — 130 references.