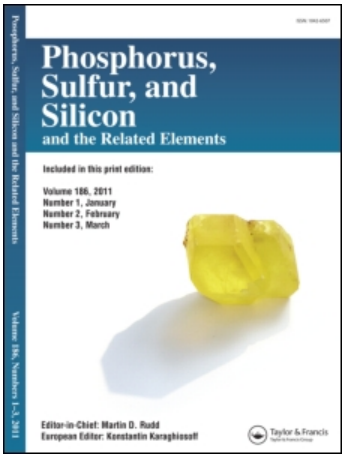

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A THEORETICAL TREATMENT OF THE SULFUR-CONTAINING ANALOGS OF CYCLOBUTADIENE, CYCLOOCTATETRAENE, BUTALENE, AND OCTALENE

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A THEORETICAL TREATMENT OF THE SULFUR-CONTAINING ANALOGS OF CYCLOBUTADIENE, CYCLOOCTATETRAENE, BUTALENE, AND OCTALENE

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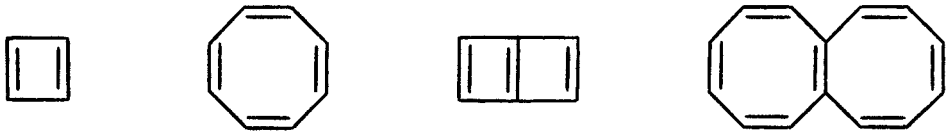
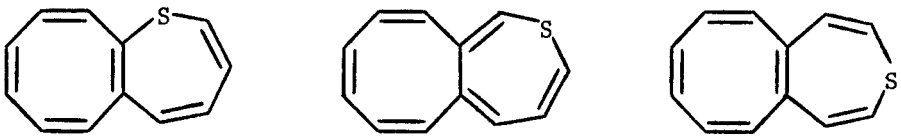
Several coordination complexes of cyclobutadiene (I) have been prepared (e.g., cyclobutadiene iron tricarbonyl [1]) and cyclooctatetraene (II) is a well-known compound (for a potentially planar form of cyclooctatetraene, see [2]). Although butalene [3] (III) has not been synthesized so far, octalene (IV) has been obtained by Vogel and co-workers [4,5]. Recently we have carried out a theoretical study of the physical and chemical properties of butalene (III) and octalene (IV), and of the various annelated butalenes and octalenes [6,7] using the HMO and SCF-MO (PPP) quantum-chemical methods as well as the structure-resonance theory and graph theoretical methods. Numerous theoretical data are available in the literature on cyclobutadiene (I) and cyclooctatetraene (II).



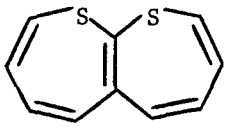
I II III IV

The present contribution will be devoted to a similar study of a group of sulfur analogs of the hydrocarbons I-IV formally derived by substituting a sulfur atom for a CH=CH group in these hydrocarbons. Among other compounds, the group includes thiirene (V), thiepin (VI), and the sulfur analogs of butalene (VII, VIII) and octalene (IX-XX).

V VI VII VIII



IX X XI



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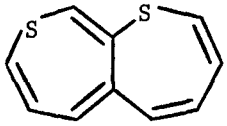

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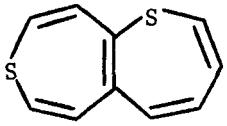

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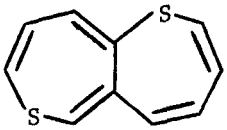

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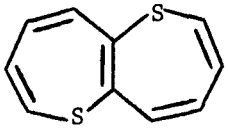

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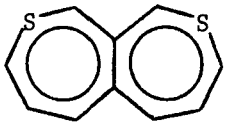

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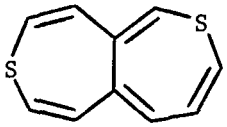

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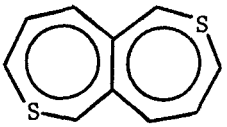

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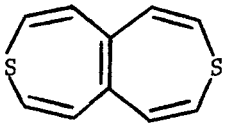

XX

Resonance energies, ionization and reduction potentials, and excited state energies from HMO (Hess and Schaad) and SCF-MO (PPP) calculations, structure-resonance theory (Herndon), graph theory (conjugated circuits - Randić), and the reference polynomial method (Aihara) will be compared. The data obtained for the heterocycles will be compared with those for the parent hydrocarbons and the calculated quantities will be used to predict their aromaticity, stability, and other physical and chemical properties.

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