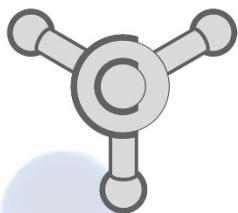


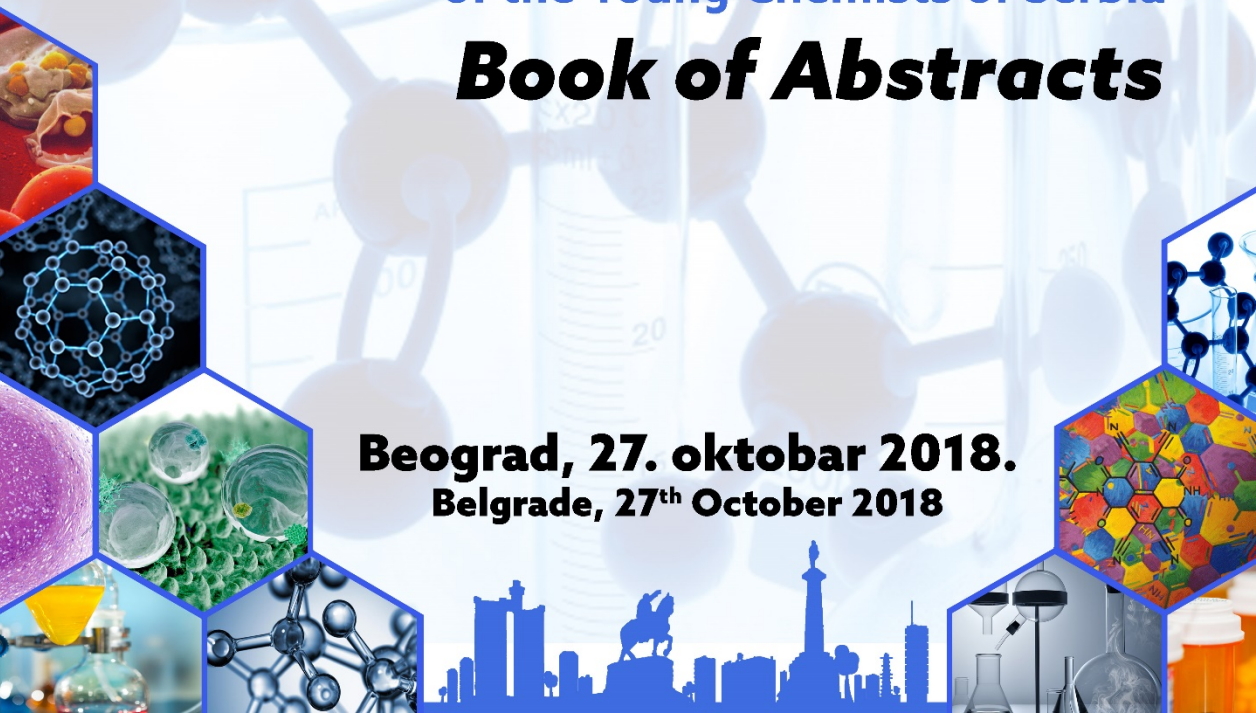
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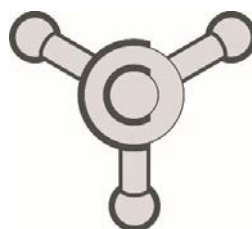
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Valence bond study of intramolecular hydrogen bonding in malondialdehyde

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Intramolecular hydrogen bonding plays a fundamental role in many fields of chemistry. In this work the resonance assisted hydrogen bonding in malondialdehyde was examined. The energy of hydrogen bonding was calculated with different methods: *cis-trans* comparative analysis method, isodesmic reaction, analysis of electron density topology (AIM method) and valence bond method. The contribution of resonance was calculated by comparison of the energy of selected valence structures of malondialdehyde at VBSCF level of theory. Our results indicate that the effect of π -electrons delocalization to hydrogen bonding is approximately 13% of the total energy.

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