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delocalization

in theoretical organic chemistry

Redistribution of the valence-shell electron density throughout a molecular entity as compared with some localized models (individual atoms in their valence states, separated bonds or fragments). Different topological modes of the electron delocalization include:

1. *ribbon delocalization* of either π- or σ-electrons (*i.e.*, electrons occupying respectively π- and σ-orbitals)
2. *surface delocalization* of σ-electrons occurring through an overlap of radially oriented σ-orbitals of a cyclic molecule, as is the case of cyclopropane; and
3. *volume delocalization* of σ-electrons through an overlap of σ-orbitals directed inside a molecular polyhedron, as is the case in tetrahedrane.

Source:

PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1933

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