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Lista publikacji

z dnia 31 października 2014

Publikacje w czasopismach

1. Szczepanik D.W., Andrzejak M., Dyduch K., Żak E., Makowski M., Mazur G., Mrozek J., 2014, **A uniform approach to the description of multicenter bonding**, *Physical Chemistry Chemical Physics* 16: 20514-20523.
2. Szczepanik D.W., Żak E., Dyduch K., Mrozek J., 2014, **Electron delocalization index based on bond order orbitals**, *Chemical Physics Letters* 593: 154-159.
3. Szczepanik D.W., Mrozek J., 2013, **Through-space and through-bridge interactions in the correlation analysis of chemical bonds**, *Computational and Theoretical Chemistry* 1026: 72-77.
4. Szczepanik D.W., Mrozek J., 2013, **Nucleophilicity index based on atomic natural orbitals**, *Journal of Chemistry* 2013: ID684134.
5. Szczepanik D.W., Mrozek J., 2013, **Minimal set of molecule-adapted atomic orbitals from maximum overlap criterion**, *Journal of Mathematical Chemistry* 51: 2687-2698.
6. Szczepanik D.W., Mrozek J., 2013, **Ground-state projected covalency index of the chemical bond**, *Computational and Theoretical Chemistry* 1023: 83-87.
7. Szczepanik D.W., Mrozek J., 2013, **On quadratic bond-order decomposition within molecular orbital space**, *Journal of Mathematical Chemistry* 51: 1619-1633.
8. Szczepanik D.W., Mrozek J., 2013, **Stationarity of electron distribution in ground-state molecular systems**, *Journal of Mathematical Chemistry* 51: 1388-1396.
9. Szczepanik D.W., Mrozek J., 2013, **On several alternatives for Löwdin orthogonalization**, *Computational and Theoretical Chemistry* 1008: 15-19.
10. Szczepanik D.W., Mrozek J., 2012, **Electron population analysis using a reference minimal set of atomic orbitals**, *Computational and Theoretical Chemistry* 996: 103-109.
11. Szczepanik D.W., Mrozek J., 2012, **Symmetrical orthogonalization within linear space of molecular orbitals**, *Chemical Physics Letters* 521: 157-160.
12. Nalewajski R.F., Szczepanik D.W., Mrozek J., 2012, **Basis set dependence of molecular information channels and their entropic bond descriptors**, *Journal of Mathematical Chemistry* 50: 1437-1457.
13. Nalewajski R.F., Szczepanik D.W., Mrozek J., 2011, **Bond differentiation and orbital decoupling in the orbital-communication theory of the chemical bond**, *Advances in Quantum Chemistry* 61: 1-48.
14. Szczepanik D.W., Mrozek J., 2011, **Entropic bond descriptors from separated output-reduced communication channels in atomic orbital resolution**, *Journal of Mathematical Chemistry* 49: 562-575.
15. Szczepanik D.W., Mrozek J., 2011, **Probing the interplay between multiplicity and ionicity of the chemical bond**, *Journal of Theoretical and Computational Chemistry* 10: 471-482.