



Features of the alkynyl ruthenium chromophore with modified anionic subsystem UV absorption

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Titre	Features of the alkynyl ruthenium chromophore with modified anionic subsystem UV absorption
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Auteur	Migalska-Zalas, Anna [1], Kityk, Ivan-V. [2], Bakasse, Mina [3], Sahraoui, Bouchta [4]
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Mots-clés	Molecular absorption spectra [5], Organometallics [6]
Résumé en anglais	<p>Theoretical simulation of UV-vis absorption for a new series of alkynyl ruthenium chromophores spectra and investigations the influence of anionic substituent on a spectral shift of UV absorption was presented. The MM+ molecular force field method was used for total energy minimization and for building of the molecular optimized geometry [S.J. Weiner, P.A. Kollman, D.A. Case, U.C. Ghio, G. Alagona, J.S. Profeta, P. Weiner, J. Am. Chem. Soc. 106 (1984) 765; S.J. Weiner, P.A. Kollman, D.T. Nguyen, D.A. Case, J. Comput. Chem. 7 (1986) 230]. All quantum chemical calculations were performed by semi-empirical ZINDO/1 method within a framework of the restricted Hartree-Fock approach and convergence limit up to 10⁻⁶ eV after 500 iterations was achieved. Good agreement between the theoretically calculated and experimentally measured spectra was observed. The largest spectral shift in position of absorption peaks was observed for compound containing the anionic (Cl), substituent. The theoretically calculated absorption maximum is blue shifted with respect to the experimental spectra for all compounds what is connected with the changes of the charge transfer determining the corresponding state dipole moments. Analysis of the theoretical spectra shows a substantial sensitivity to the backside groups.</p>
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Liens

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