Synthesis, spectroscopy and computational studies of some novel π-conjugated vinyl *N*-alkylated quinolinium salts and their precursor's.

Autorzy

Jacek E. Nycz

Karolina Czyż

Marcin Szala

Jan G. Małecki

George Shaw

Brendan Glimore

Marek Jon

Rok wydania

2016

Czasopismo

Journal of Molecular Structure

Numer woluminu

1106

Strony

416-423

DOI

10.1016/j.molstruc.2015.11.011

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

A series of π-conjugated vinyl*N*-methylated quinolinium salts (**3**) and their precursor's*N*-alkylated quinolinium salts (**2**) were prepared and characterized by NMR, IR, UV-Vis and MS spectroscopy. It was confirmed that the hydroxyl and amino derivatives of vinyl*N*-methylated quinolinium salts lead to spiro type compounds (**4**). The syntheses of*N*-alkylated quinolinium salts were successful, and even multigram scale was achievable. The structures of 1,2-dimethylquinolinium iodide (**2a**) and 1-ethyl-2-methylquinolinium iodide (**2b**) were determined by single crystal X-ray diffraction method. NMR spectra showed readily diagnostic H-1 and C-13 signals from methyl and*N*-alkyl groups for both**2**and**3**. The geometries of the studied compounds were optimized in singlet states using the density functional theory (DFT) method with B3LYP functional. In general, the predicted bond lengths and angles are in a good agreement with the values based on the X-ray crystal structure data.

Słowa kluczowe

Quinoline, Vinyl quinolinium salt, Styryl quinolinium salt, Styryl dye, Spiro, Perkin condensation

Adres publiczny

http://dx.doi.org/10.1016/j.molstruc.2015.11.011

Strona internetowa wydawcy

http://www.elsevier.com