Photophysical Behavior and Computational Investigation of Novel 1,4-Bis(2-(2-Phenylpyrimido[1,2-a]Benzimidazol-4-Yl)Phenoxy)Butan (BPPB) Macromolecule

By: Saleh, TS (Saleh, Tamer S.)[1,2] ; Hussein, MA (Hussein, Mahmoud A.)[3,4] ; Osman, OI (Osman, Osman I.)[3,5] ; Alamry, KA (Alamry, Khalid A.)[1,3] ; Mekky, AEM (Mekky, Ahmed E. M.)[1,6] ; Asiri, AM (Asiri, Abdullah M.)[3,7] ; El-Daly, SA (El-Daly, Samy A.)[8]

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JOURNAL OF FLUORESCENCE
Volume: 26 **Issue:** 5 **Pages:** 1895-1904
DOI: 10.1007/s10895-016-1884-2
Published: SEP 2016
View Journal Impact

Abstract

A new macromolecule pyrimido[l,2-a]benzimidazole derivative named 1,4-bis(2-(2-phenylpyrimido[1,2-a]benzimidazol-4-yl)phenoxy)butan (BPPB) has been synthesized in accepted yield using microwave assistance. The new compound BPPB has been formed by the interaction of 3,3'-((butane-1,4-diylbis(oxy))bis(2,1-phenylene))bis(1-phenylprop-2-en-1-one) (3) with 2- aminobenzimidazole (4) in the presence of potassium hydroxide as a basic catalyst in dimethylformamide (DMF) under microwave radiation for 20 min. The chemical structure of this novel compound was elucidated by elemental and spectral techniques including: FT-IR, H-1-NMR, C-13-NMR and mass spectra. The electronic absorption and emission spectra of BPPB were measured in different solvents. BPPB displayed a solvatochromic effect of the emission spectrum that is reflected by red shifts of its fluorescence emission maxima on increasing the solvent polarity, indicating a change of electronic charge distribution upon excitation. BPPB crystalline solids gave excimer-like emission at 535 nm with a bandwidth of ca. 60 nm. Ground and excited states electronic geometry optimizations using density functional theory (DFT) and time-dependent density functional theory (TD-DFT), respectively, complemented these spectral findings. The intramolecular charge transfer was investigated by natural bond orbital (NBO) technique.

Keywords

Author Keywords: Photoluminescence; Effect of solvent; Photostability; DFT studies; 1,4-bis(2-(2-phenylpyrimido[1,2-a]benzimidazol-4-yl)phenoxy)butan (BPPB)

KeyWords Plus: NEAR-INFRARED NIR; LASER-DYE; MOLECULAR-STRUCTURE; SPECTRAL BEHAVIOR; SOLVENT POLARITY; BODIPY DYES; FLUORESCENCE; EMISSION; IR; STATE

Author Information

Reprint Address: El-Daly, SA (reprint author)

+ Tanta Univ, Dept Chem, Fac Sci, Tanta 2173, Egypt.

Addresses:

+ [1] Jeddah Univ, Dept Chem, Fac Sci, Jeddah 80327, Saudi Arabia

+ [2] Natl Res Ctr, Green Chem Dept, Cairo 12622, Egypt

− [3] King Abdulaziz Univ, Dept Chem, Fac Sci, POB 80203, Jeddah 21589, Saudi Arabia

Organization-Enhanced Name(s)

King Abdulaziz University

[4] Assiut Univ, Dept Chem, Fac Sci, Assiut 71516, Egypt

[5] Univ Khartoum, Dept Chem, Fac Sci, POB 321, Khartoum 11111, Sudan

[6] Cairo Univ, Dept Chem, Fac Sci, Giza 12613, Egypt

[7] King Abdulaziz Univ, CEAMR, POB 80203, Jeddah 21589, Saudi Arabia

Organization-Enhanced Name(s)

King Abdulaziz University

[8] Tanta Univ, Dept Chem, Fac Sci, Tanta 2173, Egypt

E-mail Addresses: samyeldaly@yahoo.com

Publisher

SPRINGER/PLENUM PUBLISHERS, 233 SPRING ST, NEW YORK, NY 10013 USA

Categories / Classification

Research Areas: Biochemistry & Molecular Biology; Chemistry

Web of Science Categories: Biochemical Research Methods; Chemistry, Analytical; Chemistry, Physical

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000382397400039

PubMed ID: 27476069

ISSN: 1053-0509

eISSN: 1573-4994

Journal Information

Table of Contents: Current Contents Connect

Impact Factor: Journal Citation Reports

Other Information

IDS Number: DU7MD

Cited References in Web of Science Core Collection: 69

Times Cited in Web of Science Core Collection: 0