Bis-Sulfone- and Bis-Sulfoxide-Spirobifluorenes: Polar Acceptor Hosts with Tunable Solubilities for Blue-Phosphorescent Light-Emitting Devices

ID 3451771
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Year 2016
Title Bis-Sulfone- and Bis-Sulfoxide-Spirobifluorenes: Polar Acceptor Hosts with Tunable Solubilities for Blue-Phosphorescent Light-Emitting Devices
Journal European journal of organic chemistry
Number 11
Pages / **Article-Number** 2037-2047
Bis-sulfone- and bis-sulfoxide-spirobifluorenes are a promising class of high-triplet-energy electron-acceptor hosts for blue phosphorescent light-emitting devices. The molecular design and synthetic route are simple and facilitate tailoring of the solubilities of the host materials without lowering the high-energy triplet state. The syntheses and characterization (including single-crystal structures) of four electron-accepting hosts are reported; the trend in their reduction potentials is consistent with the electron-withdrawing nature of the sulfone or sulfoxide substituents. Emission maxima of 421–432 nm overlap with the MLCT absorption of the sky-blue emitter bis(4,6-difluorophenyl-pyridinato)(picolinato)iridium(III) (FIrpic), allowing effective energy transfer from the acceptor hosts to FIrpic. Theoretical calculations show that the introduction of sulfone groups leads to better electron acceptors compared to analogous phosphine oxide functionalized hosts and, at the same time, preserves the energy of the lowest-lying triplet above that of the FIrpic emitter. The new hosts have been tested in phosphorescent light-emitting electrochemical cells (LECs). Large effects of the various solubilizing moieties on the device performance are observed and discussed.
Publisher Wiley-VCH Verlag
ISSN/ISBN 1434-193X
edoc-URL http://edoc.unibas.ch/42536/
Full Text on edoc Restricted;
Digital Object Identifier DOI 10.1002/ejoc.201600247
ISI-Number WOS:000374507400015
Document type (ISI) Article