Tetrathiafulvalene-Triazine-Dipyridylamines as Multifunctional Ligands for Electroactive Complexes: Synthesis, Structures, and Theoretical Study

Titre	Tetrathiafulvalene-Triazine-Dipyridylamines as Multifunctional Ligands for Electroactive Complexes: Synthesis, Structures, and Theoretical Study
Type de publication	Article de revue
Auteur	Branzea, Diana-G. [1], Fihey, A. [2], Cauchy, Thomas [3], El-Ghayoury, Abdelkrim [4], Avarvari, Narcis [5]
Editeur	American Chemical Society
Type	Article scientifique dans une revue à comité de lecture
Année	2012
Langue	Anglais
Date	08/2012
Numéro	15
Pagination	8545-8556
Volume	51
Titre de la revue	Inorganic Chemistry
ISSN	0020-1669
Mots-clés	anion-pi interactions [6], building-blocks [7], carbonyl-complexes [8], center-dot [9], coordination chemistry [10], crystal-structures [11], donor ligands [12], magnetic-properties [13], radical-cation salt [14], transition-metal-complexes [15]
Résumé en anglais	The electroactive ligands (2,4-bis-tetrathiafulvalene[6-(dipyridin-2-ylamino)]-1,3,5-triazine) TTF2-tz-dpa (1) and (2-tetrathiafulvalene[4,6-bis-(dipyridin-2-ylamino)]-1,3,5-triazine) TTF-tz-dpa(2) (2) have been synthesized by palladium cross-coupling catalysis, and the single crystal X-ray structure for 1 was determined. In the solid state the TTF and triazine units are practically coplanar and short intermolecular S center dot center dot center dot S contacts are established. Two neutral and one tetracationic Zn(II) complexes, formulated as (TTF2-tz-dpa)ZnCl2 (3), [ZnCl2(TTF-tz-dpa(2))Zn(H2O)Cl-2] (4), and ([(H2O)(2)Zn(TTF-tz-dpa(2))](ClO4)(2)}(2) (5) have been crystallized and analyzed by single crystal X-ray analysis. A peculiar feature is the evidence for anion-pi interactions, as shown by the short Cl center dot center dot center dot triazine and O(perchlorate)center dot center dot center dot triazine distances of 3.52 and 3.00 angstrom, respectively. A complex set of intermolecular pi center dot center dot center dot pi, S center dot center dot center dot S and hydrogen bonding interactions sustain the supramolecular organizations of the complexes in the solid state. Electronic absorption spectra provide evidence for the intramolecular charge transfer from TTF to triazine, also supported by time-dependent density functional theory (TD DFT) calculations.
URL de la notice	http://okina.univ-angers.fr/publications/ua2661 [16]
DOI	10.1021/ic301117h [17]

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