Synthesis and studies of dipyrido[1,2-b:1',2'-e][1,2,4,5]tetrazine and derivatives : towards the organic electronics applications.

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π-Conjugated molecules have attracted much attention as materials for the development of organic electronics. Numerous structures have already been published[1] but the search for new architectures is still very active.

Polycyclic aromatic 1,4-dihydro-s-tetrazines, have a strong potential for such applications as electron donors because they are easily oxidized. In addition, they absorb light between 300 nm and 700 nm depending on their structure. However, these compounds have never been used in organic electronic.

The synthetic route to obtain such molecules is described in Figure 1[2,3]. The use of a so-called "electrophilic nitrogen" reagent is necessary in order to create a nitrogen-nitrogen single bond. A cyclization step follows to form the tetrazine ring.

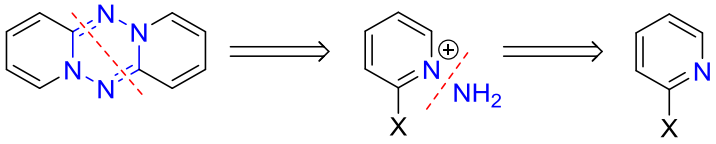

Figure 1 : Retro-synthesis of dipyrido[1,2-b:1',2'-e][1,2,4,5]tetrazine

Using this method several tetrazines have been prepared and in particular di-halogenated tetrazines (Figure 2).

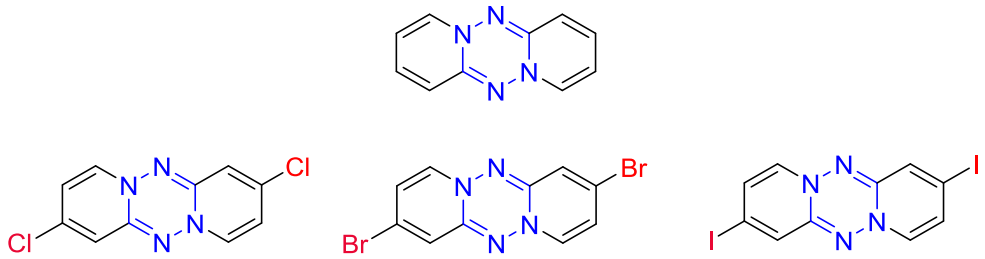

Figure 2 : dipyrido[1,2-b:1',2'-e][1,2,4,5]tetrazine and its di-halogenated derivatives.

The photophysical properties of the series have been studied in solution and rationalized with DFT calculations. These compounds represent a first step toward functional molecular materials since the halogen atoms will then be used to perform organometallic couplings

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References:

[1] *Chem. Rev.* ***2012****, 112, 4, 2208–2267.*

[2] *Liebigs Ann. Chem. 1994,* ***1994*** *(10), 1049–1053.*

[3] *Helv. Chem. Acta* ***1986****, 69 (6), 1521–1530.*