Synthesis and Characterization of New Molecular Compounds
Based on Dissymmetric Cyanobenzene TTF Donors

Afonso Varatojo\textsuperscript{a}, Dulce Simão\textsuperscript{b} and Sandra Rabaça\textsuperscript{a, *}

\textsuperscript{a} C\textsuperscript{2}TN, Centro de Ciências e Tecnologias Nucleares, Instituto Superior Técnico, Universidade de Lisboa, E.N. 10 ao km 139,7, 2695-066 Bobadela LRS, Portugal

\textsuperscript{b} Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, P1049-001 Lisboa, Portugal

Abstract

In this master’s degree dissertation, it is described the synthesis of a new donor of the type dissymmetric cyanobenzene tetrathiafulvalene, which name is cyanobenzene-pyrazine-tetrathiafulvalene (CNB-PZ-TTF) (1). This synthesis was made using a cross-coupling reaction with distilled triethyl phosphite between the compounds pyrazine-1,3-dithiol-2-thione (4) and 5-cyanobenzene-1,3-dithiol-2-one (7). This compound was characterized using NMR spectra, as well as IR and UV-visible, elemental analysis (CHNS) and cyclic voltammetry.

4 new transfer salts were also synthesized with the donors 4CNB-EDT-TTF and 5CNB-EDT-TTF. The new salts are described by a generic formula [D]\textsubscript{x}A where x=2 for the anion Au(bdt)\textsubscript{2} (14) and dianion CuCl\textsubscript{4}\textsuperscript{2-} (13), and x=1 for Br\textsubscript{3} (11) and DDQ (12). These salts were obtained using electrocrystallization ad diffusion cells, in the presence of the corresponding anion. Through X-ray diffraction techniques it was possible to determine its crystalline structures. Compound 11 is a paramagnetic compound, with dimerized donors, in units of two, arranged along the c axis. Establishes various types of short contacts, between donor molecules, which allow the formation of the R\textsubscript{2}(24) and R\textsubscript{2}(8) synthons in its structure, and short contacts with the anion present. For compound 12 it was possible to observe that along the a axis the donors were configured in a “staircase” configuration and synthons were not formed in this structure. Even so, short contacts with the anion are established within this structure. Compound 13, shows layers of donor molecules in its structure displayed along the c axis, in a wavy configuration, as well as dimers along the a axis. Short contacts between the donor molecules and the anion are established, unlike the short contacts between both donor columns. Short contacts with the anion are also established. In compound 14, dimers are also formed, along the a axis, through short contacts between donor molecules. Synthons R\textsubscript{2}(28) and R\textsubscript{2}(8) are formed in this structure as well. For compounds 11, 12 and 14 were additionally calculated the values of the |\beta_{HOMO-HOMO}| interactions between donor molecules within the charge transfer salt structure, concluding that the interactions between donor molecules that allow the formation of dimers are the strongest ones.
Introduction

For many years, it was admitted that the majority of organic compounds were insulating materials. Although ancient predictions from 1911 of McCoy and Moore[1] and 1913 from Kraus acknowledged the possibility of obtaining new substances with metallic and electrical properties from those organic compounds, it wasn’t until recently that the study of these compounds was developed.

In 1954, it was made the discovery of the first molecular compound with high electrical conductivity, perylene bromide (PerBrₓ), by H. Akamatu et al.[2], that led to the increasing interest of the study of this type of compounds.

After this point, the research on molecular compounds started to develop even more, targeting the synthesis of new materials that showed the same characteristics.

The first electron acceptor was synthetized in 1962, the 7,7,8,8-tetracyano-p-quinodimethane (TCNQ)[3]. This led to the synthesis of wide range of charge transfer salts. In 1970, the electronic donor tetrathiafulvalene (TTF) was synthetized[4]. Then in 1973, by combining this donor and the acceptor, the first charge transfer salt was made, with the name [TTF(TCNQ)]. This salt was also the first one to be exposed to a complete characterization, at different temperatures, of its electric properties.

This results propelled the investigation on this area, leading to the observation of the superconductivity phenomena in organic materials in 1980, in the Bechgaard[5] salts.

The tetrathiafulvalene molecule (TTF) and its large number of derivates has been the base of organic metals and superconductors know to date[6]. The success of these compounds as structural base for conductive materials, relies on the unique properties they present in terms of being π donors, with two oxidation states, the capability of expanding its delocalized π-system, incorporating in its periphery sulphur or other hetero-atoms and due to its chemical functionalization.

The research work done in this area has been focusing on two guidelines. The first one, focuses on the extent of the π-system, in order to create more accessible oxidation states and at the same try to maximise the intermolecular interactions between flat molecules that tend to organize themselves in layers in the solid state. The second guideline has in its core the incorporation of sulphur and other hetero-atoms in the molecule’s periphery trying to promote the lateral molecular interactions along the molecular plane, allowing this way a possible 2D or 3D character for the electronic interactions.

Since then, the TTF skeleton has been used as a basis for the synthesis of new π electronic donors, being that the compound that gave the largest number of molecular conductors was the bisetilenodithiotetrahiafulvalene (BEDT-TTF or ET)[7].

As mentioned before, the TTF derivates have been the basis for most of the organic conductors stated in the last decades[8]. A trend established right after the discovery of the first organic metals and superconductors in the development of new electronic materials of this kind was the preparation of electroactive molecules based on sulphur-rich and extended π-systems capable of establishing solid state interactions in more than one direction. The most successful constituent units for this type of electronic materials were sulphur and other TTF calcogen derivates like the bisetilenodithiotetrahiafulvalene in salts which composition as a generic formula such as (ET)ₓX, where X represents a variety of monoanions[9]. This type of molecules gave rise to the vast majority of
known organic and superconducting metals, as well as many solids with two-dimensional character with a great diversity of electronic states, for example, superconductors, insulating and antiferromagnetic.

The crystalline structures of these salts have a two-dimensional character with molecules of donors arranged with their long axes parallel to one another in layers that alternate with anionic layers. The packing of the molecules in layers can be diverse[10], leading to a large variety of electronic properties. Over the last few years, it has been found that some salts of this kind of donors have more complex structures in which two different layers of donor can alternate in the solid[11], but in all cases the layers have the thickness corresponding to the length of the donor molecule, in other words, monolayers.

The Solid State Group (GES) of the Technological and Nuclear Center (C²TN) has been developing one of the themes of investigation in the TTF research area. Most recently it was synthetized a dissymmetric derivate of the ET donor, named cyanobenzene-ethylene-dithieno-tetrathiafulvalene (CNB-EDT-TTF)[12], which through weak hydrogen bonded mediation interaction, allows the formation of dimers, which leads to the formation of charge transfer salts, using small sized anions with a new type of bilayer structure containing metallic properties and a composition of the type (CNB-EDT-TTF)X[13]. In this compound’s salts two distinct types of structural bilayer were observed. This way, two types of synths between donor molecules were verified, created by C-N…H-C interactions, which favor the association of the molecules of adjacent layers, existing then two types of synths: R_2^2(10) that only involves two types of donor molecules in its structure, and the R_4^2(10) in which four donor molecules are involved.

Through this new compound, it was possible to synthetize a large number of charge transfer salts by eletcrocrystallization, using ClO_4^−, PF_6^− and I_3^−[13] as anions. In all of these salts, it was verified the presence of two-dimensional metallic properties and in them the formation of donor bilayers as mentioned above, was observed.

The salt synthetized with the ClO_4^−[14] anion, was characterized as having a β structure. Three polymorphs* for this salt were observed, two of which have a stoichiometry of 4:1, one of them with a triclinic structure and the other with a monoclinic structure. The remaining polymorph displayed a 1:1 stoichiometry.

As for the charge transfer salt [CNB-EDT-TTF]_4[^1] [I_3^−][15], two polymorphs were observed. One corresponding to an arrangement of the donor molecules in a κ phase and the other corresponding to a β phase. Both presented a 4:1 stoichiometry, but when it came to the electrical conductivity, it was verified that the salt, whose donor molecules had a κ phase configuration, had a superconducting behaviour below 1.5 K.

In order to study the formation of bilayers observed with the hexafluorophosphate, perchlorate and iodine salts, it was attempted to obtain charge transfer salts with anions of different dimensions[16]. For this matter, two flat square anodes of type [M(mnt)_2] were used, where M=Ni or M=Au and mnt = maleonitriledithiolate., and a bulkier tetrahedral anion, FeBr_4. Charge transfer salts were obtained, which present in its structure columns with a DDADDA sequence, but said bilayers were not present. The FeBr_4 showed a 1:1 stoichiometry. However, these compounds showed very interesting magnetic characteristics, which were denominated by anions’ contributions, being these paramagnetic in the case of the anion [Ni(mnt)_2], and in the case of the FeBr_4 anion, being paramagnetic interactions, denoting donor-mediated antiferromagnetic interactions.
In this work, it was synthetized a new donor, denominated CNB-PZ-TTF, represented in figure 1 (1), that allows the combination of a cyanobenzene ring with a pyrazine ring, and two more donors, the 4CNB-EDT-TTF, figure 1(2) and 5CNB-EDT-TTF, figure 1(3), were used to try to obtain more charge transfer salts, hoping to see if the bilayers were formed.

A charge transfer salt is always composed by two types of molecules, one is the acceptor molecule and the other is the electronic π donor.

In this master’s thesis the monoanions PF$_6^-$, I$_3^-$, ReO$_4^-$, Br$_3^-$, DDQ, IBr$_2^-$, TCNQ, NaCF$_3$SO$_3^-$ and the dianion CuCl$_4^{2-}$ were used, which have small dimensions. Anions of larger dimensions were also used, the Au(bdt)$_2^-$ and the Ni(dmit)$_2^-$: These anions were used in eletrocrystallization and diffusion cells.

Only some of the combinations above showed results, by obtaining new charge transfer salts. These crystals were sent to X-ray diffraction analysis, with the donors 4-CNB-EDT-TTF and CNB-EDT-TTF, in order to determine its structures and the possible formation of synthons, polymorphs and bilayers.

**Results and Discussion**

**Donors Synthesized**

A new donor, CNB-PZ-TTF (1), was successfully synthetized and purified during this master’s thesis.

To synthesize the CNB-PZ-TTF, the following path was used:

1. The thione pyrazine-1,3-dithiol-2-thione (4) was synthesized following the procedure published in$^{[17]}$. The first step consists on the reaction between 2,3-dichloropyrazine (5) and K$_2$CS$_3$ (6), thus forming a new ring by substituting the bonds to the chlorides with bonds to the sulphur atoms of the reactant, therefore forming the thione.

2. The ketone cyanobenzene-1,3-dithiol-2-one (7) was synthesized through an oxymercuration reaction$^{[18]}$ using mercury acetate (8), that allows the thione, created in the reaction described above, to convert into a ketone.

3. The donor CNB-PZ-TTF (1) was synthesized through a cross-coupling reaction similar to the one used to synthesize the donor CNB-EDT-TTF$^{[12]}$, but in this case the reaction occurred between pyrazine-1,3-dithiol-2-thione (4) and cyanobenzene-1,3-dithiol-2-one (7) in a ratio of 1:1:1 in distilled triethylphosphite for approximately 4 hours at 130°C, with a final yield of 8.46%.

The product of the reaction is an orange precipitate, which is then recovered by filtration. To increase the recovery of the product, the flask where the reaction occurred was washed with methanol, and the mother liquid that resulted from the filtration was left under slow evaporation inside the hood, in doing so to recover the remaining product.

The reaction product contains an insoluble product in dichloromethane, therefore it is subjected to a regular filtration to remove the insoluble product.
After that it is submitted to a silica column using as eluent a 4:1 solution of dichloromethane and hexane, respectively.

For this donor, it was not possible to determine its crystalline structures, given the fact that it was not possible to obtain good enough crystals, suitable to be analysed by X-ray diffraction.

**Charge Transfer Salts**

In total, it was possible to obtain x new charge transfer salts with different anions.

The charge transfer salt \([4\text{-CNB-EDT-TTF}][\text{Br}_3]\) (11) was obtained using an electrocrystallization cell. A solution of 25 mL of dichloromethane containing 1.5 mM of donor and 4.0 mM of acceptor was prepared and subjected to an initial current of 0.5 μA and progressively raised up to 2.0 μA during approximately one month.

The crystals were then recovered by filtration and analysed under a microscope and subjected to X-ray diffraction analysis.

The obtained charge transfer salt has a 1:1 stoichiometry, which crystallized in a monoclinic system with a P2\(_1\)(1)/c space group. Being a salt with a 1:1 stoichiometry means that exists a \(\frac{1}{2}\) spin per donor, that is, a paramagnetic compound with dimerized donor. In the asymmetric unit of this structure, it can be observed two types of molecules, one is the donor molecule, represented in an ORTEP diagram in figure 3, and an anion molecule. From the ORTEP diagram it is possible to verify that the donor molecule is flat, except for the dithin ring.
The charge transfer salt [4-CNBDTET] [DDQ] (12) was obtained by a diffusion cell. For this cell a test tube was used in which solutions of dichloromethane and acetonitrile were placed in layers, trying to avoid their mixing. The bottom layer contained a 4-CNBDTET donor solution in 1.5 mL of dichloromethane, on top of this layer, a pure 1 mL acetonitrile solution is deposited, and the top layer contains a DDQ solution in 0.5 mL of acetonitrile. As the reaction was very fast, this cell was put in rest in a place absent of light during only two days.

The crystals were then recovered by filtration and analysed under a microscope and subjected to X-ray diffraction analysis.

The charge transfer salt presents a 1:1 stoichiometry, which crystalized in a P2₁ space group.

In the asymmetric unit it is possible to observe the presence of two different types of molecules. One is the donor molecule and the other is an anion molecule. Once again observing the ORTEP diagram, it is verifiable that the donor molecule is flat, the dithiin ring being the exception.

In this structure, the donors are connected through contacts of the type N−C and S−S, in the form of a “staircase”, along the a axis.
In this salt’s structure is not possible to verify the presence of any synthon. The donor and anion molecules are placed along the \( a \) axis, overlapped two by two.

This salt also shows other short contacts between donor molecules and with anion molecules of the type \( \text{S} \cdots \text{O}, \text{S} \cdots \text{N}, \text{C} \cdots \text{C}, \text{C} \cdots \text{O}, \text{H} \cdots \text{O}, \text{H} \cdots \text{N}, \text{H} \cdots \text{C}, \text{S} \cdots \text{H} \) and \( \text{H} \cdots \text{H} \).

The charge transfer salt \([4\text{-CNB-EDT-TTF}]_2\) \([\text{Cu}_2\text{Cl}_6]\) (13) was obtained through a diffusion cell. The procedure considered was similar to the one followed for the salt 12, the difference resides on the top layer of the cell, using a solution of 0,5 ml of \( \text{TPhAs}_2\text{CuCl}_4 \) with acetonitrile. The cell was put on a place with absence of light, to rest, for two days.

The crystals were then recovered by filtration and analysed under a microscope and subjected to X-ray diffraction analysis.

A stoichiometry 2:1 was observed in this salt, that crystalized in a triclinic system, with a \( \text{P1} \) space group.

The asymmetric unit of this charge transfer salt, presents two donor molecules instead of only one like the previous charge transfer salts. Both molecules are shown in the following ORTEP diagram. In the asymmetric unit is also present another molecule that corresponds to the anion. The ORTEP diagram shows that the donor molecules are flat, apart from the dithiin ring.

The structure of this charge transfer salt is composed by layers of donor molecules along the \( c \) axis, displayed in a wavy configuration. These layers are composed by dimer columns along the \( a \) axis. The columns are distinguished by the symmetry operation that generates them starting from the molecules present in the asymmetric unit and through the contacts made by the constituent molecules.

In the columns shown in blue, it is possible to observe short contacts, between donor molecules, creating that way dimers along the \( a \) axis, of the type \( \text{C} \cdots \text{C}, \text{H} \cdots \text{S} \) and \( \text{H} \cdots \text{C} \).

In the second kind of columns, shown in red, the molecules establish short contacts between them, creating dimers, of the type \( \text{C} \cdots \text{C}, \text{H} \cdots \text{S} \) and \( \text{S} \cdots \text{C} \). It is important to note that both columns do not connect between them, although both establish contacts with the anion of the type \( \text{Cl} \cdots \text{C}, \text{Cu} \cdots \text{S}, \text{Cl} \cdots \text{S} \) and \( \text{Cl} \cdots \text{H} \).

Analysing the bond lengths of the atoms present in the donor molecules in the asymmetric unit it was possible to conclude that the donor molecules showed a +1 oxidation state in the charge transfer salt structure.
The charge transfer salt [CNB-EDT-TTF]$_2$ [Au(bdt)$_2$] (14) was obtained using an electrocrystallization cell. A solution of 25 mL of dichloromethane containing 2.0 mM of donor and 6.0 mM of acceptor was prepared and subjected to an initial current of 0.5 μA and progressively raised up to 0.7 μA during approximately two weeks.

The crystals were then recovered by filtration and analysed under a microscope and subjected to X-ray diffraction analysis.

The charge transfer salt obtained, showed a stoichiometry of 2:1, that crystalized in a triclinic system, with a P-1 space group.

In the corresponding asymmetric unit, one donor molecule and half an anion molecule are present. By observing the ORTEP diagram of this salt, it is possible to verify that the donor molecule is flat, except the dithiin ring.

Other short contacts, the intercolumn contacts, are established in the structure of this salt, of the type N\(\cdot\)S and N\(\cdot\)H, allowing the formation of the synthons $R^2_2(28)$ and $R^2_4(8)$. The donor and anion molecules also establish contact between them, of the type S\(\cdot\)S and C\(\cdot\)H.

|β$_{\text{HOMO-HOMO}}$| values for the donor-Donor Interactions

In this dissertation, the donor-donor interactions values for the $|\beta_{\text{HOMO-HOMO}}|$ were also calculated, but only for the charge transfer salts 11, 12 and 14. The next figures show the contacts established between the donor in each of the salts.
The following table summarizes the obtained values for both charge transfer salts 11, 12 and 14.

Table 1 – Values of $|\beta_{\text{HOMO-HOMO}}|$ for the donor-donor interaction for salts 11, 12 and 14

| Contact | $|\beta_{\text{HOMO-HOMO}}|$ (meV) |
|---------|------------------------|
|         | Salt 11    | Salt 12    | Salt 14    |
| I       | 565,2      | 13,9       | 514,8      |
| II      | 20,6       | 188,7      | 6,7        |
| III     | 1,9        | 12,4       | 96,5       |
| IV      | 167,8      | 5,2        | -          |

Bond Length Analysis

To determine the oxidation state in which the donor molecules are found in the crystalline structures, it was used the method published in [19].

This method consists on the measuring of the specific bond lengths on the donor molecules and then using equation 1, it is possible to correlate the value of $\delta$ with the oxidation state of the donor molecules in the charge transfer salt.

$$\delta = (b + \bar{c}) - (a + \bar{d}) \quad \text{(equation 1)}$$

In the next figure it is shown the nomenclature used for the bonds, on the donors used in the charge transfer salts, and table 2 summarizes the bond length values obtained values for the various charge transfer salts.
results summary

The results obtained during this master's thesis are summarized in the following tables 3 and 4. Table 3 reviews the results for the new donor and table 4 recap's the results for the charge transfer salts.

Table 3 - Obtained results for the donor CNB-PZ-TTF

<table>
<thead>
<tr>
<th>Analysis</th>
<th>CNB-PZ-TTF</th>
</tr>
</thead>
<tbody>
<tr>
<td>'H RMN (ppm)</td>
<td></td>
</tr>
<tr>
<td>8.081</td>
<td></td>
</tr>
<tr>
<td>7.512</td>
<td></td>
</tr>
<tr>
<td>7.403</td>
<td></td>
</tr>
<tr>
<td>7.371</td>
<td></td>
</tr>
<tr>
<td>IV (cm⁻¹)</td>
<td></td>
</tr>
<tr>
<td>3080 (Ar-H); 2225 (C≡N);</td>
<td></td>
</tr>
<tr>
<td>1575 (C=C); 1555 (C=N);</td>
<td></td>
</tr>
<tr>
<td>1451 (C=C); 1335 (C-N)</td>
<td></td>
</tr>
<tr>
<td>580 (C-S)</td>
<td></td>
</tr>
<tr>
<td>UV-Vis (nm)</td>
<td></td>
</tr>
<tr>
<td>388 and 276.5</td>
<td></td>
</tr>
<tr>
<td>Cyclic Voltammetry</td>
<td></td>
</tr>
<tr>
<td>E₁/₂=1095.4</td>
<td></td>
</tr>
<tr>
<td>E₁/₂=602</td>
<td></td>
</tr>
<tr>
<td>Elemental Analysis</td>
<td></td>
</tr>
<tr>
<td>Exp: C=49.61%</td>
<td></td>
</tr>
<tr>
<td>H=1.77%</td>
<td></td>
</tr>
<tr>
<td>N=9.42%</td>
<td></td>
</tr>
<tr>
<td>S=32.24%</td>
<td></td>
</tr>
<tr>
<td>Calc: C=47.11%</td>
<td></td>
</tr>
<tr>
<td>H=1.52%</td>
<td></td>
</tr>
<tr>
<td>N=12.68%</td>
<td></td>
</tr>
<tr>
<td>S=38.69%</td>
<td></td>
</tr>
<tr>
<td>Crystalline Structure</td>
<td></td>
</tr>
<tr>
<td>Not possible to determine</td>
<td></td>
</tr>
</tbody>
</table>

Table 4 - Obtained results for the charge transfer salts

<table>
<thead>
<tr>
<th>Salt</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Donor</td>
<td>(2)</td>
<td>(2)</td>
<td>(2)</td>
<td>(3)</td>
</tr>
<tr>
<td>Anion</td>
<td>Br₃</td>
<td>DDQ</td>
<td>Cu₂Cl₆</td>
<td>Au(bdt)₂⁻</td>
</tr>
<tr>
<td>Stoichiometry</td>
<td>1:1</td>
<td>1:1</td>
<td>2:1</td>
<td>2:1</td>
</tr>
<tr>
<td>Dimer</td>
<td>Parallel to c</td>
<td>-</td>
<td>Along a</td>
<td>Along a</td>
</tr>
<tr>
<td>Synthons</td>
<td>R₂(24) and R₂(8)</td>
<td>-</td>
<td>-</td>
<td>R₂(28) and R₂(8)</td>
</tr>
</tbody>
</table>

Conclusions

A new benzo[c]anisole-substituted type donor (CNB-PZ-TTF) (1), was synthesized during this master's thesis, using a cross-coupling reaction in triethylphosphite.

Although it was impossible to determine the crystalline structure of the new donor, it was determined the electrochemical behaviour, showing a typical behaviour of the donors derived from TTF, with two redox processes, assign to the [D]²⁺/[D]⁺ and [D]⁺/D⁰ pairs.

4 new charge transfer salts were synthesized, using the donors 4-CNBP-EDT-TTF and CNB-EDT-TTF, those salts which could be described by the generic formula [D]ₓA, with 1:1 stoichiometry for A=Br₃⁻ (11), DDQ (12) and a 2:1 stoichiometry for A=Au(bdt)₂⁻ (14) and Cu₂Cl₆²⁻ (13). These salts
were obtained using elecrocrystallization and diffusion cells, in the presence of the corresponding anion. Through X-ray diffraction techniques it was possible to determine its crystalline structures. Compound 11 is a paramagnetic compound, with dimerized donors, in units of two, arranged in layers along the c axis. Establishes various types of short contacts, between donor molecules, which allow the formation of the $R_2^2(24)$ and $R_2^4(8)$ synthons in its structure, and short contacts with the anion present. For compound 12, it was observed that the donors were arranged in a “staircase” configuration, along the a axis and synthons were not formed in this structure. Even so, short contacts with the anion are established within this structure. Compound 13, shows layers of donor molecules in its structure displayed along the c axis, in a wavy configuration, as well as dimers along the a axis. Short contacts between the donor molecules and the anion are established, unlike the short contacts between both donor columns. In compound 14, dimers are also formed, along the a axis, through short contacts between donor molecules. Synthons $R_2^2(28)$ and $R_2^4(8)$ are formed in this structure as well. Short contacts with the anion are also established. For compounds 11, 12 and 14 were additionally calculated the values of the $|\beta_{\text{HOMO-HOMO}}|$ interactions between donor molecules within the charge transfer salt structure, concluding that the interactions between donor molecules that allow the formation of dimers are the strongest ones.

The motivations for the work developed in this master’s thesis was the attempt of synthesis of a new TTF type donor, with possible bilayer formation, that combined a cyanobenzene ring with a pyrazine ring.

New charge transfer salts were obtained with previously synthesized donors, in order to acquire a bigger diversity of salts with those donors and check their crystalline structures. It was possible to verify that in some of the new salts, synthons were formed between donor in adjacent chains. Some of the charge transfer salts also present dimers in its structures, although the formation of bilayers was not verified in any of the charge transfer salts.

References


