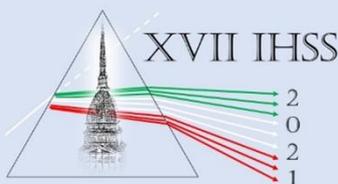


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CHARGING TRANSFER COCRYSTALS: INTERESTING PROSPECTS FOR THEIR USE IN THE ENVIRONMENTAL FIELD

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Charge-Transfer Co-Crystals (CTCCs) are a peculiar class of molecular materials whose properties emerge in a non-linear (complex) way and are not simply additive with respect to the properties of the constituent parent compounds. CTCCs are obtained from an internal redox reaction between two organic molecules, which have electronic Donor and Acceptor (D-A) properties, respectively. Thus, CTCCs synthesis is based on their different electronic affinity, on the difference between the ionization potentials and for mutual polarization [1]. Notably, CTCCs materials play an important role in optoelectronic devices, such as organic solar cells, photodetectors, and in the sensory field. In this work, CCTSs were synthesized by using 2,3,5,6-tetrafluorous-7,7,8,8,8 tetracyanoquinodimethane (F4-TCNQ) as A and dibenzotetrathiafulvalene (DBTTF) or perylene as D. CTCCs synthesis was carried out in a furnace under a temperature gradient and inert gas flow. They were characterized by spectroscopic techniques (IR, UV-Vis, Raman) and, being electronic conductors, through Cyclic Voltammetry (CV). The latter was possible with solid state electrochemistry. CVs measurements were carried out in an original-built lab-made electrochemical cell, consisting of a glass-carbon plate (Glassy Carbon, GC) as Working Electrode (WE), a CTCC thin film was formed by solvent evaporation on the WE, subsequently covered by a membrane of conductive (nafion) polymer, so as to avoid a direct CTCC solution contact. Elaboration of the CV curves allowed to estimate the energies of the Highest Occupied Molecular Orbital (HOMO) and of the Lowest Unoccupied Molecular Orbital (LUMO) of the co-crystals, and of the band-gap as well [2].

References

[1] O. Kataeva, M. Khrizanforov, Y. Budnikova, D. Islamov, T. Burganov, A. Vandyukov, K. Lyssenko, B. Mahns, M. Nohr, S. Hampel, M. Knupfel, Crystal growth, dynamic and charge transfer properties of new coronene charge transfer complexes, *Cryst. Growth Des.*, **16** (2016), 331–338.

[2] F. Solano, P. Inaudi, M. Chiesa, G. Kociok-Köhn, E. Salvadori, E. Da Como, D. Vanossi, M. Malandrino, R. Carmieli, A. Giacomino, C. Fontanesi, *J. Phys. Chem. C*, **125** (2021), 8677–8683.