Intermolecular interactions in molecular materials from the topological analysis of the electron density point of view. Mohamed Souhassou[a], Loretta Pretto[b], Paola Gilli[b], Slimane Dahaoui[a], Nicolas Claiser[a], Sebastien Pillet[a] and Claude Lecomte[a], *[a] Laboratoire de Cristallographie et Modélisation des Matériaux Minéraux et Biologiques, UMR CNRS 7036, Université Henri Poincaré-Nancy I, BP 239, 54506 Vandœuvre-lès-Nancy cedex, France. [b]Centro di Strutturistica Diffrattometrica e Dipartimento di Chimica, Universita' di Ferrara, 44100 Ferrara Italy*

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We present the characterization of different classes of materials (exhibiting molecular magnetism, charge transfer properties and resonance assisted H-bonds) containing hydrogen bonds, using experimental charge density analysis.

In the molecular magnetic materials, weak intermolecular interactions play an important role in the magnetic behavior at the macroscopic scale since they are involved in charge transfer, frontier orbital overlap and polarization mechanisms. A precise description of the electron density and its topology may help in understanding and developing new molecular magnetic materials.

The topology of the electron density is also precious for analyzing the interactions governing charge transfer between donor and acceptor in charge-transfer complexes, in peculiar in determining the pathway of the weak intermolecular interactions.

In the case of materials containing strong intramolecular hydrogen bonds, such interactions are very difficult to characterize because of the frequent dynamic and/or static (tautomerism, …) disorder affecting H atoms.

The presentation will be devoted to inter- and intra-molecular interactions in materials cited above, with an emphasis on tautomeric O-H—O/O—H-O resonance assisted hydrogen bonds. The correlation between the topological properties of the electron density at the bond critical points and the geometrical parameters characterizing hydrogen bonds will be discussed.