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Halogen Bonding-Based Crystal Engineering: From Borromean Links to Homochiral Double Helices

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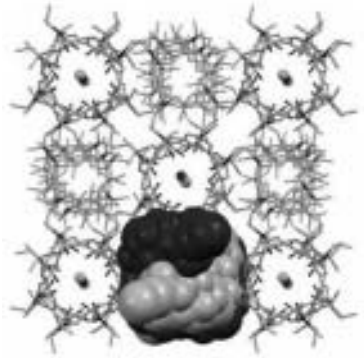
The halogen bonding (XB) (*i.e.* the attractive interaction where halogens work as electron density acceptors) is a particularly robust and directional noncovalent interaction [1]. Thanks to these properties, effective tectons tailored to XB-based crystal engineering could be successfully developed. In this communication, it will be shown how the judicious choice of electron donor and acceptor modules enables the fine control of the structural and functional properties of the formed supramolecular architectures. Topologies as complex as Borromean links [2] and homochiral double helices (figure) can be planned in a rational way [3].



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Diffuse scattering and local structure in distorted perovskite crystal $Na_{0.5}Bi_{0.5}TiO_3$

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Sodium bismuth titanate (Na0.5Bi0.5TiO3), NBT, is an A-site substituted distorted perovskite compound, which is also a ferroelectric relaxor. NBT appears to be the only crystal of perovskite family which is substituted at the A site [1]. In NBT two different cations Na and Bi occupy the *A* sites. The two cations have different charges and electronic configurations, but they possess similar ionic radii. The sequence of phase transitions from the high temperature prototypic cubic structure (above 813 K), to one of tetragonal (673±773 K) and then of rhombohedral structures (5±528 K) has been found [2]. The later phase of NBT is known to be rhombohedral with space group *R*3*c*. X-ray patterns from NBT exhibit a diffuse scattering of X-ray scattering [3]. The diffuse scattering occurs in two forms: as sharp streaks emanating from Bragg peaks and extending along the [100] direction and as a broad diffuse region around Bragg peaks. Using the high-pressure technique and a diffuse scattering Kreisel [3] has been found that the NBT undergoes a rhombohedral-to-monoclinic transition between 1.6 and 2.0 GPa and then a monoclinic-to-tetragonal transition between 9.9 and 11.1 GPa. In this paper we present the measurements of the temperature dependence of the X-ray diffuse scattering in the temperature range from 12K to 750K. Below 50K the sharp streaks despair. The redetermination of the single crystal structure at 14K confirmed the rhombohedral symmetry with space group *R*3*c*. Using Monte Carlo simulation some simple models of local structure was calculated for different temperature points.

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