Polar liquid crystals derived from boron clusters

popular science description

The subject of the proposed project is liquid crystals, which for decades have been attracting attention of scientists, technologists, as well as general public. Liquid crystals belong to the area of fascinating fundamental science, which searches for relationships between molecular structure and macroscopic properties and still discovers new unusual supramolecular structures. They have been used in and are source of modern technologies, mainly liquid crystal display technologies. Lastly, liquid crystals fascinate scientists, artists and ordinary people with their unusual textures and colors (Fig. 1).

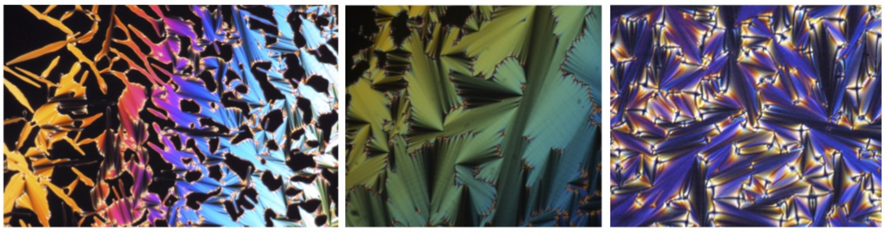

Fig. 1. Examples of liquid crystal textures (smectic phases) observed in polarized light under microscope. Photomicrographs taken in the PI's laboratory.

What are liquid crystals? They are liquids or soft wax-like substances in which molecules exhibits some degree or ordering and organization. In other words, the liquid crystalline state is characterized by a unique combination of fluidity of liquids and long-range ordering found in solid crystals. Liquid crystalline phases can be formed by substances, whose molecules, typically organic, are strongly anisomertic: they are rod-like, disk-like or their rigid core is bent. This molecular shape dictates the type of liquid crystalline phase, which is related to macroscopic properties, such as electrooptical or thermooptical.

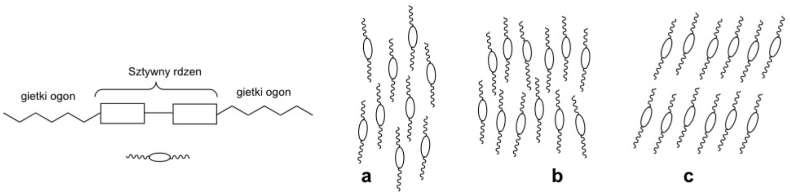

Fig. 2. From the left: schematics of a rod-like molecule which may form nematic (a) or smectic phases (e.g. b and c).

Liquid crystals have found numerous applications in a broad range of disciplines. Due to their electrooptical properties (reorientation of molecules and change of direction of polarized light upon application of electric field) these substances have been used in construction of monochromatic and color liquid crystal displays (LCD). Such displays are ubiquitous in many areas of every-day living, e.g. wrist watches, laptop computers, and at last in flat-panel TV sets. The fundamental phenomenon allowing for application of liquid crystals in information processing is the electrooptical effect, in which the applied electric field changes optical properties of a thin layer of material. The simplest example of the effect is shown in Fig. 3: elongated molecules with a longitudinal dipole moment (shown as bars) aligned parallel to the

electrodes and forming a nematic phase undergo elastic reorientation upon application of an electric field, which results in a change of optical properties. The key aspect of this effect is the presence of a sizable dipole moment, which interacts with the electric field and is appropriately oriented relative to the long molecular axis. Despite significant progress in synthesis and characterization of liquid crystals made in the past two decades, there is still continuous need for new mesogenic materials with a broad range of well-defined properties, including the magnitude of the molecular dipole moment. In this proposal, we describe specifically designed polar derivatives of boron clusters (Fig. 4) as a new generation of liquid crystals.

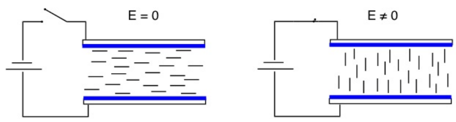

Fig. 4. Simplified schematics of electrooptical switching. Electric field causes reorientation of polar molecules having longitudinal dipole moment (shown as bars), which results in change of optical properties.

Thus, the scientific goal of the proposed project is the development of new liquid crystalline compounds with high dielectric anisotropy as modifiers of nematic and smectic materials for potential applications in LCD technology. For this purpose, specifically designed electrically neutral derivatives of three inorganic boron clusters (*closo*-borates **B** and **G**, and o-carborane **E**; Fig. 4) will be synthesized and investigated.

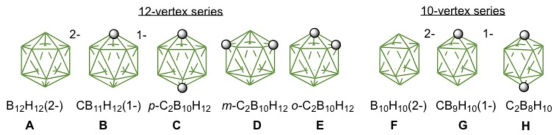

Fig. 4. Skeletal representations of selected boron clusters. In structures **A**–**H** each vertex corresponds to a B-H fragment and the CH groups are marked by filled circles

As part of the proposed investigations, thermal, optical and dielectric properties of the new derivatives will be investigated in the pure form and mixtures with other liquid crystalline compounds. Judicious selection of substituents will allow for the control of electronic properties of the boron cluster derivatives, and consequently of supramolecular structures and properties of the resulting materials. The proposed synthesis of a broad range of derivatives will result in establishing of molecular structure – properties relationships, which will permit a rational design of new structures with desired propertis.