THE INCOMMENSURATE MODULATED STRUCTURE OF A Cd-DERIVATIVE OF VALPROIC ACID, AN API USED IN THE TREATMENT OF EPILEPSY AND BIPOLAR DISORDER

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After facing a great deal of skepticism for many years, nowadays, the concept and nature of aperiodic crystals have been well established. Numerous feature articles, reviews and textbooks on this subject have paved the way for understanding this important structural characteristic of an increasing number of materials.

Despite the lack of three-dimensional periodicity in their crystal structures, these materials (which include incommensurate modulated structures, quasicrystals, and composite structures) possess a three-dimensional long-range order in the spatial arrangement of their atomic constituents. The structure of these materials can be described by the regular three-dimensional space group symmetry but modulated by a periodic deformation (*modulation*). To properly describe this type of structures a (3+*d*)-dimensional super-space approach has been developed. The main advantage of this approach is that a three-dimensional aperiodic structure can be interpreted as a periodic structure in a higher-dimensional space (*superspace*) and, in our physical 3*D* space, they are three-dimensional projections of their corresponding higher-dimensional periodic structure.

Although most of the incommensurate structure compounds investigated to date are inorganic materials or metal alloys, a growing number of molecular modulated organic and metal-organic compounds have been reported over the last few years. The study of this phenomenon may be particularly important for Active Pharmaceutical Ingredients (APIs). To the best of our knowledge, only two studies of APIs with incommensurate modulated structures have been reported in the literature.

In this contribution, preliminary results of the characterization of the incommensurate structure of a Cd-derivative of valproic acid, an API used in the treatment of epilepsy and bipolar disorder, using single crystal as well as powder diffraction data, is presented. The structure characterization of this material was carried out using single crystal data collected on a dual source (Cu, Mo) Rigaku XtaLAB PRO diffractometer equipped with a Pilatus 200K detector and powder data recorded on a Siemens D5005 diffractometer. The single crystal data were processed with CrysAlisPro 38.43 (Rigaku OD). The 3D structure was determined using SHELXT and the refinements of the modulation were carried out using Jana2006.

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