SR VALPROATE: ANOTHER METAL DERIVATIVE OF VALPROIC ACID WITH INCOMMENSURATE MODULATED STRUCTURE

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The availability of improved 2D detectors and more intense laboratory X-ray sources is allowing to detect in different laboratories around the world interesting features which were commonly overlooked in an increasing number of organic and metal-organic compounds. One of these features are weak reflections (satellites), observed near the strong (main) reflections, which cannot be indexed with the conventional Miller indices *hkl*. Compounds showing this type of phenomenon belong to the class of materials which exhibit incommensurate modulated structures. As it is well known, in incommensurate modulated structures, the constituent atoms are arranged in an aperiodic fashion. The main reflections observed in the diffraction pattern of these materials can be indexed with the Miller indices *hkl*, while the satellite reflections require the use of additional Miller indices (*m*, *n*, *o*, …) and one or more **q** vectors in addition to the three-dimensional **a**, **b**, **c** vectors. These structures can be described as periodic in more than three dimensions (3+*d* dimensions), and their projection in three-dimensional space is aperiodic. The main reflections provide information about an average 3D structure, while the satellites contain information about the modulation. The modulation comes from a variation in parameters such as atomic position, occupation, and/or anisotropic displacement from each unit cell to the next. The modulation can be described by a periodic function (sinusoidal, crenel, sawtooth, zig-zag) of irrational frequency (that does not match an integer number of unit cells).

In this contribution, the preliminary characterization by single crystal and powder diffraction of the incommensurate modulated crystal structure of a strontium derivative of valproic acid, an API used in the treatment of epilepsy and bipolar disorder, is presented. To the best of our knowledge, only two studies of active pharmaceutical ingredients (APIs) with incommensurate modulated structures have been reported in the literature.