Poster Presentation

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A new polymorphic form of Otilonium Bromide

D. Vega[1,2], R. Baggio[1]

[1]*Comisión Nacional de Energía Atómica, Centro Atómico Constituyentes, Gerencia de Investigación y Aplicaciones, Buenos Aires, Argentina,*
[2]*Universidad Nacional General San Martín, Escuela de Ciencia y Tecnología, Buenos Aires, Argentina*

Otilonium bromide (C29H43 N2 O4+.Br-) is a quaternary ammonium derivative which has been proven a potent spasmolytic drug with a good tolerability profile, used in the treatment of irritable bowel syndrome. We present herein the structural analysis of an unreported polymorphic form (I), comparing with the only one known so far and already reported [1] polymorphic form of the compound (II). The data set for I was obtained from a twinned specimen. The poor quality of the data thus available did not pose any problem in the structure resolution, but it did instead in refinement: the alkyloxy chains and ethyl branches in the quaternary ammonium groups needed some continuity restraints in their anisotropic displacement factors. In form II this effect appeared enhanced, ending up in unusually large anisotropic displacement parameters for most atoms in the chain. The main points of molecular disagreement reside in the torsion angles where the alkyloxy chains and quaternary ammonium groups leave the planar mainframe. The only notorious intermolecular contacts in both structures appear to be a number of rather weak C—H•••Br ones involving the quaternary ammonium groups somehow "wrapping" the bromide counterion. There are a few C—H•••O contacts interlinking molecules to each other. The phase transformation occurs at 124(2)ºC and can be followed by DSC and XRPD. A detailed analysis shows some features in common, viz., in both structures packing stability is mainly due to the ionic interaction between the N+ and the Br-, with the latter ion being evenly surrounded by a number of ammonium groups in a way that they define regular 2D arrays “sandwiching” the neutral part of the molecules, which thus act as spacers. These similarities allow giving a plausibility argument about the way in which the transition may take place.

[1] *P. Dapporto, A. Sega, Acta Cryst., 1986, C42, 474-478*

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