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Crystal structure solution of a new polymorph of the Agomelatine/hydroquinone cocrystal from Synchrotron X-ray data

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Although it has been traditionally suggested that cocrystals show a lower tendency to polymorphism than monocomponent crystals, the increasing number of polymorphic cocrystals described is recently questioning that old statement. The impact that this phenomenon has on the pharmaceutical industry is particularly relevant since affects to both intellectual property and formulation of new drugs. Thus, more experimental data about polymorphism of cocrystals are required to understand deeply whether the polymorphism affects in the same way to pure compounds than to multicomponent crystals. In this contribution we intend to enrich the debate by presenting the crystal structure of the second polymorph of the cocrystal between Agomelatine (an effective drug for the treatment of major depressive disorders) and hydroquinone. The structure have been determined using synchrotron X-ray powder diffraction data obtained in the high resolution powder diffraction end station of the MSPD beam line in Alba. The right data have been obtained with the sample in a 0.7 glass capillary, at 100 K, with wavelength 0.619 Å using the Mythen detector. Attempts to index high resolution powder diffraction data with Cu Kα laboratory X-ray powder diffraction data at room temperature has not been successful. The 100 K synchrotron powder diffraction data was perfectly indexed to an orthorhombic cell of about 1830 Å3 by means of Dicvol04,2 and the space group perfectly determined to be P212121 from the systematic absences. Being the asymmetric unit one molecule (1:1 agomelatine / hydroquinone stoichiometry), Z=4, the crystal structure was determined by direct space methodologies starting from a molecular model optimized with the commercial software SPARTAN by means of FOX.3 The refinement of the structure has been performed by the Rietveld method using FullProf.4 The details and difficulties of the resolution and refinement will be discussed. The final structure will be described and compared with the one of the other polymorph of Agomelatine / hydroquinone cocrystal.

References

1 A. Lemmerer, D. A. Adsmond, C. Esterhuysen, J. Bernstein, Cryst. Growth Des. 2013, 13, 3935–3952
2 A. Boultif, D. Louër, J. Appl. Crystallogr., 2004, 37, 724.
3 V. Favre-Nicolin, R. Czerny, J. Appl. Crystallogr., 2002, 35, 734-743.
4 J. Rodríguez-Carvajal, Physica B, 1993, 192, 55-69.

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