[MS24-P25] Series Isostructural Solvates of Bromocriptine Mesylate and Their Properties.

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Some molecules can form solvates with a multiple different solvents. There are two possible situations. The first one -solvate creates crystal in a new structural type -changing space group and lattice parameters. The second one -solvate creates crystal in the same space group and only the content of the cavity is occupied by another solvent. We call this case when not the space group nor lattice parameters are changed a series of isostructural solvates. This problem was studied on bromocryptine mesylate (BCM). BCM is a highly biologically active substance used in pharmacy as a dopamine agonist. Bromocriptine is used as methansulphonate salt for better pharmacokinetic properties. Up to now two structure of BCM were known; the first one was isopropanol solvate and the second one was anhydrous form. Both this structures crystallize in space group $P\ 2_1$. [1] Others solvents than isopropanol can be incorporated into the cavity in BCM and they could create a new solvates of BCM. BCM has a big potential to create noncovalent interactions with solvent to form new solvates due to many acceptors´ and donors´ groups. By the crystallization of BCM was obtained 19 new solvates that need to be clearly determined by analytical methods suitable for a solid state. We had chosen the X-ray powder diffraction for characterization because it make possible to fast characterize a big number of samples. Powder diffraction cannot offer information about exact solvent position and its noncovalent interaction. The single-crystal X-ray diffractions were used only in three cases, when information about content and noncovalent interactions was important (e.g. solvates in a new space group). Three new solvates was determined; two new solvates in space group $P\ 2_1$ and one solvate in space group $P\ 2_12_12_1$. We were trying for all solvates to find a correlation between the unit cell volume and the solvent's molecule volume. There was necessary to find suitable method for calculation for the volume of molecule solvent. We had tested correlation of the cell volume with the solvent's molecule volume calculated by five different methods. Following methods of solvent's molecule calculation were used: 1st and 2nd methods are from literature [2], where the Van der Waals (VdW) volume was extended by an envelope of 0 Å and 1.4 Å radius, respectively; 3rd and 4th are from literature [3] and the last one is generally known rule of VdW volume. The best correlation between cell volume and solvent's molecule volume was achieved when the solvent´s volume was calculated by methods number one and two. Nevertheless, the added envelope radius did not have significant influence on the results. Financial support from specific university research: MSMT No 20/2013 and 604 613 7302.

[1] The Cambridge Structural Database, version 5.34, November 2012.
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[3] Hofmannn D. W. M. (2002). *Acta Cryst.* **B57,** 489-493.

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