Structures of Cocrystals of Peganole with 6-Brompeganole

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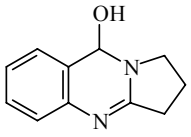
The crystal structures of two polymorphic cocrystals (I, II) of peganole (1) with 6-brompeganole (**2**) have been determined. Both forms are in the monoclinic system with space group of P2(1)/n. Cell parameters of I are a=8.232(4), b=11.768(8), c=10.156(6)Å, β=98.12(4)˚, V=974.0(10) Å^3 and II are a=7.995(6) , b=15.501(8), c=8.816(6), β=112.25(5)˚, V=1011.2(11) Å^3.

It is interesting to note that asymmetric unit of cell in both case consist of one molecule where this molecule at the same time can be **1** or **2**. Site occupation factors of molecules **1** and **2** are ~0.7 and ~0.3 (in I) and ~0.3 and ~0.7 (in II) respectively.

As well, tests on composition of single crystals by High-Performance Thin-Layer Chromatography (CAMAG, Switzerland) confirms the X-ray results.



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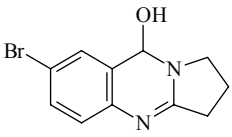

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Keywords: cocrystals, polymorphs, small-molecule single crystals