

[s7.m23.p1](#) **Searching the CSD for polymorphs.** Jacco van de Streek, *Cambridge Crystallographic Data Centre, UK.*
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Keywords: Polymorphs; CSD; Similarity

The Cambridge Structural Database (CSD, [1]) contains virtually all published crystal structures of organic and organometallic molecules, grouped by chemical compound. If two published crystal structures of the same chemical compound are different these two crystal structures are called polymorphs. Currently, polymorphs in the CSD are only flagged as such if this was explicitly mentioned in the original publication. This contribution describes how the CSD was searched for currently unflagged pairs of polymorphs based on the dissimilarity of their simulated X-ray powder diffraction (XRPD) patterns. XRPD patterns have the advantage that they are independent of the choice of origin and setting of the unit cell and, being one-dimensional, do not need to be re-oriented to find the best fit. The similarity measure used [2] is not as sensitive to peak shifts, i.e. unit-cell variations, as traditional point-by-point measures such as R-values, making comparison of crystal structures by different authors possible. The XRPD patterns were simulated using an in-house C++ library that forms the basis for e.g. the visualisation program Mercury [3]. If the similarity of the simulated XRPD patterns was "high", the two crystal structures were considered to be the same; if the similarity of the XRPD patterns was "low", the two crystal structures were inspected to see if they were true polymorphs or if the low similarity was due to an error. Details of the procedure will be described, including pitfalls and possible solutions. Time permitting, an extension to pseudo-polymorphs (polymorphs differing in solvent content) will be explained.

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[s7.m24.p1](#) **Engineering and synthesis of silyl-substituted molecular crystals of three-fold symmetry.** Nikolettta Báthori,^a László Bihátsi,^b Petra Bombicz^a and Mátyás Czugler^a, *Institute of Chemistry, Chemical Research Center, Hungarian Academy of Sciences, P.O.Box 17. H-1525, Budapest, Hungary, and*
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We synthesized special host molecules (*sym*-triaryloxy-triazines that yield to C_3 -symmetric crystalline supramolecular networks) and their crystal structures were determined by single crystal X-ray diffraction. These can form *Piedfort*-associates where the two superposed molecules of a *Piedfort*-unit serve as supramolecular *synthon* to build solid state associations [1].

The 2,4,6-tris(3-trimethylsilyl-phenoxy)-[1,3,5]-triazine (**1**) and the 2,4,6-tris(4-trimethylsilyl-phenoxy)-[1,3,5]-triazine (**2**) have been synthesized by reacting cyanuric chloride with the respective protected silylphenols [2,3]. Yellow colored crystals of the compound **1** were grown from diisopropyl-ether at room temperature and the structure was determined at 273K. It crystallized in a monoclinic unit cell with space group $P2_1/c$ ($a=8.819\text{\AA}$, $b=13.375\text{\AA}$, $c=29.192\text{\AA}$, $\beta=97.37^\circ$, $V=3415\text{\AA}^3$). In the crystal we have found *Piedfort*-pairs with the distance of the two parallel triazine rings of 3.50Å. Contrary to expectations the trimethylsilyl-groups of the molecules point towards their *Piedfort*-pairs. This leads to an alternating orientation of these substituents at the perimeter of the *Piedfort*-unit thus interlocking these units. Compound **2** is under crystallization and the synthesis of the orto-substituted version is underway.

Comparison of these structures with carbon analogues synthesized in our earlier works reveal interesting differences and similarities. An account of structural relationships between Si-organic derivatives and carbon derivatives and their related crystalline architectures will be given with special emphasis on possible solid state applications.

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