

Naming in the PDF[®]: Steps Towards a Sweeter Smelling Rose

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What's in a name? While a rose may be as sweet no matter the name, if called a daffodil we're not likely to find the flower we desire when doing a name search. The same holds true for compounds found in the Powder Diffraction File[™] (PDF[®]). Thus, a naming convention that can be applied *consistently* is paramount to the usefulness of a name search in the PDF[®]. Yet, such a convention has eluded even the most popular databases, in part because of the complexity of some compounds and because of differences amongst the various scientific camps. Using JAVA, we've attempted to address this issue and have developed a simple and efficient algorithm for turning a chemical formula into a name. Using this new method, over 19,000 PDF[®] names were assigned to entries from the Inorganic Crystal Structure Database (ICSD) and Linus Pauling File (LPF) databases in less than half the time it has taken in previous years. The new program has proven to be a step in the right direction towards a sweeter smelling rose.