

Integrating PAH databases in the VAMDC infrastructure

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Abstract. The Virtual Atomic and Molecular Data Centre (VAMDC) is a project funded by the European Union to build a unified access infrastructure to (virtually) all existing online databases of atomic and molecular data. Its aim is to offer a transparent, unified query interface to all available resources through a unique point of access (the VAMDC portal). Another part of the VAMDC infrastructure is the VAMDC registry, which keeps track of the databases which joined the infrastructure, what information they provide, the query capabilities they offer. VAMDC queries produce results in a unified format, namely the XML Schema for Atoms, Molecules and Solids, which is an international standard. Being written in XML, such results can be easily transformed in any desired format, using available libraries and tools to perform an XSL transformation. The minor drawback is that XSAMS, despite being extremely rich, due to its generality will never be able to accommodate **all** information in a specialised database. For this reasons, direct query interfaces of individual databases will continue to exist, for users requiring complete access to all available data. The possibility to simultaneously query multiple VAMDC resources, on the other hand, opens the way for (relatively) easy cross-correlation of databases.

The Cagliari/Toulouse PAH theoretical spectra database was one of the initial participants to the VAMDC project, and thus is part of the infrastructure since its initial release. This was used also as an early benchmark of the VAMDC-XSAMS format, making it possible to address some of its limitations for describing large polyatomic molecules. The preliminary release of the VAMDC interface to this database is described in this poster.

In addition, a new database of experimental data is being set up in Toulouse, which will hold (experimental) information partly overlapping but mostly complementary to that in the theoretical database. The tools developed in the VAMDC project make it a (relatively) trivial matter to turn any existing relational database into a VAMDC node (or even import a previously non-existent set of structured text dables into an automatically created, brand new relational database implemented in MySQL), and this is expected to be accomplished shortly. Preliminary information on this process is also presented, highlighting the prospective potential for cross-correlating, and merging information from, these two databases.

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