Polycyclic aromatic hydrocarbons (PAH) are thought to be omnipresent in space and are considered to be building blocks of interstellar dust grains. Although no specific PAH molecule has yet been unambiguously identified, their characteristic infrared bands at 3.3, 6.2, 7.7, 8.6, and 11.2 microns are prominent in emission from wherever dust in space is illuminated by UV-rich starlight, from protoplanetary disks to reflection nebulae, from HII regions to Planetary Nebulae. Hence, the understanding of the physics and chemistry of the interstellar medium requires the knowledge of the molecular parameters for a large sample of PAH in different fundamental, excited, ionized as well as hydrogenation states. To this end, an on-line database of computed molecular properties for a large sample of PAH in four charge states (-1, -2, 0, +1 and +2) was created to be compared with astronomical observations both in absorption in the visible and in emission in the IR.

This database, named "Cagliari/Toulouse PAH theoretical spectra database" was one of the initial participants to the Virtual Atomic and Molecular Data Centre (VAMDC) project, and thus is part of this e-infrastructure since its initial release. 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 using available libraries and tools to perform an XSL transformation. The PAH theoretical spectra database was used as an early benchmark of the VAMDC-XSAMS format, making it possible to detect and address some of its limitations for describing large polyatomic molecules. The current release of the VAMDC interface to this database is described in this poster. We also present a number of tools that have been developed to help the introduction of new data in the database directly from quantum chemical calculations and to ease the management of the database.

In addition, a new database "Cosmic PAH analogues: experimental properties and kinetics" of experimental data on PAHs is being set up in Toulouse, which will hold (experimental) information partly overlapping but mostly complementary to that in the theoretical database. It will contain the experimental results produced locally with the PIRENEA set up as well as data published by other laboratories. Gathering kinetics data is motivated by our work on modeling the chemical evolution of PAHs in astrophysical environments. 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 nonexistent set of structured text tables 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.