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# Photoelectron-photoabsorption (PePa) database*

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**Abstract.** In this paper a recently launched Photoelectron-Photoabsorption Database is presented. The database was developed in order to gather all the photoelectron and photoabsorption spectra measured by various collaborators over the years as well as to ease the access to the data to the potential users. In the paper the main features of the database were described and its outline explained.

## 1 Introduction

Spectroscopy has been central to the development of our understanding of physical and chemical phenomena. Analysis of absorption and emission spectra of atomic hydrogen and helium was central to the postulation of the Bohr hypothesis and subsequent development of quantum mechanics while our understanding of molecular structure and chemical bonding is intricately linked to analysis of vibrational and rotational spectra. The 'unique spectral fingerprint' of each atom and molecule is exploited to identify species in a wide range of environments ranging from deep space to industrial plasmas and across all phases of a matter, gas, liquid, solid and in ionic form in plasmas, indeed nearly all of our knowledge and exploration of the universe is based in spectroscopy. Many different experimental techniques have been developed to explore different spectral regions ranging from the radio through THz and IR to UV and X-ray and are necessarily combined with large scale theoretical calculations since the number of species and wide spectral range needed for each are vastly in excess of the resources of the international experimental community. Spectral data is often accumulated in large scale databases this is particularly relevant for communities in which large spectral datasets are accumulated (astronomical, aeronomical, environmental and fusion) and therefore it is these communities which have established protocols and procedures for data curation and validations. Amongst the most recognised database centres are those at NIST [1]; HITRAN (for terrestrial atmosphere) [2]; AMDIS [3] for fusion whilst most recently the VAMDC [4] project has sought to provide a common portal for some 30 databases with particular emphasis on support for the astronomical community. In addition, there are many databases assembled for and by commercial enterprises (e.g. the semiconductor and lighting industry) which are often restricted access only.

Amongst this plethora of data collections there are nevertheless atomic and molecular processes and spectral regions that to date are poorly represented. In particular those detailing photoabsorption and photoelectron spectra. Photoabsorption (PA) is one of the most fundamental atomic/molecular processes and is a direct route to chemical change in the local media since population of electronically excited states of atoms and molecules leads to the production of chemically reactive species (e.g. metastable states, dissociative fragments of absorbing molecule). Photoionization leads to production of secondary charged species (ions and electrons), which can greatly alter both the physical and chemical properties of the local media and may even have longer range effects (e.g. secondary electron induced generation of DNA damage in cellular systems [5]). Comparison of photoelectron and photoabsorption spectra provides data on the Rydberg states of atoms and molecules and may inform theoretical calculations of electronic state structure. Nevertheless since the pioneering work of Robin (for PA) [6–8] and Turner et al. [9] and Berkowitz for (PE) spectroscopy [10] there have only been a few attempts to review and construct a repository for PA and PE e.g. the VPL[1] provides spectral images of photoabsorption data many drawn from the MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules [11] which is primarily aimed at the atmospheric community where photo-fragmentation of aeronomic molecules is a precursor for much of the subsequent chemistry. Much of the PA and PE data in

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[1] http://vpl.astro.washington.edu/spectra/

these repositories was collected more than 30 years ago in the 1970s and 1980s using UV lamp sources and first generation synchrotrons and was limited to atomic and smaller polyatomics. Much of this data is displayed in graphical form without data tabulation with few, if any, uncertainties and no validation or recommendation of data where there are inconsistent datasets. For many of Robin's molecular targets PA data is in the form of solution or matrix data since the compounds are solid/liquid at room temperature while PE data was often relative with few absolute cross sections being reported.

The recent identification of the need for more data on electronic state spectroscopy and subsequent photodissociation and photoionisation pathways leading to chemical reactivity has highlighted the need for more fundamental studies of PA and PE in a wide range of molecules for which such data has not been generated these include biomolecular targets (for radiation chemistry and radiotherapy) [12]; Volatile Organic Species (VOCs) for environmental studies of atmospheric/biosphere interface [13] and a range of compounds used in next generation industries (e.g. replacements for fluorocarbons used in plasma etching) [14,15]. Accordingly new experimental programmes have been developed using synchrotron and laboratory studies to generate a wealth of data which is complemented by refined theoretical data produced by more advanced quantum chemistry based atomic/molecular structure codes.

In this short paper we outline a new database (PePa) that is based on the new data generated in these new research programmes. We hope that, in time, PePa will become the 'first stop' for any user requiring either photoabsorption or photoelectron data and will be the repository of choice for generators of such data.

## 2 Data aquisition

Data gathered here has been obtained throughout an international collaboration between scientists working at University of Liège (Belgium), Canadian Light Source (Canada), Aarhus University (Denmark), Gdańsk University of Technology (Poland), University of Lisbon (Portugal) and The Open University (United Kingdom).

Photoabsorption measurements were made at the former UK Daresbury Synchrotron facility and are now being performed at the UV1 beamline (now AU-UV) at ISA, Centre for Storage Ring Facilities, Aarhus, Denmark. Both the description of the experimental setup and the beamline details can be found in the literature [16]. Complementary PA data is being collected at the Indian INDUS synchrotron facility and BESSY synchrotron in Berlin.

Photoelectron data was recorded using laboratory and synchrotron photoionization sources. Some of the data was obtained at the University of Liege, Belgium, using He(I) UV lamp and hemispherical electron analyser [17]. The more recent measurements are being performed at VLS-PGM beamline at the Canadian Light Source facility in Saskatoon, Canada [18], using Double Toroidal Coincidence Spectrometer [19]. Complementary data is collected at BESSY Synchrotron and at the Electra Synchrotron in Trieste, Italy.

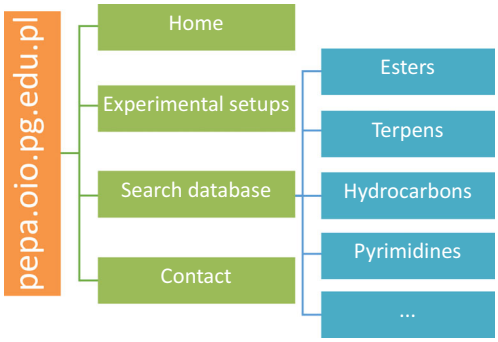


**Fig. 1.** Scheme of the PePa database.

## 3 Features of the database

The PePa Database is hosted by Gdańsk University of Technology at the web address http://pepa.oio.pg.edu.pl/. The interface of the database was designed in the simplest possible way in order to ease its functionality. Nonetheless, all the important information on the contributors, experimental apparatus and facilities used were included. The schematic outline is shown in Figure 1.

The link automatically directs the user to the Home page that contains references to the main contributors of the data included in the database (see Fig. 2). After selecting the contributor's name, database user will be directed to the web page of the contributor at his current research institution.

From there, all the general informations and links to the research facilities and experimental equipment utylized to obtained the data can be accessed by pressing the "Experimental setups" tab (Fig. 3). From there, the used can also be directed to specific web pages with detailed description of synchrotron facilities that were ised in order to perform the photoabsorption and photoelectron spectra measurements. Also, links with research papers describing the scientific apparatus were provided in this section.

The main part of the database is the "Search database" tab. The compounds that were measured and published in the scientific journals by the contributors can be accessed from the drop-down menu. For convience, the full list is also provided under this tab. Both ways of accessing the data are shown in Figure 4 – left. After choosing the compound of interest, the user will be presented with the spectra that were measured for the compound. Below the graphs, a link directing to the wesite of the publisher, containing the research article with the data can be found (Fig. 4 – right). The article can only be accessed if the user is licensed to access the website of the publisher. The research articles, apart from the data analysis, in most cases contain additional information, such as complementary theoretical data and a critical analysis of previous data (where it exists), allowing recommended datasets to be nominated. In some cases the photoabsorption spectrum is not accompanied by the photoelectron one, thus only the measured data is shown.


**Fig. 2.** Home page of the PePa Database.

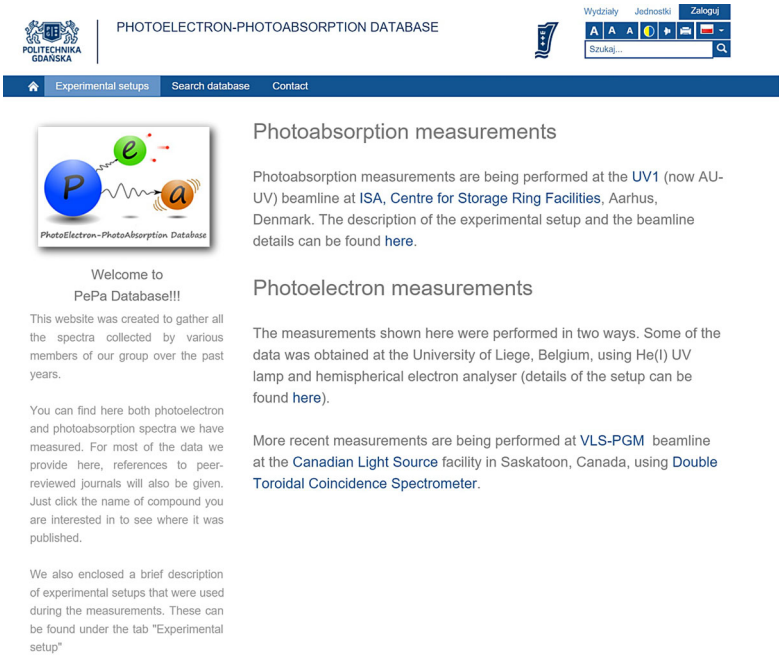


**Fig. 3.** Experimental setups tab of PePa Database.

The last tab, "Contact", allows for contacting the database administrator for data requests or comments. Users may request that the PePa team evaluates and validates new data sets, make recommendations of data sets (e.g. for models) or suggest/commission new studies.

## 4 Future development

PePa is currently in a test (beta) phase but in the near future, as more data gathered over the years by all the group members is successively included in the database, it will become a large scale resource. It is planned to extend its functionality by providing both spectra previews and direct data readouts. PePa will be made "VAMDC" compliant so it can be accessed through VAMDC portal [4] allowing its data to be compared with PA and PE data collated in other databases, for example with the solid state databases ACID [20], which reports PA cross sections and albedo (reflection) spectra in the solid (ice) phase. Furthermore, in accord with the traditions of Robin [6–8] critical reviews and comparison of PA and PE by chemical family (e.g. fluorocarbon, monoterpene,


**Fig. 4.** Search database tab of PePa Database. The compound of interest can be chosen from the drop-down menu (left); after selection, a photoabsorption and photoelectron spectrum (here – ethyl formate [21]) is shown together with a link to scientific article containing data analysis (right).

alkane, alcohol etc.) may be added with a note on theoretical calculations that accompany the experimentally measured spectra. We therefore hope other data providers will join the project and post their data in the PePa database.

## 5 Summary

In this short communication we present a recently developed Photoelectron-Photoabsorption (PePa) Database. The aim of creating this website was (1) to gather all existing data on photoabsorption and photoelectron measurements, performed over the years and (2) to made them easily accessible to scientists interested in this type of data. We hope that after the full development of additional features and completion of data collection, the database will become a reliable and complete source of information on electronic structure of molecules of environmental, industrial, biological and astrophysical interest.

## Authors contribution statement

MAŚ created the database and wrote the manuscript. NJM participated in editing and revising of the manuscript.

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## References

1. NIST Standard Reference Data, http://www.nist.gov/srd/
2. High-resolution transmission molecular absorption databas, https://www.cfa.harvard.edu/hitran/
3. Atomic Molecular Data Services, https://www-amdis.iaea.org/
4. VAMDC Consortium, http://www.portal.vamdc.eu
5. B. Boudaïffa, P. Cloutier, D. Hunting, M.A. Huels, L. Sanche, Science **287**, 1658 (2000)
6. M.B. Robin, *Higher Excited States of Polyatomic Molecules* (Academic Press, New York, 1974), Vol. 1
7. M.B. Robin, *Higher Excited States of Polyatomic Molecules* (Academic Press, New York, 1975), Vol. 2
8. M.B. Robin, *Higher Excited States of Polyatomic Molecules* (Academic Press, New York, 1985), Vol. 3
9. D.W. Turner, C. Baker, A.D. Baker, C.R. Brundle *Molecular Photoelectron Spectrsocopy* (Wiley-Interscience, London, 1970)
10. J. Berkowitz, *Photoabsorption, Photoionization and Photoelectron Spectroscopy* (Academic Press, New York, London, 1979)
11. The MPI-Mainz UV/VIS Spectral Atlas of Gaseous Molecules of Atmospheric Interest, http://satellite.mpic.de/spectral_atlas
12. N.J. Mason, AIP Conf. Proc. **1080**, 3 (2008)
13. N.J. Mason, A. Dawes, R. Mukerji, E.A. Drage, E.J. Vasekova, S.M. Webb, P. Limão-Vieira, Phys. B **38**, S893 (2005)
14. S. Samukawa et al., J. Phys. D **45**, 253001 (2012)
15. N.J. Mason, J. Phys. D **42**, 194003 (2009)
16. S. Eden, P. Limão-Vieira, S. Hoffmann, N. Mason, Chem. Phys. **323**, 313 (2006)
17. J. Delwiche, P. Natalis, J. Momigny, J.E. Collin, J. Electron Spectrosc. Relat. Phenom. **1**, 219 (1972)
18. Y.F. Hu, L. Zuin, G. Wright, R. Igarashi, M. McKibben, T. Wilson, S.Y. Chen, T. Johnson, D. Maxwell, B.W. Yates, T.K. Sham, R. Reininger, Rev. Sci. Instrum. **78**, 083109 (2007)
19. T. Reddish, G. Richmond, G. Bagley, J. Wightman, S. Cvejanovic, Rev. Sci. Instrum. **68**, 2685 (1997)
20. Astrochemical Ices Database, https://www.prl.res.in/~bhala/acid/index.php
21. M.A. Śmiałek, M. Łabuda, J. Guthmuller, M.-J. Hubin-Franskin, J. Delwiche, D. Duflot, N.J. Mason, S.V. Hoffmann, N.C. Jones, P. Limão-Vieira, J. Chem. Phys. **141**, 104311 (2014)