Issues
A user perspective of VAMDC

- How to report issues ?
- How do we know that an issue is taken under consideration ?
- And who decide about solutions ? STB ? Individuals ?

Most of the following issues have been found while debugging **the SPECTCOL tool (Y.A. Ba et al, 2024)**

→ so it is the perspective of a **VAMDC user**

Issues

- Species Database *(under investigation)*
- Query Store *(under investigation)*
- *General Issue with Stoechiometric formula*
- Exemple of case-by-case issues in Databases
  - Different cases for a molecule that seems identical in both DB
  - Current case-by-case does not cover some description of theoretical data

Issues with Species DB

Values come from another DB

DEPRECATED : NOT in BASECOL
(will stay for 45 days)

BASECOL2015: VAMDC-TAP interface (Atomic states, Atoms, Collisions, Molecular states, Molecules)

Name	Stoichiometric formula	Formula	InChI	Mass number	InChIKey	Charge
ArH+	ArH+	ArH$^+$	1S/ArH /h1H/q+1/i1-4	0	TVQSUVFYD VJWLI-AHCXROLUS A-N	0
Ar-36-H+	ArH+	^{36}ArH$^ +$	1S/ArH /h1H/q+1/i1-4	0	TVQSUVFYD VJWLI-AHCXROLUS A-N	0
36ArH+	ArH+	^{36}ArH$^ +$	1S/ArH /h1H/q+1/i1-4	0	TVQSUVFYD VJWLI-AHCXROLUS A-N	0
Ar-36-D+	ArH+	^{36}ArD$^ +$	InChI=1S/ArH /h1H/q+1 /i1-4D	38	TVQSUVFYD VJWLI-UJBPSDSUS A-N	0
36ArD+	ArH+	^{36}ArD$^ +$	InChI=1S/ArH /h1H/q+1 /i1-4D	38	TVQSUVFYD VJWLI-UJBPSDSUS A-N	0
ArD+	ArH+	ArD$^+$	1S/ArH /h1H/q+1/i1D	42	TVQSUVFYD VJWLI-MICDWDOJS A-N	0

But Pb in BASECOL node software as well

Issues with Species DB

how to report those issues ? To who ? STB ?

- Add Mass Number and Ion Charge in the output of molecular species – this is useful additional information that is displayed on “species DB”
- Improve process for “species database” in order to avoid displaying wrong information that are not provided by the databases (Mass number = 0 when DB provides the right information)
- Non-existing species stay for 45 days after it disappear from DB – Disturbing for users – Solution ?

Issues with Query Store

- It stores VAMDC queries (only for the DB where it is implemented) with various metadata, the XSAMS and the references are extracted. → Interest to get a DOI from ZENODO to identify the query, the XSAMS and the set of references
- QS impact is minor in the community right now → it is possible to find a good use but **it requests to solve issues**
- **Scientific UseCase** : Currently I am writing the SPECTCOL paper and I want to use the QS to store the result of the queries in ZENODO, have a DOI
- **Objective** :
  - →To give a snapshot at time T of what is retrieved from VAMDC
  - →The DOI allows to cite the producers of data

Issues with Query Store

Query from Portal : Stoechiometric formula = CH+

No DOI yet - Get one

VAMDC data source identifier: https://cdms.astro.uni-koeln.de/cdms/tap/

Version of the VAMDC database producing the dataset: 2019-11-27

Query originating the data: select * where (inchikey in ['wvvlbiyucxyyeu-cnrunogksa-n', 'wvvlbiyucxyyeu-micdwdojsa-n', 'wvvlbiyucxyyeu-njfspnsnsa-n', 'wvvlbiyucxyyeu-oubtzvsysa-n', 'wvvlbiyucxyyeu-uhfffaoysa-n', 'wvvlbiyucxyyeu-vvkomztbsa-n'])

Query identifier : 3fbc72f5-74e7-4e0b-b685-47b5fb3ec885

Query produced dataset: XSAMS file (if not available, please try again in a few minutes)

XSAMS version : 12.07

Query result downloaded on (UTC+1) :

- 2023-11-3 10:46:24

Bibliographic references in the dataset

Error : Invalid bibtex content

Switch references to Bibtex

This issue prevents sometimes the creation of PID and of this landing page

→ (not yet understood)

In this case the landing page is created,
But the bibliographic references are absent → QS cannot be used to cite the Producers' references !

Portal Output
(Molecular XSAMS to HTML processor)

Id	Title	Origin	Authors	Year	Link
BCDMS-429	Dipole moments and orientation polarizabilities of diatomic molecular ions for precision atomic mass measurement	journal : Phys. Rev. A (Vol : 75 , Page Begin : 012502)	Cheng, M.; Brown, J. M.; Rosmus, P.; Linguerri, R.; Komiha, N.; Myers, E. G.;	2007	
BCDMS-668	Spectroscopic parameters and rest frequencies of isotopic methylidynium, CH+	journal : Astron. Astrophys. (Vol : 514 , Page Begin : 6)	Müller, H. S. P.;	2010	
BCDMS-669	THE J= 1–0 TRANSITIONS OF12CH+,13CH+, AND12CD+	journal : Astrophys. J. (Vol : 716 , Page Begin : L1 , Page End : L3)	Amano, T.;	2010	
BCDMS-670	Some New Emission Bands of the A1Π - X1Σ+ System of CH+	journal : Phys. Scr. (Vol : 25 , Page Begin : 272 , Page End : 274)	Carrington, A.; Ramsay, D. A.;	1982	
BCDMS-671	New analysis of the Douglas-Herzberg system (A1?- X1?+) in the CH+ ion radical	journal : Eur. Phys. J. D (Vol : 38 , Page Begin : 481)	Hakalla, R.; Kepa, R.; Szajna, W.; Zachwieja, M.;	2006	
BCDMS-672	New Spectroscopic Analysis of theA1??X1?+Band System in the13CH+Radical	journal : J. Mol. Spectrosc. (Vol : 181 , Page Begin : 136)	Bembenek, Z.;	1997	
BCDMS-673	New spectroscopic analysis of the A1Π - X1Σ+band system of the CD+radical	journal : J. Phys. B (Vol : 20 , Page Begin : 6197 , Page End : 6205)	Bembenek, Z.; Cisak, H.; Kepa, R.;	1987	
BCDMS-674	Analysis of the 0–0 and 1–0 Bands of theA1Π–X1Σ+System of the13CD+Radical	journal : J. Mol. Spectrosc. (Vol : 182 , Page Begin : 439 , Page End : 443)	Bembenek, Z.;	1997	
BCDMS-675	Dipole moments and orientation polarizabilities of diatomic molecular ions for precision atomic mass measurement	journal : Phys. Rev. A (Vol : 75 , Page Begin : 012502)	Cheng, M.; Brown, J. M.; Rosmus, P.; Linguerri, R.; Komiha, N.; Myers, E. G.;	2007	
BCDMS-1771	Spectroscopic Parameters and Rest Frequencies of Isotopic Methylidynium, CH+	journal : Astron. Astrophys. (Vol : 514 , Page Begin : L6)	Müller, H. S. P. ;	2010	
BCDMS-1773	Vibration-rotation transition probabilities in CH+ and CD+	journal : Chem. Phys. Lett. (Vol : 136 , Page Begin : 562 , Page End : 565)	Follmeg, B, Rosmus, P., Werner, H.-J.;	1987	
BCDMS-1921	CDMS database	database	Müller, H. S. P.; Endres, C. P.; Schlemmer, S.; Stutzki, J.;	2012	
BCDMS-2709	The Cologne Database for Molecular Spectroscopy, CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC	journal : J. Mol. Spectrosc. (Vol : 327 , Page Begin : 95 , Page End : 104)	Endres, C. P.; Schlemmer, S.; Schilke, P.; Stutzki, J.; Müller, H. S. P.;	2016	

Portal Output (XSAMS to BIBTEX processor)


```
@misc {BCDMS-2023-11-16-10-51-4, howpublished={database}, author = {N.N.}, year = {2023}, url={https://cdms.astro.uni-koeln.de/cdms/tap/sync?LANG=VSS2&REQUEST=doQuery&
FORMAT=XSAMS&QUERY=select+*+where+%28%28InchiKey+IN+%28%27WVVLBIYUCXYYEU-OUBTZVSYSA-N%27%2C%27WVVLBIYUCXYYEU-MICDWDOJSA-N%27%2C%27WVVLBIYUCXYYEU-UHFFFAOYSA-N%27%2C
%27WVVLBIYUCXYYEU-CNRUNOGKSA-N%27%2C%27WVVLBIYUCXYYEU-VVKOMZTBSA-N%27%2C%27WVVLBIYUCXYYEU-NJFSPNSNSA-N%27%29%29%29}}

@article {BCDMS-429, author = {Cheng, M. and Brown, J. M. and Rosmus, P. and Linguerri, R. and Komiha, N. and Myers, E. G.}, title = {Dipole moments and orientation
polarizabilities of diatomic molecular ions for precision atomic mass measurement}, journal = {Phys. Rev. A}, volume = {75}, pages = {012502}, year = {2007},
doi={10.1103/PhysRevA.75.012502}}

@article {BCDMS-668, author = {Müller, H. S. P.}, title = {Spectroscopic parameters and rest frequencies of isotopic methylidynium, CH+}, journal = {Astron. Astrophys.}, volume
= {514}, pages = {6}, year = {2010}, doi={10.1051/0004-6361/201014398 }}

@article {BCDMS-669, author = {Amano, T.}, title = {THE J= 1-0 TRANSITIONS OF12CH+,13CH+, AND12CD+}, journal = {Astrophys. J.}, volume = {716}, pages = {L1,L3}, year = {2010},
doi={10.1088/2041-8205/716/1/L1}}

@article {BCDMS-670, author = {Carrington, A. and Ramsay, D. A.}, title = {Some New Emission Bands of the A1Π - X1Σ+ System of CH+}, journal = {Phys. Scr.}, volume = {25},
pages = {272,274}, year = {1982}, doi={10.1088/0031-8949/25/2/005}}

@article {BCDMS-671, author = {Hakalla, R. and Kepa, R. and Szajna, W. and Zachwieja, M.}, title = {New analysis of the Douglas-Herzberg system (A1?- X1?+) in the CH+ ion
radical}, journal = {Eur. Phys. J. D}, volume = {38}, pages = {481}, year = {2006}, doi={10.1140/epjd/e2006-00063-9}}

@article {BCDMS-672, author = {Bembenek, Z.}, title = {New Spectroscopic Analysis of theA1??X1?+Band System in the13CH+Radical}, journal = {J. Mol. Spectrosc.}, volume = {181},
pages = {136}, year = {1997}, doi={10.1006/jmsp.1996.7143}}

@article {BCDMS-673, author = {Bembenek, Z. and Cisak, H. and Kepa, R.}, title = {New spectroscopic analysis of the A1Π - X1Σ+band system of the CD+radical}, journal = {J.
Phys. B}, volume = {20}, pages = {6197,6205}, year = {1987}, doi={10.1088/0022-3700/20/23/012}}

@article {BCDMS-674, author = {Bembenek, Z.}, title = {Analysis of the 0-0 and 1-0 Bands of theA1Π-X1Σ+System of the13CD+Radical}, journal = {J. Mol. Spectrosc.}, volume =
{182}, pages = {439,443}, year = {1997}, doi={10.1006/jmsp.1996.7219}}

@article {BCDMS-675, author = {Cheng, M. and Brown, J. M. and Rosmus, P. and Linguerri, R. and Komiha, N. and Myers, E. G.}, title = {Dipole moments and orientation
polarizabilities of diatomic molecular ions for precision atomic mass measurement}, journal = {Phys. Rev. A}, volume = {75}, pages = {012502}, year = {2007},
doi={10.1103/PhysRevA.75.012502}}

@article {BCDMS-1771, author = {Müller, H. S. P. }, title = {Spectroscopic Parameters and Rest Frequencies of Isotopic Methylidynium, CH+}, journal = {Astron. Astrophys.},
volume = {514}, pages = {L6}, year = {2010}, doi={10.1051/0004-6361/201014398}}

@article {BCDMS-1773, author = {Follmeg, B, Rosmus, P., Werner, H.-J.}, title = {Vibration-rotation transition probabilities in CH+ and CD+}, journal = {Chem. Phys. Lett.},
volume = {136}, pages = {562,565}, year = {1987}, doi={10.1016/0009-2614(87)80518-3}}

@misc {BCDMS-1921, howpublished={database}, author = {Müller, H. S. P. and Endres, C. P. and Schlemmer, S. and Stutzki, J.}, title = {CDMS database}, year = {2012}}

@article {BCDMS-2709, author = {Endres, C. P. and Schlemmer, S. and Schilke, P. and Stutzki, J. and Müller, H. S. P.}, title = {The Cologne Database for Molecular Spectroscopy,
CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC}, journal = {J. Mol. Spectrosc.}, volume = {327}, pages = {95,104}, year = {2016}, doi={10.1016/j.jms.2016.03.005}}
```

Example

« New analysis of the Douglas-Herzberg system (A1?- X1?+) in the CH+ ion radical » → XSAMS content (displayed as such by the processors and by SPECTCOL)

Molecular Physics and Chemical Physics | Published: 21 March 2006

New analysis of the Douglas-Herzberg system ($A^1\Pi$-$X^1\Sigma^+$) in the CH^+ ion radical

The $A^1\Pi$- $X^1\Sigma^+$ system in the CH^+

R. Hakalla, R. Kępa, W. Szajna & M. Zachwieja

The European Physical Journal D - Atomic, Molecular, Optical and Plasma Physics **38**, 481–488 (2006) | Cite this article

179 Accesses | **31** Citations | Metrics

Example

« New analysis of the Douglas-Herzberg system (A1?- X1?+) in the CH+ ion radical » → XSAMS content (displayed as such by the processors and by SPECTCOL)

Cite this article

Hakalla, R., Kępa, R., Szajna, W. *et al.* New analysis of the Douglas-Herzberg system ($A^1\Pi$- $X^1\Sigma^+$) in the CH^+ ion radical. *Eur. Phys. J. D* **38**, 481–488 (2006). https://doi.org/10.1140/epjd/e2006-00063-9

Download citation

[No bibtex Option]

[Already different In Journal itself]

Received	Published	Issue Date
23 November 2005	21 March 2006	June 2006

DOI

https://doi.org/10.1140/epjd/e2006-00063-9

[Image]

```
TI  - New analysis of the Douglas-Herzberg system (A1Π- X1Σ+)  inthe CH+ ion radical
```

QS Issue

how to report those issues ? To who ? STB ?

- Some ideas under investigation :
  - Ask the DB to check all their references for wrong characters in the title
    - Con : Humans understand « New analysis of the Douglas-Herzberg system (A1?- X1?+) in the CH+ ion radical
    - Con : A lot of manpower
  - Make the QS the same as the 2 processors and SPECTCOL
    - Pro : Title is not commonly included in the list of references in publications and therefore does not define the uniqueness of the reference.
    - Con : we write wrong Title in ZENODO

General Issue with implementation in DB

how to report ? To STB ?

- Stoechiometric formula **has charge sign** in some databases and **no charge sign** in other databases
- For example : CDMS/JPL/BASECOL have charge sign : 'CN-' → **interesting to have charge because it narrows the search**

Questions :

  - What is the implementation in the various DB ?
  - What shall we do ?

Reported by Giacomo to MLD in June 2023

Issues with implemention in DB

how to report those issues ? To who ? STB ?

- CNCN is lpos in CDMS
- CNCN is lpcs in BASECOL
- It seems that **it is the same state** (ground state) in both databases
- *Reported to CDMS → in standby*

Current issues with case-by-case « extension »

(Annual meeting for report ?)

- Need of a process to handle changes and to follow up with the different libraries
- Currently 3 molecules have issues in BASECOL :
  - The case "hundb" has been assigned to the C$_4$ (X$^3\Sigma_g^-$) because the "SpinComponentLabel" label does not exist in the "lpos" (linear polyatomic open shell) case
    - ADD “SpinComponentLabel” To lpos

Current issues with case-by-case

- the "hunda" has been assigned to the C$_6$H (X$^2\Pi$) because the authors used (J,Ω) quantum numbers and the "lpos" case does not include Ω
  - ADD Ω to lpos
- The CH$_3$OH molecule is described with a "stcs" case in which the label "rovibSym" is used for the symmetry of the ro-torsional function
  - Symmetry of the ro-torsion is not rovibsym, should we add “rotorSym” ?