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# **vamdclib Documentation**

*Release 0.1*

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<b>1</b>	<b>Introduction</b>	<b>3</b>
1.1	About VAMDC . . . . .	3
1.2	About this library . . . . .	3
<b>2</b>	<b>Concept of this library</b>	<b>5</b>
2.1	Datamodel . . . . .	5
<b>3</b>	<b>Software prerequisites and installation</b>	<b>7</b>
3.1	Quickstart . . . . .	7
<b>4</b>	<b>The Node - Module</b>	<b>9</b>
4.1	About . . . . .	9
4.2	Library Classes and Methods . . . . .	9
4.3	Example: . . . . .	9
<b>5</b>	<b>The Request - Module</b>	<b>11</b>
5.1	About . . . . .	11
5.2	Library Classes and Methods . . . . .	11
5.3	Examples . . . . .	11
<b>6</b>	<b>The Results - Module</b>	<b>13</b>
6.1	About . . . . .	13
6.2	Library Classes and Methods . . . . .	13
<b>7</b>	<b>The Database - Module</b>	<b>15</b>
7.1	About . . . . .	15
7.2	Library Classes and Methods . . . . .	15
7.3	Examples . . . . .	15
<b>8</b>	<b>VAMDC Glossary</b>	<b>17</b>
<b>9</b>	<b>Bugs and Contact</b>	<b>19</b>
9.1	Report a bug . . . . .	19
9.2	Contact information . . . . .	19
<b>10</b>	<b>Indices and tables</b>	<b>21</b>



Contents:

This document covers the **release 0.1** of the python library *vamdclib*.

Links to HTML-versions:

- Last release: <http://>
- Latest development: <http://>

Links to PDF-versions:

- Last release: <http://>
- Latest development: <http://>



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## Introduction

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### 1.1 About VAMDC

The Virtual Atomic and Molecular Data Center is a EU FP7 research infrastructure project. A comprehensive documentation about the project, standards and related software can be found on the official webpage <http://vamdc.eu/>.

### 1.2 About this library

This library contains several modules that implement access to VAMDC's infrastructure. It allows to query the central registry service to obtain information about registered VAMDC database nodes and to send queries to these nodes as well as to process the retrieved data. The data is made available as python dictionaries. Tools to store and manage the data in a local sqlite3 database or basex - xml database are included.





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**Concept of this library**

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**2.1 Datamodel**



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## Software prerequisites and installation

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### 3.1 Quickstart



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## The Node - Module

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### 4.1 About

Information about registered VAMDC nodes are stored in the VAMDC registry service. The registry contains a list of all registered database nodes and their url's.

More information on the VAMDC registry service can be found in the documentation for the VAMDC standards: <http://www.vamdc.eu/documents/standards/registry/>

### 4.2 Library Classes and Methods

### 4.3 Example:

The following example shows how to get an node instance for CDMS:

```
>>> import nodes
>>> nl = nodes.Nodelist()
>>> cdms = nl.getnode('ivo://vamdc/cdms/vamdc-tap-dev')
>>> cdms.url
u'http://cdms.ph1.uni-koeln.de/cdms/tap/'
```

The 'getnode' method can be replaced by findnode if the 'searchstring' is unique:

```
>>> nl.findnode ('CDMS')
```



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## The Request - Module

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### 5.1 About

### 5.2 Library Classes and Methods

### 5.3 Examples

```
>>> import request
>>> req = request.Request()
>>> req.setnode(cdms)
>>> req.setquery("Select Species")
>>> result = req.dorequest()
```

req contains now an instance of the Request class. The database CDMS is selected (see example in nodes.py) and a query which selects all species available at the CDMS database is formulated. The last command performs the request and returns an instance of results.Result which contains the return raw xml string and the data parsed into dictionaries whose layout has been defined in spectmodel.py





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**The Results - Module**

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**6.1 About**

**6.2 Library Classes and Methods**



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## The Database - Module

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### 7.1 About

### 7.2 Library Classes and Methods

### 7.3 Examples

```
>>> import database
>>> db = database.Database()
```



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## VAMDC Glossary

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### **VAMDC nodes**

A “node” within VAMDC is a data service that offers its data using the standards and protocols defined by the VAMDC. They are web services with a simple API, the specification of which can be found in the documentation for the VAMDC standards: <http://vamdc.org/documents/standards/>

### **VAMDC central registry service**

The registry service contains the list of VAMDC nodes and the capabilities of each node.



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## Bugs and Contact

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### 9.1 Report a bug

The vamdclib library is in active development and there are some rough edges still. We very much appreciate your feedback and complaints are usually resolved quickly.

Please file an issue at <https://github.com/VAMDC/vamdclib/issues>

This can be used for bugs on both, the software itself and the documentation.

### 9.2 Contact information

You can write to the VAMDC developers email list: `vamdc.developer <AT> sympa.obspm.fr`





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**Indices and tables**

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- `genindex`
- `modindex`
- `search`



## V

VAMDC central registry service, [17](#)

VAMDC nodes, [17](#)