

CDB Documentation

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Chapter 1

CDB Documentation

1.1 Welcome to CDB

CDB - CHEMICAL DATABASE V 1.05

IDEA TEAM Science & Tech Collection.

Science & Tech is a collection of scientific programs written by S. ←
Peruzzi.

For more informations on currently available programs, up-to-date versions
and future plans, just contact the author.

1. INTRODUCTION

1.1

Short description

.....What is ←
CDB ?

1.2

System Requirements

.....What you need to run CDB

1.3

Features list

.....Complete CDB ←
feature list

1.4

Greetings

.....Greetings ←
from the author

2. INSTALLATION

2.1

Installing CDB

.....How to ←
install CDB

3. USER GUIDE

3.1

	User Interface	
GUI complete	↔
	reference	
3.2	ARexx Interface	
Controlling CDB via ARexx	
4.	TECHNICAL GUIDE	
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1.2 Short Description

Short Description

CDB (Chemical Database) is a general purpose database for chemistry. At the present time it provides data about all chemical elements easily accessible from a graphical user interface (gui) and from ARexx.

CDB interface recalls the classic "periodic table", just to make easier to find and select elements (every student knows this table!).

Thanks to ARexx interface CDB is fully operational even from ARexx programs and macros, it is possible to ask for a single physical value of an element or getting a complete synoptic table.

In future versions there will be other databases related to chemistry.

I really don't know how many people need such tools on Amiga but if so many molecular biology & physics tools are yet present for Mac & PC I really wonder why not so for Amiga (given such a powerful O.S.).

I really need a feedback from students and biomol/biophys guys that think I am on the right way. :-)

So e-mail comments & suggestions to peru@maya.dei.unipd.it

1.3 System Requirements

System Requirements

CDB need MUI 3.x, Amiga O.S. 3.x.

Element database is not very big but some memory is required for asynchronous user interface, more windows you use at the same time and more free memory you need. To avoid memory fragmentation CDB makes use of system memory pools.

MUI 3.x can be found on every AMINET site, CD, and many BBS.

1.4 Features List

Features List

- o Fully multitasking.
- o MUI fully configurable user interface
- o On line bubble help.
- o Asynchronous user interface.
- o Easy saving and printing of every window content.
- o ARexx port for power users with a complete set of ARexx commands.
- o CX exchange broker for better control.

1.5 Greetings

Greetings

Many thanx to Stefan Stuntz for MUI, buy it, it does really worth the price! I coded other GUI's using intuition,

gadtools and BOOPSI but are all nothing respect to MUI easy of use and configurability, its best feature is surely the auto-layer-rescaling and positioning feature.

Thanks to my friends:

Andsk (Andrea Rafreider) that has written the installer script and that constantly updates my internet A4000 setup, now he's working on new stuff he will release on Aminet as an IDEA TEAM product.

Amex (Amedeo Petrella) and Ire (Ireneo Toffano) for debugging and ideas for future releases. Ireneo is working on a new program but we have to wait to know more about it.

Zanna (Claudio Zanella) that we usually meet at his AmiProBBS for Pizza&Amiga parties. Claudio will enter other databases that I shall implement in future releases, so you must thank Claudio for next databases.

Atreju (Antonio Guerra) my personal movie adviser, a guy that sold off his A1200 and CD32 for a brand new Pentium 90 one year ago for some 4000 USD, and that now whispers for P-166 at half the price - he really can't go on with such a slowly P-90 ... maybe next year he'll be braked by a mere P-166 and will be forced to look for P-200 :-). We call him SVGA as this word has been proved to be the most used interlocution by PC guys, Atreju in particular!

Martino Pornaro & Gianluca Coppo for soccer matches (real one I mean!).

Guys at Ederle N.A.T.O. base for their great work for Italy. I spent a very nice July 4th at Ederle (North East Italy) this year (1996), you're OK - go on this way !!!

PS) Call AmiProBBS! Gb of Amiga files on line, every AMINET CD and much other stuff:

AmiProBBS 24/24h Zyxel Elite 28.8K
BBS +39-49-604488 Voice +39-49-8641713

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1.6 Installing CDB

Installing CDB

Installation is very simple thanks to Amiga Technologies official installer. Simply run the installer script and follow on line requests and instructions.

If you want do it manually then follow these steps:

- Copy CDB drawer where you want in your hard disk.

PS) CDB looks for databases in "PROGDIR:data/", so no assignments are needed.

1.7 Getting Started

1.8 User Interface

User Interface

Shell & Workbench

To start program iconified simply set tooltype ICONIFY=YES in program icon or use ICONIFY=YES option in the CLI command line.

Another useful tooltype is LANGUAGE to enter the localized elements database path & filename. Default is LANGUAGE=data/english.loc.

Gadgets

Help Leaving the mouse pointer resting on any GUI gadget will popup a bubble help text.

Element gadgets open windows with data for selected elements, data can be saved and printed with three gadgets available in every element window. User can open many windows asynchronously and operate freely without worrying about double selection that is ignored by CDB. Every window provides print, save and save as gadgets for printing and saving data.

Synoptic table frame groups show button and a cycle gadget that allows selection out of 20 cross-reference databases. Use cycle gadget to make your choice and then open the correlated window. You can open many windows asynchronously without worrying about double selection that is automatically ignored by CDB. Every window provides print, save and save as gadgets for printing and saving data.

Database table frame groups show button and a cycle gadget that allows selection of databases. Use cycle gadget to make your choice and then open the correlated window. You can open many windows asynchronously without worrying about double selection that is automatically ignored by CDB. Every window provides print, save and save as gadgets for printing and saving data.

The "Tips" database is accessible in two distinct ways:

It is possible to enter the element tips by simply clicking on the header of any element window, the header displays the element name and electronic configuration but it is itself a button.

A second way is to toggle "tips" on program menu, when this menu item is checked
 every selection on the periodic table will display tips instead of element data.

Menus

About CDB Information on version of CDB, author and ARexx port.

User Info Information on the registered user.

Tips A checked menu that toggles between data and tips mode.

MUI Prefs Opens a window to modify CDB user interface.

Iconify iconifies application. This action is possible also via CX exchanger utility, shell, tooltypes and ARexx.

Quit Exits CDB.

1.9 ARexx Interface

ARexx Interface

CDB include an ARexx interface. Port name consists of basename plus an index number. This allows multiple CDB windows to work in multitasking without sharing the same public message port for ARexx messages exchange.

The first time CDB is run the public port name will be "CDB.1", but you can check the current ARexx port name just selecting "About CDB" menu item.

For ARexx interprocess communication with CDB just send commands to CDB ARexx port and check return variable RC for errors and RESULT for return values.

Here's a little example:

```
ADDRESS CDB.1      -> to select CDB ARexx port.
OPTIONS RESULTS   -> to get results values.
COMMAND PARAM     -> CDB internal command + parameter if needed.
SAY RC            -> 0=OK, 5=WARN, 10=ERROR, 20=FATAL
                  WARN when requested operation could not
                  be
                  completed for memory or other problems.
SAY RESULT        -> Check return string if needed.
```

So to iconify CDB just open a shell and type:
 rx "ADDRESS CDB.1; ICONIFY" (enter)

To get electronic configuration of Iron just enter:

```
rx " ADDRESS CDB.1; OPTIONS RESULTS; GETDATA Fe 0; SAY RC; SAY RESULT" (enter)
```

ARexx Commands

WinToFront Puts CDB window to front.

WinToBack Puts CDB window to back.

ActivateWin Activate CDB window.

LockGUI Locks user interface.

UnLockGUI Unlocks user interface.

Iconify Iconifies CDB window.

UnIconify Uniconifies CDB window.

GetVersion Returns complete CDB version string.

GetAuthor Returns CDB author string.

Quit Exits CDB without any requester.

OpenWinEl symbol/A Opens the element window selected by symbol.

CloseWinEl symbol/A Closes the element window selected by symbol.

SaveEl symbol/A Saves the data for element selected by symbol.

SaveAsEl symbol/A name/A/K Saves, with name, the data for element selected by symbol. ↵

SaveReqEl symbol/A Saves, with requester, the data for element selected by symbol ↵
.

PrintEl symbol/A Prints the data for element selected by symbol.

OpenWinTab code/N Opens the synoptic table selected by code.

CloseWinTab code/N Closes the synoptic table selected by code.

SaveTab code/N Saves the synoptic table selected by code.

SaveAsTab code/N name/A/K Saves, with name, the synoptic table selected by code.

SaveReqTab code/N Saves, with requester, the synoptic table selected by code.

PrintTab code/N Prints the synoptic table selected by code.

GetData symbol/A code/N Get data selected by code for element symbol.

OpenWinDB database/N Opens the database table selected by code.

CloseWinDB database/N Closes the database table selected by code.

SaveDB database/N Saves the database table selected by code.

SaveAsDB database/N name/A/K Saves, with name, the database table selected by code. ←

SaveReqDB database/N Saves, with requester, the database table selected by code.

PrintDB database/N Prints the database table selected by code.

OpenTipsWin symbol/A Opens the element tips window selected by symbol.

CloseTipsWin symbol/A Closes the element tips window selected by symbol.

Symbol could be any standard element symbol, selection is case insensitive.

Symbol table:

H He Li Be B C N O F Ne Na Mg Al Si P S Cl Ar K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn ←
 Ga
 Ge As Se Br Kr Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe Cs Ba La Hf ←
 Ta
 W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn Fr Ra Ac Ku Ha Ce Pr Nd Pm Sm Eu Gd Tb Dy
 Ho Er Tm Yb Lu Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Implemented Databases:

0 - Isotopes

Codes for synoptic tables:

0 - Electronic Configuration
 1 - Atomic Weight
 2 - Oxidation State
 3 - Melting Point
 4 - Boiling Point
 5 - Volumic Mass
 6 - Electronegativity
 7 - Ionization Energy
 8 - Heat of Fusion
 9 - Heat of Vaporization
 10 - Thermal Conductivity
 11 - Electrical Resistivity
 12 - Specific Heat Capacity
 13 - Atomic Radius
 14 - Covalent Radius
 15 - Ionic radius
 16 - Atomic Volume
 17 - Crystal Structure
 18 - Acidic-Basic Properties
 19 - Steady Phase

1.10 Inside CDB

References for CDB

- o Elements data and isotopes table have been extracted from
"Tavola periodica degli elementi" by Prof. R.Barbucci
V.Morelli Edition - Firenze, Italy.
- o Tips textfiles has been downloaded from LANL WWW archive
(<http://mwanal.lanl.gov/CST/imagemap/periodic/periodic.html>)
and then stripped of HTML tags and partially modified.
The sources of all data are
"CRC Handbook of Chemistry and Physics" and the
"American Chemical Society".

Other references from other databases will be notified
as soon as such databases will be implemented.

1.11 Inside CDB

Inside CDB

CDB has been developed with A4000 platform, SAS 6.56, MUI 3.3
GoldED and many other tools that runs in multitasking and that
makes great Amiga and Amiga O.S.

CDB makes use of memory pools method in order to avoid memory
fragmentation. No memory loss or enforcer hit has been detected.

CDB on startup tries to load databases in "CDB:data/" and if not present
quits and releases resources.

Loaded databases are kept in memory with linked lists for fast and
reliable access, this way it is possible to get a single value via ARexx.

Other databases are not yet been implemented for technical problems
with fonts. Chemistry databases need particular symbols that are not
present in standard ASCII set (0-128). It could be possible to provide
a special font with needed symbols but this would interfere with GUI
cofigurability that, at the present time, allows font selection through
MUI button font selector.

I hope problem will be solved as soon as possible, it is not on top of
my to-do list because I am working to other 3 programs and I can work only
in my spare time.

1.12 History

History

Many thanx to all of you for your feedback, bug-reporting and suggestions.

Version 1.00

- o First AMINET release.

Version 1.01

- o Now loading and saving to PROGDIR, no assign needed. (Albert-Jan Brouwer)
- o Removed a stupid bug on memory allocation. (Michael Currie)

Version 1.02

- o Added database routines.
- o Added isotopes database and 6 new ARexx commands.

Version 1.03

- o Element Ha was incorrect, database element.dat fixed. (Gianluca Coppo)
- o Internal minor changes. Recompiled with latest version of SAS-C.
- o New naming style for distribution: now CDB_xyy.lha, xyy=version-revision.

Version 1.04

- o Added 7 new elements, from 106 to 112. (Esa Haapaniemi & Ingo Paulsen)
- o Added a new database of 250Kb with history and tips on all elements.
- o Added new ARexx commands for the new database.
- o Added separate database for localized element names. (Ingo Paulsen)
- o New menu item and new tooltype LANGUAGE for selection of language.

Version 1.05

- o Fixed LANGUAGE tooltype bug, it didn't work.
- o Elements Ns,S,Ku,W,Pa were not correctly linked to tips database.
- o Double selection of an element tips gadget didn't work correctly.
- o Increased program stack to 50Kb.

TO DO LIST

- o Radioactive elements database.
- o Red-Ox pairs database.
- o Full localization.

1.13 Bugs

Bugs & bug reporting

For bug reporting, be sure that bug is reproducible at given conditions. Report the exact configuration of your platform, the version of CDB used and of AOS (Amiga O.S.) and the circumstances that trigger the buggy behaviour.

Some strange behaviour may be due to MUI library and, were it the case, it could be present in other MUI applications.

Bugs could be reported via postal service or (much better) via e-mail to the following address:

Stefano Peruzzi
Via S. Dall'Arzere, 23
I-35132 Padova - ITALY
peru@maya.dei.unipd.it

Possible bugs & other stuff

- * Using MCP multi-commodity with SaveGIRPort option, could severely slow down CDB video refresh, causing the gadget imagery to be damaged when moving the sliders or using the popup gadget.

1.14 Copyright

Copyright

CDB © Copyright 1996 by Stefano P.R. Peruzzi. All rights reserved.

This software has been entirely developed by the author who owns all rights on his product. The author is free to change the copyright conditions at any moment.

1.15 Licence

Licence

CDB is SHAREWARE.

Now CDB does use a keyfile protection system, this and my other products required time and work, everyone who tried coding anything in whatever computer language, knows very well how long it is the way from concept to alfa, beta and final release, and how much time is needed for debugging, for documents & installer and all other stuff.

So, help me continuing developing science & tech programs for Amiga, send just 15 USD (U.S. Dollars).

The registration is not intended for CDB only but for all programs of my science & tech collection. This means that you pay once for more programs and registration fee is very low, quite a good deal!

Thanx in advance for your supporting.

CDB is freely distributable provided that no more than a nominal fee is charged to cover costs of media or network transmission and that the CDB distribution archive is kept intact.

CDB could be included in any CD, BBS, Internet and Aminet site.

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1.16 Disclaimer

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