INFORMATION SOCIETY TECHNOLOGIES
(IST)
PROGRAMME

OpenMolGRID

DESCRIPTION OF NTP

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Abstract: This document is to describe the NTP data source that will be integrated into the OpenMolGRID data warehouse (MOLDW) and to indicate what information present is useful.

Delivery Slip

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Files

Files in this section relate to actual storage locations on the BSCW server located at https://hermes.chem.ut.ee/bscw/bscw.cgi. The URL below describes the location on BSCW from the root OpenMolGRID directory

Software Products	User files / URL
Word 2000/XP	OpenMolGRID/Workpackage 1/Deliverables/ OpenMolGRID-1-D1.4b-0110-2-1-DescNTP

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Contents

1. Introduction

1.1. Purpose and Scope

The main purpose of this document is to describe the NTP data source that will be integrated into the OpenMolGRID data warehouse (MOLDW) and to indicate what information present is useful. It is to be used as a reference document for other documents that are written.

1.2. Document Overview

The main aim of the MOLDW is to integrate data relevant to molecular engineering from disparate repositories. These repositories are held in different systems, at different locations and in different formats. Integration of each source into the MOLDW will be specific to that source, meaning that the adaptation of formats and access procedures will be required. Each source must therefore be described in detail. This document aims to describe the NTP data source.

1.3. Document Structure

In addition to this section the document contains the following sections:

- Section 2 – a description of NTP.
- Appendix A – Appendix used to support the document.

2. NTP

The US National Toxicology Program (NTP) was established in 1978 by the Department of Health and Human Services (DHHS) to coordinate toxicological testing programs within the Department, strengthen the science base in toxicology; develop and validate improved testing methods; and provide information about potentially toxic chemicals to health regulatory and research agencies, the scientific and medical communities, and the public. The NTP database on chemical health and safety information contains over 2000 chemicals. It is located at http://ntp-server.niehs.nih.gov/Main_Pages/Chem-HS.html. There are a number of ways to retrieve data from these NTP files via the Web.

1) View a list of the chemicals with Health & Safety data with links to the individual chemical H & S data, i.e. navigating hyperlinks (list also includes primary synonyms and CAS numbers).
2) Search the entire H & S database. This is a full text search and retrieves a list of all the files with matches to the search term(s). Search items are CAS number(s), chemical name(s) or synonym.
3) Download Macintosh (sea) or PC (zip) archives of these data.

2.1. Data Download

The details associated with the NTP archive are as follows:

Update frequency	Last Update	URL
Unknown	02-12-1996	http://ntp-db.niehs.nih.gov/NTP_Reports/ NTP_Chem_H&S/H&S_Archive.zip

Within this archive all data is located in `.txt` files. Each file is labelled according to its CAS (Chemical Abstracts Service) number e.g. `71432.txt` is the file associated with the chemical benzene. A CAS number is unique and specific to only one substance regardless of how the substance may characterised or defined. An abbreviated sample output from NTP for the chemical benzene is shown in Appendix A.

Information is in NTP largely text-based and is organised into categories. Each category is defined as follows:

```
-CATEGORY NAME
===============
```

One or more subcategories follows the main category. These are expressed as follows:

```
*SUBCATEGORY NAME: Data
```

In some cases, the data associated with the subcategories is categorised further. In such cases information may be structured or unstructured. If unstructured it appears as free text, otherwise it is as follows:

```
NAME (UPPERCASE, Title Case or Sentence case): Data
```

In this way it is possible to extract the relevant information from the database.

2.2. General Notes

Typically users navigate hyperlinks if they know what they are looking for, or they use the simple keyword search. Neither approach is suitable for MOLDW. The third data access method however is conceivable. The data from NTP is available in one archive that is freely downloadable via HTTP.

Appendix A – NTP Output Example

NB! Where "…" appears in this section this means data has been edited and that more information is available in the original source.

<--START OF OUTPUT EXAMPLE-->

```
        NTP CHEMICAL REPOSITORY (RADIAN CORPORATION, AUGUST 29, 1991)
                                  BENZENE


-IDENTIFIERS
 ===========
*CATALOG ID NUMBER: 000477

*CAS NUMBER: 71-43-2

*BASE CHEMICAL NAME: BENZENE

*PRIMARY NAME: BENZENE

*CHEMICAL FORMULA: C6H6

*STRUCTURAL FORMULA: C6H6

*WLN: RH

*SYNONYMS:
  (6)ANNULENE
  BENZOL
  CYCLOHEXATRIENE
  PHENE
……..


-PHYSICAL CHEMICAL DATA
 ======================

*PHYSICAL DESCRIPTION: LITERATURE: Clear, colorless to light yellow liquid
                       REPOSITORY: Clear colorless liquid

*MOLECULAR WEIGHT: 78.11

*SPECIFIC GRAVITY: 0.8765 @ 20/4 C [017,047]

*DENSITY: 0.905 g/mL @ 21 C (RAD)

*MP (DEG C): 5.5 C [017,058,395,421]

*BP (DEG C): 80.1 C [017,031,055,395]

*SOLUBILITIES:
       WATER : 1-5 mg/mL @ 18 C (RAD)
        DMSO : >=100 mg/mL @ 22 C (RAD)

OTHER SOLVENTS:
  Cyclohexane: >=100 mg/mL @ 21 C (RAD)
……..

*VOLATILITY:
    Vapor pressure: 60 mm Hg @ 15 C [038,055]; 76 mm Hg @ 20 C [055]
    Vapor density : 2.77 [043,051,055,058]

*FLAMMABILITY(FLASH POINT):
```

```
      This chemical has a flash point of -11 C (12 F) [031,036,058,275].  It is
flammable.  Fires involving this material can be controlled with a dry chemical,
carbon dioxide or Halon extinguisher.  The autoignition temperature is 562 C
(1044 F) [036,043,058,062].

*UEL: 8% [036,043,058,062]                 LEL: 1.4% [036,043,058,430]

*REACTIVITY:
      This chemical is incompatible with oxidizers [036,058,269,346].  It is
also incompatible with strong acids [058].  It can react with chlorine, ozone,
permanganates, sulfuric acid, peroxides, perchlorates, nitrating acid, nitric
acid, chromic acid anhydride and chromium trioxide [051]. ……..

 *STABILITY:
      This chemical is hygroscopic [269].  It is also sensitive to heat [058].
Solutions of this chemical in water, DMSO, 95% ethanol or acetone should be
stable for 24 hours under normal lab conditions (RAD).

*OTHER PHYSICAL DATA:
  Specific gravity: 0.8787 @ 15/4 C [031,395]; 0.879 @ 15/15 C [058]
……..


-TOXICITY
 ========

*NIOSH REGISTRY NUMBER: CY1400000

*TOXICITY: (abbreviations)
        typ. dose    mode     specie      amount     units     other
          LCLo       ihl       hmn           2      pph/5M
          LCLo       ihl       hmn        2000      ppm/5M
          TCLo       ihl       man         150      ppm/1Y-I
          TCLo       ihl       hmn         100      ppm
          LCLo       ihl       hmn          65      mg/m3/5Y
          LDLo       unr       man         194      mg/kg
          LD50       orl       rat        3306      mg/kg
          LC50       ihl       rat       10000      ppm/7H
          LD50       ipr       rat        2890      ug/kg
          LD50       orl       mus        4700      mg/kg
          LC50       ihl       mus        9980      ppm
          LD50       ipr       mus         340      mg/kg
          LDLo       orl       dog        2000      mg/kg
          LCLo       ihl       dog      146000      mg/m3
          LCLo       ihl       cat      170000      mg/m3
          LCLo       ihl       rbt       45000      ppm/30M
          LDLo       ivn       rbt          88      mg/kg
          LDLo       ipr       gpg         527      mg/kg
          LDLo       scu       frg        1400      mg/kg
          LCLo       ihl       mam       20000      ppm/5M
          LDLo       ipr       mam        1500      mg/kg
          LDLo       orl       man          50      mg/kg

*SAX TOXICITY EVALUATION:
  THR: A human poison by inhalation. An experimental poison by skin contact,
intraperitoneal, intravenous and possibly other routes. ……

*CARCINOGENICITY:
  Tumorigenic Data:
    TCLo: ihl-man    200 mg/m3/78W-I
    TCLo: ihl-hmn     10 ppm/8H/10Y-I
    TDLo: orl-rat     52 gm/kg/52W-I
……

*MUTATION DATA:
```

```
       test          lowest dose      |      test          lowest dose
    -----------   -----------------   |   -----------   -----------------
    dns-rat:lvr        1 mmol/L       |   dni-hmn:leu     2200 umol/L
    cyt-rat-ihl      300 mg/m3/16W-I  |   cyt-hmn:leu        1 mmol/L/72H
……..

*TERATOGENICITY:
  Reproductive Effects Data:
    TCLo: ihl-rat    670 mg/m3/24H (15D pre/1-22D preg)
    TCLo: ihl-rat  56600 ug/m3/24H (1-22D preg)
……..

*STANDARDS, REGULATIONS & RECOMMENDATIONS:  OSHA: Federal Register (1/19/89) and
29 CFR 1910.1000 Subpart Z
        Transitional Limit: PEL-TWA 10 ppm; Ceiling Limit 25 ppm; ……

*OTHER TOXICITY DATA:
  Skin and Eye Irritation Data: ……


-OTHER DATA (Regulatory)
 ========================

*PROPER SHIPPING NAME (IATA): Benzene

*UN/ID NUMBER: UN1114

*HAZARD CLASS: 3             SUBSIDIARY RISK: None    PACKING GROUP: II

*LABELS REQUIRED: Flammable liquid

*PACKAGING: PASSENGER: PKG. INSTR.: 305, Y305       MAXIMUM QUANTITY: 5 L, 1 L
            CARGO    : PKG. INSTR.: 307             MAXIMUM QUANTITY: 60 L

*SPECIAL PROVISIONS: None

*USES:
      This chemical is used as a solvent.  It is used in the manufacture of
medicines, dyes, artificial leather, linoleum, oil cloth, pesticides,…….

*COMMENTS:
      This chemical occurs in coal tar and petroleum naphtha and is also a
constituent of gasoline.  …….


-HANDLING PROCEDURES
 ====================

*ACUTE/CHRONIC HAZARDS:
      This compound is highly toxic by ingestion, inhalation and skin contact
[036,165,295,395].  Poisoning may occur through skin absorption ……

*MINIMUM PROTECTIVE CLOTHING:
      If Tyvek-type disposable protective clothing is not worn during handling
of this chemical, wear disposable Tyvek-type sleeves taped to your gloves.

*RECOMMENDED GLOVE MATERIALS:
 Permeation Test Results For The Neat (Undiluted) Chemical:
      The permeation test results for the neat (undiluted) chemical are given
below.  …….

*RECOMMENDED RESPIRATOR:
      When working with this chemical, wear a NIOSH-approved full face positive
pressure supplied-air respirator or a self-contained breathing apparatus (SCBA).
[651]
```

```
*OTHER:
      Since this chemical is a known or suspected carcinogen you should contact
a physician for advice regarding the possible long term health effects and …….

*STORAGE PRECAUTIONS:
      You should store this chemical in an explosion-proof refrigerator, …..

*SPILLS AND LEAKAGE:
      If you spill this chemical, FIRST REMOVE ALL SOURCES OF IGNITION.  Then,
use absorbent paper to pick up all liquid spill material ……

*DISPOSAL AND WASTE TREATMENT: Not available


-EMERGENCY PROCEDURES
 ====================

*SKIN CONTACT:
      IMMEDIATELY flood affected skin with water while removing and isolating
all contaminated clothing.  Gently wash all affected skin areas ……..

*INHALATION:
      IMMEDIATELY leave the contaminated area; take deep breaths of fresh air.
IMMEDIATELY call a physician and be prepared to transport the victim to a
hospital ……

*EYE CONTACT:
      First check the victim for contact lenses and remove if present.  Flush
victim's eyes with water or normal saline solution for 20 to 30 minutes while ….

*INGESTION:
      DO NOT INDUCE VOMITING.  Volatile chemicals have a high risk of being
aspirated into the victim's lungs during vomiting which increases the medical ……


-SOURCES
 =======

*SOURCES:
 [015] Lewis, R.J., Sr. and R.L. Tatken, Eds.  Registry of Toxic Effects of
Chemical Substances.  On-line Ed.  National Institute for Occupational Safety
and Health.  Cincinnati, OH.  CY1400000. January 9, 1990.
….
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