ECHA
EUROPEAN CHEMICALS AGENCY

Poison Centres Notification Format

Part B: Developer's Guide to IUCLID Format

Version	Changes	
1.0	1st version	April 2018

Title: Poison Centres Notification Format Part B: Developer's Guide to IUCLID format

Reference: ECHA-18-H-09-EN
ISBN: 978-92-9020-534-0
Cat. Number: ED-01-18-464-EN-N
DOI: 10.2823/540354
Publ.date: April 2018
Language: EN

If you have questions or comments in relation to this document please send them (quote the reference and issue date) using the information request form. The information request form can be accessed via the Contact ECHA page at:
http://echa.europa.eu/contact

European Chemicals Agency

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland
Visiting address: Annankatu 18, Helsinki, Finland

Table of Contents

1. Introduction

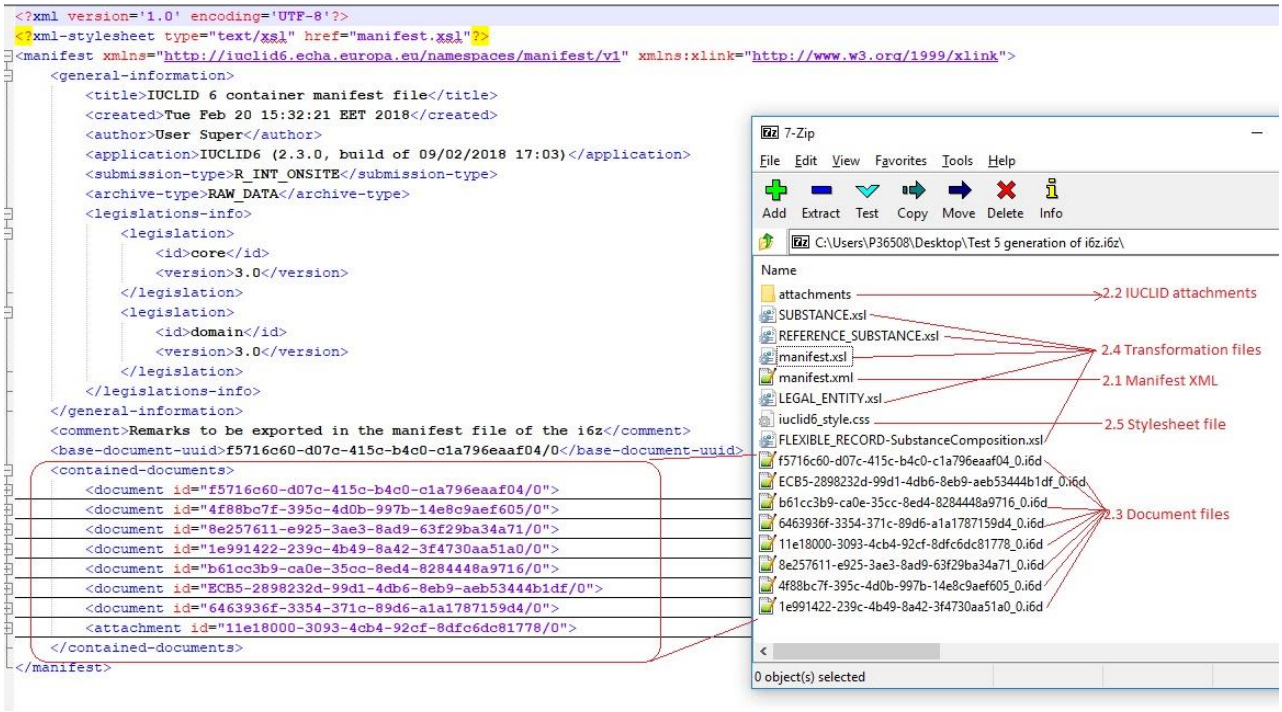
In IUCLID6, the exchange of chemical information (raw datasets or dossiers) is facilitated via a zip/archive file with the extension .i6z (IUCLID6 zip). The chemical information can be exported from one IUCLID6 installation and imported into another. This archive contains information concerning all (inter)related IUCLID6 entities (documents and attachments), in a well-defined and structured format. IUCLID6 provides a rather advanced filtering mechanism so the user could decide which interrelated entities to be excluded from the archive.

2. Content of i6z file

This section analyzes the contents of an i6z archive file in greater detail. An i6z file contains the following types of content:

- **manifest file (manifest.xml)**: A single XML file providing top-level metadata of the archive and summarizing the archive's contents.
- **IUCLID document files (*.i6d)**: IUCLID6 XML files including information about the IUCLID6 entities. By entities, we refer to:
  - documents: containing top-level information concerning the document along with the actual chemical information content;
  - attachments: containing metadata concerning the actual attachment content linked to the documents (directly or via its enclosing fields).
- **IUCLID attachments**: The actual content in its original format (.doc, .pdf, etc.) that is attached to the documents and placed under the **/attachments** directory.
- **eXtensible Stylesheet Language files (*.xsl)**: The files that describe how to display the XML content of IUCLID document into a human readable, HTML-based format via a web browser.
- **Stylesheet (iuclid6_style.css)**: A single .css file in order to customize the presentation of the HTML elements.

Each of the aforementioned types are further explained below. As a reference, please have a look at the following screenshot:



I6z mandatory contents

Exporting a dataset/dossier via IUCLID6 results in an .i6z archive that contains all the aforementioned types. However, import operation does **not** require the existence of the ***.xsl** and ***.css** files. In other words, these files are optional and could be omitted from the archive.

2.1 Manifest

All IUCLID 6 archives (i.e. i6z files) are meant to have **a manifest file describing their contents**. The *manifest.xml* file contains a table of contents of all data files that are available in the i6z file. It is important to notice what is included in the manifest and how the information is roughly split:

- **general-information**: section that describes the top-level information of the container file;
- **comment:** optional field that contains the user-defined text during the export operation of the specific dataset/dossier;
- **base-document**: The key of the document the export operation was initiated from;
- **contained-documents**: section listing the metadata of all the documents and attachments included in the archive.

2.1.1 Sample of manifest.xml

Manifest xml file for a Substance dataset
<?xml version='1.0' encoding='UTF-8'?> <?xml-stylesheet type="text/xsl" href="manifest.xsl"?>

```
<manifest xmlns="http://iuclid6.echa.europa.eu/namespaces/manifest/v1"
xmlns:xlink="http://www.w3.org/1999/xlink">
  <general-information>
    <title>IUCLID 6 container manifest file</title>
    <created>Tue Feb 20 15:32:21 EET 2018</created>
    <author>User Super</author>
    <application>IUCLID6 (2.3.0, build of 09/02/2018 17:03)</application>
    <submission-type>R_INT_ONSITE</submission-type>
    <archive-type>RAW_DATA</archive-type>
    <legislations-info>
      <legislation>
        <id>core</id>
        <version>3.0</version>
      </legislation>
      <legislation>
        <id>domain</id>
        <version>3.0</version>
      </legislation>
    </legislations-info>
  </general-information>
  <comment>Remarks to be exported in the manifest file of the i6z</comment>
  <base-document-uuid>f5716c60-d07c-415c-b4c0-c1a796eaaf04/0</base-document-uuid>
  <contained-documents>
    <document id="f5716c60-d07c-415c-b4c0-c1a796eaaf04/0">
      <type>SUBSTANCE</type>
      <name xlink:type="simple" xlink:href="f5716c60-d07c-415c-b4c0-c1a796eaaf04_0.i6d">Test substance for
checking the i6z</name>
      <first-modification-date>2018-02-20T09:09:17Z</first-modification-date>
      <last-modification-date>2018-02-20T11:16:53Z</last-modification-date>
      <uuid>f5716c60-d07c-415c-b4c0-c1a796eaaf04/0</uuid>
      <links>
        <link>
          <ref-uuid>4f88bc7f-395c-4d0b-997b-14e8c9aef605/0</ref-uuid>
          <ref-type>REQUIRED_LEGAL_ENTITY</ref-type>
        </link>
        <link>
          <ref-uuid>4f88bc7f-395c-4d0b-997b-14e8c9aef605/0</ref-uuid>
          <ref-type>REFERENCE</ref-type>
        </link>
        <link>
          <ref-uuid>8e257611-e925-3ae3-8ad9-63f29ba34a71/0</ref-uuid>
          <ref-type>REFERENCE</ref-type>
        </link>
      </links>
      <representation>
        <reference-substance>
          <name>25167-70-8      </name>
          <IUPAC-name>25167-70-8      </IUPAC-name>
          <CAS-number/>
          <inventory-number/>
        </reference-substance>
        <legal-entity>
          <name>Predefined Legal entity</name>
          <town/>
          <country/>
        </legal-entity>
      </representation>
```

```
    </document>
    <document id="4f88bc7f-395c-4d0b-997b-14e8c9aef605/0">
      <type>LEGAL_ENTITY</type>
      <name xlink:type="simple" xlink:href="4f88bc7f-395c-4d0b-997b-14e8c9aef605_0.i6d">Predefined Legal
entity</name>
      <first-modification-date>2017-12-18T10:01:44Z</first-modification-date>
      <last-modification-date>2017-11-15T11:19:39Z</last-modification-date>
      <uuid>4f88bc7f-395c-4d0b-997b-14e8c9aef605/0</uuid>
      <links/>
      <representation>
        <name>Predefined Legal entity</name>
        <town/>
        <country/>
      </representation>
    </document>
    <document id="8e257611-e925-3ae3-8ad9-63f29ba34a71/0">
      <type>REFERENCE_SUBSTANCE</type>
      <name xlink:type="simple" xlink:href="8e257611-e925-3ae3-8ad9-63f29ba34a71_0.i6d">25167-70-8
</name>
      <first-modification-date>2018-01-12T15:26:44Z</first-modification-date>
      <last-modification-date>2012-12-05T13:16:44Z</last-modification-date>
      <uuid>8e257611-e925-3ae3-8ad9-63f29ba34a71/0</uuid>
      <links/>
      <representation>
        <name>25167-70-8      </name>
        <IUPAC-name>25167-70-8      </IUPAC-name>
        <CAS-number/>
        <inventory-number/>
      </representation>
    </document>
    <document id="1e991422-239c-4b49-8a42-3f4730aa51a0/0">
      <type>FLEXIBLE_RECORD</type>
      <subtype>SubstanceComposition</subtype>
      <name xlink:type="simple" xlink:href="1e991422-239c-4b49-8a42-
3f4730aa51a0_0.i6d">Composition.001</name>
      <first-modification-date>2018-02-20T09:46:31Z</first-modification-date>
      <last-modification-date>2018-02-20T09:47:12Z</last-modification-date>
      <uuid>1e991422-239c-4b49-8a42-3f4730aa51a0/0</uuid>
      <links>
        <link>
          <ref-uuid>f5716c60-d07c-415c-b4c0-c1a796eaaf04/0</ref-uuid>
          <ref-type>CHILD</ref-type>
        </link>
        <link>
          <ref-uuid>b61cc3b9-ca0e-35cc-8ed4-8284448a9716/0</ref-uuid>
          <ref-type>REFERENCE</ref-type>
        </link>
        <link>
          <ref-uuid>ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df/0</ref-uuid>
          <ref-type>REFERENCE</ref-type>
        </link>
        <link>
          <ref-uuid>6463936f-3354-371c-89d6-a1a1787159d4/0</ref-uuid>
          <ref-type>REFERENCE</ref-type>
        </link>
      </links>
      <representation>
```

```
        <parent>
          <type>SUBSTANCE</type>
          <name>Test substance for checking the i6z</name>
        </parent>
        <reference-substance>
          <name>25167-70-8      </name>
          <IUPAC-name>25167-70-8      </IUPAC-name>
          <CAS-number/>
          <inventory-number/>
        </reference-substance>
        <legal-entity>
          <name>Predefined Legal entity</name>
          <town/>
          <country/>
        </legal-entity>
      </representation>
    </document>
    <document id="b61cc3b9-ca0e-35cc-8ed4-8284448a9716/0">
      <type>REFERENCE_SUBSTANCE</type>
      <name xlink:type="simple" xlink:href="b61cc3b9-ca0e-35cc-8ed4-8284448a9716_0.i6d">Automatically
generated during migration to IUCLID 6, no data available</name>
      <first-modification-date>2018-01-12T15:26:44Z</first-modification-date>
      <last-modification-date>2009-12-09T08:02:39Z</last-modification-date>
      <uuid>b61cc3b9-ca0e-35cc-8ed4-8284448a9716/0</uuid>
      <links/>
      <representation>
        <name>Automatically generated during migration to IUCLID 6, no data available</name>
        <IUPAC-name>Automatically generated during migration to IUCLID 6, no data available</IUPAC-name>
        <CAS-number/>
        <inventory-number/>
      </representation>
    </document>
    <document id="ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df/0">
      <type>REFERENCE_SUBSTANCE</type>
      <name xlink:type="simple" xlink:href="ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df_0.i6d">2,4,4-
trimethylpentene</name>
      <first-modification-date>2018-01-12T15:26:44Z</first-modification-date>
      <last-modification-date>2016-05-26T06:43:41Z</last-modification-date>
      <uuid>ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df/0</uuid>
      <links/>
      <representation>
        <name>2,4,4-trimethylpentene</name>
        <IUPAC-name>2,4,4-trimethylpentene</IUPAC-name>
        <CAS-number>25167-70-8</CAS-number>
        <inventory-number>246-690-9</inventory-number>
      </representation>
    </document>
    <document id="6463936f-3354-371c-89d6-a1a1787159d4/0">
      <type>REFERENCE_SUBSTANCE</type>
      <name xlink:type="simple" xlink:href="6463936f-3354-371c-89d6-a1a1787159d4_0.i6d">Mixed xylenes (in
hydrocarbons)</name>
      <first-modification-date>2018-01-12T15:26:44Z</first-modification-date>
      <last-modification-date>2015-03-04T09:04:48Z</last-modification-date>
      <uuid>6463936f-3354-371c-89d6-a1a1787159d4/0</uuid>
      <links/>
      <representation>
        <name>Mixed xylenes (in hydrocarbons)</name>
```

```
          <IUPAC-name>Mixed xylenes (in hydrocarbons)</IUPAC-name>
          <CAS-number/>
          <inventory-number/>
        </representation>
      </document>
      <attachment id="11e18000-3093-4cb4-92cf-8dfc6dc81778/0">
        <name xlink:type="simple" xlink:href="11e18000-3093-4cb4-92cf-8dfc6dc81778_0.i6d">Balsamiq Mockups
3.lnk</name>
        <first-modification-date>2018-02-20T11:16:48Z</first-modification-date>
        <last-modification-date>2018-02-20T11:16:48Z</last-modification-date>
        <uuid>11e18000-3093-4cb4-92cf-8dfc6dc81778/0</uuid>
        <container-uuid>f5716c60-d07c-415c-b4c0-c1a796eaaf04/0</container-uuid>
        <linked-attachments>
          <linked-doc xlink:type="simple"
xlink:href="attachments/070818f5e12266e6ac74bbf799bc15ae.lnk">Balsamiq Mockups 3.lnk</linked-doc>
        </linked-attachments>
      </attachment>
    </contained-documents>
</manifest>
```

2.1.2 <general-information> section

As already stated, this section contains the top-level information of the container file.

Element	Type	Description	Required
title	xs:string	The name that should be displayed as a first element, once opening the XML file via a web browser. For the time being, it is hardcoded to "IUCLID 6 container manifest file"	Yes
created	xs:string	The creation date of the i6z file	Yes
author	xs:string	The IUCLID user (i.e. concatenation of "First name " and "Last name") that created the i6z file	Yes
application	xs:string	It is by default "IUCLID6" and in a parenthesis the release version and build date/time are mentioned	Yes
submission-type	xs:string	The submission type of the dataset: • For the dossier it is extremely useful; • For raw datasets it is less useful; anyhow, choosing a submission type prior to exporting a raw dataset is mandatory, hence this information will exist.	Yes
archive-type	(RAW_DATA | DOSSIER_DATA | CHEMICAL_INVENTORY)	Indicates the type of the documents included in the archive	Yes

Element	Type	Description	Required
legislations-info	complexType: list(legislation)	Contains an optional list of **legislation** elements. This section mentions information relevant to the **IUCLID legislations**; in this section, the legislations that provide the documents (found within the i6z file) are listed. For instance, in the example mentioned above, the documents found within the respective i6z file are provided by two IUCLID legislations: CORE and DOMAIN.	Yes
→ legislation	complexType: sequence(id, version)	The name and version of the legislation provider whose at least one document is included in the archive	No
→ → id	xs:string	The name of the legislation provider	Yes
→ → version	xs:string	The version of the legislation provider	Yes

Below a sample of the **general-information** section

Example of <general-information> section

```
<general-information>
  <title>IUCLID 6 container manifest file</title>
  <created>Tue Feb 20 15:32:21 EET 2018</created>
  <author>User Super</author>
  <application>IUCLID6 (2.3.0, build of 09/02/2018 17:03)</application>
  <submission-type>R_INT_ONSITE</submission-type>
  <archive-type>RAW_DATA</archive-type>
  <legislations-info>
    <legislation>
      <id>core</id>
      <version>3.0</version>
    </legislation>
    <legislation>
      <id>domain</id>
      <version>3.0</version>
    </legislation>
  </legislations-info>
</general-information
```

2.1.3 <comment> section

This is an optional field that contains the user-defined text during the export operation of the specific dataset or dossier.

Example of <comments> section

```
<comment>Remarks to be exported in the manifest file of the i6z</comment>
```

2.1.4 2.1.4 <base-document-uuid> section

This field keeps the key of the document the export operation was initiated from. For additional information concerning the document key/identifier, see section 3.1 Document identification. The following cases should be mentioned:

1. Dossier export: the key of the dossier header <document_uuid>/<snapshot_uuid>;
2. Entity export: the key of the entity (substance, mixture, template, legal entity, reference substance, etc.) to be exported;
3. Document export: the key of the section document the export operation initiated from.

Example of <base-document> section

```
<base-document-uuid>f5716c60-d07c-415c-b4c0-c1a796eaaf04/0</base-document-uuid>
```

2.1.5 <contained-documents> section

As already stated, this section lists the metadata of all the documents and attachments included in the archive. It consists of a list of the following two subsection elements:

- document: This element contains the metadata and top-level information of all IUCLID6 documents included in the archive;
- attachment: This element contains the metadata of all the attachments included in the archive.

2.1.5.1 <document> subsection

Below an analysis of the attributes and elements included in the document subsection.

Element/Attribute	Type	Description	Required
@id	xs:string	The unique identifier of the document. See section 3.1 Document identification.	Yes

Element/Attribute	Type	Description	Required
type	xs:string - Eligible values are: • ANNOTATION • CATEGORY • DOSSIER • FIXED_RECORD • FLEXIBLE_RECORD • ENDPOINT_STUDY_RECORD • FLEXIBLE_SUMMARY • ENDPOINT_SUMMARY • ASSESSMENT_ENTITY • LEGAL_ENTITY • MIXTURE • REFERENCE_SUBSTANCE • SITE • CONTACT • LITERATURE • SUBSTANCE • TEMPLATE • TEST_MATERIAL_INFORMATION • INVENTORY • CUSTOM_ENTITY • CUSTOM_SECTION	The type of the *document*	Yes
subtype	xs:string	The subtype in case of section document. This information is not applicable for entity documents. *<type>.<subtype>* uniquely identify the section document type and represent the document definition identifier.	No
name	xs:string with two required attributes • xlink:type • xlink:href	It is the name of the document as specified by the user. The *xlink:href* attribute of the element specifies the name of the XML file (*.i6d) that contains the actual content of this document	No
first-modification-date	xs:dateTime	The date that the document was created	Yes

Element/Attribute	Type	Description	Required
last-modification-date	xs:dateTime	The last modification date of the document	Yes
uuid	xs:string	The unique identifier of the document. See section 3.1 Document identification.	Yes
links	linksType: list(link)	It contains a list of the documents that are referenced from/linked to the given document	No
→ link	complexType: sequence(ref-uuid, ref-type)	A single link between two documents	No
→ → ref-uuid	xs:string	The unique identifier of the document that is referenced from/linked to the given document	Yes
→ → ref-type	xs:string - Eligible values are: • PARENT • CHILD • REFERENCE • USES_TEMPLATE • REQUIRED_LEGAL_ENTITY • CATEGORY • ATTACHMENT • DOSSIER_SUBJECT • ANNOTATION	Specifies the type of the relationship between the given and the linked document	Yes

Element/Attribute	Type	Description	Required
representation	A complex element containing a sequence of the following optional elements: • subject-type • last-name • first-name • organisation • parent • reference-substance • name • town • country • legal-entity • IUPAC-name • CAS-number • inventory-number • title • author • reference-type	Additional metadata per document needed to produce the document's representation in the IUCLID 6 Swing UI. Not all elements are applicable for all document types. Only a subset of them are filled per case.	No

Manifest-document mandatory contents

The elements *links* and *representation* are used to facilitate the generation of an archive summary without the need to read/parse any document xml file (*.i6d).

Although per XSD definition, these elements are optional, the current IUCLID6.2 version requires their presence. Otherwise an error during import process occurs. Eventually, however, the mechanism will be updated to work without the existence of these elements.

Below an example of the **document** subsection under <contained-documents> section.

Example of <document> section under <<contained-documents>

```
<document id="1e991422-239c-4b49-8a42-3f4730aa51a0/0">
  <type>FLEXIBLE_RECORD</type>
  <subtype>SubstanceComposition</subtype>
  <name xlink:type="simple" xlink:href="1e991422-239c-4b49-8a42-
3f4730aa51a0_0.i6d">Composition.001</name>
  <first-modification-date>2018-02-20T09:46:31Z</first-modification-date>
  <last-modification-date>2018-02-20T09:47:12Z</last-modification-date>
  <uuid>1e991422-239c-4b49-8a42-3f4730aa51a0/0</uuid>
  <links>
    <link>
      <ref-uuid>f5716c60-d07c-415c-b4c0-c1a796eaaf04/0</ref-uuid>
      <ref-type>CHILD</ref-type>
    </link>
    <link>
      <ref-uuid>b61cc3b9-ca0e-35cc-8ed4-8284448a9716/0</ref-uuid>
      <ref-type>REFERENCE</ref-type>
    </link>
    <link>
      <ref-uuid>ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df/0</ref-uuid>
      <ref-type>REFERENCE</ref-type>
```

```
    </link>
    <link>
      <ref-uuid>6463936f-3354-371c-89d6-a1a1787159d4/0</ref-uuid>
      <ref-type>REFERENCE</ref-type>
    </link>
  </links>
  <representation>
    <parent>
      <type>SUBSTANCE</type>
      <name>Test substance for checking the i6z</name>
    </parent>
    <reference-substance>
      <name>25167-70-8</name>
      <IUPAC-name>25167-70-8</IUPAC-name>
      <CAS-number/>
      <inventory-number/>
    </reference-substance>
    <legal-entity>
      <name>Predefined Legal entity</name>
      <town/>
      <country/>
    </legal-entity>
  </representation>
</document>
```

2.1.5.2 <attachment> subsection

Below an analysis of the attributes and elements included in the attachment subsection.

Element/Attribute	Type	Description	Required
@id	xs:string	The unique identifier of the attachment. See section 3.1 Document identification.	Yes
name	xs:string with two required attributes • xlink:type • xlink:href	It is the name of the document as specified by the user. The *xlink:href* attribute of the element specifies the name of the XML file (*.i6d) that contains the actual content of this document	No
first-modification-date	xs:dateTime	The date that the attachment was created	Yes
last-modification-date	xs:dateTime	The last modification date of the attachment	Yes
uuid	xs:string	The unique identifier of the attachment. See section 3.1 Document identification.	Yes
container-uuid	xs:string	The unique identifier of the document the attachment is linked to	Yes

Element/Attribute	Type	Description	Required
linked-attachments	list(linked-doc)		No
→ linked-doc	xs:string with two required attributes • xlink:type • xlink:href	The name of the attachment. The *xlink:href* attribute specifies the actual attachment content file under the **attachments** directory	No

Below an example of the **attachment** subsection under <contained-documents> section.

Example of <attachment> section under <contained-documents>

```
<attachment id="ECB5-d3a3b15d-d83f-4b21-acc9-001c31505c6d/0">
  <name xlink:type="simple" xlink:href="ECB5-d3a3b15d-d83f-4b21-acc9-001c31505c6d_0.i6d">110-54-3-V2.jpeg</name>
  <first-modification-date>2017-10-06T13:08:00Z</first-modification-date>
  <last-modification-date>2017-10-06T13:08:00Z</last-modification-date>
  <uuid>ECB5-d3a3b15d-d83f-4b21-acc9-001c31505c6d/0</uuid>
  <container-uuid>ECB5-27a8cb0b-5cb5-4ab8-ac18-4eab59415f7f/0</container-uuid>
  <linked-attachments>
    <linked-doc xlink:type="simple" xlink:href="attachments/e3cde6b1d8fba4ac4ce414ebe9610ccf.jpeg">110-54-3-V2.jpeg</linked-doc>
  </linked-attachments>
</attachment>
```

2.2 IUCLID Attachment files

As already stated, the XML documents (.i6d) contain metadata information about the attachments included in the archive. Below an analysis of the attributes and elements included in the **Attachment** element inside the attachment-related .i6d files.

Element/Attribute	Type	Description	Required
documentKey	xs:string	The unique identifier of the attachment. See section 3.1 Document identification.	Yes
name	xs:string	It is the name of the uploaded attachment	Yes
creationDate	xs:dateTime	The date that the attachment was created	Yes
lastModificationDate	xs:dateTime	The last modification date of the attachment	Yes
remarks	xs:string	The remarks provided by the user during the attachment uploading	No

Element/Attribute	Type	Description	Required
md5	xs:string	The MD5 hash of the uploaded attachment content	Yes
mimetype	xs:string	The media type of the attachment content	No
content	xs:string with two required attributes • xlink:type • xlink:href	The name/location of the attachment binary under the "**attachments**"	Yes

Below an example of the **Attachment** subsection under <contained-documents> section.

Example of <attachment> section under <contained-documents>

```
<?xml version='1.0' encoding='UTF-8'?>
<Attachment xmlns="http://iuclid6.echa.europa.eu/namespaces/platform-attachment/v1"
xmlns:xlink="http://www.w3.org/1999/xlink" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <documentKey>ECB5-65104712-25bd-4366-bbd6-2d085a0c4eb3/0</documentKey>
  <name>108-88-3-V2.jpeg</name>
  <creationDate>2017-10-06T21:08:00.675+08:00</creationDate>
  <lastModificationDate>2017-10-06T21:08:00.675+08:00</lastModificationDate>
  <md5>8c930da8a8967b53dc73b919a2309c1b</md5>
  <mimetype>image/jpeg</mimetype>
  <content xlink:href="attachments/8c930da8a8967b53dc73b919a2309c1b.jpeg" xlink:type="simple"/>
</Attachment>
```

2.3 IUCLID Document files

Besides attachments, there are also XML-based documents (.i6d) that contain top-level information concerning the IUCLID6 document along with the document's actual chemical information content. The name of the i6d file is based on the document identifier that is <document_uuid>_<snapshot_uuid>.i6d. In case this is a raw document, and not part of a dossier, the **snapshot_uuid = 0**

Below an analysis of the elements included in the **Document** element within the document-related .i6d files.

- **PlatformMetadata:** section that contains the top-level information of a IUCLID6 document such as document identifier, name, type and subtype, etc;
- **Content:** section that contains the chemical information of the specific document;
- **Attachments:** section that lists the attachments that are directly linked to the document;
- **ModificationHistory:** section that lists the entries of the document's modification history.

2.3.1 <PlatformMetadata> section

Element	Type	Description	Required
iuclidVersion	xs:string	The current IUCLID version used for exporting the .i6z archive	Yes
documentKey	xs:string	The unique identifier of the document. See section 3.1 Document identification.	Yes
documentType	xs:string - Eligible values are: • ANNOTATION • CATEGORY • DOSSIER • FIXED_RECORD • FLEXIBLE_RECORD • ENDPOINT_STUDY_RECORD • FLEXIBLE_SUMMARY • ENDPOINT_SUMMARY • ASSESSMENT_ENTITY • LEGAL_ENTITY • MIXTURE • REFERENCE_SUBSTANCE • SITE • CONTACT • LITERATURE • SUBSTANCE • TEMPLATE • TEST_MATERIAL_INFORMATION • INVENTORY • CUSTOM_ENTITY • CUSTOM_SECTION	The type of the document	Yes
definitionVersion	xs:string	The definition version of the exported document. This value: • indicates that the content section follows the document format of the specified version' • during import operation, this value drives the resolution of the proper document's .xsd to run the validation with.	Yes
creationDate	xs:dateTime	The date that the document was created	Yes

Element	Type	Description	Required
lastModificationDate	xs:dateTime	The last modification date of the document	Yes
name	xs:string	It is the name of the document as specified by the user.	Yes
documentSubType	xs:string	The subtype in case of section document. This information is not applicable for entity documents. *<type>.<subtype>* uniquely identify the section document type and represent the document definition identifier.	Yes
parentDocumentKey	xs:string	In case this document is a section document, this element keeps the unique identifier of its parent document. See section 3.1 Document identification.	Yes
orderInSectionNo	xs:nonNegativeInteger	In case this is a section document, the order of the document with the specific definition identifier (type, subtype) under the provided parent entity	Yes
submissionType	xs:string	Applicable only for dossier archives. Indicates the submission type used during dossier generation. The value is specified in case the XML concerns: • the dossier document • the composite documents (SUBSTANCE/MIXTURE) under the dossier with a submission type different than the one of the dossier document	Yes

Element	Type	Description	Required
submissionTypeVersion	xs:string	The version of the submission type used to generate the dossier for	Yes
submittingLegalEntity	xs:string	The legal entity document identifier that originated the dossier creation	Yes
dossierSubject	xs:string	In case this is the dossier document, it contains the document key (unique identifier) of the dossier subject document (SUBSTANCE, MIXTURE, CATEGORY) which is the document the dossier was created from	Yes
i5Origin	xs:boolean	Flag indicating whether this document originated from a IUCLID5 instance and migrated to the current IUCLID6 format or not	Yes
creationTool	xs:string	Element that specifies the application this document was first created with. Default value "IUC6" should be provided for IUCLID6-documents	Yes
snapshotCreationTool	xs:string	In case of dossier archive, element that specifies the application this dossier was created from. Upon dossier creation this is filled in with "IUC6"	Yes

Below an example of the **PlatformMetadata** subsection.

XML example of <platform metadata> section of a DOSSIER HEADER document

```
<i6c:PlatformMetadata xmlns:i6m="http://iuclid6.echa.europa.eu/namespaces/platform-metadata/v1"
xsi:schemaLocation="http://iuclid6.echa.europa.eu/namespaces/platform-container/v1 platform-container.xsd">
  <i6m:iuclidVersion>2.5.0</i6m:iuclidVersion>
  <i6m:documentKey>98051ac9-53d0-45b0-acae-42c28665de54/98051ac9-53d0-45b0-acae-
42c28665de54</i6m:documentKey>
  <i6m:parentDocumentKey/>
  <i6m:name/>
  <i6m:documentType>DOSSIER</i6m:documentType>
  <i6m:documentSubType>R_1-10_PC</i6m:documentSubType>
  <i6m:orderInSectionNo/>
```

```
  <i6m:definitionVersion>3.0</i6m:definitionVersion>
  <i6m:creationDate>2018-03-09T12:22:55Z</i6m:creationDate>
  <i6m:lastModificationDate>2018-03-09T12:22:55Z</i6m:lastModificationDate>
  <i6m:submissionType>R_1-10_PC</i6m:submissionType>
  <i6m:submissionTypeVersion>reach 3.0</i6m:submissionTypeVersion>
  <i6m:submittingLegalEntity/>
  <i6m:dossierSubject>50672294-fceb-4ff4-9321-bc19c1bc9224/98051ac9-53d0-45b0-acae-
42c28665de54</i6m:dossierSubject>
  <i6m:i5Origin>false</i6m:i5Origin>
  <i6m:creationTool>IUC6</i6m:creationTool>
  <i6m:snapshotCreationTool>IUC6</i6m:snapshotCreationTool>
</i6c:PlatformMetadata>
```

2.3.2 <Content> section

This section contains the chemical information of the specific document. At this point, we should describe in short the key concepts of IUCLID6 document types and structure. In IUCLID6 every structure that keeps chemical information is called document. There are the following type of documents:

- Entity: This is a top-level document without temporal or other dependencies to other documents. Examples are: ANNOTATION, CATEGORY, LEGAL_ENTITY, MIXTURE, REFERENCE_SUBSTANCE, SITE, CONTACT, LITERATURE, SUBSTANCE, TEMPLATE, TEST_MATERIAL_INFORMATION. A sub-category of the entities is the composite entities that refer to documents, which hold additional children documents underneath. Examples of composite entities are: SUBSTANCE, MIXTURE, TEMPLATE.
- Section: This document lives only under a composite entity and can be any of the following types: FIXED_RECORD, FLEXIBLE_RECORD, ENDPOINT_STUDY_RECORD, FLEXIBLE_SUMMARY, ENDPOINT_SUMMARY. The section documents are further categorized based on the kind of information they hold. The extra categorization is described by the document subtype.

Every document, entity or section, has a specific and well-defined structure. This hierarchical, tree-based data structure consists of the following nodes:

- root: the document itself
- leaf: the document fields of the various types. IUCLID6 supports numerous data types, primitives and composite. The data types are:
    - Text
    - Picklist (single/multiple)
    - Physical quantity
    - Physical quantity range
    - Data protection / confidentiality
    - Attachments (single/multiple)
    - Address
    - Boolean
    - Date
    - Number
    - Document reference (single/multiple)
    - Section types

- internal nodes: the blocks that specify a set of fields or nested blocks (blocks inside blocks) under a specific header. This header acts as an aggregator of related chemical information. There are two types of blocks:
    - single blocks: a block with a single occurrence per document. This block can be uniquely identified by its path
    - repeatable blocks: a block with an unbounded number of occurrences. These blocks have the same document path and exist multiple times so to uniquely identify them, there are assigned with block identifiers. See section 3.1 Document identification.

Every node has a type/identifier. The identifier of the root node is the concatenation of its document type/subtype information. By node path we mean the location of the node inside the tree. Its value is the concatenation of all the identifiers from the root node up to the node itself.

The **Content** section contains the XML-based representation of the hierarchical document structure where leaf elements provide the values of the document fields and internal nodes are blocks consisting of other fields or nested blocks. There is a standard XML representation of the composite field elements. In case of repeatable blocks, the **UUID** attribute is utilized to uniquely identify the block inside the document.

An example that illustrates the XML format for a document definition is given below. Let's consider the following sample endpoint study record, which contains a single and a repeatable block, each containing various types of fields:

- ENDPOINT_STUDY_RECORD.Density
    - AdministrativeData: single block
        - DataProtection: data protection field
        - Endpoint: picklist field
        - AttachedJustification: repeatable block
            - AttachedJustification: attachment field
            - ReasonPurspose: picklist field

XML example for ENDPOINT_STUDY_RECORD.Density

```
<i6c:Content>
  <ENDPOINT_STUDY_RECORD.Density
xmlns="http://iuclid6.echa.europa.eu/namespaces/ENDPOINT_STUDY_RECORD-Density/2.0"
xmlns:i6="http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1">
    <AdministrativeData>
      <DataProtection>
        <i6:confidentiality/>
        <i6:justification>Justification_text</i6:justification>
      </DataProtection>
      <Endpoint>
        <i6:value>2311</i6:value>
        <i6:remarks>REMARKS_ENDPOINT_STUDY_RECORD.Density.AdministrativeData.Endpoint</i6:remarks>
      </Endpoint>
      …
      <AttachedJustification>
        <entry i6:uuid="66687d92-2220-4b95-9b21-61cc692a9a8c">
          <AttachedJustification>599777e4-6619-4863-bb1f-02cd2dc913fc/3cfc96de-e097-4b1d-a7ac-
39b1d108593d</AttachedJustification>
          <ReasonPurpose>
```

```
            <i6:value>60006</i6:value>

<i6:remarks>REMARKS_ENDPOINT_STUDY_RECORD.Density.AdministrativeData.AttachedJustification.ReasonPurpose</i6:remarks>
          </ReasonPurpose>
        </entry>
        <entry i6:uuid="74f0fafb-aaee-49ab-853c-3de1da94ab5d">
          <AttachedJustification>7424406b-eb1a-4ccf-a625-ea272a106d2d/3cfc96de-e097-4b1d-a7ac-39b1d108593d</AttachedJustification>
          <ReasonPurpose>
            <i6:value>60010</i6:value>

<i6:remarks>REMARKS_ENDPOINT_STUDY_RECORD.Density.AdministrativeData.AttachedJustification.ReasonPurpose</i6:remarks>
          </ReasonPurpose>
        </entry>
        <entry i6:uuid="9c8425c5-7630-494d-9f63-99d98ad6ae75">
          <AttachedJustification>396555fa-795b-461c-b83d-a297830f3726/3cfc96de-e097-4b1d-a7ac-39b1d108593d</AttachedJustification>
          <ReasonPurpose>
            <i6:value>60009</i6:value>

<i6:remarks>REMARKS_ENDPOINT_STUDY_RECORD.Density.AdministrativeData.AttachedJustification.ReasonPurpose</i6:remarks>
          </ReasonPurpose>
        </entry>
      </AttachedJustification>
      ...
    ...
  </ENDPOINT_STUDY_RECORD.Density>
</i6c:Content>
```

Important notes

It should be highlighted that:

- The content of this section depends on the definition format of the document under the specific version. The structure of the example contains the sequence of fields as specified for document ENDPOINT_STUDY_RECORD.Density in IUCLID6.1 version;
- During export, the generated XML documents (*.i6d) contain the full document structure (all fields and blocks) regardless of whether a value is specified or not.

During import, an XSD-based validation verifies that the structure of the i6d document of the specific version is the correct one that means that the sequence of elements is the expected one and all field values match the XSD-defined types.

2.3.3 <Attachments> section

Section that lists the attachments that are directly linked to the document. The content of this section is an unbounded list of references to attachment identifiers that this document is linked to.

The following example indicates that there is an attachment with identifier **b9800746-5007-3ad7-b2c8-cd8a544bbdf9/0** that is directly linked to this document. By directly, we mean that this content is directly linked to the document itself and not included in any of the document's fields.

XML example of <Attachments> section

```
<i6c:Attachments xmlns:i6a="http://iuclid6.echa.europa.eu/namespaces/platform-attachment/v1"
xsi:schemaLocation="http://iuclid6.echa.europa.eu/namespaces/platform-attachment/v1 platform-
attachment.xsd">
  <i6a:AttachmentRef>b9800746-5007-3ad7-b2c8-cd8a544bbdf9/0</i6a:AttachmentRef>
</i6c:Attachments>
```

2.3.4 <ModificationHistory> section

This section lists the entries of the document's modification history. Every entry is a single operation that took place on the specific document and specifies the date of the action, the user that run the action, the submitting legal entity of the user and the modification remarks if any**.**

Element	Type	Description	Required
Date	xs:dateTime	The date the action was performed on the document	Yes
Author	xs:string	The userName of the user that performed the modification	Yes
LegalEntity	xs:string	The description of the submitting legal entity of the user. This information contains the concatenated value of the LE name, city and localized country information	Yes
Remarks	xs:string	The modification comment	Yes

Below a sample of the modification history section.

XML example of < ModificationHistory > section

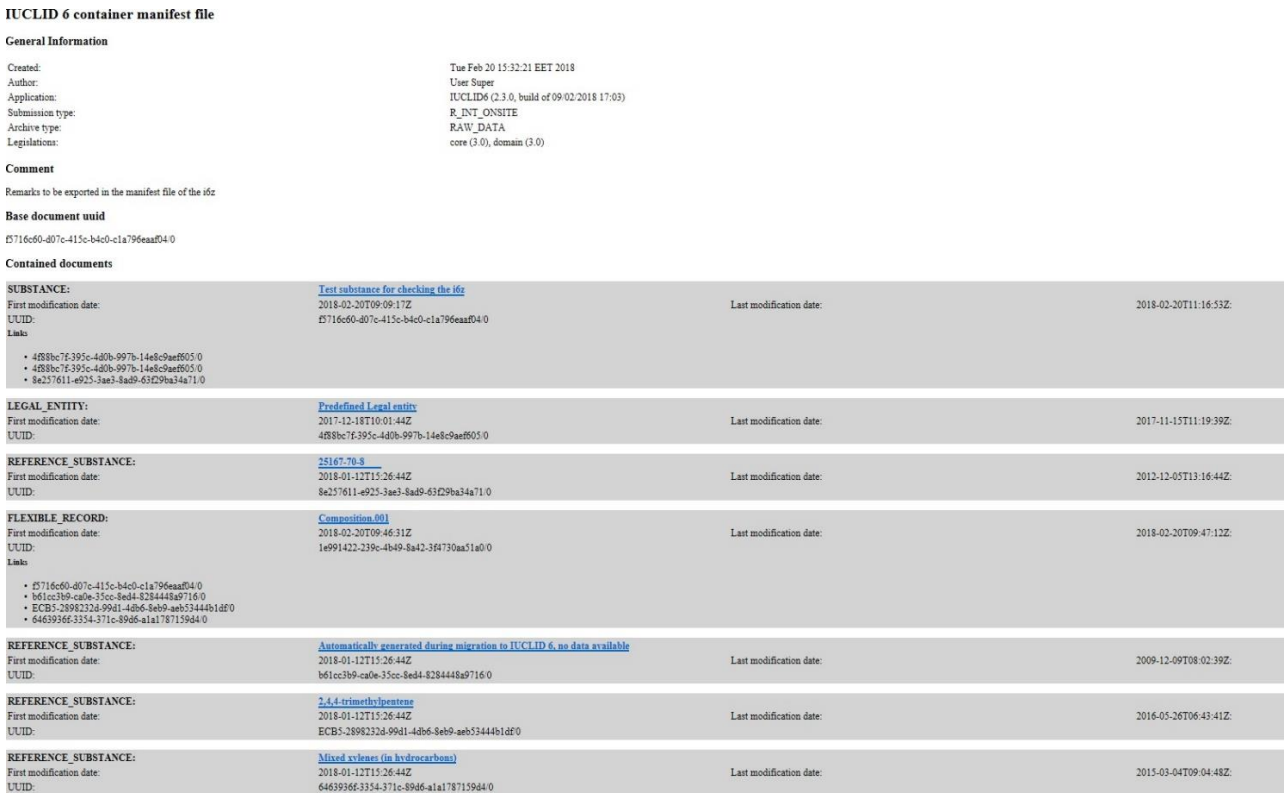
```
<i6c:ModificationHistory xmlns:i6h="http://iuclid6.echa.europa.eu/namespaces/platform-modification-history/v1"
xsi:schemaLocation="http://iuclid6.echa.europa.eu/namespaces/platform-modification-history/v1 platform-
modification-history.xsd">
  <i6h:Modification>
    <i6h:Date>2017-12-15T10:59:18Z</i6h:Date>
    <i6h:Author>MuylaertJoris</i6h:Author>
    <i6h:LegalEntity>Folat B.V. / Haarlem / Netherlands</i6h:LegalEntity>
    <i6h:Remarks/>
  </i6h:Modification>
  <i6h:Modification>
    <i6h:Date>2017-12-15T10:59:09Z</i6h:Date>
    <i6h:Author>MuylaertJoris</i6h:Author>
    <i6h:LegalEntity>Folat B.V. / Haarlem / Netherlands</i6h:LegalEntity>
    <i6h:Remarks/>
```

```
    </i6h:Modification>
    <i6h:Modification>
      <i6h:Date>2017-12-15T10:58:38Z</i6h:Date>
      <i6h:Author>MuylaertJoris</i6h:Author>
      <i6h:LegalEntity>Folat B.V. / Haarlem / Netherlands</i6h:LegalEntity>
      <i6h:Remarks>Created</i6h:Remarks>
    </i6h:Modification>
</i6c:ModificationHistory>
```

2.4 Transformation files of IUCLID documents (i.e. XSL files)

There is a business need, to be able to **open** an I6Z archive and **browse** its contents **without** necessarily importing it in an IUCLID 6 installation. The solution to this scenario revolves around using XSLs and viewing the archive contents on a browser.

For example, the *manifest.xsl* combined with the *manifest.xml* should be accessible in human readable format via a web browser. Via the use of a stylesheet (i.e. CSS file), the outcome of the *manifest.xml* looks like the following mock-up.



IUCLID 6 container manifest file

General Information

Created:	Tue Feb 20 15:32:21 EET 2018
Author:	User Super
Application:	IUCLID6 (2.3.0, build of 09/02/2018 17:03)
Submission type:	R_INT_ONSITE
Archive type:	RAW_DATA
Legislations:	core (3.0), domain (3.0)

Comment

Remarks to be exported in the manifest file of the i6z

Base document uuid

f5716c60-d07c-415c-b4c0-c1a796eaaf04/0

Contained documents

SUBSTANCE:	Test substance for checking the i6z		
First modification date:	2018-02-20T09:09:17Z	Last modification date:	2018-02-20T11:16:53Z:
UUID:	f5716c60-d07c-415c-b4c0-c1a796eaaf04/0		
Links			
• 4f88bc7f-395c-4d0b-997b-14e8c9aef605/0 • 4f88bc7f-395c-4d0b-997b-14e8c9aef605/0 • 8e257611-e925-3ae3-8ad9-63f29ba34a71/0			
LEGAL_ENTITY:	Predefined Legal entity		
First modification date:	2017-12-18T10:01:44Z	Last modification date:	2017-11-15T11:19:39Z:
UUID:	4f88bc7f-395c-4d0b-997b-14e8c9aef605/0		
REFERENCE_SUBSTANCE:	25167-70-8		
First modification date:	2018-01-12T15:26:44Z	Last modification date:	2012-12-05T13:16:44Z:
UUID:	8e257611-e925-3ae3-8ad9-63f29ba34a71/0		
FLEXIBLE_RECORD:	Composition 001		
First modification date:	2018-02-20T09:46:31Z	Last modification date:	2018-02-20T09:47:12Z:
UUID:	1e991422-239c-4b49-8a42-3f4730aa51a0/0		
Links			
• f5716c60-d07c-415c-b4c0-c1a796eaaf04/0 • b61cc3b9-ca0e-35cc-8ed4-8284448a9716/0 • ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df/0 • 6463936f-3354-371c-89d6-a1a178159d4/0			
REFERENCE_SUBSTANCE:	Automatically generated during migration to IUCLID 6, no data available		
First modification date:	2018-01-12T15:26:44Z	Last modification date:	2009-12-09T08:02:39Z:
UUID:	b61cc3b9-ca0e-35cc-8ed4-8284448a9716/0		
REFERENCE_SUBSTANCE:	2,4,4-trimethylpentene		
First modification date:	2018-01-12T15:26:44Z	Last modification date:	2016-05-26T06:43:41Z:
UUID:	ECB5-2898232d-99d1-4db6-8eb9-aeb53444b1df/0		
REFERENCE_SUBSTANCE:	Mixed xylenes (in hydrocarbons)		
First modification date:	2018-01-12T15:26:44Z	Last modification date:	2015-03-04T09:04:48Z:
UUID:	6463936f-3354-371c-89d6-a1a178159d4/0		

2.5 Stylesheet (i.e. CSS file)

As mentioned above, a CSS file is used as a stylesheet for displaying an XML file (via a web browser) in a human readable format.

3. Hints for developers

3.1 Document identification

A textual key is utilized to uniquely identify IUCLID6 documents and attachments. In the IUCLID6 domain, this structure is called **DocumentKey** and its format is **<document_uuid>/<snapshot_uuid>**

- document_uuid: It is the unique identifier of the document or attachment
- snapshot_uuid: Indicates the UUID of the dossier that the document or attachment belongs to. If the document is not yet part of the dossier, which means it is a **raw** and editable document, then the **snapshot_uuid = 0**

The content of every subpart is a **universally unique identifier** (**UUID**) being a 128-bit number. In its canonical textual representation, the UUID is represented as 32 hexadecimal (base 16) digits, displayed in five groups separated by hyphens, in the form `8-4-4-4-12` for a total of 36 characters (32 alphanumeric characters and four hyphens).

☞ For additional information, please check Universally unique identifier - wikipedia and RFC 4122: A Universally Unique IDentifier (UUID) URN Namespace.

Finally, the information concerning the application this document originated from is stored in the corresponding metadata elements **creationTool** and **snapshotCreationTool**.

Below, a code snippet for UUID generation.

UUID generation

```
java.util.UUID.randomUUID().toString();
```

3.2 Block identification

IUCLID6 domain also contains blocks. A block is a collection of elements (fields or blocks) defined under this block's path. There are two types of blocks:

1. Single block: A block with maximum one occurrence in the document context
2. Repeatable block: A block with multiple occurrences within the same document

Single blocks are uniquely identified per document via its path. Repeatable blocks however have the same path so they are assigned with UUID identifiers. The identifier does not follow the document identification pattern so there is no snapshot_uuid kept in the block entries.

In the sample of the exported document below, one can see that every entry of a repeatable block contains the UUID identifier.

Repeatable block identification

```
<i6c:Content>
  <ENDPOINT_STUDY_RECORD.Density
xmlns="http://iuclid6.echa.europa.eu/namespaces/ENDPOINT_STUDY_RECORD-Density/3.0"
xmlns:i6="http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1">
```

```
<!-- Single block -->
<AdministrativeData>
  ...
  <!-- Repeatable block -->
  <AttachedJustification>
    <entry i6:uuid="66687d92-2220-4b95-9b21-61cc692a9a8c">
      ...
    </entry>
    <entry i6:uuid="74f0fafb-aaee-49ab-853c-3de1da94ab5d">
      ...
    </entry>
  </AttachedJustification>
```

3.3 Cross-referencing XML documents

As already specified, an i6z archive includes a single **manifest.xml** file. This file provides some top-level metadata of the archive along with metadata of the documents and attachments included in the archive.

One of the main metadata information is the reference to the XML document (.i6d) that contains the actual document content. Check below:

Referencing XML documents

```
<document id="fb199594-8b87-426b-a21d-eac5f1c930a9/3cfc96de-e097-4b1d-a7ac-39b1d108593d">
  ...
  <name xlink:type="simple" xlink:href="fb199594-8b87-426b-a21d-eac5f1c930a9_3cfc96de-e097-4b1d-a7ac-39b1d108593d.i6d">DSD - DPD.001</name>
  ...
```

Similar for the reference to the XML attachment information (.i6d):

Referencing XML attachments

```
<attachment id="96072c4b-bb63-4d24-81f5-53747ddb7e3c/3cfc96de-e097-4b1d-a7ac-39b1d108593d">
  <name xlink:type="simple" xlink:href="96072c4b-bb63-4d24-81f5-53747ddb7e3c_3cfc96de-e097-4b1d-a7ac-39b1d108593d.i6d">Excel-icon.jpg</name>
  ...
</attachment>
```

As already indicated, XLink (*XML Linking Language*) is used to create hyperlinks within XML documents. This is the official W3C solution for XML linking.

XLink defines a set of attributes that may be added to elements of other XML namespaces. To get access to the XLink features, the XLink namespace must be declared at the top of the manifest document (xmlns:xlink="http://www.w3.org/1999/xlink")

The **xlink:type="simple"** attribute creates a simple "HTML-like" link

The **xlink:href** attribute specifies the URL to link to. In our case, this is the .i6d XML document that contains the document or attachment content.

3.4 Null or empty-value fields

An i6z archive should contain documents specifying only the fields with actual content; null or empty-value fields should be omitted.

If a required field is missing from the XML document, the proper XSD validation error will be thrown.

3.5 Multilingual support

IUCLID6 supports multilingual content (in its latest version). All fields that include any kind of textual information have been modified to accept content in multiple languages. The affected fields are:

1. Text fields
2. Picklist fields (with and without remarks)
3. Data protection fields
4. Physical quantity fields
5. Physical quantity range fields

Except of the Text field that is a single-value field, all other fields are composite and consist of multiple subfields. For example the picklist field contains textual information on the **"other"** and **"remarks"** subfields. The physical quantity and quantity range fields consist, among others, of a picklist field so the "other" textual subfield is also present.

From the XML point of view, the implemented approach is to allow multiple occurrences of the same textual field/subfield. In addition to that, any multilingual field, could optionally contain the **@xml:lang** attribute that specifies the language and (optional) locale of the element content. The `@xml:lang` attribute is described in the XML Recommendation. Note that the recommended style for the `@xml:lang` attribute is lowercase language and (optional) uppercase, separated by a hyphen, for example, "en-US" or "sp-SP" or "fr".

Below some examples of the content of the multilingual fields.

Multilingual XML content

```
<!-- Text field -->
<JustificationForTypeOfInformation>this is the default text</JustificationForTypeOfInformation>
<JustificationForTypeOfInformation xml:lang="en">This is the english text</JustificationForTypeOfInformation>
<JustificationForTypeOfInformation xml:lang="it">This is the italian text</JustificationForTypeOfInformation>

<!-- Single picklist field -->
<StudyResultType>
   <i6:value>1342</i6:value>
   <i6:other>this is the default other text</i6:other>
   <i6:other xml:lang="en">This is the english other text</i6:other>
   <i6:other xml:lang="it">This is the italian other text</i6:other>
   <i6:remarks>this is the default remarks</i6:remarks>
   <i6:remarks xml:lang="en">This is the english remarks text</i6:remarks>
   <i6:remarks xml:lang="it">This is the italian remarks text</i6:remarks>
</StudyResultType>

<!-- Multiple picklist field -->
<SpecificSubmissions>
```

```
   <RegulatoryProgramme>
      <i6:value>209</i6:value>
      <i6:remarks>this is the default remarks</i6:remarks>
   </RegulatoryProgramme>
   <RegulatoryProgramme>
      <i6:value>210</i6:value>
      <i6:remarks>this is the default remarks</i6:remarks>
      <i6:remarks xml:lang="en">This is the english remarks text</i6:remarks>
      <i6:remarks xml:lang="it">This is the italian remarks text</i6:remarks>
   </RegulatoryProgramme>
</SpecificSubmissions>

<!-- Physical quantity field -->
<Conc>
   <unitCode>1342</unitCode>
   <unitOther>this is the default text</unitOther>
   <unitOther xml:lang="en">This is the english text</unitOther>
   <unitOther xml:lang="it">This is the italian text</unitOther>
   <value>1</value>
</Conc>

<!-- Physical quantity range field -->
<Tension>
   <i6:unitCode>1342</i6:unitCode>
   <i6:unitOther>this is the default text</i6:unitOther>
   <i6:unitOther xml:lang="en">This is the english other text</i6:unitOther>
   <i6:unitOther xml:lang="it">This is the italian other text</i6:unitOther>
   <i6:lowerQualifier>&gt;</i6:lowerQualifier>
   <i6:upperQualifier>&lt;</i6:upperQualifier>
   <i6:lowerValue>1</i6:lowerValue>
   <i6:upperValue>2</i6:upperValue>
</Tension>

<!-- Data protection field -->
<DataProtection>
   <i6:confidentiality>3441</i6:confidentiality>
   <i6:justification>this is the default justification text</i6:justification>
   <i6:justification xml:lang="en">This is the english justification text</i6:justification>
   <i6:justification xml:lang="it">This is the italian justification text</i6:justification>
   <i6:legislation>
      <i6:value>1342</i6:value>
      <i6:other>other legislation text</i6:other>
      <i6:other xml:lang="en">This is the english other text</i6:other>
      <i6:other xml:lang="it">This is the italian other text</i6:other>
   </i6:legislation>
</DataProtection>
```

Below some examples of the XSDs concerning multilingual fields. Please note that all the multilingual complexTypes assigned to the document fields are specified inside **platform-fields.xsd** and declared under the http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1 namespace. That is the reason of the i6 prefix when specifying these elements at the XML document as shown above.

Multilingual XSD content

```
<!-- Text field -->
<xs:element name="JustificationForTypeOfInformation" minOccurs="1" maxOccurs="unbounded"
type="i6:multiLingualTextFieldLarge"/>

<!-- Single picklist field -->
<xs:element name="StudyResultType" type="i6:multiLingualPicklistFieldWithSmallTextRemarks"/>
<xs:complexType name="multiLingualPicklistFieldWithSmallTextRemarks">
  <xs:complexContent>
    <xs:restriction base="picklistFieldWithSmallTextRemarks">
      <xs:sequence>
        <xs:element name="value" minOccurs="0" type="textFieldSmall" />
        <xs:element name="other" minOccurs="0" maxOccurs="unbounded" type="multiLingualTextFieldSmall" />
        <xs:element name="remarks" minOccurs="0" maxOccurs="unbounded"
type="multiLingualTextFieldSmall"/>
      </xs:sequence>
    </xs:restriction>
  </xs:complexContent>
</xs:complexType>

<!-- Multiple picklist field -->
<xs:element name="RegulatoryProgramme" minOccurs="0" maxOccurs="unbounded"
type="i6:multiLingualPicklistFieldWithMultiLineTextRemarks"/>
<xs:complexType name="multiLingualPicklistFieldWithMultiLineTextRemarks">
  <xs:complexContent>
    <xs:restriction base="picklistFieldWithMultiLineTextRemarks">
      <xs:sequence>
        <xs:element name="value" minOccurs="0" type="textFieldSmall" />
        <xs:element name="other" minOccurs="0" maxOccurs="unbounded" type="multiLingualTextFieldSmall" />
        <xs:element name="remarks" minOccurs="0" maxOccurs="unbounded"
type="multiLingualTextFieldMultiline"/>
      </xs:sequence>
    </xs:restriction>
  </xs:complexContent>
</xs:complexType>

<!-- Physical quantity field -->
<xs:element name="Conc" type="i6:multiLingualPhysicalQuantityField"/>
<xs:complexType name="multiLingualPhysicalQuantityField">
  <xs:complexContent>
    <xs:restriction base="physicalQuantityField">
      <xs:sequence>
        <xs:element name="unitCode" minOccurs="0" type="textFieldSmall" />
        <xs:element name="unitOther" type="multiLingualTextFieldSmall" minOccurs="0"
maxOccurs="unbounded"/>
        <xs:element name="value" type="xs:decimal" minOccurs="0"/>
      </xs:sequence>
    </xs:restriction>
  </xs:complexContent>
</xs:complexType>

<!-- Physical quantity range field -->
<xs:element name="Tension" type="i6:multiLingualPhysicalQuantityRangeField"/>
<xs:complexType name="multiLingualPhysicalQuantityRangeField">
  <xs:complexContent>
```

```
      <xs:restriction base="physicalQuantityRangeField">
        <xs:sequence>
          <xs:element name="unitCode" minOccurs="0" type="textFieldSmall" />
          <xs:element name="unitOther" minOccurs="0" maxOccurs="unbounded"
type="multiLingualTextFieldSmall"/>
          <xs:group ref="physicalQuantityRangeGroup"/>
        </xs:sequence>
      </xs:restriction>
    </xs:complexContent>
</xs:complexType>

<!-- Data protection field -->
<xs:element name="DataProtection" type="i6:multiLingualDataProtectionField"/>
<xs:complexType name="multiLingualDataProtectionField">
  <xs:complexContent>
    <xs:restriction base="dataProtectionField">
      <xs:sequence>
        <xs:element name="confidentiality" type="xs:string"/>
        <xs:element name="justification" maxOccurs="unbounded" type="multiLingualTextFieldLarge"/>
        <xs:element name="legislation" minOccurs="0" maxOccurs="unbounded">
          <xs:complexType>
            <xs:sequence>
              <xs:element name="value" type="xs:string"/>
              <xs:element name="other" minOccurs="0" maxOccurs="unbounded"
type="multiLingualTextFieldSmall"/>
            </xs:sequence>
          </xs:complexType>
        </xs:element>
      </xs:sequence>
    </xs:restriction>
  </xs:complexContent>
</xs:complexType>
```

It should be noted that the requirement for the multilingual support created a lot of new platform-specific types that are deviations of the existing ones in order to increase the element's occurrence and account for the optional @xml:lang attribute.

Examples of the new types added in the platform-fields.xsd are:

Field	Type
multilingualTextField	textual value with no size restriction
multilingualTextFieldSmall	textual value with 255 characters length restriction
multilingualTextFieldMultiLine	textual value with 2000 characters length restriction
multilingualTextFieldLarge	textual value with 32768 characters length restriction
multilingualPicklistField	complex type specifying value and other elements

Field	Type
multilingualPicklistFieldWithSmallTextRemarks	complex type specifying value, other and remarks elements restricting the latter to 255 characters
multilingualPicklistFieldWithLargeTextRemarks	complex type specifying value, other and remarks elements restricting the latter to 32768 characters
multilingualPicklistFieldWithMultiLineTextRemarks	complex type specifying value, other and remarks elements restricting the latter to 2000 characters
multilingualDataProtectionField	complex type specifying sub-elements (confidentiality, justification and legislation) of data protection field
multilingualPhysicalQuantityRangeField	complex type specifying sub-elements (unitCode, unitOther, lowerQualifier, upperQualifier, lowerValue, upperValue) of physical quantity range fields with decimal lower and upper values
multilingualPhysicalQuantityIntegerRangeField	complex type specifying sub-elements (unitCode, unitOther, lowerQualifier, upperQualifier, lowerValue, upperValue) of physical quantity range fields with integer lower and upper values
multilingualPhysicalQuantityHalfBoundedField	complex type specifying sub-elements (unitCode, unitOther, qualifier, value) of physical quantity half bounded fields with decimal value
multilingualPhysicalQuantityIntegerHalfBoundedField	complex type specifying sub-elements (unitCode, unitOther, qualifier, value) of physical quantity half bounded fields with decimal value

3.6 Encoding picklist phrases

Part of the IUCLID6 definition is the picklist-related fields along with their applicable phrase codes. These fields include single/multiple picklist, physical quantity, physical quantity range and data protection fields.

IUCLID6 includes an XSD generation mechanism so that:

- Every element holding a picklist phrase code value is linked to a custom, text-based type listing the eligible phrase codes for the given picklist field.
- The eligible values are identified based on the phrase group code that is linked to the specific picklist field

Encoding picklist phrases in XSD of OECD v3 legislation

```
<!-- XSD for v3 document with type ENDPOINT_STUDY_RECORD.BioaccumulationAquaticSediment -->
<?xml version="1.0" encoding="UTF-8" standalone="no"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
xmlns="http://iuclid6.echa.europa.eu/namespaces/ENDPOINT_STUDY_RECORD-
BioaccumulationAquaticSediment/3.0" xmlns:ct="http://iuclid6.echa.europa.eu/namespaces/oecd/v3"
xmlns:i6="http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1" attributeFormDefault="qualified"
elementFormDefault="qualified"
targetNamespace="http://iuclid6.echa.europa.eu/namespaces/ENDPOINT_STUDY_RECORD-
BioaccumulationAquaticSediment/3.0">

<!-- Import the commonTypes.xsd that contains the phrasegroup-specific types that are included in the
commonTypes.xsd and are part of the specific namespace for OECD v3 legislation -->
<xs:import namespace="http://iuclid6.echa.europa.eu/namespaces/oecd/v3"
schemaLocation="commonTypes.xsd"/>

<xs:element name="ENDPOINT_STUDY_RECORD.BioaccumulationAquaticSediment">
  ...
  <!-- Confidentiality value of data protection field -->
  <xs:element minOccurs="0" name="confidentiality" type="ct:N64"/>

  <!-- Regulatory programme value of data protection field -->
  <xs:element minOccurs="0" name="value" type="ct:N78"/>

  <!-- Phrase code of a picklist field -->
  <xs:element minOccurs="0" name="value" type="ct:PG6_60496"/>

  <!-- unitCode value of a physical quantity (range) field -->
  <xs:element minOccurs="0" name="unitCode" type="ct:E04"/>
  ...
</xs:element>
</xs:schema>
```

Below a part of the commonTypes.xsd listing the various phrase group-specific types per legislation provider.

OECD v3 legislation commonTypes.xsd

```
<!-- Every type defined is part of the OECD v3 name space (http://iuclid6.echa.europa.eu/namespaces/oecd/v3) -->
<?xml version="1.0" encoding="UTF-8" standalone="no"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema"
xmlns="http://iuclid6.echa.europa.eu/namespaces/oecd/v3"
xmlns:i6="http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1" attributeFormDefault="qualified"
elementFormDefault="qualified" targetNamespace="http://iuclid6.echa.europa.eu/namespaces/oecd/v3">
  <xs:import namespace="http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1"
schemaLocation="platform-fields.xsd"/>

  <xs:simpleType name="N64">
    <xs:restriction base="i6:textFieldSmall">
      <xs:enumeration value=""/>
      <xs:enumeration value="2732"/>
      <xs:enumeration value="2859"/>
      <xs:enumeration value="3441"/>
```

```
    </xs:restriction>
  </xs:simpleType>

  <xs:simpleType name="N78">
    <xs:restriction base="i6:textFieldSmall">
      <xs:enumeration value=""/>
      <xs:enumeration value="733"/>
      <xs:enumeration value="9000"/>
      <xs:enumeration value="5793"/>
      <xs:enumeration value="735"/>
      <xs:enumeration value="209"/>
      <xs:enumeration value="210"/>
      <xs:enumeration value="919"/>
      <xs:enumeration value="1313"/>
      <xs:enumeration value="1646"/>
      <xs:enumeration value="1647"/>
      <xs:enumeration value="1648"/>
      <xs:enumeration value="1342"/>
    </xs:restriction>
  </xs:simpleType>

  <xs:simpleType name="PG6_60496">
    <xs:restriction base="i6:textFieldSmall">
      <xs:enumeration value=""/>
      <xs:enumeration value="62504"/>
      <xs:enumeration value="62505"/>
      <xs:enumeration value="62507"/>
      <xs:enumeration value="3437"/>
      <xs:enumeration value="58256"/>
      <xs:enumeration value="2282"/>
      <xs:enumeration value="62470"/>
    </xs:restriction>
  </xs:simpleType>

  <xs:simpleType name="E04">
    <xs:restriction base="i6:textFieldSmall">
      <xs:enumeration value=""/>
      <xs:enumeration value="2113"/>
      <xs:enumeration value="1976"/>
      <xs:enumeration value="1839"/>
      <xs:enumeration value="2468"/>
    </xs:restriction>
  </xs:simpleType>
</xs:schema>
```

3.7 XML namespaces

IUCLD6 makes heavy use of namespaces in order to break up the various XML schemas (platform- and document-specific). In that way, we are able to define re-usable definitions and avoid conflicts of element and attribute names. Defining a default namespace for an element also saves us from using prefixes in all its child elements.

Below an analysis of:

- The namespaces supported by IUCLID6;

- The alias for each namespace in order to fully qualify elements and types that are defined in the corresponding XSD and are part of this namespace;
- The XSD file defining the entities that are part of this namespace;
- The XML file inside the i6z archive where this namespace is used.

Namespaces	Namespace alias	XSD file	XML document usage
http://iuclid6.echa.europa.eu/namespaces/manifest/v1	-	manifest.xsd Specifies the elements included in the manifest.xml along with their types	manifest.xml
http://iuclid6.echa.europa.eu/namespaces/platform-container/v1	i6c	platform-container.xsd Specifies the sub-elements (PlatformMetadata, Content, Attachments, ModificationHistory) of the **Document** element	Document-specific XML files (.i6d)
http://iuclid6.echa.europa.eu/namespaces/platform-metadata/v1	i6m	platform-metadata.xsd Specifies the sub-elements of the **PlatformMetadata** element under the **Document** element	Document-specific XML files (.i6d)
http://iuclid6.echa.europa.eu/namespaces/platform-attachment/v1	i6a	platform-attachment.xsd Specifies the sub-elements of the **Attachment** element along with their types. This is also a sub-element of the **Attachments** under the **Document** element	Attachment-specific XML files (.i6d) Document-specific XML files (.i6d)
http://iuclid6.echa.europa.eu/namespaces/platform-modification-history/v1	i6h	platform-modification-history.xsd Specifies the **ModificationEntry** sub-elements and types under the **ModificationHistory** which lies under the **Document** element	Document-specific XML files (.i6d)
http://iuclid6.echa.europa.eu/namespaces/platform-fields/v1	i6	platform-fields.xsd Specifies all the common types of the IUCLID fields Imported by the auto-generated XSDs to gain access to its definitions/types	Document-specific XML files (.i6d)

Namespaces	Namespace alias	XSD file	XML document usage
http://iuclid6.echa.europa.eu/namespaces/<ENTITY_TYPE>/<DEFINITION_VERSION> e.g. http://iuclid6.echa.europa.eu/namespaces/SUBSTANCE/3.0	-	Auto-generated XSD files <ENTITY_TYPE>-<DEFINITION_VERSION>.xsd e.g. SUBSTANCE-3.0.xsd Specifies the element with name <ENTITY_TYPE> under the **Content** element	Document-specific XML files (.i6d)
http://iuclid6.echa.europa.eu/namespaces/<DOCUMENT_TYPE>-<DOCUMENT_SUBTYPE>/<DEFINITION_VERSION> e.g. http://iuclid6.echa.europa.eu/namespaces/ENDPOINT_STUDY_RECORD-WaterSolubility/3.0	-	Auto-generated XSD files <DOCUMENT_TYPE>-<DOCUMENT_SUBTYPE>-<DEFINITION_VERSION>.xsd e.g. ENDPOINT_STUDY_RECORD-WaterSolubility-3.0.xsd Specifies the element with name <DOCUMENT_TYPE>.<DOCUMENT_SUBTYPE> under the **Content** element	Document-specific XML files (.i6d)

3.8 IUCLID6 document references

IUCLID6 provides many data types to assign to every document field. One of these types allows a field to reference another IUCLID6 document. These types are the DocumentReferenceField and DocumentReferenceMultipleField based on whether the field keeps a reference to a single or multiple documents respectively. The value of this field is the identifier of the referenced document.

Below, the XML presentation of the document references which makes clear that a weak reference exists.

IUCLID6 document references

```
<?xml version='1.0' encoding='UTF-8'?>

<!-- Field SUBSTANCE.OwnerLegalEntity referencing a single LEGAL ENTITY document -->
<OwnerLegalEntity>4f88bc7f-395c-4d0b-997b-14e8c9aef605/0</OwnerLegalEntity>

<!-- Field ENDPOINT_STUDY_RECORD.DermalAbsorption.DataSource.Reference referencing multiple LITERATURE documents -->
<Reference>
   <i6:key>d247ab3f-2393-36f2-a603-48ec1a84d694/0</i6:key>
   <i6:key>f574f4b0-af68-300b-9aa2-85c6071280f7/0</i6:key>
</Reference>
```

3.9 Attachment content

The **Attachment** XML document (.i6d) has the following structure.

Attachment document (.i6d)

```
<?xml version='1.0' encoding='UTF-8'?>
<Attachment xmlns="http://iuclid6.echa.europa.eu/namespaces/platform-attachment/v1"
xmlns:xlink="http://www.w3.org/1999/xlink" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
   <documentKey>ee038911-4d8c-4532-ba71-ca95716a6464/3cfc96de-e097-4b1d-a7ac-
39b1d108593d</documentKey>
   <name>Excel-icon.jpg</name>
   <creationDate>2016-09-13T10:15:47.427+02:00</creationDate>
   <lastModificationDate>2016-09-13T10:15:47.427+02:00</lastModificationDate>
   <remarks>Remarks value</remarks>
   <md5>6001a8c2832408420073f53543d7e2fe</md5>
   <mimetype>image/jpeg</mimetype>
   <content xlink:href="attachments/6001a8c2832408420073f53543d7e2fe.jpg" xlink:type="simple"/>
</Attachment>
```

3.9.1 Cross-referencing attachment content

The Attachment XML document contains only the metadata information of the actual attachment file. Instead of embedding the actual content inside the document, the **content** element provides the link to the actual attachment content. During import operation, the parser resolves the link and loads the attachment from the i6z archive.

3.9.2 MD5 hash calculation

The **Attachment** document contains a required **md5** element. The element's value is the MD5 hash of the actual attachment content linked to the specific Attachment document and included in the i6z archive under the **attachments** directory. During import operation, the attached content is parsed and its MD5 hash value is calculated. The calculated value is checked against the one specified in the document. In case of any discrepancy, the import operation fails with the corresponding error message.

Below, a code snippet to generate the MD5 hash value in Java. Exception handling is omitted.

MD5 generation

```
import java.io.InputStream;
import java.security.DigestInputStream;
import java.security.MessageDigest;

import javax.xml.bind.DatatypeConverter;

import org.apache.tika.io.TemporaryResources;
import org.apache.tika.io.TikaInputStream;

// The loaded attachment content
InputStream attachmentContent = null;
```

```
// Object implementing the MD5 digest algorithm in charge of running the hash computation of the attachment
// content
MessageDigest md5Digest = java.security.MessageDigest.getInstance("MD5");

// Creates a digest input stream, using the specified input stream and message digest
DigestInputStream digestInputStream = new DigestInputStream(attachmentContent, md5Digest);

// Read the digest input stream to properly update the md5Digest...

// The array of hex bytes for the resulting hash value
byte[] bytes = md5Digest.digest();

// The textual representation of the MD5 hash value
String md5 = javax.xml.bind.DatatypeConverter.printHexBinary(bytes).toLowerCase();
```

3.9.3 Mime type calculation

The **Attachment** document contains an optional **mimetype** element. The value indicates the media type of the actual attachment content linked to the specific Attachment document and included in the i6z archive under the **attachments** directory. During import operation, the media type of the attached content is recalculated. The latter value is checked against the one specified in the document. In case of any discrepancy, the import operation proceeds normally and the corresponding **warning** message is displayed to the user. The database eventually keeps the media type calculated from the application itself thus overriding the one included in the i6d document.

Below, a code snippet to generate the media type of an attachment in Java. Exception handling is omitted.

Media type generation

```
import org.apache.tika.config.TikaConfig;
import org.apache.tika.detect.Detector;
import org.apache.tika.metadata.Metadata;
import org.apache.tika.mime.MediaType;

// ...

// The loaded attachment content
InputStream attachmentContent = null;

// Provides a default configuration
TikaConfig config = TikaConfig.getDefaultConfig();

// Returns the configured detector instance
Detector detector = config.getDetector();
```

```
// Constructs a new, empty metadata
Metadata metadata = new Metadata();

// Detects the content type of the given input document. Returns <code>application/octet-stream</code>
// if the type of the document cannot be detected.
MediaType mediaType = detector.detect(attachmentContent, metadata);

// The textual representation of the media type object
String mimeType = mediaType.toString();
```