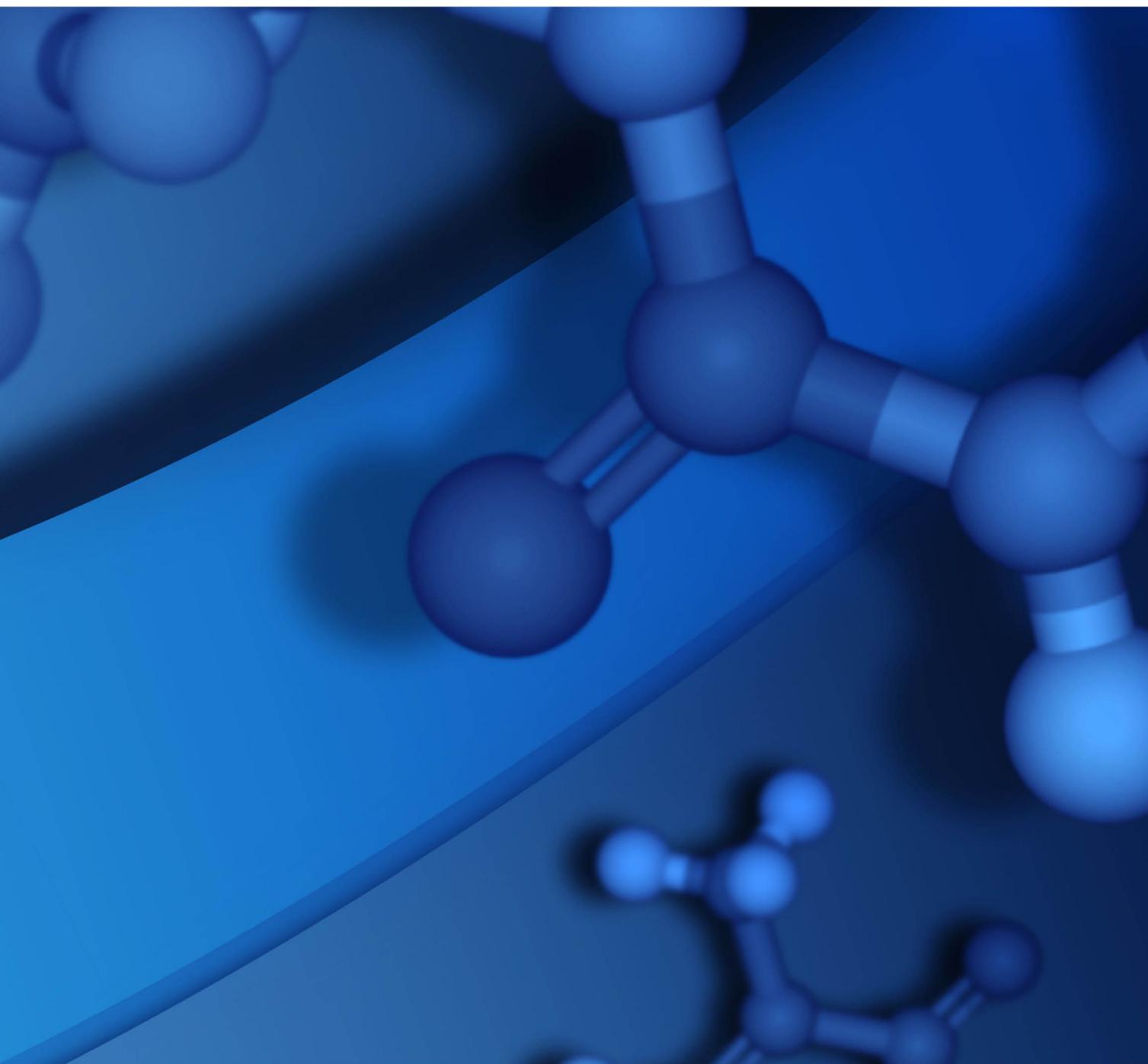


# **ERROR MESSAGES GUIDE**

BIOVIA DIRECT 2021



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# Chapter 1:

## Introduction

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### The Direct Error Messages Guide

This guide documents error messages that might display in BIOVIA Direct. It applies to all platforms on which Direct is supported: Red Hat Linux, SUSE Linux, and Microsoft Server.

### Limitations of This Guide

The information in this guide is intended for guidance only. It is the best advice available at the time of publication on error situations that produce error messages and on corrective actions.

This guide explains the probable causes of errors and corrective actions you can take.

If an explanation or corrective action does not prove useful, or if it does not appear to apply to the circumstances in which the error message occurred, contact Dassault Systèmes Customer Support for assistance.

### Additional Information

For more information about Direct and other BIOVIA software products, visit <https://3ds.com/products-services/biovia/communities/>.

# Chapter 2:

## Direct Error Messages

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**Tip:** An "E" indicates that an exception is raised.

### Direct Error Messages

1 unable to read file "%s"

**Explanation:** A file whose name was provided as a query or insert/update argument could be opened, but an error occurred while reading the file.

**Action:** This is an unusual error. Contact Dassault Systèmes Customer Support.

4 unable to read converted Chime string as a rxnfile

**Explanation:** A query or insert/update argument that is a valid Chime string was successfully unpacked, but the contents are not a valid rxnfile.

**Action:** Provide an rxnfile Chime string instead of a molfile Chime string as an argument.

7 unable to convert rxnfile string to binary rxn

**Explanation:** An error occurred while converting a string containing a file name, rxnfile, or Chime string to an internal format.

**Action:** Check for a more specific error message to help diagnose the problem.

8 unable to convert rxnfile CLOB to binary rxn

**Explanation:** An error occurred while converting a CLOB containing a file name, rxnfile, or Chime string to an internal format.

**Action:** Check for a more specific error message to help diagnose the problem.

9 unable to convert internal handle to rxnfile string

**Explanation:** An error occurred while creating an rxnfile string from an internal reaction format.

**Action:** This is unusual. Contact Dassault Systèmes Customer Support.

10 unable to unpack binary rxn to internal handle

**Explanation:** An error occurred while unpacking a binary reaction object (BLOB) into an internal format. This could indicate a corrupted BLOB.

**Action:** This is unusual. Contact Dassault Systèmes Customer Support.

11 Error converting rxnfile string to Chime string

**Explanation:** An error occurred while converting an rxnfile to Chime format.

**Action:** This is unusual. Contact Dassault Systèmes Customer Support.

12 Unable to copy contents of file "%s" to CLOB

**Explanation:** An error occurred in the READFILE operator.

**Action:** Check for a more specific error message to help diagnose the problem.

13 Unable to write contents of CLOB to file "%s"

**Explanation:** An error occurred in the WRITEFILE operator.

**Action:** Check for a more specific error message to help diagnose the problem.

14 Invalid component type, specify (1) for reactants, (2) for products

**Explanation:** The value of the component type argument to the NCOMPONENTS operator was invalid.

**Action:** Correct the argument. It must be an integer of (1) or (2).

15 Invalid component type, specify (1) for reactants, (2) for products

See error message 14.

16 Invalid component index, specify (1) or greater

**Explanation:** The value of the component index argument to the NCOMPONENTS operator was invalid.

**Action:** Correct the argument. It must be an integer of (1) or larger.

17 Invalid RXNAUTOMAP mode: %s

**Explanation:** The value of the mode argument to the AUTOMAP function or RXNAUTOMAP operator is incorrect.

**Action:** See the *Direct Reference* for the allowed values.

18 Unable to open file "%s": %s

**Explanation:** The file name argument to the WRITEFILE operator is invalid; the file could not be opened for writing. The most common reason for this error is specifying a directory in which files cannot be created by the Oracle external procedure (extproc) process.

**Action:** Check the system error message is included in the text to help diagnose the problem.

19 Unable to write to file "%s": %s

**Explanation:** Any error occurred while writing to the file whose name was specified as an argument to the WRITEFILE operator.

**Action:** Check the system error message that is included in the text to help diagnose the problem.

20 Error reading LOB, nread too small

**Explanation:** An error occurred while reading characters from a BLOB.

**Action:** Check the Oracle error message that is included to help diagnose the problem. This is an unusual error.

21 Unable to copy LOB to string

**Explanation:** An error occurred while reading a CLOB or BLOB.

**Action:** Check for another error message that provides more information. This is an unusual error.

22 Unable to copy string to LOB

**Explanation:** An error occurred while writing to a CLOB or BLOB.

**Action:** Check for another error message that provides more information. This is an unusual error.

23 Unable to convert string CLOB to Chime CLOB

**Explanation:** An error occurred in the CLOBTOCHIME function.

**Action:** Check for a more specific error message to help diagnose the problem.

24 Unable to convert Chime CLOB to string CLOB

**Explanation:** An error occurred in the CHIMETOCLOB function.

**Action:** Check for a more specific error message to help diagnose the problem.

25 Unable to allocate call memory

**Explanation:** An error occurred while allocating memory.

**Action:** This error usually indicates a serious problem. End your Oracle session since any subsequent operations are likely to fail as well.

29 Unable to set global environment item from file

**Explanation:** An error occurred in the SETENVFILE function.

**Action:** Check for a more specific error message to help diagnose the problem.

31 Unable to write global environment item to file

**Explanation:** An error occurred in the GETENVFILE function.

**Action:** Check for a more specific error message to help diagnose the problem.

34 Unable to write index environment item to file

See error message 31.

35 Too many files are open

**Explanation:** This message occurs when running the RDCAPPS.READRXNRDF or RDCAPPS.READMOLRDF functions.

**Action:** Contact Dassault Systèmes Customer Support and report this error.

36 Unable to open file "%s": %s

**Explanation:** An error occurred while trying to open the file whose file name was provided as an argument to RDCAPPS.READRXNRDF or RDCAPPS.READMOLRDF. The most likely cause is a misspelled file name, or a file whose permissions do not allow the Oracle extproc process to read it.

**Action:** See the system error message that is included to help diagnose the error.

### 37 Invalid file handle

**Explanation:** An error occurred when running the RDCAPPS . READRXNRDF or RDCAPPS . READMOLRDF functions.

**Action:** Contact Dassault Systèmes Customer Support to report this error.

### 38 Line in file is too long

**Explanation:** The Rdf file whose name was provided as an argument to RDCAPPS . READRXNRDF or RDCAPPS . READMOLRDF contains a line that is too long.

**Action:** Ensure that the file is a valid Rdf file.

### 39 Unable to open file "%s": %s

**Explanation:** An error occurred while opening a file for reading.

**Action:** Check the file name and system error message that are included to help diagnose the problem.

### 40 Unable to open file "%s": %s

**Explanation:** An error occurred while trying to create a file or open an existing file so that it can be overwritten.

**Action:** Check system error message that are included to help diagnose the problem.

### 54 Unable to insert into table, ROWID=%s, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the *indexname\_CONV* table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

### 55 Unable to delete from table, ROWID=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the *indexname\_CONV* table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

### 56 Unable to prepare ROWID to REGNO search, ROWID=%s, SQL=%s

**Explanation:** An error occurred while attempting to fetch value from the <indexname>\_CONV table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

### 57 Unable to prepare MAX(REGNO) search, SQL=%s

**Explanation:** An error occurred while attempting to fetch a maximum value from the <indexname>\_CONV table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

### 59 Unable to initialize FSlib

**Explanation:** An error occurred while initializing the FSlib component. This indicates a serious problem.

**Action:** End your Oracle session because any subsequent operations are likely to fail as well. Contact Dassault Systèmes Customer Support.

### 61 Unable to initialize process data area

**Explanation:** This error can occur if Direct is not correctly installed.

**Action:** If this error persists, uninstall, and then reinstall Direct. Verify that the installation was successful. If the error still occurs, Contact Dassault Systèmes Customer Support.

### 62 Unable to initialize local environment

**Explanation:** An error occurred while fetching or initializing the per-index environment.

**Action:** Check for a more specific error message to help diagnose the problem.

### 64 Logging disabled, unable to open log file "%s" for append: %s Severity Warning, the program will continue to operate but without any debug logging.

**Explanation:** The user has enabled logging (the MDL\_DC\_LOGGING table exists and contains a file name), but the log file cannot be opened.

The probable cause is either an invalid file name, or the file name includes a directory that cannot be written to by the Oracle extproc process.

### 66 Molecule contains an invalid Sgroup data field: %s %s

**Explanation:** A molecule contains an Sgroup data field name that is not in the allowed list of names as specified by the SETENVFILE('SGROUPFIELDS',...) function.

**Action:** This molecule or reaction cannot be used in an insert, update, or query. Correct the molecule so that it contains an allowed Sgroup data field name.

### 80 There must be a global %s set up

**Explanation:** The global cartridge environment table (MDL\_INDEX\_PROPERTIES) does not contain an entry for the specified environment item. This indicates an omission or error during installation of the cartridge.

**Action:** If this error persists, uninstall, and then reinstall Direct. Verify that the installation was successful. If the error still occurs, Contact Dassault Systèmes Customer Support for information on allowed Sgroup field operators.

### 81 Unable to get local %s for index %s.%s

**Explanation:** An error occurred while fetching an environment item from the local index-specific environment table.

**Action:** Check for the more specific error message to help diagnose the problem.

### 85 No environment name specified

**Explanation:** The environment name argument to SETENVFILE or GETENVFILE is blank or NULL.

**Action:** Specify a valid environment name.

86 Invalid environment name specified: %s

**Explanation:** The environment name argument to SETENVFILE or GETENVFILE is invalid.

**Action:** Specify a valid environment name.

91 Error reading environment file "%s"

**Explanation:** An error occurred while opening or reading an environment file.

**Action:** Use the file name and check for a more specific error to diagnose the problem.

92 Error reading default environment

**Explanation:** This probably indicates a memory allocation error.

**Action:** Check for another specific error message to help diagnose the problem.

94 No file name specified

**Explanation:** The file name argument to GETENVFILE is blank or NULL.

**Action:** Specify a valid file name.

95 Unable to fetch CLOB for envname %s

See error message 79.

96 Unable to open file "%s": %s

**Explanation:** The file name specified to the GETENVFILE function could not be opened for writing.

**Action:** Use the file name and check the system error message to help diagnose the problem.

97 Error writing environment CLOB to file "%s"

**Explanation:** An error occurred while writing an environment item to a file.

**Action:** Check for a more specific error message to help diagnose the problem.

101 Unable to fetch CLOB from index %s for envname %s

See error message 81.

118 Invalid line for SGROUPFIELDS

**Explanation:** The Sgroup fields environment CLOB contains invalid data. The data should have been validated when written to the CLOB. This error can indicate a corrupted MDL\_INDEX\_PROPERTIES table.

**Action:** Contact Dassault Systèmes Customer Support.

119 Two fields have the same name: %s

**Explanation:** The Sgroup fields environment file that was used to load the CLOB contains two lines with the same Sgroup field name, but with different field types.

**Action:** This is an invalid file, and must be corrected by reloading the corrected file with SETENVFILE ('SGROUPFIELDS',...).

123 Invalid field type: %s

**Explanation:** The Sgroup field environment file contains an invalid field type. Valid types are NUMERIC (or N) and TEXT (or T).

**Action:** Correct the Sgroup file.

132 Index name must be unique to the first 24 characters

**Explanation:** This error occurs with this command:

```
CREATE INDEX <indexname> ON <table> (<column>) INDEXTYPE IS  
C$MDLICHEM60.RXIXMDL;
```

or

```
CREATE INDEX <indexname> ON <table> (<column>) INDEXTYPE IS  
C$MDLICHEM60.MXIXMDL;
```

The error indicates that the first 24 characters of the index name are the same as the first 24 characters of some other index name. Because objects are created with the name <indexname>\_<XXXXX> (where XXXXX are 4 or 5 letters and numbers), the first 24 characters of the index name must be unique. Even though this error occurs, Oracle still creates the index.

**Action:** Drop the index:

```
DROP INDEX <indexname>;
```

Then re-create the index using an index name of which the first 24 characters are unique.

133 Molecule index must be created on a column of type BLOB

**Explanation:** This error occurs with the command:

```
CREATE INDEX <indexname> ON <table> (<column>) INDEXTYPE IS  
C$MDLICHEM60.MXIXMDL;
```

The error indicates that the column type is not BLOB. Even though this error occurs, Oracle still creates the index.

**Action:** Drop the index:

```
DROP INDEX <indexname>;
```

Then recreate the index using the correct table.

134 Reaction index must be created on a column of type BLOB

**Explanation:** This error occurs with the command:

```
CREATE INDEX <indexname> ON <table> (<column>) INDEXTYPE IS  
C$MDLICHEM60.RXIXMDL;
```

The error indicates that the column type is not BLOB. Even though this error occurs, Oracle still creates the index.

**Action:** Drop the index:

```
DROP INDEX <indexname>;
```

Then re-create it using the correct table.

135 Objects exist whose names conflict with ones which would be created during the creation of this index, names of the form '%sxxxxx'

**Explanation:** This error occurs with this command:

```
CREATE INDEX <indexname> ON <table> (<column>) INDEXTYPE IS
C$MDLICHEM60.RXIXMDL;
```

or

```
CREATE INDEX <indexname> ON <table> (<column>) INDEXTYPE IS
C$MDLICHEM60.MXIXMDL;
```

The error indicates that there are already tables that have names that will conflict with the names created by the cartridge, for example:

```
<indexname>_PROP
```

```
<indexname>_CONV
```

```
<indexname>_FSIX
```

These are not "left over" reaction index tables, they contain column names that are not known to the cartridge.

Choose a different name for the index where the first 24 characters of the name, with the suffixes above, do not conflict with any other tables. Even though this error occurs, Oracle still creates the index.

**Action:** Drop the index:

```
DROP INDEX <indexname>;
```

Then recreate the index using a different index name.

139 Unable to allocate memory

See error message 25.

142 Invalid ALTER INDEX parameter: %s

**Explanation:** This error occurs with the following command and indicates that one of the parameter values is incorrect.

```
ALTER INDEX <indexname> [REBUILD] PARAMETERS ('<parameters>');
```

No alteration to the index has occurred.

**Action:** Reissue the command with the correct parameter value(s).

143 The domain index is now marked as unusable.

Severity Information, and occurs with the command:

```
ALTER INDEX <indexname> [REBUILD] PARAMETERS ('<parameters>');
```

**Explanation:** This message is posted because the ALTER INDEX command failed, and Oracle has marked the index as "invalid" or "unusable". Generally, the index should be completely rebuilt when this occurs. However, this message provides a command that can be used to mark the index as "valid" or "usable".

**Action:** Mark it "usable" using the command that follows. However, this does not fix any errors and can leave the index in an indeterminate state (requiring a full rebuild to fix):

```
ALTER INDEX %s.%sREBUILD PARAMETERS('NOACTION');
```

**Note:** Note: Underlying objects created by the cartridge might still not be valid. BIOVIA recommends a full rebuild in this case.

### 149 unable to initialize local environment

**Explanation:** An error occurred while initializing the local index-specific environment after an ALTER INDEX command.

**Action:** Check for a more specific error message to help diagnose the problem.

### 150 Error in COMMIT

**Explanation:** An error occurred while trying to commit an autonomous transaction.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

### 151 Too many reaction errors, key generation terminated

**Explanation:** During reaction key generation (from ALTER INDEX REBUILD), up to 100 errors are allowed during reaction fetching. This error message indicates that more errors have occurred, and that key generation will be terminated with an error.

**Action:** Check for more specific error messages to help diagnose the problem.

### 152 Error in COMMIT

See error message 150.

### 153 E Reaction domain index creation failed

**Explanation:** This is the general exception that is posted when CREATE INDEX fails. Oracle creates the index, even though the cartridge has indicated an error to Oracle.

**Action:** Drop the index because it is unusable:

```
DROP INDEX indexname;
```

### 154 E Reaction index alter failed

**Explanation:** This is the general exception that is posted when ALTER INDEX fails.

**Action:** See error message 143.

### 155 E Reaction index truncate failed

**Explanation:** This is the general exception that is posted when the index truncation, which occurs during TRUNCATE TABLE, fails.

**Action:** Check for more specific error messages to help diagnose the problem.

### 156 E Reaction index drop failed

**Explanation:** This is the general exception that is posted when the index drop, which occurs during DROP TABLE or DROP INDEX, fails.

**Action:** Check for more specific error messages to help diagnose the problem.

157 E Reaction index insert failed

**Explanation:** This is the general exception that is posted when the index insert, which occurs during INSERT INTO table ..., fails.

**Action:** Check for more specific error messages to help diagnose the problem.

158 E Reaction index delete failed at ROWID=%s

**Explanation:** This is the general exception that is posted when the index delete fails during DELETE FROM table ... .

**Action:** Check the ROWID of the reaction that is provided to help diagnose the problem.

159 E Reaction index update failed at ROWID=%s

**Explanation:** This is the general exception that is posted when the index update fails during UPDATE table ... .

**Action:** Check the ROWID of the reaction that is provided to help diagnose the problem.

162 E Reaction index search initialization failed

**Explanation:** This is the general exception that is posted when an indexed search fails during initialization. Generally, the failure is due to an invalid query.

**Action:** Check for a more specific error that can be used to diagnose the problem.

163 Error in OCIStrAssignText

**Explanation:** An Oracle error occurred while returning search hits to Oracle.

**Action:** Check for a more specific error that can be used to diagnose the problem.

164 Error in OCICollAppend

See error message 163.

165 Error in OCIStrAssignText

See error message 163.

166 Error in OCICollAppend

See error message 163.

167 E Reaction index search fetch failed

**Explanation:** This is a general exception that is posted when an indexed search fails while fetching hits.

**Action:** Check for a more specific error message to help diagnose the problem.

171 Unable to insert into table, PROP=%s, VAL=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the MDL\_INDEX\_PROPERTIES table.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

172 Unable to insert into table, PROP=%s, VAL=%s, SQL=%s

See error message 171.

173 Unable to insert into table, PROP=%s, VAL=%s, SQL=%s

See error message 171.

175 Unable to delete from table, PROP=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the MDL\_INDEX\_PROPERTIES table.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

176 Unable to get inverted key chunksize

**Explanation:** An error occurred while fetching a row from the local property table (indexname\_PROP).

**Action:** Check for a more specific error message to help diagnose the problem.

177 Unable to prepare sequential keys fetch, SQL=%s

**Explanation:** An error occurred while preparing to fetch sequential keys.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

178 Unable to fetch inverted keys, SQL=%s

**Explanation:** An error occurred while fetching the inverted keys BLOB.

**Action:** Check for a more specific error message to help diagnose the problem.

179 Error converting INT to NUMBER

**Explanation:** An error occurred in the Oracle routine that converts an int to an Oracle NUMBER datatype.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

181 Error converting FLOAT to NUMBER

**Explanation:** An error occurred in the Oracle routine that converts a float to an Oracle NUMBER datatype.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

183 Error converting INT to existing NUMBER

See error message 179.

184 Error converting NUMBER to INT

**Explanation:** An error occurred in the Oracle routine that converts an Oracle NUMBER datatype to an int.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

195 E Unable to get user handle for memory allocation

See error message 25.

196 E Unable to allocate session memory

See error message 25.

198 Unable to open LOB

**Explanation:** An error occurred while opening a LOB for write access.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

199 Unable to get length of LOB

**Explanation:** An error occurred while trying to determine the length of a LOB.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

201 Unable to read from BLOB

**Explanation:** An error occurred while reading from a BLOB.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

202 Unable to write to LOB

**Explanation:** An error occurred while writing to a LOB during UPDATEPENDINGFASTSEARCH.

**Action:** Check the Oracle error message that is included to help diagnose the problem. Ensure that DB\_SECUREFILE is not set to ALWAYS or FORCE.

203 Unable to read from CLOB (csfrm=%d, csid=%d)

**Explanation:** An error occurred while reading from a CLOB. This error can occur when using EMPTY\_CLOB as an argument, for example, INSERT INTO ... (CTAB) VALUES (MOL(EMPTY\_CLOB())).

**Action:** Check the Oracle error message that is included to help diagnose the problem. If this error is due to using (MOL(EMPTY\_CLOB())), change the application so that it inserts a molecule or reaction instead of an empty CLOB.

204 Unable to write to CLOB (csfrm=%d, csid=%d)

**Explanation:** An error occurred while writing to a CLOB.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

205 Failed to allocate statement handle

**Explanation:** An error occurred while allocating an SQL statement handle.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

206 Failed to prepare statement: %s

**Explanation:** An error occurred while preparing an SQL statement.

**Action:** Check the SQL statement and Oracle error message that are included to help diagnose the problem.

208 Unable to allocate LOB locator

**Explanation:** An error occurred while allocating a LOB locator.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

209 Unable to define fetch parameter

**Explanation:** An error occurred while allocating an SQL statement fetch parameter.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

210 Unable to bind variable

**Explanation:** An error occurred while binding a variable to an SQL statement.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

211 Unable to allocate LOB locator

See error 208.

212 Unable to bind variable

See error 210.

213 Error in statement fetch

**Explanation:** An error occurred while fetching from a SQL statement.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

214 Unable to select long value, SQL=%s

**Explanation:** An error occurred while selecting a value from a table.

**Action:** Check for a more specific error message to help diagnose the problem.

215 Unable to select string value, SQL=%s

See error 214.

216 Error logging to table

Warning

**Explanation:** An error occurred while logging debug information to a file and does not affect the normal cartridge operation.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

220 Unable to insert into table, PROP=%s, VAL=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_PROP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

221 Unable to insert into table, PROP=%s, VAL=%s, SQL=%s

See error 220.

222 Unable to insert into table, PROP=%s, VAL=%s, SQL=%s

See error 220.

223 Unable to delete from table, PROP=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_PROP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

235 Unable to generate fragment hash values

**Explanation:** An error occurred while generating pre-screen information about the reaction, prior to a RXNFLEXMATCH search. This is an unusual error.

**Action:** Contact Dassault Systèmes Customer Support.

236 Unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_RFLX table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

237 Unable to delete from table, REGNO=%s, SQL=%

**Explanation:** An error occurred while deleting a row from the indexname\_RFLX table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

251 Unable to insert into table, REGNO=%s, SQL=%

**Explanation:** An error occurred while inserting a row into the indexname\_SRKY table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

252 Unable to delete from table, REGNO=%s, SQL=%

**Explanation:** An error occurred while deleting a row from the indexname\_SRKY table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

255 Unable to generate reaction keys for REGNO=%s

**Explanation:** An error occurred while generating reaction keys for a reaction.

**Action:** Check for a more specific error message to help diagnose the problem.

256 WARNING: %s key inversion succeeded but sequential key truncation failed

**Note:** %s is replaced by "reaction", "2d molecule", or "3d molecule".

Warning

**Explanation:** This message indicates that all of the sequential keys were successfully "inverted" and copied into the inverted keys BLOB. However, at the end of that operation, the truncation of the sequential key table failed.

This is serious, but the index should still be usable.

**Action:** Check for a more specific error message to help diagnose the problem. Or you might want to try truncating the table manually:

```
TRUNCATE TABLE indexname_SRKY;
```

or

```
TRUNCATE TABLE indexname_SKY2;
```

```
TRUNCATE TABLE indexname_SKY3;
```

257 unable to prepare COUNT(\*) search, SQL=%s

**Explanation:** An error occurred while preparing an SQL statement to determine the number of sequential keys pending inversion.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

258 unable to convert rxnfile string to Chime string

**Explanation:** An error occurred in RSSHIGHLIGHT while converting a rxnfile string to a Chime string.

**Action:** Check for a more specific error message to help diagnose the problem.

259 ScanCtx is NULL

**Action:** This is an internal error. Contact Dassault Systèmes Customer Support to report the problem.

260 Error in OCIRawAssignBytes for ScanCtx

**Explanation:** An Oracle error occurred while trying to copy bytes to a RAW object.

**Action:** Check the Oracle error message to help diagnose the problem.

261 ScanCtx is NULL

See error 259.

262 Error in OCIRawPtr for ScanCtx

See error 259.

263 unable to get indexed table information

**Explanation:** An Oracle error occurred while trying to get index information.

**Action:** Check the Oracle error message to help diagnose the problem.

264 E Reaction search initialization failed

**Explanation:** This is the general exception that is posted when a non-indexed search fails during initialization. Generally, the failure is due to an invalid query.

**Action:** Check for a more specific error to help to diagnose the problem.

265 Unable to create sequence, SQL=%s

**Explanation:** An error occurred while creating the indexname\_SQNC sequence.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

267 Unable to rename sequence, SQL=%s

**Explanation:** An error occurred while renaming the indexname\_SQNC sequence.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

268 Unable to select from sequence, SQL=%s

**Explanation:** An error occurred while fetching the next value from the indexname\_SQNC sequence.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

269 Unable to analyze table, SQL=%s

**Explanation:** An error occurred while analyzing an internal table to compute its statistics.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

272 A LOB may be opened for update only once

**Explanation:** This error indicates that two concurrent Oracle connections to the same session are attempting to invert pending keys or to rebuild the index.

**Action:** Ensure that only one such operation is allowed at one time in a session.

273 Unable to fetch or open LOB, SQL=%s

**Explanation:** An error occurred while fetching or opening a LOB.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

274 Unable to close LOB

**Explanation:** An error occurred while closing a LOB.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

275 Line in string or file is too long, exceeds 32768 characters

**Explanation:** A line in a molfile or rxnfile string is too long, which indicates that a string argument does not contain a valid molfile or rxnfile.

**Action:** Use a valid molfile or rxnfile.

276 Line in file is too long, exceeds 32768 characters

**Explanation:** A line in a molfile or rxnfile is too long; this indicates that the argument is not a valid molfile or rxnfile.

**Action:** Use a valid molfile or rxnfile.

277 String to be written to file is too long, exceeds 32768 characters

**Explanation:** A line being written to a file is too long.

**Action:** Report this error to Dassault Systèmes Customer Support.

278 Error writing file "%s": %s

**Explanation:** An error occurred while writing a file.

**Action:** Check the system error the help diagnose the problem. One cause might be that the disk is full.

280 CDBLib Error %ld:%s%s

**Explanation:** This error message is used to report all error messages from the CDBlib component.

**Action:** Use this low-level error message to help diagnose the general problem indicated by a higher-level message.

280 CDBLib Error 2918:unpackCtab:Invalid packed ctab header

**Explanation:** This error can happen if you pass a binary reaction to a function that expects a molecule.

**Action:** Use the appropriate function or select from the proper column.

291 Error fetching sequential keys

**Explanation:** An error occurred while fetching sequential keys.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

292 Unable to close inverted key LOB

**Explanation:** An error occurred while closing the inverted keysLOBafter writing to it.

**Action:** Check for a more specific error message to help diagnose the problem.

293 Error in COMMIT

See error message 150.

296 Not enough bytes written to CLOB: %u instead of %u

**Action:** Report this error to Dassault Systèmes Customer Support

299 No operation other than RXNFLEXMATCH() $=$ 1 is valid

**Explanation:** The RXNFLEXMATCH query was not posed as:

```
SELECT cols FROM table WHERE  
RXNFLEXMATCH(rxn,query,opts) = 1;
```

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc, was used.

**Action:** Correct query as shown above.

300 unable to create RXNFLEXMATCH data area

See error 25.

301 RXNFLEXMATCH search query can not be NULL

**Explanation:** A RXNFLEXMATCH query must be a reaction, and cannot be NULL.

**Action:** Correct the query.

302 Unable to initialize RXNFLEXMATCH matching

**Explanation:** An error occurred while preparing the RXNFLEXMATCH query.

Two common causes for failure are that the query:

- Contains RSS query features.
- Has only reactants or products (but not both), and the subset flag is not included in the options.

**Action:** Check for a more specific error message to help diagnose the problem. If either of these causes are the problem, correct the query.

303 Unable to prepare hash select, SQL=%s

**Explanation:** An error occurred while preparing the an SQL statement for a RXNFLEXMATCH search.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

304 Unable to fetch fetch hash value

**Explanation:** An error occurred while fetching during a RXNFLEXMATCH search.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

305 unable to allocate reaction flexmatch data area

See error 25.

306 No operation other than RXNSIM() $=$ 1 is valid

**Explanation:** The RXNSIM query was not posed as:

```
SELECT cols FROM table WHERE
```

```
RXNSIM(rxn,query,opts) = 1;
```

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc., was used.

**Action:** Correct the query as shown above.

307 Unable to create RXNSIM data area

See error 25.

308 RXNSIM search query can not be NULL

**Explanation:** A RXNSIM query must be a reaction, it cannot be NULL.

**Action:** Correct the query.

309 No operation other than RSS() $=$ 1 is valid

**Explanation:** The RSS query was not posed as:

SELECT cols FROM table WHERE

RSS(rxn,query) = 1;

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc., was used.

**Action:** Correct the query as shown above.

310 Unable to create RSS data area

See error 25.

311 RSS search query can not be NULL

**Explanation:** An RSS query must be a reaction and cannot be NULL.

**Action:** Correct the query.

312 Unable to initialize RSS matching

**Explanation:** An error occurred while preparing the RSS query. It is likely that the query contains some feature which is incompatible with RSS, and the query must be corrected.

**Action:** Check for a more specific error message to help diagnose the problem.

313 Rxnstructure search query is not a valid reaction

**Explanation:** The query argument to the RSS, RXNSIM, or RXNFLEXMATCH operator could not be converted into an internal format.

Common problems are that:

- An rxnfile file name is either misspelled
- The file is not readable by the Oracle extproc process.

**Action:** Correct the query.

319 Invalid call to rxntable\_fetchinit

**Action:** Contact Dassault Systèmes Customer Support.

320 Invalid value for nregnos: %d

**Action:** Contact Dassault Systèmes Customer Support.

321 unable to prepare SQL: %s

**Explanation:** An error occurred while preparing a fetch from either the structure table or from the structure table joined with the ROWID conversion table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

322 Error executing ROWIDs select

**Explanation:** An error occurred while fetching rows from either the structure table or from the structure table joined with the ROWID conversion table.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

324 Unable to unpack reaction at ROWID/REGNO=%s

**Explanation:** This error indicates that a binary packed reaction (BLOB) has become corrupted.

**Action:** Check for the ROWID or REGNO of the row containing the reaction to help diagnose the problem.

**Note:** The reaction should be updated from a backup source. (The reaction might need to be deleted first, and/or the index might need to be dropped before updating the reaction, and then re-created after the update).

325 ROWID is NULL

**Action:** Contact Dassault Systèmes Customer Support.

327 Unable to unpack reaction at ROWID=%s

See error 324.

328 Unable to read from temporary file "%s": %s

**Explanation:** An error occurred while reading from a temporary file.

**Action:** Check the file name and system error message to help diagnose the problem.

329 Unable to write to temporary file "%s": %s

**Explanation:** An error occurred while writing to a temporary file.

**Action:** Check the file name and system error message to help diagnose the problem.

330 Unable to allocate memory for temporary file

See error 25.

335 Input string is empty or NULL

**Explanation:** This error message indicates that a string molfile or rxnfile (input to a query, insert, or update) is empty or NULL.

**Action:** Specify the correct molfile or rxnfile as input.

336 Input string is empty

**Explanation:** This error message indicates that a string molfile or rxnfile (input to a query, insert, or update) contains only line-feed characters.

**Action:** Specify the correct molfile or rxnfile as input.

337 Input file "%s" is empty

**Explanation:** This error message indicates that a file (whose name was input to a query, insert, or update) contains only line-feed characters.

**Action:** Specify the correct molfile or rxnfile name as input.

340 Unable to read converted Chime string from file "%s" as a rxnfile

**Explanation:** A query or insert/update argument that is a file containing a valid Chime string was successfully unpacked, but the contents are not a valid rxnfile.

A possible cause is that the provided rxnfile file contains a molfile Chime string instead of an rxnfile Chime string.

**Action:** Correct the rxnfile.

345 E Error inverting pending reaction keys

**Explanation:** An error occurred while running MDLAUX.UPDATEPENDINGINVERSIONS to invert any pending reaction keys.

**Action:** Check for a more specific error message to help diagnose the problem.

346 unable to lock table, SQL=%s

**Explanation:** This error occurs when running MDLAUX.UPDATEPENDINGINVERSIONS while trying to lock the sequential key table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

347 unable to delete sequential keys at regno = %lu

**Explanation:** This error occurs when running MDLAUX.UPDATEPENDINGINVERSIONS while trying to delete a sequential key record.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

348 Error in COMMIT

**Explanation:** This error occurs when running MDLAUX.UPDATEPENDINGINVERSIONS while trying to commit changes to the sequential and inverted key tables.

**Action:** Check the Oracle error message to help diagnose the problem.

349 Error in ROLLBACK

**Explanation:** This occurs when running MDLAUX.UPDATEPENDINGINVERSIONS while trying to rollback changes to the sequential and inverted key tables.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

350 Error in COMMIT

See error 348.

351 unable to prepare or bind sequential key delete SQL

**Explanation:** This occurs when running MDLAUX.UPDATEPENDINGINVERSIONS while trying to prepare the delete for sequential key records.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

353 unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing an insert into the indexname\_CONV table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

354 unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing to insert a row into the indexname\_RFLX table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

355 Unable to prepare sequence select, SQL=%s

**Explanation:** An error occurred while preparing to fetch the next value from the indexname\_SQNC sequence.

**Action:** Check the SQL command and Oracle error message are included to help diagnose the problem.

360 Unable to obtain key chunksize or count

**Explanation:** An error occurred while obtaining environment information for the index being scanned by MDLAUX.SCANINDEX.

**Action:** Contact Dassault Systèmes Customer Support.

361 Unable to initialize scan over structure table

**Explanation:** An error occurred while preparing for an index scan in MDLAUX.SCANINDEX.

**Action:** Check for a more specific error message to help diagnose the problem.

362 Unable to initialize key scan

See error 361.

364 Reaction KEYS scan has errors, use MDLAUX.LOGTABLE to view errors

**Explanation:** This error indicates that the scan in MDLAUX.SCANINDEX generated one or more errors messages. Normally this indicates a problem in a specific scan.

**Action:** Check for more specific error messages to help diagnose the problem.

**Note:** Scan problems are not indicated in the error messages but instead are stored in the log table. Use MDLAUX.LOGTABLE to view the errors.

366 Unable to initialize hash table lookup, SQL=%s

**Explanation:** An error occurred when preparing to fetch index data while executing MDLAUX.SCANINDEX.

**Action:** Check the SQL statement and Oracle error message that are provided to help diagnose the problem.

369 Unable to prepare hash value fetch, SQL=%s

See error 366.

370 Unable to fetch hash value at ROWID=%s, SQL=%s

**Explanation:** An error occurred when fetching index data while executing MDLAUX.SCANINDEX.

**Action:** Check the ROWID and SQL statement that are provided to help in diagnosing the problem. There should also be a more specific error message.

371 Reaction FLEXMATCH hash scan has errors, use MDLAUX.LOGTABLE to view

errors

See error 364.

372 Unable to interpret RXNFLEXMATCH switches

**Explanation:** The switches argument to the RXNFLEXMATCH operator is not valid.

**Action:** Reissue the query using the correct RXNFLEXMATCH switches.

373 RXNFLEXMATCH query contains invalid data Sgroups

**Explanation:** A molecule within a reaction query for a RXNFLEXMATCH search contains an Sgroup data field name that is not in the allowed list of names as specified by the SETENVFILE('SGROUPFIELDS',...) function. This reaction cannot be used as a query.

**Action:** Check for a more specific error that provides the invalid field name.

384 Unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing to insert a row into the indexname\_RSGP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

385 Unable to get Sgroup data for REGNO=%s

**Explanation:** An error occurred while fetching Sgroup data from a reaction during an index rebuild operation. This is an unusual error and probably indicates some sort of corruption, since the data were checked when the reaction was inserted into the table in the first place.

**Action:** Check for a more specific error message to help diagnose the problem or locate the reaction that is in the error message. You might need to re-register one or more reactions to correct the problem.

386 Unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_RSGP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

387 Unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_RSGP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

388 Index rebuild failed at ROWID=%s, REGNO=%s

**Explanation:** If an error occurs during an index build or rebuild operation, this message is output. It gives the reaction table ROWID of the reaction where the error occurred, and might also give the conversion table regno.

**Action:** If the error occurred due to an invalid reaction, use the ROWID to obtain the reaction, and then correct it.

389 Error converting FLOAT to existing NUMBER (NULL value)

**Explanation:** An error occurred in the Oracle routine that converts a float to an Oracle NUMBER datatype.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

390 Error converting FLOAT to existing NUMBER

See error 389.

391 Error converting NUMBER to FLOAT

**Explanation:** An error occurred in the Oracle routine that converts an Oracle NUMBER datatype to a float.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

392 Unable to close LOB

**Explanation:** An error occurred while closing a LOB after writing to it.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

393 Unable to determine length of rowid in index-organized-table

**Explanation:** An error occurred while fetching information from Oracle data dictionary tables for an index organized table on which a reaction index is being created.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

394 ALTER INDEX MODIFY is not supported for a reaction index

**Explanation:** According to Oracle 9.2 documentation, this mode is never passed to the cartridge. But in case it is, this message indicates that this mode is not supported.

401 Unable to allocate snapshot descriptor

**Explanation:** This indicates an error executing a SQL statement.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

409 Unable to invert keys while another user is performing maintenance

**Explanation:** This error occurs when you try to run the procedure MDLAUX.UPDATEPENDINGINVERSIONS, and

another user is already running MDLAUX.UPDATEPENDINGINVERSIONS, MDLAUX.RECREATEKEYS, MDLAUX.SCANINDEX, ALTER INDEX, DROP INDEX, DROP TABLE, or TRUNCATE TABLE.

**Action:** Wait until the other user has finished, and then run this procedure.

410 Unable to allocate handle for resource %s

**Explanation:** This is not a fatal error, but it prevents the cartridge from locking the index during the MDLAUX.UPDATEPENDINGINVERSIONS maintenance operation. The inability to lock means that another user could also run MDLAUX.UPDATEPENDINGINVERSIONS at the same time, which would corrupt the inverted keys.

The most common cause of this error is that user has not been granted access to the SYS.DBMS\_LOCK package. If this is the case, the full error text will be:

RDC-0410: unable to allocate handle for resource <name>: ORA-06550:line 1,

column 7:PLS-00201: identifier 'DBMS\_LOCK' must be declaredORA-06550: line 1, column 7:PL/SQL: Statement ignored

**Action:** To correct this error, the Oracle DBA must grant execute on SYS.DBMS\_LOCK to this user or to PUBLIC.

For example:

```
GRANT EXECUTE ON SYS.DBMS_LOCK TO PUBLIC;
```

411 Unable to request lock %s in mode %d

**Explanation:** This is not a fatal error, but it does prevent the user from executing the MDLAUX.UPDATEPENDINGINVERSIONS procedure. An error occurs during a request for an Oracle lock.

**Action:** Check the Oracle error message to help diagnose the failure.

412 Unable to release lock %s

**Explanation:** An error has occurred while trying to release an Oracle lock.

**Action:** Check the Oracle error message that is included to help diagnose the failure.

**Note:** This is not a fatal error, but if the lock is still held it can prevent other users from executing the MDLAUX.UPDATEPENDINGINVERSIONS procedure. If this is the case, Oracle utilities can be used to release the lock.

413 Unable to access SYS.DBMS\_LOCK package

See error 410.

**Note:** This is the final error in the sequence of errors which start with 410.

414 Rxnstructure search query is not a valid molecule

**Explanation:** The molecule query argument to the RSS operator in SSS-as-component mode could not be converted into an internal format. One common problem is that a molfile file name is either misspelled, or the file is not readable by the Oracle extproc process. Because a molfile is required here, another problem is that an rxnfile is mistakenly provided.

**Action:** Correct the query.

415 Unable to read converted Chime string from file "%s" as a molfile

**Explanation:** A query argument that is an file containing a valid Chime string was successfully unpacked, but the contents are not a valid molfile. One cause is that a file containing a rxnfile Chime string instead of a molfile Chime string was provided.

**Action:** Correct the query.

416 Unable to read converted Chime string as a molfile

**Explanation:** A query argument that is a valid Chime string was successfully unpacked, but the contents are not a valid molfile. One cause is that a rxnfile Chime string instead of a molfile Chime string as an argument was provided.

**Action:** Correct the query.

417 Input file "%s" does not contain a valid molfile string:

**Explanation:** A query argument that is a file which is supposed to contain either a molfile string or a Chime string could not be interpreted as either of those. The most common cause of this error is providing the wrong file name.

**Action:** Use the first 66 characters of the file that are provided to help diagnose the problem.

418 Input string is not a valid filename or molfile string:

**Explanation:** A query argument that is supposed to be either a file name, a molfile string, or a chime string could not be interpreted as any of those. The most common reason for this error is a misspelled file name.

**Action:** Use the first 66 characters of the file or string that are provided to help diagnose the problem.

419 Input string is not a valid molfile string:

**Explanation:** A query argument that is supposed to be either a molfile string or a chime string could not be interpreted as either of those.

**Action:** Use the first 66 characters of the string that are provided to help diagnose the problem.

420 Input file "%s" does not contain a valid molfile string or Chime string:  
See error 417.

421 Input string is not a valid filename, molfile string or Chime string:  
See error 419.

422 Input string is not a valid molfile string or Chime string:  
See error 418.

424 Unable to convert molecule component to reaction

**Explanation:** An error occurred while converting the RSS "SSS-as-component" query molecule into a reactant-only reaction.

**Action:** Contact Dassault Systèmes Customer Support.

425 Unable to convert molecule component to reaction

**Explanation:** An error occurred while converting the RSS "SSS-as-component" query molecule into a product-only reaction.

**Action:** Contact Dassault Systèmes Customer Support.

426 RSS search query in 'SSS-as-component' mode requires 'PRODUCT [NOT REACTANT]' or 'REACTANT [NOT PRODUCT]' argument.

**Explanation:** The third argument to the RSS operator is not correct. To run an "SSS-as-component" search, the component must be a string containing one of the following (case does not matter):

- PRODUCT
- PRODUCT NOT REACTANT
- REACTANT
- REACTANT NOT PRODUCT

**Action:** Specify the correct argument.

428 Rxnfile containing Rgroup atoms is not supported

**Explanation:** This error indicates that this version of the cartridge does not support reactions containing R# atoms.

**Action:** Remove the Rgroup components from your reaction before using it with Direct.

601 TEMPDIR parameter "%s" is invalid, cannot create temporary file: %s

**Explanation:** The TEMPDIR=dirname parameter specifies an invalid directory name. Either the directory does not exist, or the Oracle extproc process does not have rights to create a file in the directory.

**Action:** Check operating system error message that is included in the error text. Specify a directory that exists and that is writable by the extproc process.

**Note:** On Microsoft Windows, the extproc process is probably not logged in to any domain, and might not be able to access network drives.

602 unable to get primary key column name from conversion table during import

**Explanation:** This error is not likely to occur, but if it does, it indicates a problem trying to get column names for a table that is known to exist.

**Action:** Use the more specific information that is included with the message to diagnose the problem.

603 Error updating table during import, SQL: %s

**Explanation:** This indicates an error has occurred while correcting ROWID values during import. One possibility is that the rollback segment is too small. There should be a more specific error message giving more detail.

**Action:** Check for a more specific Oracle error message to help diagnose and correct the problem, then reissue the import operation.

605 ALTER INDEX RENAME requires that the index schema match the user's schema

**Explanation:** This error message indicates an attempt to rename a domain index when connected to a schema different from the one that owns the domain index.

**Action:** Connect to the index owner's schema before using ALTER INDEX RENAME.

606 Invalid ALTER INDEX REBUILD parameter(s)

**Explanation:** This error message indicates that one or more parameters in the PARAMETERS argument to ALTER INDEX REBUILD was invalid.

**Action:** Check for a more specific message indicating exactly which parameters caused the error. Correct the parameter and reissue the command.

608 UNIQUE constraint cannot be applied, there would be duplicates

**Explanation:** This error message indicates that the UNIQUE constraint cannot be applied to the domain index because there are duplicate molecules or reactions.

**Action:** Remove all duplicates before using the UNIQUE parameter.

611 Error converting molfile string to Chime string

**Explanation:** An error occurred while converting a molfile to Chime format.

**Action:** Contact Dassault Systèmes Customer Support.

612 Unable to compute number of specifics

**Explanation:** An error occurred while attempting to count the number of specifics for a generic molecule.

**Action:** Check for a more specific error message to help diagnose the problem.

613 Unable to fetch molname

**Explanation:** An error occurred while attempting to fetch the molname from a molecule.

**Action:** Contact Dassault Systèmes Customer Support.

615 Unable to set molname

**Explanation:** An error occurred while attempting to set the molname for a molecule.

**Action:** Contact Dassault Systèmes Customer Support.

616 Unable to convert molfile string to Chime string

See error message 611.

617 E Error inverting pending 2D molecule keys

**Explanation:** An error occurred while running MDLAUX.UPDATEPENDINGINVERSIONS to invert any pending 2D molecule keys.

**Action:** Check for a more specific error message to help diagnose the problem.

619 E Error executing INVERTPENDING partition loop SQL: %s

**Explanation:** This indicates an error getting partition information in MDLAUX.UPDATEPENDINGINVERSIONS.

**Action:** Contact Dassault Systèmes Customer Support.

621 E Error updating pending FASTSEARCH

**Explanation:** An error occurred while running MDLAUX.UPDATEPENDINGFASTSEARCH.

**Action:** Check for a more specific error message to help diagnose the problem.

624 E Error recreating FASTSEARCH

**Explanation:** An error occurred while running MDLAUX.RECREATEFASTSEARCH.

**Action:** Check for a more specific message that will provide the reason for the failure.

627 E Invalid argument to MDLAUX.SCANINDEX

**Explanation:** This error message indicates that one or more parameters in the argument string to MDLAUX.SCANINDEX were incorrect.

**Action:** Check for a more specific message indicating the incorrect parameter. Correct the argument, and reissue the command.

632 Molfile containing Rgroup atoms is not supported

**Explanation:** Indicates that this version of the cartridge does not support registration of molecules containing R# atoms. These molecules can only be used as SSS queries.

**Action:** Remove the Rgroup components from the molecule before trying to register it with Direct.

633 E Unable to convert molfile string to binary molecule ctab

**Explanation:** An error occurred while converting a string containing a file name, molfile, or Chime string to an internal format.

**Action:** Check for a more specific error to help diagnose the problem.

634 E Unable to convert molfile CLOB to binary molecule ctab

**Explanation:** An error occurred while converting a CLOB containing a file name, molfile, or Chime string to an internal format.

**Action:** Check for a more specific error to help diagnose the problem.

635: Unable to convert internal handle to molfile string

**Explanation:** An error occurred while creating a molfile string from an internal molecule format.

**Action:** Contact Dassault Systèmes Customer Support.

636: Unable to unpack binary molecule ctab to internal handle

**Explanation:** An error occurred while unpacking a binary molecule object (BLOB) into an internal format. This could indicate a corrupted BLOB.

**Action:** Contact Dassault Systèmes Customer Support.

639: E Sgroup field names will not fit into a VARCHAR2

**Explanation:** This error message indicates that there are so many Sgroup field names that they cannot be stored in a 4000 character string.

**Action:** The application needs to directly access the SGROUPFIELDS environment item contained in indexname\_PROP in order to enumerate the Sgroup field names.

651 Error locking classcode (insert)

**Explanation:** An error occurred while inserting a record into the indexname\_CCLK table.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

652 Error locking classcode (update)

**Explanation:** An error occurred while updating a record in the indexname\_CCLK table.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

653 LIKE operator may not be used with MOLSIM

**Explanation:** The LIKE operator cannot be applied to MOLSIM(ctab).

**Action:** Use numeric comparison operators (<, <=, etc.) and BETWEEN.

654 Unable to convert MOLSIM threshold to float

**Explanation:** The numeric operand used with MOLSIM(ctab) could not be converted to a 32-bit floating point number.

**Action:** Specify an operand between 0.0 and 100.0.

655 MOLSIM threshold must be between 0 and 100: %f

**Explanation:** The numeric operand used with MOLSIM(ctab) must be between 0.0 and 100.0 inclusive.

**Action:** Check the error message for the incorrect value.

656 Unable to convert MOLSIM maximum threshold to float

See error message 654.

657 MOLSIM maximum threshold must be between 0 and 100: %f

See error message 655.

658 MOLSIM maximum threshold must be greater or equal to minimum threshold

**Explanation:** When MOLSIM(ctab) is used with BETWEEN, the threshold values must be ordered with the smaller value first. (Oracle enforces this for non-domain-index predicates as well, but does not give any error; rather it returns no records.)

**Action:** Specify the query as MOLSIM(...) BETWEEN minimum-threshold AND maximum-threshold

674 Local %s is NULL for index %s.%s

**Explanation:** This error message indicates that an environment item in the local index-specific environment table (indexname\_PROP) is NULL, and that the indexname\_PROP table is corrupted.

**Action:** Drop the index and recreate it, or Contact Dassault Systèmes Customer Support for assistance in correcting the property table.

675 Unable to fetch global %s environment CLOB

**Explanation:** An error occurred while accessing the global environment table.

**Action:** Check for a more specific error message to help diagnose the problem.

696 Unable to create FLEXMATCH data area

See error 25.

697 FLEXMATCH search query can not be NULL

**Explanation:** Generally, this error is caught at a higher level. But if it does occur, it indicates that a FLEXMATCH query must be a molecule and cannot be NULL.

**Action:** Correct the query and reissue it.

698 Unable to interpret FLEXMATCH switches: %s

**Explanation:** The FLEXMATCH options are not valid. The invalid argument is included in the error message.

**Action:** Correct the argument and reissue the query.

700 FLEXMATCH query contains invalid data Sgroups

**Explanation:** The molecule query contains an Sgroup data field name that is not in the allowed list of names as specified by the SETENVFILE('SGROUPFIELDS',...) function.

**Action:** Check for a more specific error that provides the invalid field name. This molecule cannot be used as a query.

701 Unable to initialize FLEXMATCH matching

**Explanation:** An error occurred while preparing the FLEXMATCH query. A common cause for failure is if the query contains SSS query features.

**Action:** Check for a more specific error message to help diagnose the problem.

702 Unable to prepare hash select, SQL=%s

**Explanation:** An error occurred while preparing an SQL statement for a FLEXMATCH search.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

703 Unable to fetch fetch hash value

**Explanation:** An error occurred while executing an SQL statement for a FLEXMATCH search.

**Action:** Check the SQL command and Oracle error message are included to help diagnose the problem.

706 WARNING: A timeout occurred when searching against the molecule at ROWID=%s

**Explanation:** This warning occurs during a CREATE INDEX or ALTER INDEX duplicate check prior to insert or update of a molecule. This error message indicates that there is a molecule present in the table that might be a duplicate. The matching algorithm times out when comparing the molecule being registered with this one.

The ROWID of the potential duplicate is shown in the message.

**Action:** Specify /ALLOW\_TIMEOUT in the FLEXMATCH switches used for the duplicate check if you do not want to consider molecules that time out as duplicates. If this option is not specified, the time out is treated as a duplicate, and the molecule is not registered.

707 WARNING: Timeouts occurred when searching molecules, the first at ROWID=%s

See error 706.

721 Unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing to insert a row into the indexname\_FLEX table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

722 Unable to generate fragment hash values

**Explanation:** An error occurred while generating pre-screen information about the molecule, prior to registration.

**Action:** Contact Dassault Systèmes Customer Support.

723 Unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_FLEX table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

724 Unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_FLEX table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

725 No operation other than %s() $\neq$ 1 is valid

**Explanation:** The FMLAMATCH or FMLALIKE query was not posed as:

SELECT cols FROM table WHERE FMLAMATCH(ctab,query) = 1;

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc. was used.

**Action:** Correct the query and reissue it.

726 Unable to fetch fetch formula index value

**Explanation:** An error occurred while fetching a row from the indexname\_FMLA table.

**Action:** Check the Oracle error message to help diagnose the problem.

727 Unable to fetch fetch formula index value

See error 726.

728 Unable to initialize molecule fetch during formula search

**Explanation:** An error occurred while preparing to fetch molecules during a formula search.

**Action:** Check for a more specific error message to help diagnose the problems.

729 Unable to fetch molecule fetch during formula search

**Explanation:** An error occurred while fetching molecules during a formula search.

**Action:** Check for a more specific error message to help diagnose the problem.

730 Unable to create FMLAMATCH data area

See error 25.

731 %s search query can not be NULL

**Explanation:** Generally, this error should be caught at a higher level and will never appear. However, if it does display, it indicates a FMLAMATCH or FMLALIKE query string might not be NULL.

**Action:** Correct the query.

732 Unable to initialize %s matching

**Explanation:** An error occurred while preparing a FMLAMATCH or FMLALIKE formula search. The most likely cause of the error is an incorrectly formatted query.

**Action:** Check for a more specific error message to help diagnose the problem. Correct the query as necessary.

733 unable to prepare %s index lookup

**Explanation:** An error occurred while preparing a FMLAMATCH or FMLALIKE formula search.

**Action:** Check for a more specific error message to help diagnose the problem.

734 unable to initialize molecule fetch during formula search

See error 728.

744 unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing to insert a row into the indexname FMLA table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

745 unable to generate formula atom counts

**Explanation:** An error occurred while generating formula information for the molecule, prior to registration.

**Action:** Contact Dassault Systèmes Customer Support.

746 unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname FMLA table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

747 unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname FMLA table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

748 Can not get formula index information for query

**Explanation:** An error occurred while fetching query information.

**Action:** Contact Dassault Systèmes Customer Support.

749 unable to prepare formula query, SQL=%s

**Explanation:** An error occurred while preparing to search the indexname FMLA table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

750 unable to execute formula query, SQL=%s

**Explanation:** An error occurred while searching the indexname FMLA table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

751 unable to prepare formula scan, SQL=%s

**Explanation:** An error occurred while preparing to fetch from the indexname\_FMLA table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

752 Unable to fetch formula record

**Explanation:** An error occurred while fetching from the indexname\_FMLA table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

753 Unable to generate formula atom counts

**Explanation:** An error occurred while fetching formula information from a molecule.

**Action:** Contact Dassault Systèmes Customer Support.

762 Unable to insert empty BLOB, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_FSIX table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

763 Unable to set up FS index

See error message 25.

764 Unable to initialize FS index

**Explanation:** An error occurred while initializing an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

775 Error inserting structure into FS update area: %d: %s

**Explanation:** An error occurred inserting a molecule into the FS update area. (This message includes FSLIB error text.)

**Action:** Check for a more specific message that provides the reason for the failure.

776 Error inserting structure into FS update area: %d: %s

See error 775.

777 Error inserting structure into FS delete area: %d: %s

**Explanation:** An error occurred inserting a molecule into the FS delete area. (This message includes FSLIB error text.)

**Action:** Check for a more specific message that provides the reason for the failure.

778 Error inserting structure into FS delete area: %d: %s

See error 777.

779 Unable to determine number of FS index segments, SQL=%s

**Explanation:** An error occurred while querying the FS index table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

781 Unable to initialize FS index

**Explanation:** An error occurred while initializing an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

782 Unable to open FS index

**Explanation:** An error occurred while opening an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

784 Unable to prepare FS update/delete select, SQL=%s

**Explanation:** An error occurred while preparing an FS update or delete area select statement.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

785 Unable to prepare FS update/delete select, SQL=%s

See error 784.

786 Unable to prepare FS update/delete select, SQL=%s

See error 784.

787 Unable to execute FS update/delete select, SQL=%s

**Explanation:** An error occurred while executing an FS update or delete area select statement.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

788 Unable to fetch FS update/delete row, SQL=%s

**Explanation:** An error occurred while fetching from an FS update or delete area SELECT statement.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

789 Unable to allocate buffer while fetching FS update/delete record

See error 25.

790 Unable to fetch FS update/delete row, SQL=%s

See error 788.

791 Unable to execute FS update/delete select, SQL=%s

See error 787.

792 Unable to execute FS update/delete select, SQL=%s

See error 787.

793 Unable to prepare FS update/delete count select, SQL=%s

See error message 784.

794 Unable to execute FS update/delete insert, SQL=%s

**Explanation:** An error occurred while inserting a record into the FS update or delete area.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

795 unable to execute FS update/delete delete, SQL=%s

**Explanation:** An error occurred while deleting a record from the FS update or delete area.

**Action:** Check the SQL command and Oracle error message are included to help diagnose the problem.

796 unable to execute FS update/delete delete, SQL=%s

See error 795.

797 unable to prepare FS update/delete delete, SQL=%s

**Explanation:** An error occurred while preparing a statement to delete a record from the FS update or delete area.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

798 unable to execute FS update/delete delete, SQL=%s

**Explanation:** An error occurred while deleting a record from the FS update or delete area.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

805 unable to prepare fetch of FS index lob

**Explanation:** An error occurred while preparing to fetch a row from the indexname\_FSIX table.

**Action:** Check for a more specific message that provides the reason for the failure.

806 unable to open FS index for rebuilding

**Explanation:** An error occurred while opening an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

807 unable to merge structures in FS index, FS error %d: %s

**Explanation:** An error occurred while merging molecules into the FS index. (This message includes FSLIB error text.)

**Action:** Check for a more specific message that provides the reason for the failure.

808 unable to reopen FS index for rebuilding

See error 806.

809 unable to add structure to FS index, FS error %d: %s

**Explanation:** An error occurred while adding molecules to the FS index. (This message includes FSLIB error text.)

**Action:** Check for a more specific message giving the reason for the failure.

810 unable to open FASTSEARCH index for updating

**Explanation:** An error occurred while opening an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

811 unable to initialize FASTSEARCH structure fetch

**Explanation:** An error occurred while preparing to fetch structures.

**Action:** Check for a more specific message that provides the reason for the failure.

812 Error updating FASTSEARCH index, FS error %d: %s

**Explanation:** An error occurred while updating molecules in the FS index. (This message includes FSLIB error text.)

**Action:** There should be a more specific message giving the reason for the failure.

813 Error closing FASTSEARCH index after update

**Explanation:** An error occurred while closing an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

814 Error incrementing ACCESSNO

**Explanation:** An error occurred while updating the ACCESSNO column in the FS indexname\_FSIX table.

**Action:** Check the Oracle error message to help diagnose the problem.

815 Unable to update pending FASTSEARCH while another user is performing maintenance

**Explanation:** This error occurs when the procedure MDLAUX.UPDATEPENDINGFASTSEARCH is run and another user is already running MDLAUX.UPDATEPENDINGFASTSEARCH, MDLAUX.RECREATEFASTSEARCH, MDLAUX.SCANINDEX, ALTER INDEX, DROP INDEX, DROP TABLE, or TRUNCATE TABLE.

**Action:** Wait until the other user has finished before running this procedure.

816 Unable to open FASTSEARCH index for updating

See error 810.

817 Unable to reopen FASTSEARCH index for updating

See error 810.

818 Error closing FASTSEARCH index after update

See error 813.

819 Error in FASTSEARCH ROLLBACK

**Explanation:** An error occurred while rolling back after a previous failure.

**Action:** Check the Oracle error message to help diagnose the problem.

820 Error in FASTSEARCH COMMIT

**Explanation:** An error occurred while committing after an otherwise successful MDLAUX.UPDATEPENDINGFASTSEARCH operation.

**Action:** Check the Oracle error message to help diagnose the problem.

823 Unable to insert empty BLOB, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_FSIX table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

824 Unable to add more FS segments to datastructure

See error 25.

827 Unable to recreate FASTSEARCH while another user is performing maintenance

**Explanation:** This error message occurs when the procedure MDLAUX.RECREATEFASTSEARCH is run, and another user is already running MDLAUX.UPDATEPENDINGFASTSEARCH, MDLAUX.RECREATEFASTSEARCH, MDLAUX.SCANINDEX, ALTER INDEX, DROP INDEX, DROP TABLE, or TRUNCATE TABLE.

**Action:** Wait until the other user has finished then run this procedure.

830 Error deleting old negative SEGNO FS index rows, SQL=%s

**Explanation:** An error occurred while deleting left over temporary FS index rows.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

831 Unable to insert empty BLOB, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_FSIX table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

832 Unable to initialize FS index

**Explanation:** An error occurred while initializing an FS index.

**Action:** Check for a more specific message that provides the reason for the failure.

833 Unable to open FS index

**Explanation:** An error occurred while opening an FS index.

**Action:** Check for a more specific message giving the reason for the failure.

834 Unable to get update timestamp

**Explanation:** An error occurred while selecting from the indexname\_FSUP table.

**Action:** Check the Oracle error message to help diagnose the problem.

835 Unable to get delete timestamp

**Explanation:** An error occurred while selecting from the indexname\_FSDL table.

**Action:** Check the Oracle error message to help diagnose the problem.

836 Unable to add structure to FS index, FS error %d: %s

See error 809.

837 Error in COMMIT

**Explanation:** An error occurred while trying to commit changes to the FS index during MDLAUX.RECREATEFASTSEARCH.

**Action:** Check the Oracle error message to help diagnose the problem.

838 Unable to reopen FS index for rebuilding

See error 833.

839 Recreate FASTSEARCH failed at ROWID=%s, REGNO=%s

**Explanation:** An error occurred in MDLAUX.RECREATEFASTSEARCH.

**Action:** Check for a more specific error message that provides the reason for the failure and includes the ROWID of the molecule at which the error occurred is included in the message. The molecule at this ROWID is not necessarily the cause of the failure.

840 Unable to merge structures in FS index, FS error %d: %s

**Explanation:** An error occurred while merging molecules into the FS index. (This message includes FSLIB error text.)

**Action:** Check for a more specific message that provides the reason for the failure.

842 Error deleting old FS index rows, SQL=%s

**Explanation:** An error occurred while deleting the old FS index segment(s).

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

843 Error updating negative SEGNO values, SQL=%s

**Explanation:** An error occurred while trying to update the temporary FS index segment(s) to be the permanent segment(s).

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

844 Error in COMMIT

See error 837.

845 Unable to delete old FS update rows

Warning

**Explanation:** This error message indicates an error occurred while trying to remove rows from the FS update area (indexname\_FSUP) that have been successfully updated in the FS index. The presence of these rows can affect SSS searching, resulting in missed or extra hits.

**Action:** Check the Oracle error message to help diagnose the problem. BIOVIA recommends that you rebuild the FS index if this error occurs.

846 Unable to commit after delete of old FS update rows

See error 845.

847 Unable to delete old FS delete rows

Warning

**Explanation:** This error message indicates an error occurred while trying to remove rows from the FS delete area (indexname\_FSDL) that have been successfully delete from the FS index. The presence of these rows can affect SSS searching, resulting in missed or extra hits.

**Action:** Check the Oracle error message to help diagnose the problem. BIOVIA recommends that you rebuild the FS index if this error occurs.

848 Unable to commit after delete of old FS delete rows

See error 847.

852 Unable to fetch generic exact match index value

**Explanation:** An error occurred while fetching from the indexname\_GENX table.

**Action:** Check the Oracle error message to help diagnose the problem.

853 Unable to initialize molecule fetch during generic exact match search

**Explanation:** An error occurred while preparing to fetch molecules during a generic exact match search.

**Action:** Check for a more specific error message to help diagnose the problem.

854 Unable to fetch molecule during generic exact match search

**Explanation:** An error occurred while fetching molecules during a generic FLEXMATCH search.

**Action:** Check for a more specific error message to help diagnose the problem.

855 Cannot perform a generic exact match search against non-generic molecule table

**Explanation:** The generic FLEXMATCH search can only be used if the domain index was created with the GENERICS parameter.

858 Unable to initialize generic exact match search

**Explanation:** An error occurred while preparing the generic FLEXMATCH match QUERY.

**Action:** Check for a more specific error message to help diagnose the problem.

859 Unable to get generic range data for generic exact match search

**Explanation:** An error occurred while fetching information from the query molecule.

**Action:** This is an unusual error. Report the error to Dassault Systèmes Customer Support

860 Unable to prepare generic exact match molecule lookup

**Explanation:** An error occurred while preparing to fetch molecules during a generic FLEXMATCH search.

**Action:** Check for a more specific error message to help diagnose the problem.

874 Unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing an insert into the indexname\_GENX table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

875 Unable to generate generic range data

**Explanation:** An error occurred while fetching information from the molecule during registration.

**Action:** This is an unusual error. Report the error to Dassault Systèmes Customer Support

876 Unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_GENX table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

877 Unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_GENX table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

878 Unable to prepare or execute generic exact match query, SQL=%s

**Explanation:** An error occurred while preparing or executing a query against the indexname\_GENX table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

879 Unable to prepare ISGENERIC query, SQL=%s

**Explanation:** An error occurred while preparing a query over the indexname\_GENX table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

880 Unable to prepare generic exact match scan, SQL=%s

**Explanation:** An error occurred while preparing a query over the indexname\_GENX table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

881 Unable to fetch generic exact match record

**Explanation:** An error occurred while fetching a row from the indexname\_GENX table.

**Action:** Check the Oracle error message to help diagnose the problem.

882 Unable to generate generic range data

**Explanation:** An error occurred while fetching information from the molecule during scanning.

**Action:** This is an unusual error. Report the error to Dassault Systèmes Customer Support

883 Unable to initialize OVERLAP matching

**Explanation:** An error occurred while preparing the OVERLAP query.

**Action:** Check a more specific error message to help diagnose the problem.

884 No operation other than OVERLAP() $\neq$ 1 is valid

**Explanation:** The OVERLAP query was not posed as:

```
SELECT <cols> FROM <table> WHERE  
OVERLAP(<ctab>,<query>) = 1;
```

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc., was used.

**Action:** The query must be posed as above.

885 OVERLAP search may only be used with a GENERICS index

**Explanation:** The OVERLAP search can only be used if the domain index was created with the GENERICS parameters.

886: Unable to create OVERLAP data area

See error 25.

887 OVERLAP search query can not be NULL

**Explanation:** An OVERLAP query must be a molecule, it cannot be NULL.

**Action:** This error is usually caught at a higher level and should not appear. However, it does, the query must be corrected.

888 Unable to determine query information

**Explanation:** An error occurred while fetching information from the molecule during OVERLAP query preparation.

**Action:** This is an unusual error. Report the error to Dassault Systèmes Customer Support

889 Unable to open FS index for OVERLAP search

**Explanation:** An error occurred while opening an FS index.

**Action:** Check a more specific error message that gives the reason for the failure.

890 Unable to initialize OVERLAP matching

See error 883.

892 Cannot not perform a generic SSS search against a non-generic molecule table

**Explanation:** The generic SSS search can only be used if the domain index was created with the GENERICS parameters.

895 Unable to determine generic SSS query information

**Explanation:** An error occurred while fetching information from the molecule during generic SSS query preparation.

**Action:** This is an unusual error. Report the error to Dassault Systèmes Customer Support

896 This query cannot be used in a generic SSS search

**Explanation:** This error indicates that the query contains feature that make it unusable as a generic SSS query. For example, a generic SS query cannot itself be generic, nor can it contain Sgroups.

**Action:** See the Direct documentation for the complete list of restriction.

897 unable to open FS index for generic SSS search

**Explanation:** An error occurred while opening an FS index.

**Action:** Check a more specific error message that gives the reason for the failure.

898 unable to initialize generic SSS matching

**Explanation:** An error occurred while preparing the generic SSS query.

**Action:** Check a more specific error message that gives the help to diagnose the problem.

904 unable to determine free space, SQL=%s

**Explanation:** An error occurred while selecting from the USER\_FREE\_SPACE view.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

905 unable to get default tablespace

**Explanation:** An error occurred while selecting the default tablespace of the user.

**Action:** Contact Dassault Systèmes Customer Support.

906 unable to prepare or execute SQL: %s

**Explanation:** An error occurred while selecting from the USER\_FREE\_SPACE view.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem. If you require further assistance, Contact Dassault Systèmes Customer Support.

907 unable to fetch from SQL: %s

**Explanation:** An error occurred while fetching from the USER\_FREE\_SPACE view.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem. If you require further assistance, Contact Dassault Systèmes Customer Support.

916 unable to compute molecular weight

**Explanation:** An error occurred while computing the molecular weight of a molecule.

**Action:** Contact Dassault Systèmes Customer Support.

917 unable to compute molecular formula

**Explanation:** An error occurred while computing the molecular formula of a molecule.

**Action:** Contact Dassault Systèmes Customer Support.

918 There are no SUBSET key definitions available

**Explanation:** This error indicates that the user has specified a SUB or SUBSET argument to the MOLKEYS operator. However, the environment does not include any MOLSKEYDEFS entry to define what the key subset is.

**Action:** The SUB argument cannot be used in this case. Correct the argument.

919 unable to obtain molecule 2D key weights

**Explanation:** An error occurred while fetching the SSS key weights from the environment.

**Action:** Contact Dassault Systèmes Customer Support.

924 unable to generate 2D molecule keys for REGNO=%s

**Explanation:** An error occurred while generating 2D keys for a molecule.

**Action:** Check for a more specific error message to help diagnose the problem.

927 Previous message occurred while inserting molecule at ROWID=%s

**Explanation:** This message is printed after other molecule insertion errors, and provides the ROWID of the insertion.

929 Previous message occurred while updating molecule at ROWID=%s

**Explanation:** This message is printed after other molecule update errors, and provides the ROWID of the update.

935 Error in COMMIT

**Explanation:** An error occurred while periodically committing during an index build or rebuild operation.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

936 Index rebuild failed at ROWID=%s, REGNO=%s

**Explanation:** When an error occurs during an index build or rebuild operation, this message is output. It gives the reaction table ROWID of the molecule where the error occurred; it might also give the conversion table regno.

**Action:** If the error occurred due to a invalid molecule, the ROWID can be used to obtain the molecule and correct it.

937 Too many molecule errors, key generation terminated

**Explanation:** During molecule key generation (from ALTER INDEX REBUILD), up to 100 errors are allowed during molecule fetching. This message indicates that more errors have occurred, and that key generation will be terminated with an error.

**Action:** Check for more specific errors messages to help diagnose the problem.

938 Error in COMMIT

See error 935.

939 Error in COMMIT

See error 935.

942 UNIQUE parameter does not specify valid FLEXMATCH switches: %s

**Explanation:** The FLEXMATCH argument specified with the UNIQUE parameter is not valid. The invalid argument is included in the message.

**Action:** Correct the argument.

944 Unable to get UNIQUE setting for index

**Explanation:** This error message indicates an error fetching the current duplicate setting.

**Action:** Contact Dassault Systèmes Customer Support.

945 Molecule duplicate check failed

**Explanation:** An error occurred while preparing the molecule duplicate check.

**Action:** Check more specific error messages to help diagnose the problem.

946 Molecule duplicate check lock failed

**Explanation:** An error occurred while trying to lock a bucket prior to performing a molecule duplicate check.

**Action:** Check for more specific error messages to help diagnose the problem.

947 molecule duplicate check failed

**Explanation:** An error occurred while performing a molecule duplicate check.

**Action:** Check for more specific error messages to help diagnose the problem.

948 Duplicate molecule found at ROWID=%s

**Explanation:** This error message indicates that a duplicate molecule already exists in the index, and the current molecule cannot be registered. The ROWID of the duplicate molecule is included in the message.

**Action:** If this message occurs while inserting a new molecule, or updating an existing molecule, the molecule at the given ROWID is a duplicate of the molecule being inserted or used for updating. If this message occurs while creating a new domain index or rebuilding an existing domain index, use error message 949 Duplicate molecule found for ROWID=%s, which follows, to find the query molecule for this molecule that is a duplicate.

949 Duplicate molecule found for ROWID=%s

**Explanation:** This error message indicates that the molecule whose ROWID is given has duplicates, and the index cannot be created or rebuilt.

**Action:** Check the one or more errors with number 948 Duplicate molecule found at ROWID=%s, which precedes this one. Use these messages to find the ROWID of the molecule that is a duplicate of this one. There might be more than one duplicate.

967 molecule domain index creation failed

**Explanation:** This is the general exception error that is posted when CREATE INDEX fails.

**Note:** Oracle created the index, even though the cartridge has indicated an error to Oracle.

**Action:** Drop the index because it is unusable. Use the following command: `DROP INDEX indexname;`

968 molecule index alter failed

**Explanation:** This is the general exception error that is posted during index alter, which occurs during ALTER INDEX, fails.

**Action:** See error 143.

969 molecule index truncate failed

**Explanation:** This is the general exception error that is posted when the index truncation, which occurs during TRUNCATE TABLE, fails.

**Action:** Check for a more specific error message to help diagnose the problem.

970 molecule index drop failed

**Explanation:** This is the general exception error that is posted when the index drop, which occurs during DROP TABLE or DROP INDEX, fails.

**Action:** Check for a more specific error message to help diagnose the problem.

## 971 Molecule index insert failed

**Explanation:** This is the general exception error that is posted when the index insert, which occurs during INSERT INTO table ..., fails.

**Action:** Check for a more specific error message to help diagnose the problem.

## 972 Molecule index delete failed at ROWID=%s

**Explanation:** This is the general exception error that is posted when the index delete, which occurs during DELETE FROM table ..., fails.

**Action:** Use the ROWID of the reaction that is provided to help diagnose the problem.

## 973 Molecule index update failed at ROWID=%s

**Explanation:** This is the general exception error that is posted when the index update, which occurs during UPDATE table ..., fails.

**Action:** Use the ROWID of the reaction that is provided to help diagnose the problem.

## 974 Operator '%s' does not have an indexed implementation

**Explanation:** This error usually indicates that the MOLWT, MOLFMLA, or MOLKEYS operator is being used in the WHERE clause of a query.

**Action:** These operators do not have a high-speed indexed implementation, so to use these in the WHERE clause, force Oracle to bypass the index by using them in a function, for example:  
SELECT ... FROM ... WHERE (MOLWT(ctab) + 0) > 200;

## 976 Molecule index search initialization failed

**Explanation:** This is the general exception error that is posted when an indexed search fails during initialization.

**Action:** Generally, this failure is due to an invalid query. Check for a more specific error message to help diagnose the problem. Then correct the query.

## 978 Error in OCIStringAssignText

**Explanation:** An Oracle error occurred while returning search hits to Oracle.

**Action:** Check the Oracle error message to help diagnose the problem.

## 979 Error in OCICollAppend

See error 978.

## 980 Error in OCIStringAssignText

See error 978.

## 981 Error in OCICollAppend

See error 978.

## 982 E Molecule index search fetch failed

**Explanation:** This is the general exception error that is posted when an indexed search fails while fetching hits.

**Action:** Check for a more specific error to help diagnose the problem.

990 Unable to allocate LOB descriptor

**Explanation:** An error occurred while allocating an Oracle descriptor.

**Action:** Check the Oracle error to help diagnose the problem.

991 Unable to create temporary LOB

**Explanation:** An error occurred while creating a temporary LOB.

**Action:** Check the Oracle error to help diagnose the problem.

992 Unable to free temporary LOB

**Explanation:** An error occurred while freeing a temporary LOB.

**Action:** Check the Oracle error to help diagnose the problem.

993 Unable to define object fetch parameter

**Explanation:** An error occurred while preparing a SQL statement.

**Action:** Check the Oracle error to help diagnose the problem.

994 Unable to get type descriptor for %s.%s

See error 993.

995 Unable to define object

See error 993.

996 Invalid value for %s: %s

**Explanation:** This error indicates that the user has specified an invalid value for a PARAMETERS argument. The parameter name (keyword) and the invalid value are included in the message.

**Action:** Correct the value, and reissue the command.

998 Invalid parameter keyword or value: %s

**Explanation:** This error message indicates that the parameter name (keyword) or value in a PARAMETERS argument is invalid.

**Action:** Correct the parameter name and/or value, and reissue the command.

999 Invalid parameter keyword: %s

See error 998.

1000 Keyword not valid for CREATE INDEX: %skeyword not valid for ALTER INDEX REBUILD: %skeyword not valid for ALTER INDEX: %skeyword not valid for MDLAUX.SCANINDEX: %skeyword not valid for MDLAUX.UPDATEPENDINGFASTSEARCH: %skeyword not valid for MDLAUX.RECREATEFASTSEARCH: %skeyword not valid for MDLAUX.RECREATEKEYS: %skeyword not valid for MDLAUX.UPDATEPENDINGINVERSIONS:

%skeyword not valid for CREATE INDEX on reactions: %skeyword not valid for CREATE INDEX on molecules: %skeyword not valid for CREATE INDEX on models: %s

**Explanation:** This error indicates that the parameters name (keyword) is valid, but does not apply to the current operation.

For example, the EXTENTS keyword is only valid with CREATE INDEX, not with ALTER INDEX. An additional clause can be added to the error if the option is only invalid for a particular type, for example, reactions.

**Action:** Remove or correct the invalid parameter name, and reissue the command.

1001 keyword is missing value: %s

**Explanation:** The specified parameter name (keyword) requires a value, and none was provided.

**Action:** Provide a value for the parameter name, and reissue the command.

1002 keyword must not have value: %s

**Explanation:** The specified parameter name (keyword) does not take a value, but one was provided.

**Action:** Remove the value for the parameter name, and reissue the command.

1007 Invalid value for MAXROWS parameter: %s

**Explanation:** An invalid argument to the MAXROWS parameter name was used.

**Action:** Specify an integer, optionally followed by the multiplier K (1024) or M (1048576).

1008 Invalid value for %s parameter: %s

**Explanation:** An invalid argument to one of the integer parameter names was used. The parameter name is provided in the message, and it might one of several.

**Action:** Specify an integer, optionally followed by the multiplier K (1024) or M (1048576).

1009 Invalid value for PREALLOCATE parameter: %s

**Explanation:** An invalid argument to the PREALLOCATE parameter name was used.

**Action:** Specify one of NONE, NOSTORAGECHECK, or ALL.

1015 WARNING: A timeout occurred when searching against the reaction at ROWID=%s

Warning

**Explanation:** This warning occurs during a CREATE INDEX or ALTER INDEX duplicate check prior to insert or update of a reaction. This error message indicates that there is a reaction present in the table that might be a duplicate. The matching algorithm times out when comparing the reaction being registered with this one. The ROWID of the potential duplicate is shown in the message.

**Action:** Specify /ALLOW\_TIMEOUT in the FLEXMATCH switches used for the duplicate check if you do not want to consider reactions that time out as duplicates. If this option is not specified, the time out is treated as a duplicate, and the reaction is not registered.

1016 WARNING: Timeouts occurred when searching reactions, the first at ROWID=%s

See error 1015.

1017 unable to prepare storage clause for %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create the indexname\_RFLX table.

**Action:** Check for a more specific message that provides the reason for the failure. See also error 642.

1018 unable to prepare storage clause for %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create the indexname\_RFLX1 index.

**Action:** Check for a more specific message that provides the reason for the failure. See also error 642.

1019 unable to prepare storage clause for %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create the indexname\_RFLX2 index.

**Action:** Check for a more specific message that provides the reason for the failure. See also error e 642.

1020 unable to prepare storage clause for %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create the indexname\_RSGP table.

**Action:** Check for a more specific message that provides the reason for the failure. See also error 642.

1021 unable to prepare storage clause for %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create the indexname\_RSGP1 index.

**Action:** Check for a more specific message that provides the reason for the failure. See also error 642.

1022 unable to prepare storage clause for %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create the indexname\_RSGP2 index.

**Action:** Check for a more specific message that provides the reason for the failure. See also error 642.

1029 Error in COMMIT

See error 150.

1041 UNIQUE parameter does not specify valid RXNFLEXMATCH switches: %s

**Explanation:** The RXNFLEXMATCH argument specified with the UNIQUE parameter are not valid, the invalid argument is included in the message.

**Action:** Correct the argument.

1042 UNIQUE parameter can not include SUBSET flag

**Explanation:** The RXNFLEXMATCH argument specified with the UNIQUE parameter may not include the SUBSET flag.

**Action:** Remove the SUBSET option, and reissue the command.

1043 Unable to get UNIQUE setting for index

**Explanation:** This error indicates an error fetching the current duplicate setting.

**Action:** Contact Dassault Systèmes Customer Support.

1045 Reaction duplicate check lock failed

**Explanation:** An error occurred while trying to lock a bucket prior to performing a reaction duplicate check.

**Action:** Check for more specific errors to help diagnose the problem.

1046 Reaction duplicate check failed

**Explanation:** An error occurred while performing a reaction duplicate check.

**Action:** Check for a more specific errors to help diagnose the problem.

1047 Duplicate reaction found at ROWID=%s

**Explanation:** This error message indicates that a duplicate molecule already exists in the index, and the current molecule cannot be registered. The ROWID of the duplicate molecule is included in the message.

**Action:** If this message occurs while inserting a new reaction or updating an existing reaction, the reaction at the given ROWID is a duplicate of the reaction being inserted or used for updating. If this message occurs while creating a new domain index or rebuilding an existing domain index, use error message, which follows, to find the query reaction for this reaction that is a duplicate.

1048 Duplicate reaction found for ROWID=%s

**Explanation:** This error message indicates that the reaction whose ROWID is given has duplicates, and the index cannot be created or rebuilt.

**Action:** Check the one or more errors with number 1047, which precedes this one. Use these messages to find the ROWID of the reaction that is a duplicate of this one. There might be more than one duplicate.

1049 Unable to unpack molecule at ROWID/REGNO=%s

**Explanation:** This error message indicates that a binary packed molecule (BLOB) has become corrupted. The ROWID or REGNO of the row containing the molecule is provided.

**Action:** Update the molecule from a backup source. The molecule might need to be deleted first, and/or the index might need to be dropped before updating the molecule and re-created after the update.

1050 Unable to unpack molecule at ROWID=%s

See error 1049.

1051 Molstructure search query is not a valid molecule

**Explanation:** The query argument to the SSS, FLEXMATCH, etc. operator could not be converted into an internal format.

One common problem is that a molfile file name is either misspelled, or the file is not readable by the Oracle extproc process.

**Action:** Correct the problem, and reissue the query.

1053 Molecule 2D KEYS scan has errors, use MDLAUX.LOGTABLE to view errors  
See error 364.

1057 Unable to initialize hash table lookup, SQL=%s  
See error 366.

1059 Unable to prepare hash value fetch, SQL=%s  
See error 366.

1060 Unable to fetch hash value at ROWID=%s, SQL=%s

**Explanation:** This error occurs when a molecule key search indicates that there is an error in the molecule keys.

**Action:** View the output from MDLAUX.SCANINDEX using MDLAUX.LOGTABLE, and then rebuild the molecule keys using ALTER INDEX REBUILD PARAMETERS ('KEYS') or MDLAUX.RECREATEKEYS.

1061 Molecule FLEXMATCH hash scan has errors, use MDLAUX.LOGTABLE to view errors  
See error 364.

1063 Unable to initialize formula table scan  
See error 366.

1065 FORMULA index scan has errors, use MDLAUX.LOGTABLE to view errors  
See error 364.

1067 Unable to initialize generic exact match table scan  
See error 366.

1069 Generic exact-match index scan has errors, use MDLAUX.LOGTABLE to view errors  
See error 364.

**Note:** You might need to rebuild FLEXMATCH to correct the problem.

1070 Unable to open FASTSEARCH index for validation

**Explanation:** This error occurs when a reaction scan indicates that there is an error in the searching aid used for the SSS search.

**Action:** View the output from MDLAUX.SCANINDEX using MDLAUX.LOGTABLE, and then rebuild the searching aid using ALTER INDEX REBUILD PARAMETERS ('FASTSEARCH').

1071 FASTSEARCH validation has errors, use MDLAUX.LOGTABLE to view errors  
See error 364.

1073 Unable to open molecule FASTSEARCH index for scan

See error 366.

1076 No operation other than SIMILAR() $=$ 1 is valid

**Explanation:** The SIMILAR query was not posed as:

```
SELECT cols FROM table WHERE SIMILAR(ctab,query,opts) = 1;
```

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc., was used.

**Action:** Correct query as shown above.

1077 SIMILAR search query can not be NULL

**Explanation:** This error should be caught at a higher level and never appear. However, if it does appear, a SIMILAR query must be a molecule, it cannot be NULL.

**Action:** Correct the query and reissue it.

1078 unable to initialize %s matching

**Explanation:** An error occurred while preparing an SSS or SSS3D query.

**Action:** Check for a more specific error message to help diagnose the problem.

1081 unable to convert molfile string to Chime string

**Explanation:** An error occurred in SSSHIGHLIGHT or SSS3DHIGHLIGHT while converting a molfile string to a Chime string.

**Action:** Check for a more specific error message to help diagnose the problem.

1082 No operation other than %s() $=$ 1 is valid

**Explanation:** The SSS or SSS3D query was not posed as:

```
SELECT cols FROM table WHERE SSS[3D](ctab,query[,opts]) = 1;
```

Instead, an operator such as less than (<), greater than (>), equal to some number other than 1, etc., was used.

**Action:** Correct the query as shown above.

1083 unable to create SSS data area

See error 25.

1084 SSS search query can not be NULL

**Explanation:** This error should be caught at a higher level and never appear. However, if it does appear, an SSS or SSS3D query must be a molecule, it cannot be NULL.

**Action:** Correct the query.

1087 Unable to determine query information

**Explanation:** An error occurred while fetching information from the molecule during SSS query preparation.

**Action:** Contact Dassault Systèmes Customer Support.

1088 unable to open FS index for %s search

**Explanation:** An error occurred while opening an FS index prior to an SSS search.

**Action:** Check for a more specific message that provides the reason for the failure.

1089 Unable to initialize %s matching

See error 1078.

1092 Unable to open global buffer client

**Explanation:** An error occurred during LOB buffering.

**Action:** Check for a more specific message that provides the reason for the failure.

1093 Unable to close global buffer client

See error 1092.

1095 Unable to flush global buffer client

See error 1092.

1108 Unable to initialize FASTSEARCH structure fetch

See error 811.

1109 Error updating FASTSEARCH index, FS error %d: %s

See error 812.

1110 Error closing FASTSEARCH index after update

See error 813.

1111 Error in FASTSEARCH COMMIT

**Explanation:** An error occurred while committing during MDLAUX.RECREATEFASTSEARCH.

**Action:** Use the Oracle error message that is included to help diagnose the problem.

1112 E MDLAUX.SCANINDEX scan(s) failed

**Explanation:** One or more of the scan operations in MDLAUX.SCANINDEX failed.

**Action:** Check the log table (MDLAUX.LOGTABLE) and errors (MDLAUX.ERRORS) for detailed information about which scan failed and where. Use ALTER INDEX REBUILD to rebuild all or part of the index to correct the problem.

1113 E Error converting packed reaction to rxnfile or Chime CLOB

**Explanation:** An error occurred while converting a packed binary reaction to a rxnfile or Chime CLOB.

**Action:** Check for a more specific message that provides the reason for the failure.

1114 E Error converting packed molecule to molfile or Chime CLOB

**Explanation:** An error occurred while converting a packed binary molecule to a molfile or Chime CLOB.

**Action:** Check for a more specific message that provides the reason for the failure.

1115 E Error setting molname

**Explanation:** An error occurred in MDLAUX.SETMOLNAME.

**Action:** Check for a more specific message that provides the reason for the failure.

1116 Error converting string to Chime

**Explanation:** An error occurred while converting an uncompressed string to a Chime string.

**Action:** Contact Dassault Systèmes Customer Support.

1117 Error converting Chime to string

**Explanation:** An error occurred while converting a Chime string to an uncompressed string.

**Action:** Contact Dassault Systèmes Customer Support.

1119 WARNING: FLEXMATCH index is disabled - doing full table scan

Warning

**Explanation:** This error message indicates that the flexmatch hash index has been disabled, and that the molecule flexmatch search will thus use a full table scan.

The search will complete, but can be very slow.

1120 WARNING: Formula index is disabled - doing full table scan

Warning

**Explanation:** This error message indicates that the formula index has been disabled, and that the molecule formula search will thus use a full table scan.

The search will complete, but can be very slow.

1121 Generic exact match index is disabled - cannot perform indexed search

**Explanation:** This error indicates that the generic exact-match index has been disabled, and that the molecule formula search will thus use a full-table scan.

**Action:** You can run the search using a full-table scan by either using a hint to disable the domain index, or by adding zero to the query, for example:

```
... WHERE FLEXMATCH(CTAB, 'QUERY', 'GENERIC') + 0 = 1;
```

**Note:** This search will be very slow if using a full-table scan.

1124 WARNING: RXNFLEXMATCH index is disabled - doing full table scan

Warning

**Explanation:** This is a warning message, it indicates that the reaction flexmatch hash index has been disabled and that the reaction flexmatch search will thus use a full table scan.

The search will complete, but might be very slow.

1125 RXNKEYS index is disabled - cannot perform indexed search

**Explanation:** This error indicates that the reaction keys index has been disabled, and that the reaction similarity search cannot be completed.

**Action:** Run the search using a full table scan by either using a hint to disable the domain index, or by adding zero to the query, for example:

```
... WHERE RXNSIM(ctab, 'query', 'opts') + 0 = 1;
```

This search can be very slow if using a full table scan.

1126 WARNING: Reaction keys index is disabled - doing full table scan

Warning

**Explanation:** This is error message indicates that the reaction keys index has been disabled, and that the RSS search will thus use a full table scan.

The search will complete, but might be very slow.

1127 MOL2DKEYS index is disabled - cannot perform indexed search

Warning

**Explanation:** This error indicates that the molecule 2D keys index has been disabled, and that the molecule similarity search cannot be completed.

**Action:** Run the search using a full table scan by either using a hint to disable the domain index, or by adding zero to the query, for example:

```
... WHERE SIMILAR(ctab, 'query', 'opts')+0 = 1;
```

This search can be very slow if using a full table scan.

1128 WARNING: Molecule keys index is disabled - doing full table scan

Warning

**Explanation:** This is error message indicates that both the FASTSEARCH index and the molecule 2D keys index have been disabled, and that the SSS or SSS3D search will thus use a full table scan.

The search will complete, but might be very slow.

1131 Cannot have the same ENABLE and DISABLE option

**Explanation:** This error indicates that the same argument was provided to both ENABLE= and DISABLE= in an ALTER INDEX statement. You cannot both enable and disable the same item.

**Action:** Correct the ALTER INDEX statement and reissue the statement.

1132 UNIQUE can not be combined with DISABLE=FLEXMATCH

**Explanation:** You cannot specify molecule duplicate checking and disable the molecule flexmatch index at the same time. The flexmatch index is required in order to perform the duplicate check.

**Action:** Remove one of these options from your CREATE INDEX or ALTER INDEX command.

1133 UNIQUE can not be combined with DISABLE=FLEXMATCH

**Explanation:** You cannot specify reaction duplicate checking and disable the reaction flexmatch index at the same time. The flexmatch index is required in order to perform the duplicate check.

**Action:** Remove one of these options from your CREATE INDEX or ALTER INDEX command.

1139 Invalid internal option for DISABLE: %s

**Explanation:** This error should not occur, it indicates that a row in the index' property table contains an invalid value.

**Action:** Drop and recreate the domain index.

1140 ROWID conversion table scan has errors, use MDLAUX.LOGTABLE to view

errors

See error 364.

1141 Unable to allocate memory for KEYS scan

See error 25.

1142 Unable to allocate memory for reaction FLEXMATCH scan

See error 25.

1143 Unable to allocate memory for molecule FLEXMATCH scan

See error 25.

1144 Unable to allocate memory for FORMULA scan

See error 25.

1145 Unable to allocate memory for generic exact match scan

See error 25.

1146 Unable to allocate memory for molecule FASTSEARCH scan

See error 25.

1147 Unable to allocate memory for molecule CTAB scan

See error 25.

1148 Unable to allocate memory for reaction CTAB scan

See error 25.

1151 FASTSEARCH index scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

1152 Molecule CTAB scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

1153 Reaction CTAB scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

1160 Unable to create SIMILAR data area

See error 25.

1164 Error fetching from structure table just past REGNO=%s

See error message 1166. Only the conversion table REGNO is available.

1165 Error fetching from structure table just past ROWID=%s

See error message 1166. Only the structure table ROWID is available.

1166 Error fetching from structure table just past ROWID=%s, REGNO=%s

**Explanation:** An error occurred while fetching structures from either the structure table or from the structure table joined with the ROWID conversion table.

**Action:** The ROWID and conversion table REGNO of the row that had been processed just before the failure is given to help in diagnosing the problem. Also check for a more specific error message to help diagnose the problem.

1167 Error fetching from structure table

**Explanation:** See error message 1166. Because the fetch was not ordered, there is no information available to indicate which row was being fetched.

**Action:** Check for a more specific error message to help diagnose the problem.

1168 WARNING, Error unpacking reaction at ROWID=%s, record will not be considered a duplicate

**Explanation:** The reaction at the specified ROWID cannot be unpacked, and will not be used as a query to check for duplicates.

**Action:** The reaction is corrupted in some way, and should be re-registered.

1169 WARNING: Error unpacking molecule at ROWID=%s, record will not be considered a duplicate  
Warning

**Explanation:** The molecule at the specified ROWID cannot be unpacked, and will not be used as a query to check for duplicates.

**Action:** The molecule is corrupted in some way, and should be re-registered.

1170 WARNING: Ignoring previous unpack errors during molecule delete  
Warning

**Explanation:** The molecule being deleted at the specified ROWID cannot be unpacked, and will not be removed from the FASTSEARCH index. This should not result in incorrect SSS search results.

**Action:** The molecule is corrupted in some way, and should be re-registered.

1171 WARNING: Ignoring previous unpack errors during molecule update  
Warning

**Explanation:** The old molecule being updated at the specified ROWID cannot be unpacked, and will not be removed from the FASTSEARCH index. This might result in incorrect SSS search results.

**Action:** The molecule is corrupted in some way, and should be re-registered.

1172 Unable to allocate memory for SGROUPDATA scan  
See error 25.

1173 Unable to initialize Sgroup data lookup, SQL=%s  
See error 366.

1174 Unable to fetch Sgroup data at ROWID=%s, SQL=%s

See error 370.

1175 SGROUPDATA scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

1176 Unable to truncate table, SQL=%s

**Explanation:** An error occurred while truncating a table belonging to the domain index.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1179 Unable to rename table, SQL=%s

**Explanation:** An error occurred while renaming a table belonging to the domain index.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1180 Unable to rename index, SQL=%s

**Explanation:** An error occurred while renaming an index belonging to the domain index.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1183 Previous MDLAUX.RECREATEFASTSEARCH operation was interrupted, FASTSEARCH index cannot be updated until recreate is complete

**Explanation:** This error occurs with ALTER INDEX [REBUILD] PARAMETERS ('UPDATEPENDINGFASTSEARCH') and indicates that the FASTSEARCH index cannot be updated at this time. A previous attempt to recreate the index using MDLAUX.RECREATEFASTSEARCH failed, and the index must be successfully recreated before pending records can be updated.

**Action:** Use either MDLAUX.RECREATEFASTSEARCH or ALTER INDEX REBUILD PARAMETERS ('FASTSEARCH') to recreate the index.

1184 Previous MDLAUX.RECREATEFASTSEARCH operation was interrupted, FASTSEARCH index cannot be updated until recreate is complete

**Explanation:** This error occurs with MDLAUX.UPDATEPENDINGFASTSEARCH and indicates that the FASTSEARCH index cannot be updated at this time. A previous attempt to recreate the index using MDLAUX.RECREATEFASTSEARCH failed, and the index must be successfully recreated before pending records can be updated.

**Action:** Use either MDLAUX.RECREATEFASTSEARCH or ALTER INDEX REBUILD PARAMETERS ('FASTSEARCH') to recreate the index.

1185 Unable to determine number of negative FS index segments, SQL=%s

**Explanation:** An error occurred while fetching the row count in the indexname\_FSIX table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1186 Unable to restart loop for FS index rebuild

**Explanation:** An error occurred while preparing a SQL statement to loop over molecules or reactions in the MDLAUX.RECREATEFASTSEARCH function.

**Action:** Check for a more specific error message to help diagnose the problem.

1187 Unable to determine number of negative FS index segments, SQL=%s

See error message 1185.

1190 Unable to determine query information

**Explanation:** An error occurred while fetching information from the molecule during RSS query preparation.

**Action:** Contact Dassault Systèmes Customer Support.

1191 Unable to initialize RSS highlighting

**Explanation:** An error occurred while preparing an RSSSSSHIGHLIGHT query.

**Action:** Check for a more specific error message to help diagnose the problem.

1192 Unable to open FS index for RSS search

**Explanation:** An error occurred while opening an FS index prior to an RSS search.

**Action:** Check for a more specific message giving the reason for the failure.

1193 Unable to allocate memory for reaction FASTSEARCH scan

See error 25.

1194 Unable to open reaction FASTSEARCH index for scan

See error 366.

1199 E Error recreating keys

**Explanation:** An error occurred while running MDLAUX.RECREATEKEYS.

**Action:** Check for a more specific message that provides the reason for the failure.

1202 Unable to recreate keys while another user is performing maintenance

**Explanation:** This error occurs when you try to run the procedure MDLAUX.RECREATEKEYS, and another user is already running MDLAUX.UPDATEPENDINGINVERSIONS, MDLAUX.RECREATEKEYS, MDLAUX.SCANINDEX, ALTER INDEX, DROP INDEX, DROP TABLE, or TRUNCATE TABLE.

**Action:** Wait until the other user has finished before running this procedure.

1203 Error deleting old negative key chunks, SQL=%s

**Explanation:** An error occurred during processing of the inverted key table while executing MDLAUX.RECREATEKEYS.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1204 Error deleting old negative 3D key chunks, SQL=%s

See error 1203.

1205 Unable to get sequential key timestamp

**Explanation:** An error occurred while selecting from the sequential key table.

**Action:** Check the Oracle error message to help diagnose the problem.

1206 Recreate keys failed at ROWID=%s, REGNO=%s

**Explanation:** An error occurred in MDLAUX.RECREATEKEYS.

**Action:** Check for a more specific error message that provides the reason for the failure. The ROWID of the molecule at which the error occurred is included in the message. The molecule at this ROWID is not necessarily the cause of the failure.

1207 Unable to restart loop for key index rebuild

**Explanation:** An error occurred while preparing a SQL statement to loop over molecules or reactions in the MDLAUX.RECREATEKEYS function.

**Action:** Check for a more specific error message to help diagnose the problem.

1208 Error deleting old inverted key index rows, SQL=%s

See error 1203.

1210 Error updating negative CHUNKNO values, SQL=%s

See error 1203.

1213 WARNING: Unable to delete old sequential key rows

Warning

**Explanation:** This indicates that an error occurred while trying to remove rows from the sequential keys which have been successfully processed into the inverted keys.

**Action:** Check the Oracle error message that is included to help diagnose the problem. This is only a warning, not an error. The presence of these rows may affect SSS searching, resulting in missed or extra hits. It would be best to rebuild the keys if this occurs.

1218 Previous MDLAUX.RECREATEKEYS operation was interrupted, keys cannot be inverted until recreate is complete.

See error 1217.

1219 Unable to execute search, SQL=%s

See error 1213.

1221 Unable to execute search, SQL=%s

See error 1213.

1225 Unable to insert empty BLOB, SQL=%s

See error 1213.

1227 Error executing ALL\_LIBRARIES SQL: %s

**Explanation:** This error would occur while determining the Direct cartridge schema name. If it occurs, this error is ignored and the cartridge schema is determined by querying the current synonyms.

**Action:** No user action is required. Report this error to Dassault Systèmes Customer Support

1231 Invalid value for FS\_BUFFER\_POOL parameter: %s

**Explanation:** An invalid argument to the FS\_BUFFER\_POOL parameter name was used.

**Action:** Specify one of 'DEFAULT', 'KEEP', or 'RECYCLE'.

1244 OVERLAP search query can not be a NOSTRUCT or unconnected H or LP atom

**Explanation:** The query molecule cannot be NOSTRUCT (no-structure), it must contain one or more non-hydrogen atoms.

**Action:** Correct and reissue the query.

1246 RSS search query can not contain NOSTRUCT molecules

**Explanation:** None of the molecules in this query reaction can be a NOSTRUCT (no-structure), all molecules must contain one or more non-hydrogen atoms.

**Action:** Correct and reissue the query.

1247 SSS-as-component search query can not be a NOSTRUCT

**Explanation:** The query molecule cannot be a NOSTRUCT (no-structure), it must contain one or more atoms.

**Action:** Correct and reissue the query.

1248 SSS search query can not be a NOSTRUCT

See error 1247.

1249 RXNSIM search query can not be composed entirely of NOSTRUCT molecules

**Explanation:** At least one of the molecules in this query reaction cannot be a NOSTRUCT (no-structure), at least one molecule must contain one or more non-hydrogen atoms.

**Action:** Correct and reissue the query.

1250 SIMILAR search query can not be a NOSTRUCT

See error 1247.

1260 Cannot get creation parameters for NOACTION index create

**Explanation:** An error occurred while reading the indexname\_PROP table during processing of the command:

```
CREATE INDEX indexname ON tablename
```

```
INDEXTYPE IS indextype PARAMETERS ('NOACTION')
```

There should also be a more specific error message. Oracle may still create the index, however it will be invalid.

**Action:**

Either:

- Drop the index and completely recreate it.

or

- Drop the index without dropping the underlying objects, and attempt to recreate the index with the 'NOACTION' parameter after correcting the problem preventing access from the indexname\_PROP table. Do this by using the MDLAUX.NODROP function, for example:

```
SELECT MDLAUX.NODROP FROM DUAL;
```

```
DROP INDEX <indexname>;
```

1261 E Cannot create index with NOACTION parameters unless domain index objects already exist

**Explanation:** An attempt was made to use the command:

```
CREATE INDEX indexname ON tablename
```

```
INDEXTYPE IS indextype PARAMETERS ('NOACTION')
```

However, there were not underlying domain index objects present, thus the index could not be created.

**Action:** Do not use the 'NOACTION' parameter in this case.

1262 E Cannot create index with NOACTION parameters, unable to ensure tables are secondary

**Explanation:** An error occurred during processing of the command:

```
CREATE INDEX indexname ON tablename
```

```
INDEXTYPE IS indextype PARAMETERS ('NOACTION')
```

As part of this command, underlying domain index tables are made "secondary" so that they can be exported correctly. The attempt to make of the tables "secondary" failed. Check for a more specific error message that details the problem. Oracle can still create the index, however, it will be invalid.

**Action:**

Either:

- Drop the index and completely recreate it, or
- Drop the index without dropping the underlying objects, and attempt to recreate it with the 'NOACTION' parameter after correcting the problem preventing access from the indexname\_PROP table. Drop the index using the MDLAUX.NODROP function, for example:

```
SELECT MDLAUX.NODROP FROM DUAL;
```

```
DROP INDEX indexname;
```

1264 Unable to mark table as secondary

See error 1262.

1269 Cannot get creation parameters for index import

**Explanation:** This error occurs when importing a molecule or domain index, and indicates that the program is unable to fetch the original index creation parameters from the index.

This error should not occur, and it might indicate corruption of the original index or some other reason.

**Action:** Check for other errors to help diagnose the problem.

1275 unable to create indexes on new CONV table

**Explanation:** This error message indicates that Oracle was unable to create an index on a table during an IMPORT operation.

**Action:** Check for additional errors to help diagnose the problem.

1277 unable to select CLOB value from environment table, SQL=%s

**Explanation:** An error occurred while reading a CLOB from a user-specified table of environment CLOBs. This is currently only used by the conversion programs `convertcrg` and `converttxn`.

**Action:** Check for additional errors to help diagnose the problem. Report this error to Dassault Systèmes Customer Support

1278 Unable to select CLOB value from environment table, no rows: %s

See error 1277.

1279 Unable to convert CLOB value from environment table to string: %s

See error 1277.

1280 Unable to select CLOB value from environment table, more than one row: %s

See error 1277.

1285 WARNING: Unable to modify FS index LOB caching, SQL=%s

**Explanation:** An Oracle error occurred while trying to modify the FS index LOB caching mode. This is not treated as an error, the index is still usable; however the LOB caching mode will not be changed.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

1289 keyword can not be present twice: %s

**Explanation:** This error indicates that the parameter string to CREATE INDEX or ALTER INDEX contains the same parameter more than once.

**Action:** Re-issue the command with a parameter string that contains each parameter only once.

1290 Tablespace %s does not contain sufficient free space, need %d Kbytes

**Explanation:** A tablespace name specified in the PARAMETERS argument in CREATE INDEX or ALTER INDEX does not contain enough free space.

**Action:** Specify a different tablespace, or use the `PREALLOCATE=NOSTORAGECHECK` parameter to disable the check for sufficient free space.

1291 Unable to alter index while another user is performing maintenance

**Explanation:** This error occurs when ALTER INDEX is run while another user is running MDLAUX.UPDATEPENDINGFASTSEARCH, MDLAUX.RECREATEFASTSEARCH, MDLAUX.UPDATEPENDINGINVERSIONS, or MDLAUX.RECREATEKEYS.

**Action:** Wait until the other user has finished before running this command.

1292 Unable to truncate index while another user is performing maintenance

**Explanation:** This error occurs when TRUNCATE TABLE is run with a table that has a molecule or reaction domain index, and another user is running MDLAUX.UPDATEPENDINGFASTSEARCH, MDLAUX.RECREATEFASTSEARCH, MDLAUX.UPDATEPENDINGINVERSIONS, or MDLAUX.RECREATEKEYS.

**Action:** Wait until the other user has finished before running this command.

1297 E Index name is invalid: %s

**Explanation:** The argument to MDLAUX.DROPINDEXOBJECTS is not a valid object name.

**Action:** Specify the name of an Direct domain index that does not currently exist.

1298 E Unable to select index count

**Explanation:** An Oracle error occurred while trying to select index names.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

1299 E Index exists, cannot drop objects: %s.%s

**Explanation:** The argument to MDLAUX.DROPINDEXOBJECTS must not name an index that currently exists.

**Action:** Contact Dassault Systèmes Customer Support.

1300 unable to generate formula atom counts

See error 745.

1301 Unable to prepare update of table, SQL=%s

**Explanation:** An error occurred while preparing to update a row in the indexname\_FMLA table.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1302 Unable to update table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while updating a row in the indexname\_FMLA table.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1303 unable to fetch property lob, SQL=%s

**Explanation:** An error occurred while fetching a LOB from the global property table.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1304 unable to fetch property lob, SQL=%s

**Explanation:** An error occurred while fetching a LOB from the local index property table.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1305 unable to update table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while updating a row into the indexname\_SRKY table.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1306 unable to initialize RSS NOT matching

See error message 312.

1310 Unable to prepare or execute index name select, SQL=%s

**Explanation:** An error occurred while trying to fetch index names.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1312 Unable to prepare or execute index object name select, SQL=%s

**Explanation:** An error occurred while trying to fetch index object names.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1315 Unable to prepare or execute column name select, SQL=%s

**Explanation:** An error occurred while trying to fetch index object column names.

**Action:** Check the SQL command and Oracle error messages to help diagnose the problem.

1316 Unable to trim LOB

**Explanation:** An error occurred while trimming the length of a LOB to zero.

**Action:** Check the Oracle error message to help diagnose the problem.

1317 Unable to get CLOB characters set form

**Explanation:** An error occurred while getting CLOB character set information. This error can occur when using EMPTY\_CLOB as an argument, for example, INSERT INTO ... (CTAB) VALUES (MOL(EMPTY\_CLOB())).

**Action:** Check Oracle error message to help diagnose the problem. If this error is due to using MOL(EMPTY\_CLOB()) or RXN(EMPTY\_CLOB()), change the application so that it inserts a molecule or reaction instead of an empty CLOB.

1318 Unable to get CLOB characters set id

See error 1317.

1319 Error ending statement

**Explanation:** An error occurred while ending a SQL statement.

**Action:** Check the Oracle error message to help diagnose the problem.

1320 Unable to get client character set ID

**Explanation:** An error occurred while fetching the default client character set.

**Action:** Check the Oracle error message to help diagnose the problem.

1321 Unable to convert character set from csid=%d to csid=%d

**Explanation:** An error occurred while converting an NCLOB to the default client character set.

**Action:** Check the Oracle error message to help diagnose the problem.

1322 Unable to scan index while another user is performing maintenance

**Explanation:**

This occurs when you try to run the procedure MDLAUX.SCANINDEX, and another user is already running MDLAUX.UPDATEPENDINGFASTSEARCH, MDLAUX.RECREATEFASTSEARCH, MDLAUX.UPDATEPENDINGINVERSIONS, MDLAUX.RECREATEKEYS, MDLAUX.SCANINDEX, ALTER INDEX, DROP INDEX, DROP TABLE, or TRUNCATE TABLE.

If this error occurs and no other user is performing maintenance, it can mean that Oracle failed to clear a lock. This can sometimes happen when an operation is interrupted.

**Action:**

Wait until the other user has finished before running this procedure.

The DBA needs to log in as SYS and delete rows from SYS.DBMS\_LOCK\_ALLOCATED. For example, if the Direct molecule or reaction table is stored in schema SMITH and the domain index is MYMOL\_MDLIX, then the DBA needs to delete rows with NAME LIKE 'MDL.SMITH.MYMOL\_MDLIX%';

Log in to SQL\*Plus with /nolog, and then enter the following commands:

```
SQL> connect / as sysdba
SQL> delete from dbms_lock_allocated2 where name like 'MDL.SMITH.MYMOL_MDLIX%';
SQL> commit;
```

1325 Table scan prepare failed, SQL=%s

**Explanation:** An error occurred while preparing a fetch from either the structure table or from the structure table joined with the ROWID conversion table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1326 Table scan reprepare failed, SQL=%s

See error 1325.

1327 E Unable to write global environment item to CLOB

**Explanation:** An error occurred in the GETENV function.

**Action:** Check for a more specific error message to help diagnose the problem.

1328 E Unable to write index environment item to CLOB

See error 1327.

1329 Error reading environment CLOB

**Explanation:** An error occurred while reading the environment CLOB which is the argument to the MDLAUX.SETENV function.

**Action:** Check for a more specific error message to help diagnose the problem.

1330 Error reading environment CLOB

**Explanation:** An error occurred while reading and environment CLOB within a molecule or reaction domain index, or in the global cartridge environment.

**Action:** Check for a more specific error message to help diagnose the problem.

1331 Error writing environment string to output CLOB

**Explanation:** An error occurred while writing and environment string to the temporaryCLOB returned by the GETENV or GETINDEXENV function.

**Action:** Check for a more specific error message to help diagnose the problem.

1334 WARNING: MDL BIOVIA cartridge schema "%s" does not match schema in synonyms "%s"

Warning

**Explanation:** This warning indicates that the domain index being created or operated on is owned by a different schema than the cartridge synonyms in the user account. The warning prints first the schema that owns the index, and second the schema to which the cartridge synonyms point.

**Action:** Set up the synonyms for the schema using the same Direct cartridge schema as the schema that owns the domain index.

1335 unable to determine MDL Direct cartridge schema name

**Explanation:** This error indicates that BIOVIA is unable to determine the schema name for the cartridge.

**Action:** First try to set up the cartridge synonyms correctly:  
execute `c$mdl\chem60.mdl\auxop.setup;`

If this fails to resolve the problem, Contact Dassault Systèmes Customer Support.

1336 Error inserting rows into CONV table, SQL: %s

**Explanation:** This message indicates an error has occurred while inserting ROWID values during an index build or rebuild operation.

**Action:** Check for a more specific error message that provides more detail. Use the more specific Oracle error message to diagnose and correct the problem, and then re-run the import operation.

1337 Error in COMMIT

**Explanation:** This message indicates an error has occurred in the COMMIT following insertion of ROWID values during an index build or rebuild operation.

**Action:** Check for a more specific error message that provides more detail. Use the more specific Oracle error message to diagnose and correct the problem, and then re-run the import operation.

1338 Error in COMMIT

See error s 1337.

1339 unable to get length of LOB for copy

**Explanation:** An error occurred while trying to determine the length of a LOB.

**Action:** Check the Oracle error message to help diagnose the problem.

1340 unable to trim LOB for copy

**Explanation:** An error occurred while trimming the length of a LOB to zero.

**Action:** Check the Oracle error message to help diagnose the problem.

1341 unable to copy LOB

**Explanation:**

An error occurred while copying a LOB. The most likely cause of this error is that the temporary tablespace does not contain sufficient space to hold a copy of the FS index segment as a temporary LOB.

Another cause for the error is that the tablespace which is used to hold the Fastsearch LOB column in your domain index does not have sufficient space.

**Action:**

If the additional Oracle error messages that are include indicate this to be the problem, increase the size of your temporary tablespace and re-run the operation.

If the additional Oracle error message that is include indicates this to be the problem, increase the size of the tablespace used to hold this LOB column. (The table is named `indexname_FSIX`, and the column is named `FSINDEX`.)

1343 TABLESPACE parameter is invalid

**Explanation:** The TABLESPACE=name parameter specifies an invalid tablespace name.

**Action:** Specify a valid tablespace name.

1344 TABLE\_TABLESPACE parameter is invalid

**Explanation:** The TABLE\_TABLESPACE=name parameter specifies an invalid tablespace name.

**Action:** Specify a valid tablespace name.

1345 INDEX\_TABLESPACE parameter is invalid

**Explanation:** The INDEX\_TABLESPACE=name parameter specifies an invalid tablespace name.

**Action:** Specify a valid tablespace name.

1346 LOB\_TABLESPACE parameter is invalid

**Explanation:** The LOB\_TABLESPACE=name parameter specifies an invalid tablespace name.

**Action:** Specify a valid tablespace name.

1347 Filename cannot be NULL or blank

**Explanation:** The filename argument to the READFILE operator cannot be NULL or a string containing only blanks.

**Action:** Specify a valid filename with the READFILE operator.

1348 Filename cannot be NULL or blank

**Explanation:** The filename argument to the WRITEFILE operator cannot be NULL or a string containing only blanks.

**Action:** Specify a valid filename with the WRITEFILE operator.

1349 FSBLOCKSIZE parameter (%d) must be no more than 1/16 of the FSCACHE parameter (%d)

**Explanation:** The FSBLOCKSIZE parameter cannot exceed 1/16th of the FSCACHE parameter.

**Action:** Retry the command with a smaller value for the FSBLOCKSIZE parameter and/or a larger value for the FSCACHE parameter.

1350 FSUPDBLOCKSIZE parameter (%d) must be no more than 1/16 of the FSUPDCACHE parameter (%d)

**Explanation:** The FSUPDBLOCKSIZE parameter cannot exceed 1/16th of the FSUPDCACHE parameter.

**Action:** Retry the command with a smaller value for the FSUPDBLOCKSIZE parameter and/or a larger value for the FSUPDCACHE parameter.

1355 Unable to grant, SQL=%s

**Explanation:** An error occurred while granting SELECT on the indexname\_FSUP or indexname\_FSDL table to public.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1356 Unable to grant, SQL=%s

**Explanation:** An error occurred while granting SELECT on the indexname\_SKY2, indexname\_SKY3, or indexname\_RSKY table to public.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1357 Unable to grant, SQL=%s

**Explanation:** An error occurred while granting select on the indexname\_PROP table to public.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1358 E MDLAUX.UPDATEPENDINGFASTSEARCH is not valid with a MODELS index

**Explanation:** Model (3D) indexes do not use Fastsearch when searching.

**Action:** Do not use this command with a model index.

1359 E MDLAUX.RECREATEFASTSEARCH is not valid with a MODELS index

See error 1358.

1361 Invalid data Sgroup field flag: %s

**Explanation:** The SGROUPFIELDS file contains an invalid flag following the data Sgroup field type. Only FIELDID=n and IGNORECASE are valid entries following the field type.

**Action:** Remove the invalid text in the file, or use the correct flag. Do not add a FIELDID=n entry, this is only needed when an RCG database is converted by convertrcg.

1362 Invalid IDXTYPE parameter: %s

**Explanation:** This is an internal error and should not occur, but if it does appear, it indicates that the IDXTYPE parameter should only be used when creating any index during import, and should have come from a valid domain index.

**Action:** Contact Dassault Systèmes Customer Support.

1363 E Packed connection table is a reaction, when a molecule is expected

**Explanation:** This error indicates that an SSS, FLEXMATCH, or other molecule search operator is being used on a table that contains reactions.

**Action:** Correct the table name in the application so that the name refers to a table containing molecules.

1364 E Packed connection table is a molecule, when a reaction is expected

**Explanation:** This error indicates that a RSS, RXNFLEXMATCH, or other reaction search operator is being used on a table that contains molecules.

**Action:** Correct the table name in the application so that the name refers to a table containing reactions.

1368 RXNSIM query must contain both reactant and product molecules

**Explanation:** This error indicates that an SSS, FLEXMATCH, or other molecule search operator is being used on a table that contains molecules.

**Action:** Correct the table name in the application so that the name refers to a table containing reactions.

1369 unable to allocate sgroup formula hash memory

See error 25.

1370 Unable to prepare sgroup formula hash select, SQL=%s

**Explanation:** This error occurred while preparing a SQL statement for a FLEXMATCH "IGNORE=MSU" search.

**Action:** Review the SQL command and see the Oracle error message to help diagnose the problem.

1371 Unable to fetch sgroup formula hash value

**Explanation:** This error occurred while preparing a SQL statement for a FLEXMATCH "IGNORE=MSU" search.

**Action:** Review the SQL command and see the Oracle error message to help diagnose the problem.

1372 Attempt to open FS index after I/O error

**Explanation:** This error is secondary, and occurs after an I/O error has occurred during a FASTSEARCH maintenance operation.

**Action:** See more specific errors indicating the original problem source.

1373 FS index unit not found when closing

See error 1372.

1374 FS index unit not found when getting I/O callbacks

See error 1372.

1385 Unable to allocate memory for molecule monomer/SRU formula hash scan

See error 25.

1386 Unable to initialize monomer /SRU formula hash table lookup, SQL=%s

See error 366.

1387 Unable to prepare monomer /SRU formula hash table lookup, SQL=%s

See error 366.

1388 Unable to fetch monomer /SRU formula hash value at ROWID=%s, SQL=%s

See error 370.

1399 Molecule monomer/SRU formula hash scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

1416 Unable to prepare insert into table, SQL=%s

**Explanation:** This error occurs while preparing to insert a row into the indexname\_NEC table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1417 Unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** This error occurs while deleting a row into the indexname\_NEC table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1418 Unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** This error occurs while inserting a row into the indexname\_NEC table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1419 Unable to prepare update of table, SQL=%s

**Explanation:** This error occurs while preparing to update a row into the indexname\_NEC table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1420 Unable to update table, REGNO=%s, SQL=%s

**Explanation:** This error occurs while preparing to update a row into the indexname\_NEC table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1421 NEMA key generation failed

**Explanation:** This error occurs when NEMA stereochemical and symmetry perception of a molecule failed.

**Action:** Contact Dassault Systèmes Customer Support.

1424 Unable to prepare NEMAKEY query, SQL=%s

**Explanation:** This error occurs while preparing an NEMAKEY table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1425 Error fetching NEMAKEY value

**Explanation:** This error occurs while fetching from the NEMAKEY table.

**Action:** Check the SQL command and the Oracle error message to help diagnose the problem.

1426 Error retrieving molecule at REGNO %s

**Explanation:** This error occurs while fetching a molecule for verification.

**Action:** The internal regno of the molecule is provided to help identify the problem. Contact Dassault Systèmes Customer Support for help in determining which molecule in database this is.

1433 Unable to allocate memory for molecule NEMAKEY scan

See error 25.

1434 Unable to initialize NEMAKEY hash table lookup, SQL=%s.2000s

See error 366.

1435 Unable to prepare NEMAKEY fetch at ROWID=%s, SQL=%s.2000s

See error 366.

1436 Molecule NEMAKEY scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

1437 Unable to compute NEMAKEY

**Explanation:** This error occurs while computing the NEMAKEY for a molecule.

**Action:** Check for a more specific error message to help diagnose the problem.

1438 Unable to get user handle for NLS call

**Explanation:** This error occurs while calling an Oracle routine prior to fetching the NLS decimal separator.

**Action:** Check the Oracle error message to help diagnose the problem.

1439 Unable to get NLS decimal separator

**Explanation:** This error occurs while fetching the NLS decimal separator.

**Action:** Check the Oracle error message to help diagnose the problem.

1442 E Index export failed

**Explanation:** This error indicates MDLAUX.INDEXEXPORT failed.

**Action:** Check for a more specific error message to help diagnose the problem.

1443 E Index import failed

**Explanation:** This error indicates MDLAUX.INDEXIMPORT failed.

**Action:** Check the more specific error message giving the reason for the failure. The failure can be corrected:

- If no data was imported, you can run MDLAUX.INDEXIMPORT again.
- If data was imported before the failure, you need to drop the molecule or reaction table, re-import it, and run MDLAUX.INDEXIMPORT again.

If the failure cannot easily be corrected, you must drop the domain index and create it from data in the molecule or reaction table.

1445 Too many primary-key columns, the maximum is 7

**Explanation:** This error indicates the number of primary-key columns in the argument to MDLAUX.INDEXEXPORT cannot exceed seven.

**Action:** If the table has more than seven columns that make up the primary key, create a key with fewer columns.

1446 Primary-key column does not end in quote: %s

**Explanation:** This error indicates the primary-key column argument to MDLAUX.INDEXEXPORT is incorrect. The argument contains a column with a starting double quote, but no ending double quote.

**Action:** Correct the argument and reissue the command.

1447 Expecting ',' following column name, found: %s

**Explanation:** This error indicates the primary-key column argument to MDLAUX.INDEXEXPORT is incorrect. The argument does not contain a comma between column names.

**Action:** Correct the argument and reissue the command.

1448 unable to fetch from table to check row count, SQL=%s

**Explanation:** This error occurs in MDLAUX.INDEXIMPORT while checking the count of one of the domain index secondary tables.

**Action:** Check for a specific Oracle error to help diagnose the problem.

If the secondary table does not exist, the index was not created correctly. In this case, you must drop the molecule or reaction table and then re-import it.

1450 Import file contains invalid header line

**Explanation:** This error indicates that the MDLAUX.INDEXIMPORT has the wrong format. The file is probably not a Direct domain index .dmp file.

**Action:** Reissue the command with the correct file name.

1452 Import file is not the first file of a multipart file set: %s

**Explanation:** This error indicates that the import file provided to MDLAUX.INDEXIMPORT is a continuation file from a multi-part export file set.

**Action:** Reissue the command with the correct file name.

1457 Import file key column name %s does not exist in table %s

**Explanation:** This error indicates that the import file contains the “key” column names in it. At least one of the columns does not exist in the molecule or reaction table on which the domain index was created. This might indicate to MDLAUX.INDEXIMPORT, or that the wrong domain index .dmp file has been modified.

**Action:** Use the correct import file, or alter the table to match the original column names.

1458 Import file is empty or contains only unknown header files

See error 1450.

1459 Import file does not contain correct header files

See error 1450.

1460 Import file does not contain BIOVIA Direct build ID

**Explanation:** This error might indicate an invalid file name.

**Action:** See error 1450.

1461 Import file created with BIOVIA Direct build %s, not compatible with current build

**Explanation:** This error indicates that this version of MDLAUX.INDEXIMPORT is the wrong version to process the domain index .dmp file.

**Action:** Import the .dmp file into a schema that is enabled for use with the correct version of Direct.

1462 Import file does not contain primary-key column count header line

See errors 1450 and 1460.

1463 Import file does not contain correct number of primary-key column header

lines

See errors 1450 and 1460.

1464 Import file FILESIZE value does not match the value provided with the filename

**Explanation:** MDLAUX.IMPORTINDEX does not need a FILESIZE=n keyword in the filename, as the domain index .dmp file contains the file size limitation value. However if you do specify the FILESIZE=n keyword, it must match the value stored in the .dmp file.

**Action:** Reissue the command without specifying the FILESIZE=n keyword in the filename argument.

1465 Import file FILESIZE value does not match the value provided with the filename

See error 1464.

1466 Unable to get creation parameters for import

**Explanation:** This error message occurred in MDLAUX.INDEXIMPORT while fetching domain index parameters from one of the domain index secondary tables.

**Action:** Check for a more specific error message to help diagnose the problem. If the secondary table does not exist, the index was not created correctly. In this case, you must drop the molecule or reaction table and re-import it.

1467 Import header line is missing TYPE: %s

**Explanation:** This error message occurs when the domain index .dmp file is missing a header line indicating the start of a new secondary table.

**Action:** This error might indicate an internal error in MDLAUX.INDEXIMPORT, or it might indicate a corrupted .dmp file. If you can obtain a new copy of the .dmp file, you can drop the molecule or reaction table, re-import it, and then reissue the MDLAUX.INDEXIMPORT command.

1469 Missing TYPE header line in import file

See error 1467.

1470 Unable to initialize local environment after import

**Explanation:** This error occurred initializing the domain index environment after the import succeeded.

**Action:** The import data might be correct. Try reconnecting to SQL\*Plus and issuing an SSS or RSS search to test the cartridge. For example:  
`select count(*) from moltable wheresss(ctab, (select ctab from moltable where id='value'))=1;`

If the search succeeds without errors, the domain index has been imported correctly. If the search fails, especially with errors which indicate an environment problem, try dropping the molecule or reaction table, re-import it, and then reissue the MDLAUX.INDEXIMPORT command.

1471 Unable to fetch column count, SQL=%s

**Explanation:** An error occurred while verifying the existence of a "key" column in the molecule or reaction table.

**Action:** Check for a more specific Oracle error to help diagnose the problem.

1472 No file name argument provided

**Explanation:** The filename argument to MDLAUX.INDEXEXPORT or MDLAUX.INDEXIMPORT was NULL.

**Action:** Reissue the command with the correct filename argument.

1473 Invalid value for FILESIZE parameter, too big: %s

**Explanation:** This error indicated that the value of n in the keyword FILESIZE=n in the filename argument is too large.

**Action:** Specify a value for n between 2000 and 4294967295.

1474 Invalid value for FILESIZE parameter, must be at least 2000: %s

See error 1473.

1475 No file name argument provided

**Explanation:** This error indicated that the filename argument to MDLAUX.INDEXEXPORT or MDLAUX.INDEXIMPORT contains only a FILESIZE=n keyword, it does not contain a file name.

**Action:** Reissue the command with the correct filename argument.

1476 File name is too long: %s

**Explanation:** This error indicated that the filename in MDLAUX.INDEXEXPORT or MDLAUX.INDEXIMPORT cannot exceed 1024 characters.

**Action:** Shorten the filename and reissue the command.

1477 Unable to create or open file %s for export: %s

**Explanation:** MDLAUX.INDEXEXPORT could not create the domain index dump file.

**Action:** Check the operating system error message to help diagnose the problem.

- Include the full pathname in the argument.
- Be sure that the directory in which the file is to be created is writable by the Oracle listener process.
- If a file already exists, MDLAUX.INDEXEXPORT attempts to overwrite it. The file must be writable by the Oracle listener process.

1478 Error writing %s import data to file %s: %s

**Explanation:** This error occurred while MDLAUX.INDEXEXPORT was writing to the domain index .dmp file.

**Action:** Check the operating system error message to help diagnose the problem. Correct the problem and reissue the command.

1479 Error writing %s import data to file %s: %s

**Explanation:** This error occurred while MDLAUX.INDEXEXPORT was writing to a domain index continuation .dmp file.

**Action:** Check the operating system error message to help diagnose the problem. Correct the problem and reissue the command.

1480 Unable to create or open file %s for export: %s

**Explanation:** This error indicates that MDLAUX.INDEXEXPORT could not create a domain index continuation .dmp file.

**Action:** See error 1477.

1481 Error exporting %s, cannot determine length of BLOB

**Explanation:** This error occurred in MDLAUX.INDEXEXPORT exporting a BLOB.

**Action:** Check the more specific error to help diagnose the problem.

1482 Error exporting %s, error reading BLOB

See error 1481.

1483 unable to open file %s for import: %s

**Explanation:** This error indicates that MDLAUX.INDEXIMPORT could not open the domain index .dmp file.

**Action:** Check the operating system error message to help diagnose the problem.

- Include the full pathname in the argument.
- Be sure that the file is readable by the Oracle listener process.

1484 Invalid import data (datatype) for %s

**Explanation:** This error indicates that the domain index .dmp file used with MDLAUX.INDEXIMPORT contains invalid data.

**Action:** See error 1467.

1485 Invalid import data (length) for %s

See error 1484.

1486 Invalid import data (header length) for %s

See error 1484.

1487 Internal import error, header string is NULL for %s

See error 1484.

1488 Invalid import data (length) for %s

See error 1484.

1489 Invalid import data (length) for %s

See error 1484.

1490 Invalid import data (datatype) for %s

See error 1484.

1491 Error reading %s import data from file %s: %s

**Explanation:** An error occurred while MDLAUX.INDEXEXPORT was reading from the domain index .dmp file.

**Action:** Check the operating system error message to help diagnose the problem.

1492 Error reading %s import data from file %s: %s

**Explanation:** This error occurred while MDLAUX.INDEXEXPORT was reading from a domain index continuation .dmp file.

**Action:** Check the operating system error message to help diagnose the problem.

1493 Error importing %s, unable to open BLOB

**Explanation:** This error occurred in MDLAUX.INDEXIMPORT importing a BLOB.

**Action:** Check for a more specific error to help diagnose the problem.

1494 Error importing %s, error writing BLOB

See error 1493.

1495 Error importing %s, unable to close BLOB

See error 1493.

1496 Unable to open file %s for import: %s

**Explanation:** This error indicates that MDLAUX.INDEXIMPORT could not open a domain index continuation .dmp file.

**Action:** Check the operating system error message to help diagnose the problem. The most likely problem is that the continuation file was not copied into the same directory as the first file.

1497 Import file %s is not a valid import continuation file

**Explanation:** This error indicates a continuation file opened by MDLAUX.INDEXIMPORT did not contain the correct header.

**Action:** Either the file is not the correct file, or it is corrupted.

1499 Unable to create temporary table for import of CONV, SQL=%s

**Explanation:** This error indicates that MDLAUX.INDEXIMPORT was not able to create a temporary table for use in creating a domain index secondary table.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1500 Unable to prepare insert for CONV, SQL=s

**Explanation:** This error occurred when MDLAUX.INDEXIMPORT was preparing a SQL insert.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1501 Unexpected end-of-file marker for CONV

See error 1467.

1502 Error inserting into temp table for CONV at row %s, SQL=%s

**Explanation:** This error indicates that MDLAUX.INDEXIMPORT was not able to insert into a temporary table used in creating a domain index secondary table.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1503 Error inserting into CONV at row %s, SQL=%s

**Explanation:** This error occurred when MDLAUX.INDEXIMPORT was performing a SQL insert.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1504 Error truncating temp table for CONV at row %s, SQL=%s

**Explanation:** MDLAUX.INDEXIMPORT was not able to truncate a temporary table used in creating a domain index secondary table.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1505 Error committing CONV at row %s

**Explanation:** An error occurred when MDLAUX.INDEXIMPORT was performing a COMMIT.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1506 Error committing CONV

See error 1505.

1507 Unable to drop FLEX indices before import

**Explanation:** MDLAUX.INDEXIMPORT was not able to drop existing indexes on a domain index secondary table, prior to importing data into that table.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1508 Unable to create FLEX indices after import

**Explanation:** MDLAUX.INDEXIMPORT was not able to create new indexes on a domain index secondary table, after importing data into that table.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1509 Unable to drop FMLA indices before import

See error 1507.

1510 Unable to create FMLA indices after import

See error 1508.

1511 Unable to drop GENX indices before import

See error 1570.

1512 Unable to create GENX indices after import

See error 1580.

1514 Unable to create MSU indices after import

See error 1580.

1515 Unable to drop NEC indices before import

See error 1570.

1516 Unable to create NEC indices after import

See error 1508.

1517 Unable to drop RFLX indices before import

See error message 1507.

1518 Unable to create RFLX indices after import

See error message 1508.

1520 Unable to truncate FSIX table during import

**Explanation:** MDLAUX.INDEXIMPORT was not able to truncate a domain index secondary table, prior to importing data into that table.

**Action:** Check the accompanying Oracle error message to help diagnose the problem.

1521 Unable to fetch value from PROP table during import

**Explanation:** MDLAUX.INDEXIMPORT was not able to fetch index parameters from the property secondary table, prior to importing data into that table.

**Action:** Check the accompanying error messages to help diagnose the problem.

1522 Unable to truncate PROP table during import

See error 1520.

1523 WARNING: Unable to process PROP table after import, index may contain invalid TABLESPACE and/or TEMPDIR parameters

**Explanation:** This is a warning, it indicates that the TABLESPACE and/or TEMPDIR parameters stored in the domain index were not removed and might not be valid for the current Oracle instance.

**Action:** Try using ALTER INDEX to modify these parameters to desired values. Note that the current values can be displayed using MDLAUX.INDEXPARAMETERS.

1524 Unable to fetch sequence number for export, SQL=%s

**Explanation:** MDLAUX.INDEXEXPORT was not able to fetch the next value for the domain index sequence.

**Action:** Check the accompanying error messages to help diagnose the problem.

1525 Import header line for SQNC is missing START value: %s

See error 1467.

1526 Unable to drop sequence during import, SQL=%s

**Explanation:** MDLAUX.INDEXIMPORT was not able to drop the existing sequence during the import operation.

**Action:** Check the accompanying error messages to help diagnose the problem.

1527 Unable to create sequence during import, SQL=%s

**Explanation:** MDLAUX.INDEXIMPORT was not able to create a new sequence during the import operation.

**Action:** Check the accompanying error messages to help diagnose the problem.

1528 Unable to prepare export fetch for %s, SQL=%s

**Explanation:** MDLAUX.INDEXEXPORT was not able to fetch data from a domain index secondary table.

**Action:** Check the accompanying error messages to help diagnose the problem.

1529 Unable to perform export fetch for %s, SQL=%s

See error 1528.

1530 Error writing %s export line %s to file: %s

See error 1478.

1533 Error writing %s CLOB to string

See error 1528.

1534 Unable to prepare insert for %s, SQL=%s

See error 1500.

1535 Unexpected end-of-file marker for %s

See error 1467.

1536 Error inserting into %s at row %s, SQL=%s

See error 1500.

1537 Error committing %s at row %s

See error 1505.

1538 Error committing %s

See error 1505.

1539 Unable to prepare insert for %s, SQL=%s

See error 1500.

1540 Unexpected end-of-file marker for %s

See error 1467.

1541 Error inserting into %s at row %s, SQL=%s

See error 1500.

1542 Expecting BLOB data in import file for %s

See error 1467.

1543 Error committing %s at row %s

See error 1505.

1544 Error committing %s

See error 1505.

1545 Unable to allocate %u bytes while importing %s

See error 25.

1546 Invalid or missing column data in %s import file: %d

See error 1467.

1547 Missing %s import data row terminator

See error 1467.

1548 Import header line for %s is missing VERSION value: %s

See error 1467.

1549 Unable to fetch table count, SQL=%s

**Explanation:** An error occurred fetching the row count from the molecule or reaction table.

**Action:** Check the Oracle error message to help diagnose the problem. Note that if this error occurs, it probably indicates a more serious problem within Oracle.

1552 Unable to allocate memory for parameters

See error 25.

1555 E Packed connection table is a reaction, when a molecule is expected

**Explanation:** This error indicates that an SSS, FLEXMATCH, or other molecule search operator is being used on a table that contains reactions.

**Action:** Correct the table name in the application so that the name refers to a table containing molecules.

1556 Unable to create index, SQL=%s

**Explanation:** An error occurred while creating an index on a secondary table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1557 Unable to prepare storage clause for table %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create a secondary table.

**Action:** Check for a more specific message giving the reason for the failure.

One reason for this error is that the USER\_FREE\_SPACE view indicates that there is insufficient free space available. See the cartridge extent management documentation for information about how the cartridge allocates storage during object creation.

1558 unable to prepare storage clause for index %s

**Explanation:** An error occurred while creating the STORAGE clause needed to create an index on a secondary table.

**Action:** Check for a more specific message that gives the reason for the failure. See also error 1557.

1559 WARNING: Unable to delete unused chunks greater than %d

**Explanation:** This warning occurs at the end of MDLAUX.RECREATEKEYS, and it indicates that an error occurred when deleting unused rows from the inverted key table. Some SSS searches and similarity searches might perform slower, but results will not be affected.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1566 unable to prepare insert into table, SQL=%s

**Explanation:** An error occurred while preparing to insert a row into the indexname\_CTAB table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1567 unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_CTAB table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1568 unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_CTAB table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1569 unable to update table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while updating a row in the indexname\_CTAB table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1570 unable to insert into table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while inserting a row into the indexname\_CTAB table during an update operation.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1577 unable to delete from table, REGNO=%s, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_FSUP table.

**Action:** Check the SQL command and Oracle error message to help diagnose the problem.

1584 UNIQUE parameter can not be used with a BUILDINGBLOCK index

**Explanation:** This error indicates that you cannot use duplicate checking with a molecule column which contains building block structures (molecules with attachment points).

**Action:** Remove the UNIQUE parameter in order to create the index.

1585 Unable to initialize FLEXMATCH matching

**Explanation:** This error occurred while re-preparing a previously prepared FLEXMATCH query for a non-indexed match.

**Action:** Check for a more specific error message to help diagnose the problem.

1586 Unable to initialize RXNFLEXMATCH matching

**Explanation:** This error occurred while re-preparing a previously prepared RXNFLEXMATCH query for a non-indexed match.

**Action:** Check for a more specific error message to help diagnose the problem.

1588 Unable to initialize RSS matching

**Explanation:** This error occurred while re-preparing a previously prepared RSS query for a non-indexed match.

**Action:** Check for a more specific error message to help diagnose the problem.

1589 Reaction FASTSEARCH index scan has errors, use MDLAUX.LOGTABLE to view errors

See error 364.

**Note:** You might need to rebuild FASTSEARCH to correct the problem.

1599 unable to reinitialize FSlib

**Explanation:** This error occurred after an error during a Fastsearch maintenance operator such as MDLAUX.RECREATEFASTSEARCH.

**Action:** The cartridge is not reliable after this error. Disconnect from Oracle and reconnect to establish a new session.

1600 Invalid value for USENEMAKEKEY parameter: %s (valid values are YES or NO)

**Explanation:** An invalid argument to the USENEMAKEKEY parameter name was used.

**Action:** Specify either no parameter at all (same as 'YES'), 'YES' or 'NO'.

1613 Unable to convert internal handle to rxnfile in CLOB

**Explanation:** An error occurred writing a rxnfile to a temporary CLOB.

**Action:** Check for a more specific error message to help diagnose the problem.

1614 unable to convert internal handle to molfile in CLOB

**Explanation:** An error occurred writing a molfile to a temporary CLOB.

**Action:** Check for a more specific error message to help diagnose the problem.

1618 unable to initialize %s matching

See error 1078.

1621 Input file "%s" is not a valid %s:

**Explanation:** This error indicates that a filename containing a molecule or reaction, as a molfile, rxnfile, etc., does not contain valid data.

The filename and type of data the cartridge was looking for are provided in the error message. The most common cause of this error is providing the wrong file name.

**Action:** Check the first 66 characters of the file to help diagnose the problem.

1622 Input string is not a valid %s:

**Explanation:** This error indicates that a molecule or reaction argument could not be interpreted as a valid molecule or reaction, for example as a valid molfile. The type of data the cartridge was looking for is provided in the error message.

**Action:** Check the first 66 characters of the file to help diagnose the problem.

1623 SMILES generation failed: Molecule contains polymer SGroups

**Explanation:** This error indicates that a SMILES string cannot be generated for a molecule containing polymer SGroups.

1624 SMILES generation failed: Molecule contains Rgroups

**Explanation:** This error indicates that a SMILES string cannot be generated for a molecule containing Rgroups.

1626 %s

**Explanation:** This error indicates that the OpenEye function to generate SMILES from a molfile failed.

**Action:** Check the OpenEye error message, if one is available, to help diagnose the problem.

1628 Name generation failed: Molecule contains polymer SGroups

**Explanation:** This error indicates that an IUPAC name string cannot be generated for a molecule containing polymer SGroups.

1629 Name generation failed: Molecule contains Rgroups

**Explanation:** This error indicates that an IUPAC name string cannot be generated for a molecule containing Rgroups.

1631 %s

**Explanation:** This error indicates that the OpenEye function to generate an IUPAC name from a molfile failed.

**Action:** Check the OpenEye error message, if one is available, to help diagnose the problem.

1738 NEMAKEY version in index does not match version in this program

**Explanation:** The NEMAKEY version for the NEMA keys stored in the index is not the same as the NEMAKEY version for keys which would be created by the current version of Direct.

**Action:** See error 1739.

1739 You must rebuild NEMAKEY before using FLEXMATCH searches in this index: ALTER INDEX "%s"."%s" REBUILD PARAMETERS('NEMAKEY');

**Explanation:** The NEMAKEY version for the NEMA keys stored in the index either cannot be determined, or it is not the same as the NEMAKEY version for keys that are created by the current version of Direct.

**Action:** In order to use FLEXMATCH searching with this index, the NEMA keys must first be rebuilt. The command to rebuild the NEMA keys is provided as part of the error message text.

1740 Filename cannot be NULL or blank

**Explanation:** This error occurs if the filename argument to the READBINARYFILE operator is NULL or is a string containing only blanks.

**Action:** Specify a valid filename with the READBINARYFILE operator.

1741 E Unable to copy contents of file "%s" to BLOB

**Explanation:** An error occurred in the READBINARYFILE operator. There should be a more specific error message.

**Action:** Check for a more specific error message to help diagnose the problem.

1742 Filename cannot be NULL or blank

See error 1348.

1743 E Unable to write contents of BLOB to file "%s"

See error 13.

1747 Unable to open file "%s": %s

**Explanation:** This error occurred while opening a binary file for reading.

**Action:** Check the file name and system error message that are included in the error message to help diagnose the problem.

1748 Unable to open file "%s": %s

**Explanation:** This error occurred while trying to create a binary file or open an existing binary file so that it can be overwritten.

**Action:** Check the file name and system error message that are included in the error message to help diagnose the problem.

1749 Error writing file "%s": %s

**Explanation:** This error occurred while writing a binary file.

**Action:** Check the file name and system error message that are included in the error message to help diagnose the problem. One cause might be that the disk is full.

1765 Sequence molecule query FLEXMATCH switches must be MATCH=ALL or IGNORE=DAT

**Explanation:** A FLEXMATCH search in which the query is a sequence molecule can be done only if the Flexmatch switches are 'MATCH=ALL' or 'IGNORE=DAT'.

**Action:** Correct the FLEXMATCH switches, and rerun the query.

1766 GENERIC switch may not be used with a sequence molecule search

**Explanation:** The GENERIC switch, which causes FLEXMATCH to perform a generic exact-match search, cannot be used when the query is a sequence molecule.

**Action:** Remove the GENERIC switch and rerun the query.

1777 WRITEFILE argument cannot be NULL

**Explanation:** The first (CLOB) argument to WRITEFILE cannot be NULL.

**Action:** Specify a non-NULL argument and rerun the query.

1778 WRITEBINARYFILE argument cannot be NULL

**Explanation:** The first (BLOB) argument to WRITEBINARYFILE cannot be NULL.

**Action:** Specify a non-NULL argument and rerun the query.

1780 system command produced no binary output file: %s

**Explanation:** This error occurs when the program WriteImage, called by MDLAUX.MOLIMAGE or MDLAUX.RXNIMAGE, does not create an output image file. Generally, this error occurs when users do not have privileges to create files in the system temporary directory.

**Action:** Ensure that any user can create files in the system temporary directory. This is especially important on the Microsoft Windows 2008 OS.

1782 WARNING: Unable to change CTAB LOB compression, SQL=%s

**Explanation:** An Oracle error occurred while trying to modify the compression of the CTAB LOB column in the indexname\_CTAB table.

This is not treated as an error, the index is still usable. However, the LOB compression will not be changed.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

1783 Invalid value for COMPRESS parameter: %s

**Explanation:** An invalid argument to the COMPRESS parameter name was used.

**Action:** Specify either 'YES' or 'NO'. You can also specify COMPRESS with no argument, which is the same as COMPRESS=YES.

1784 MDLGetwrapLob called with invalid buffer or block size

1785 Invalid value for blocksize

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1786 Unable to allocate memory

See error 25.

1787 Invalid handle

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1788 Invalid handle

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1789 Invalid handle

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1790 Invalid handle

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1791 Invalid handle

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1792 Unable to locate block on LRU list

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1793 Unable to allocate memory

See error 25.

1794 Unable to seek to position %d

**Explanation:** An error occurred while accessing Fastsearch data.

**Action:** Check for a more specific error message to help diagnose the problem.

1795 Unable to read %d bytes at position %d

See error 1794.

1796 Unable to seek to position %d

**Explanation:** An error occurred while trying to write Fastsearch data.

**Action:** Check for a more specific error message to help diagnose the problem.

1797 Unable to write %d bytes at position %d

See error 1796.

1798 Unable to seek to EOF

See error 1794.

1799 Unable to determine EOF

See error 1794.

1800 Unable to allocate memory

See error 25.

1801 Unable to allocate memory

See error 25.

1802 Block does not exist in temp device

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1803 Unable to allocate memory

See error 25.

1804 Block exists in temp device

**Explanation:** An internal error occurred.

**Action:** Contact Dassault Systèmes Customer Support.

1805 Error positioning to position %d

**Explanation:** An error occurred while accessing Fastsearch data stored in a temporary file.

**Action:** Check for a more specific error message to help diagnose the problem.

1806 Error reading %d bytes at position %d

See error 1805.

1807 Unable to create temporary file

**Explanation:** An error occurred while trying to create a temporary file to hold Fastsearch data.

**Action:** Check for a more specific error message to help diagnose the problem. The most likely problem is that the Oracle listener process does not have permission to create a file in the directory.

1808 Error positioning to position %d

**Explanation:** An error occurred while trying to write Fastsearch data to a temporary file.

**Action:** Check for a more specific error message to help diagnose the problem.

1809 Error writing %d bytes at position %d",

**Explanation:** An error occurred while trying to write Fastsearch data to a temporary file.

**Action:** Check a more specific error message to help diagnose the problem. The most likely problem is that the disk contains insufficient space to extend the file.

1810 Unable to prepare or execute SELECT: %s

**Explanation:** An error occurred while inserting ROWIDs and internal ID numbers into the indexname\_CONV table, this occurs at the beginning of a CREATE INDEX statement.

The SQL statement and Oracle error are included in the error message. Setting the COMMITCOUNT parameter in the CREATE INDEX statement to a smaller value may solve the problem. (The default value is 50000.)

**Action:** Contact Dassault Systèmes Customer Support.

1811 Unable to prepare SELECT: %s

See error 1810.

1812 Unable to prepare INSERT: %s

See error 1810.

1813 Unable to execute SELECT: %s

See error 1810.

1814 Error in SELECT: %s

See error 1810.

1815 Error in INSERT: %s

See error 1810.

1816 Error in COMMIT

See error 1810.

1824 Unable to recreate sequence

**Explanation:** This error is related to error 1810 because it is the last step in creating the indexname\_CONV table.

**Action:** See error 1810.

1825 No boost file directory is available, specify parameter BOOSTDIR=directory-path

**Explanation:** When creating a boost file with MDLAUX.CREATEBOOSTFILE, a directory name must be specified. The directory name can be set globally for all Direct cartridge users with MDLAUX.SETPROPERTY, it can be set when the index is created with a parameter BOOSTDIR=directory-name, or it can be set in the argument to MDLAUX.CREATEBOOSTFILE by including a parameter BOOSTDIR=directory-name.

**Action:** Specify a directory name and rerun the command.

1826 No boostnames argument provided

**Explanation:** The second argument to MDLAUX.CREATEBOOSTFILE does not contain one the required keywords.

**Action:** Correct the argument and reissue the command.

1827 MDLAUX.CREATEBOOSTFILE failed

**Explanation:** MDLAUX.CREATEBOOSTFILE has failed.

**Action:** Check for a more specific error to help diagnose the problem.

1829 Cannot create KEYS boost file: KEYS are disabled

**Explanation:** Substructure keys are disabled for the index, thus a boost file cannot be created.

**Action:** To create a boost file, first enable keys using either MDLAUX.RECREATEKEYS or ALTER INDEX REBUILD PARAMETERS ('ENABLE=KEYS'), then reissue the MDLAUX.CREATEBOOSTFILE command.

1830 Cannot create KEYS boost file: Another user is performing index maintenance

**Explanation:** Another user is performing index maintenance (ALTER INDEX, MDLAUX.RECREATEKEYS, etc.).

**Action:** Wait until the other user has finished, then rerun the command.

1831 Cannot create KEYS boost file

**Explanation:** An error has occurred while creating the KEYS boost file,

**Action:** Check for a more specific error to help diagnose the problem.

1832 Cannot create FASTSEARCH boost file: Index type does not support FASTSEARCH

**Explanation:** Fastsearch is not used by this index type, thus a boost file cannot be created.

1833 Cannot create FASTSEARCH boost file: FASTSEARCH is disabled

**Explanation:** Fastsearch is disabled for the index, thus a boost file cannot be created.

**Action:** To create a boost file, first enable Fastsearch using either MDLAUX.RECREATEFASTSEARCH or ALTER INDEX REBUILD PARAMETERS ('ENABLE=FASTSEARCH'), and then reissue the MDLAUX.CREATEBOOSTFILE command.

1834 Cannot create FASTSEARCH boost file: Another user is performing index maintenance

**Explanation:** Another user is performing index maintenance (ALTER INDEX, MDLAUX.RECREATEKEYS, etc.).

**Action:** Wait until the other user has finished, then reissue the command.

1835 Cannot create FASTSEARCH boost file

**Explanation:** An error has occurred while creating the FASTSEARCH boost file.

**Action:** Check for a more specific error to help diagnose the problem.

1836 Cannot create CTAB boost file: Another user is performing index maintenance

**Explanation:** Another user is performing index maintenance (ALTER INDEX, MDLAUX.RECREATEKEYS, etc.).

**Action:** Wait until the other user has finished, then reissue the command.

1837 Cannot create CTAB boost file

**Explanation:** An error has occurred while creating the CTAB boost file.

**Action:** Check for a more specific error to help diagnose the problem.

1838 No boostnames argument provided

**Explanation:** The second argument to MDLAUX.REMOVEBOOSTFILE does not contain one the required Keywords.

**Action:** Correct the argument and reissue the command.

1839 MDLAUX.REMOVEBOOSTFILE failed

**Explanation:** MDLAUX.REMOVEBOOSTFILE has failed.

**Action:** Check for a more specific error to help diagnose the problem.

1841 Cannot remove KEYS boost file: KEYS are disabled

**Explanation:** Substructure keys are disabled for the index, thus a boost file is not in use.

1842 Cannot remove KEYS boost file: Another user is performing index maintenance

**Explanation:** Another user is performing index maintenance (ALTER INDEX, MDLAUX.RECREATEKEYS, etc.).

**Action:** Wait until the other user has finished, then reissue the command.

1843 Cannot remove FASTSEARCH boost file: Index type does not support FASTSEARCH

**Explanation:** Fastsearch is not used by this index type, thus a boost file is not in use.

1844 Cannot remove FASTSEARCH boost file: FASTSEARCH is disabled

**Explanation:** Fastsearch is disabled for the index, thus a boost file is not in use.

1845 Cannot remove FASTSEARCH boost file: Another user is performing index maintenance

**Explanation:** Another user is performing index maintenance (ALTER INDEX, MDLAUX.RECREATEKEYS, etc.).

**Action:** Wait until the other user has finished, then reissue the command.

1846 Cannot remove CTAB boost file: Another user is performing index maintenance

**Explanation:** Another user is performing index maintenance (ALTER INDEX, MDLAUX.RECREATEKEYS, etc.).

**Action:** Wait until the other user has finished, then reissue the command.

1847 Property name cannot be NULL

**Explanation:** The first argument to MDLAUX.SETPROPERTY cannot be NULL.

**Action:** Correct the argument and reissue the command.

1848 Invalid property name: %s

**Explanation:** The first argument to MDLAUX.SETPROPERTY does not specify a valid keyword.

**Action:** Correct the argument and reissue the command.

1849 Error setting global property %s

**Explanation:** An error occurred setting the specified global property.

**Action:** Check for a more specific error to help diagnose the problem.

1850 Error setting global property

**Explanation:** MDLAUX.SETPROPERTY has failed.

**Action:** Check for a more specific error to help diagnose the problem.

1851 Property name cannot be NULL

**Explanation:** The first argument to MDLAUX.GETPROPERTY cannot be NULL.

**Action:** Correct the argument and reissue the command.

1852 Invalid property name: %s

**Explanation:** The first argument to MDLAUX.GETPROPERTY does not specify a valid keyword.

**Action:** Correct the argument and reissue the command.

1853 Error getting global property %s

**Explanation:** An error occurred getting the specified global property.

**Action:** Check for a more specific error to help diagnose the problem.

1854 Error getting global property

**Explanation:** MDLAUX.GETPROPERTY has failed.

**Action:** Check for a more specific error to help diagnose the problem.

1855 Unable to allocate memory

See error 25.

1856 Unable to create index boost file "%s": %s

**Explanation:** Direct is not able to create the boost file.

**Action:** Check the complete file path name and the operating system error that are provided to help diagnose the problem. This problem most often occurs when the Oracle "extproc" process does not have permission to create files in the directory. Ensure that the operating system user which owns the "extproc" process has rights to create files in this directory.

1857 Unable to create data boost file "%s": %s

See error 1856.

1858 Unable to create boost file "%s": %s

See error 1856.

1859 Unable to read BLOB

**Explanation:** An error occurred reading binary data from an Oracle table (either KEYS, FASTSEARCH, or CTAB data).

**Action:** Check for a more specific error to help diagnose the problem.

1860 Error writing data to boost file "%s": %s

**Explanation:** Direct is not able to write data to the boost file.

**Action:** Check the complete file path name and the operating system error that are provided to help diagnose the problem. Ensure that there is sufficient disk space for the files. For information on how to determine how much disk space will be required, see the *Direct 2021 Administration Guide > BIOVIA Direct Boost Files*.

1861 Error writing boost file index data to file "%s": %s

See error 1860.

1862 [error text]

**Explanation:** An error has occurred while mapping a boost file into memory. The error message will list one of the following errors:

Unable to open file "%s": %s  
Unable to memory-map file "%s": %s  
Unable to create file mapping for file "%s": %s  
Unable to get address of memory-mapped file "%s": %s

**Action:** In each case, the complete file path name and the operating system error are provided to help diagnose the problem. Verify that the file exists. If it was inadvertently deleted by an administrator, you must recreate the boost file using MDLAUX.CREATEBOOSTFILE.

1863 [error text]

See error 1862.

1864 Invalid boost file mode

**Explanation:** This is an internal error.

**Action:** Contact Dassault Systèmes Customer Support.

1865 Boost file pathname exceeds 2001 characters

**Explanation:** This is an internal error.

**Action:** Contact Dassault Systèmes Customer Support.

1866 Unable to allocate memory

See error 25.

1867 Unable to prepare or execute SQL: %s

**Explanation:** An error occurred while fetching Fastsearch data to write to the FASTSEARCH boost file.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

1868 Unable to fetch SQL: %s

See error 1867.

1869 Unable to prepare or execute SQL: %s

See error 1867.

1870 Unable to allocate memory

See error 25.

1871 Unable to prepare or execute SQL: %s

**Explanation:** An error occurred while fetching key data to write to the KEYS boost file.

**Action:** Check the SQL command and Oracle error messages are included to help diagnose the problem.

1872 Unable to fetch SQL: %s

See error 1871.

1873 Unable to prepare or execute SQL: %s

See error 1871.

1874 Unable to allocate memory

See error 25.

1875 Error fetching CTAB

**Explanation:** An error occurred while fetching molecule or reaction ctab data to write to the CTAB boost file.

**Action:** Check for a more specific error to help diagnose the problem.

1876 BOOSTDIR directory name is too long: %s

**Explanation:** The directory name in a BOOSTDIR=directory-name parameter is too long. The name cannot exceed 1000 characters.

**Action:** Correct the directory name and reissue the command.

1877 Invalid argument to MDLGetWrapLob

**Explanation:** This is an internal error.

**Action:** Contact Dassault Systèmes Customer Support.

1878 MDLGetWrapLob can not use boost file with index

**Explanation:** This is an internal error.

**Action:** Contact Dassault Systèmes Customer Support.

1879 MDLGetWrapLob cannot write to boost file

**Explanation:** This is an internal error.

**Action:** Contact Dassault Systèmes Customer Support.

1880 SSS search query can not contain only global template atoms

**Explanation:** The SSS query molecule cannot be composed only of global template atoms, there must be one or more real atoms or local template atoms.

**Action:** Correct the query and then reissue it.

1881 Tablespace "%s" does not exist (not found in USER\_TABLESPACES)

**Explanation:** This error precedes errors 1343-1346 and indicates that the tablespace does not exist or that the user does not have the required privileges to access the tablespace.

**Action:** Either specify a valid tablespace or assign access privileges to the user.

1882 Tablespace "%s" status is not ONLINE, status is: %s

**Explanation:** This error precedes errors 1343-1346, and indicates that the tablespace is not online, and thus not available to be used.

**Action:** The status of the tablespace is included in the error message, for example the status might be "READ ONLY". Correct status issue.

1883 WARNING: Unable to open CTAB boost file or to map it into memory, search will not use boost file

**Explanation:** The domain index is set up to use a CTAB boost file to enhance search performance, however the search could either not open the file or it could not map the file into memory. The search will continue, but will not use the boost file.

**Action:** Check for a more specific error message giving the reason that the file could not be opened or mapped, for example, someone might have deleted the file.

You can remove the use of this boost file from the domain index with:

```
EXECUTE MDLAUX.REMOVEBOOSTFILE('indexname', 'CTAB');
```

Or you can recreate the boost file with:

```
EXECUTE MDLAUX.CREATEBOOSTFILE('indexname', 'CTAB [BOOSTDIR=directory]');
```

1884 WARNING: Unable to open FASTSEARCH boost file or to map it into memory, search will not use boost file

**Explanation:** The domain index is set up to use a FASTSEARCH boost file to enhance search performance, however the search could either not open the file or it could not map the file into memory. The search will continue, but will not use the boost file.

**Action:** There will be a more specific error message giving the reason that the file could not be opened or mapped, for example someone may have deleted the file.

You can remove the use of this boost file from the domain index with:

```
EXECUTE MDLAUX.REMOVEBOOSTFILE('indexname', 'FASTSEARCH');
```

Or you can recreate the boost file with:

```
EXECUTE MDLAUX.CREATEBOOSTFILE('indexname', 'FASTSEARCH [BOOSTDIR=directory]');
```

1885 WARNING: Unable to open KEYS boost file or to map it into memory, search will not use boost file

**Explanation:** The domain index is set up to use a KEYS boost file to enhance search performance, however the search could either not open the file or it could not map the file into memory. The search will continue, but will not use the boost file.

**Action:** Check for a more specific error message giving the reason that the file could not be opened or mapped, for example someone might have deleted the file.

You can remove the use of this boost file from the domain index with:

```
EXECUTE MDLAUX.REMOVEBOOSTFILE('indexname', 'KEYS');
```

Or you can recreate the boost file with:

```
EXECUTE MDLAUX.CREATEBOOSTFILE('indexname', 'KEYS [BOOSTDIR=directory]');
```

1892 Unable to read packed ctab from boost file at REGNO=%d

**Explanation:** An error occurred while reading data from the memory-mapped file containing molecule or reaction binary connection table data.

**Action:** Check for an additional error providing an operating system error message. If the error is caused by insufficient virtual memory, you can either increase the amount of physical or virtual memory on the computer, or you can remove the boost file with MDLAUX.REMOVEBOOSTFILE.

1893 Unable to read packed ctab at ROWID=%s

**Explanation:** An error occurred reading the packed binary molecule or reaction connection table from the molecule or reaction table.

**Action:** Check for additional messages to help diagnose the problem.

1894 Unable to read packed ctab at REGNO=%d

**Explanation:** See error 1893.

**Action:** The internal registry number of the record is provided in the error message, this can be converted to a ROWID in the molecule or reaction table with the following SQL query:  
SELECT ROWID FROM molecule-or-reaction-table A, domain-index\_CONV B WHERE  
A.ROWID=B.RID and B.REGNO=regno-from-error-message

1895 Unable to read packed ctab from boost file at ROWID=%s

See error 1892.

1896 Unable to read packed ctab from boost file at REGNO=%d

See error 1892.

1897 Unable to read packed ctab at ROWID=%s

See error 1893.

1898 Unable to allocate memory for ctab data

See error 25.

1899 Unable to read ctab BLOB

**Explanation:** An error occurred reading the contents of the BLOB column containing the packed binary molecule or reaction connection table.

**Action:** Check for additional messages to help diagnose the problem.

1900 Unable to unpack reaction at ROWID=%s

See error 324.

1901 Unable to unpack reaction at REGNO=%d

See error 324.

1902 Unable to unpack reaction

See error 324.

1903 Unable to unpack molecule at ROWID=%s

See error 1049.

1904 Unable to unpack molecule at REGNO=%d

See error 1049.

1905 Unable to unpack molecule

See error 1049.

1910 Cannot remove KEYS boost file: No boost file in use

**Explanation:** This error occurred because there is no boost file for this index, and so there is nothing to remove.

**Action:** Do not include the KEYS keyword when calling MDLAUX.REMOVEBOOSTFILE.

1911 Cannot remove FASTSEARCH boost file: No boost file in use

**Explanation:** This error occurred because there is no boost file for this index, and so there is nothing to remove.

**Action:** Do not include the FASTSEARCH keyword when calling MDLAUX.REMOVEBOOSTFILE.

1912 Cannot remove CTAB boost file: No boost file in use

**Explanation:** This error occurred because there is no boost file for this index, and so there is nothing to remove.

**Action:** Do not include the CTAB keyword when calling MDLAUX.REMOVEBOOSTFILE.

1913 TEMPDIR value "%s" is invalid, cannot create temporary file: %s

**Explanation:** The TEMPDIR parameter either stored in the domain index or in the global cartridge settings contains an invalid directory name.

Either the directory does not exist, or the Oracle external procedure process does not have rights to create a file in the directory. The directory specification was valid when it was first set (either by ALTER INDEX or by MDLAUX.SETPROPERTY), the most likely cause of this error is that the directory has been deleted.

**Action:** Use MDLAUX.INDEXPARAMETERS to see the current setting of TEMPDIR for the index. If not set for the index, use MDLAUX.GETPROPERTY('TEMPDIR') to see the current setting for the cartridge. Whichever is invalid should be corrected. To correct the index setting, use ALTER INDEX PARAMETERS ('TEMPDIR=new-directory').

To correct the global cartridge setting, use MDLAUX.SETPROPERTY('TEMPDIR', 'new-directory').

1914 Invalid ALTER INDEX REBUILD 'ENVIRONMENT' parameter(s)

**Explanation:** This indicates that one or more parameters in the PARAMETERS argument to ALTER INDEX REBUILD is invalid. There will be a more specific message indicating exactly which parameters caused the error.

**Action:** Correct the parameter and rerun the command.

#### 1915 Error in COMMIT

**Explanation:** An error occurred while committing work after a successful ALTER INDEX REBUILD operation.

**Action:** Check the Oracle error message to help diagnose the problem.

#### 1916 Error in COMMIT

**Explanation:** An error occurred while committing work after a successful RECREATEFASTSEARCH operation.

**Action:** Check the Oracle error message to help diagnose the problem.

#### 1917 Error in COMMIT

**Explanation:** An error occurred while committing work after a successful RECREATEKEYS operation.

**Action:** Check the Oracle error message to help diagnose the problem.

#### 1918 Unable to get index creation parameters

**Explanation:** An error occurred while fetching index creation parameters for display in MDLAUX.INDEXPARAMETERS.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

#### 1919 Molecule failed registration check: %s

**Explanation:** This error indicates that the molecule cannot be registered; the reason for the failure is included in the error message. A common reason is that the molecule contains substructure query features.

**Action:** Correct the molecule and try again.

#### 1920 Molecule registration check failed: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

#### 1921 Reaction failed registration check: %s

**Explanation:** This error indicates that the reaction cannot be registered, the reason for the failure is included in the error message. A common reason is that the reaction not contain both reactant and product molecules.

**Action:** Correct the reaction and try again.

#### 1922 Reaction registration check failed: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

#### 1923 Invalid arguments to ANALYZE TABLE

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1924 Unable to rename table, SQL=%s

**Explanation:** An error occurred renaming a domain index table while trying to ensure that it is a secondary table.

**Action:** Check the Oracle error message to help diagnose the problem.

1925 Unable to rename table, SQL=%s

See error 1924.

1926 Invalid call to tableStorage

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1927 Invalid call to indexStorage

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1928 Invalid call to lobStorage

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1929 unable to prepare storage clause for lob %s in table %s

**Explanation:** An error occurred preparing a SQL statement to create a domain index secondary table.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1930 Invalid call to tableSql

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1931 Invalid call to indexSql

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1932 Error updating table during import, SQL: %s

**Explanation:** This indicates an error has occurred while correcting ROWID values during import. One possibility is that the rollback segment is too small; there should be a more specific error message giving more detail.

**Action:** Use the more specific Oracle error message to diagnose and correct the problem, then re-run the import operation.

1933 unable to read binary molecule

**Explanation:** An error occurred unpacking a molecule binary connection table. This could indicate an attempt to unpack a molecule created by Direct 8 or an earlier version of Direct, or it could indicate an attempt to unpack a reaction binary connection table when the operation is expecting a molecule.

1934 unable to read binary molecule: %s

See error 1933.

1935 unable to set global templates in binary molecule

**Explanation:** An error occurred while setting up global and local template definitions in a sequence molecule.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1936 unable to read binary reaction

**Explanation:** An error occurred unpacking a reaction binary connection table. This could indicate an attempt to unpack a reaction created by Direct 8 or an earlier version of Direct, or it could indicate an attempt to unpack a molecule binary connection table when the operation is expecting a reaction.

1937 unable to read binary reaction: %s

See error 1936.

1938 unable to set global templates in binary reaction

**Explanation:** An error occurred while setting up global and local template definitions in a sequence reaction.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1939 unable to write binary molecule

**Explanation:** An error occurred creating a molecule binary connection table.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1940 unable to write binary molecule: %s

See error 1939.

1941 Error in molecule perception: %s

**Explanation:** An error occurred while perceiving information about a molecule.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1942 unable to write binary reaction

**Explanation:** An error occurred creating a reaction binary connection table.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1943 Unable to write binary reaction: %s

See error 1942.

1944 Error in reaction perception: %s

**Explanation:** An error occurred while perceiving information about a reaction.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1945 Error in reaction automap: %s

**Explanation:** An error occurred while generating atom-atom maps and bond change marks for a reaction.

**Action:** There should be a more specific error that can be used to help diagnose the problem.

1946 Unable to set global templates

**Explanation:** An error occurred while setting up global and local template definitions in a sequence molecule read in from a molfile.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1947 Unable to read rxnfile: Error in file

**Explanation:** An error occurred while reading a rxnfile.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1948 Unable to read rxnfile: Empty file

**Explanation:** An rxnfile was provided to Direct but the file was empty.

**Action:** Correct the file and try again.

1949 Unable to read rxnfile

See error 1947.

1950 Unable to read rxnfile: %s

See error 1947.

1951 Unable to write rxnfile

**Explanation:** An error occurred while writing a rxnfile.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1952 Unable to write rxnfile: %s

See error 1951.

1953 Unable to read molfile: Error in file

**Explanation:** An error occurred while reading a molfile.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1954 Unable to read molfile: Empty file

**Explanation:** A molfile was provided to Direct but the file was empty.

**Action:** Correct the file and try again.

1955 Unable to read molfile

See error 1953.

1956 Unable to read molfile: %s

See error 1953.

1957 Unable to write molfile

**Explanation:** An error occurred while writing a molfile.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1958 Unable to write molfile: %s

See error 1957.

1959 Error initializing global %s

**Explanation:** An error occurred while installing the global environment for the specified item (for example, PTABLE).

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1960 Error initializing index-specific %s

**Explanation:** An error occurred while installing an index environment for the specified item (for example, PTABLE).

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1961 Environment item %s can not be empty

**Explanation:** An attempt was made to set the environment item to an empty file with MDLAUX.SETENVFILE.

**Action:** Try again with a valid, non-empty, environment file.

1962 No filename for upgrade environment %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1963 Error writing PTABLE environment string to output CLOB

**Explanation:** An error occurred while writing the PTABLE environment to a CLOB.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1964 Unable to fetch %s CLOB from index %s

**Explanation:** An error occurred fetching an environment lob from a domain index while trying to compare the environment with that of another index.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1965 Unable to fetch %s CLOB from index %s

See error 1964.

1966 %s environments are different

**Explanation:** The environments for two domain indexes are different, and the operation (for example, EXCHANGE PARTITION) cannot be done.

**Action:** Ensure that the environments for the two domain indexes are the same.

1967 No local environment available

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1968 Unable to initialize global environment

**Explanation:** An error occurred while initializing the global environment in preparation for ALTER INDEX REBUILD PARAMETERS ('ENVIRONMENT').

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1969 Invalid environment type

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1970 Custom element "%s" is not contained in the global environment; the environment cannot be used with this domain index

**Explanation:** This message occurs with ALTER INDEX REBUILD PARAMETERS ('ENVIRONMENT'). It indicates that the current global environment PTABLE does not contain a custom element (pseudoatom) symbol that is present in the current local domain index environment.

**Action:** Add the custom element to the global PTABLE before you use ALTER INDEX REBUILD PARAMETERS ('ENVIRONMENT').

1971 Error reading global PTABLE

**Explanation:** An error occurred reading the global PTABLE environment.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1972 Error reading global PTABLE: %s

See error 1971.

1973 Data sgroup field "%s" is not contained in the global environment, the environment cannot be used with this domain index

**Explanation:** This message occurs with ALTER INDEX REBUILD PARAMETERS ('ENVIRONMENT'). It indicates that the current global environment SGROUPFIELDS does not contain a data Sgroup field that is being used in the current local domain index.

**Action:** Add the data Sgroup field to the global SGROUPFIELDS before you use ALTER INDEX REBUILD PARAMETERS ('ENVIRONMENT').

1974 unable to get molecule keys from environment

**Explanation:** An error occurred fetching the local and global MOL2DKEYDES environment.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1975 unable to get reaction keys from environment

**Explanation:** An error occurred fetching the local and global RXNCTRKEYDEFS environment.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1976 Unknown type in SetEnvItem

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

1977 Error reading PTABLE

**Explanation:** An error occurred reading the global or local environment PTABLE environment data.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1978 Error reading PTABLE: %s

See error 1977.

1979 warning: Error initializing SALTS definitions

**Explanation:** An error occurred reading the global or local environment SALTS environment data.

**Action:** There should be a more specific error that can be used to help diagnose the problem.

If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1980 warning: Error initializing SALTS definitions: %s

See error 1979.

1981 MOLSKEYDEFS contains invalid header

**Explanation:** An error occurred reading the global or local environment MOLSKEYDEFS environment data, the initial (header) data are invalid.

**Action:** If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1982 MOLSKEYDEFS contains invalid key number at line %d

**Explanation:** An error occurred reading the global or local environment MOLSKEYDEFS environment data, there is an invalid key number in the data.

**Action:** If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1983 MOLSKEYDEFS does not contain enough entries

**Explanation:** An error occurred reading the global or local environment MOLSKEYDEFS environment data, the number of key entries does not match the length specified in the header.

**Action:** If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1984 molecule key definitions cannot be empty

**Explanation:** An error occurred reading the global or local environment MOL2DKEYDEFS environment data, there are no data present at all.

**Action:** If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1985 Reacting center key definitions cannot be empty

**Explanation:** An error occurred reading the global or local environment RXNCTRKEYDEFS environment data, there are no data present at all.

**Action:** If this occurs while calling MDLAUX.SETENVFILE, it indicates an error in the contents of the file. Correct the file and try again.

If this error occurs during an index operation it indicates a general problem with the domain index environment.

1986 Unable to initialize FLEXMATCH matching

**Explanation:** An error occurred while preparing a FLEXMATCH mapping so that the query can be oriented to the target.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

1987 Unable to truncate, SQL=%s

**Explanation:** An error occurred while truncating the <indexname>\_FSIX table.

**Action:** Check the Oracle error message that is included to help diagnose the problem.

1988 Unable to create temporary file name: %s

**Explanation:** An error occurred while trying to generate a temporary file name.

**Action:** The system error message is included to help diagnose the problem. There might be insufficient disk space, or the TEMPDIR parameter might point to a directory that does not exist.

1989 Unable to create temporary file "%s": %s

**Explanation:** An error occurred while creating a temporary file.

**Action:** The file name and system error message are included to help diagnose the problem. There might be insufficient disk space, or the TEMPDIR parameter might point to a directory which does not exist.

1990 Unable to create temporary file name: All possible names already exist

**Explanation:** An error occurred while trying to generate a temporary file name, too many files already exist and a new name cannot be generated.

**Action:** Remove unused temporary files and try again, or specify a TEMPDIR parameter that points to a different directory.

**Note:** Temporary files are named DIRECT\_x where "x" is one or more random characters.

1991 Unable to select from import property table, SQL=%s

**Explanation:** An error occurred selecting rows from the <indexname>\_CRPRM table during an import operation.

**Action:** Check the Oracle error message to help diagnose the problem.

1992 Unable to select from import property table, SQL=%s

See error 1991.

1993 Import property table is missing PARAMETERS data

**Explanation:** The <indexname>\_CRPRM table does not contain the correct information needed to create the domain index during an import operation. This might indicate an internal error during domain index export.

**Action:** Contact Dassault Systèmes Customer Support.

1994 Import property table contains invalid ITEMTYPE value: %d  
See error 1993.

1995 Unable to fetch from import property table, SQL=%s  
See error 1991.

1996 Error during read from import property table: %s  
See error 1993.

1997 Error in import property table  
See error 1993.

1998 Missing import data for %s  
See error 1993.

1999 Unable to compute isotopic formula  
**Explanation:** An error occurred while computing the molecular formula of a molecule.

2000 Unable to compute mono-isotopic mass  
**Explanation:** An error occurred while computing the molecular mass of a molecule.

2001 Unable to get number of keys  
**Explanation:** This is an internal error, and should never occur.  
**Action:** Contact Dassault Systèmes Customer Support.

2002 Unable to get number of keys  
**Explanation:** This is an internal error, and should never occur.  
**Action:** Contact Dassault Systèmes Customer Support.

2003 Error in COMMIT  
See error 1727.

2004 Unable to allocate memory for molecule: %s  
See error 25.

2005 Unable to allocate memory for molecule: %s  
See error 25.

2006 Error preparing molecule for index operation: %s  
**Explanation:** An error occurred while preparing a molecule for indexing.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2007 Unable to allocate memory for reaction: %s

See error 25.

2008 Error preparing reaction for index operation: %s

**Explanation:** An error occurred while preparing a reaction for indexing.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2009 NEMA key error: %s

**Explanation:** An error occurred while generating a NEMA key.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2010 warning: Removed invalid Chiral flag

**Explanation:** This message is informational, not an error. It indicates that during registration the Chiral flag was removed from the molecule or reaction. This occurs when there is symmetry in the structure that prevents it from actually being chiral.

**Action:** To preserve the original molecule or reaction, add a new column and store the original molfile, rxnfile, or Chimestring in it.

2011 warning: Removed invalid non-tetrahedral stereo center(s)

**Explanation:** This message is informational, not an error. It indicates that during registration one or more up or down (non-tetrahedral stereo center) bond marks was removed from the molecule or reaction. This occurs when there is symmetry in the structure which prevents the atom from being a stereo center.

**Action:** To preserve the original molecule or reaction, add a new column and store the original molfile, rxnfile, or Chimestring in it.

2012 warning: Removed invalid atom stereo center(s)

**Explanation:** This message is informational, not an error. It indicates that during registration one or more up or down (tetrahedral stereo center) bond marks was removed from the molecule or reaction. This occurs when there is symmetry in the structure which prevents the atom from being a stereo center.

**Action:** To preserve the original molecule or reaction, add a new column and store the original molfile, rxnfile, or Chimestring in it.

2016 Unable to allocate memory for parameter partitions

See error 25.

2017 Invalid range "%s", use ROWS=min-max

**Explanation:** The ROWS argument to MDLAUX.SCANINDEX is not correct. It must be ROWS=min-max where min is the minimum row number and max is the maximum row number, or it can be ROWS=min-

where only the minimum row number is specified (maximum will be the total number of rows in the table).

**Action:** Correct the argument and try again.

2018 %s filename is missing

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2019 %s filename is too long: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2020 Error generating SMILES

**Explanation:** An error occurred generating the SMILES string for a molecule.

2021 Error generating SMILES: %s

See error 2020.

2022 Error converting SMILES to molecule: %s

**Explanation:** An error occurred converting a SMILES string into a molecule.

2023 warning: Error calculating coordinates for molecule: %s

**Explanation:** An error occurred computing 2D coordinates for a molecule that was converted from a SMILES string. This is only a warning. The molecule will be present but will not have any coordinate information.

2024 Error installing OpenEye license: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2028 Error converting molecule to name

**Explanation:** OpenEye was unable to create an IUPAC name for the molecule.

2029 Error converting molecule to name: %s

See error 2028.

2030 Error installing OpenEye license: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2034 Error converting name to molecule

**Explanation:** OpenEye was unable to create a molecule from the input name.

2035 Error converting name to molecule: %s

See error 2034.

2036 Error generating InChI: %s

**Explanation:** An error occurred generating an InChI string from a molecule.

2037 Error generating InChI: %s

See error 2036.

2038 %s generation failed: Molecule contains Rgroups

**Explanation:** This error indicates that the molecule is a Markush molecule with Rgroups and members, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2039 %s generation failed: Molecule contains polymer Sgroups

**Explanation:** This error indicates that the molecule contains polymer features, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2040 %s generation failed: Molecule contains sequence atoms

**Explanation:** This error indicates that the molecule contains sequence template atoms, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2041 %s generation failed: Molecule contains dative bonds

**Explanation:** This error indicates that the molecule contains dative bonds, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2042 %s generation failed: Molecule contains hydrogen bonds

**Explanation:** This error indicates that the molecule contains hydrogen bonds, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2043 %s generation failed: Molecule contains haptic bonds

**Explanation:** This error indicates that the molecule contains haptic ( $\pi$ -system) bonds, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2044 %s generation failed: Molecule contains markush bonds

**Explanation:** This error indicates that the molecule contains markush bonds, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2045 %s generation failed: Molecule contains pseudo-atoms

**Explanation:** This error indicates that the molecule contains pseudo-atoms, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2046 %s generation failed: Molecule contains enhanced stereochemistry

**Explanation:** This error indicates that the molecule contains enhanced stereochemistry, and a SMILES string, InChI key or IUPAC name cannot be generated from it.

2047 Error drawing molecule

**Explanation:** An error occurred while creating an image of the molecule.

**Action:** If the problem is an invalid parameter, use the more specific error to diagnose the problem.

2048 Error drawing molecule: %s

See error 2047.

2049 Error drawing reaction

**Explanation:** An error occurred while creating an image of the reaction.

**Action:** If the problem is an invalid parameter, use the more specific error to diagnose the problem.

2050 Error drawing reaction: %s

See error 2049.

2051 Invalid value for ImageType (%s), allowed values are PNG, SVG, BMP, EMF, GDJPEG

**Explanation:** An invalid parameter value for MOLIMAGE or RXNIMAGE was specified.

**Action:** Correct the parameter value and try again.

2052 Invalid value for width (%s), must be integer

See error 2051.

2053 Invalid value for Height (%s), must be integer

See error 2051.

2054 Invalid value for ColorAtomsByType (%s), allowed values are TRUE, FALSE

See error 2051.

2055 Invalid value for HydrogenDisplayMode (%s), allowed values are HYDROGEN\_OFF, HYDROGEN\_HETERO, HYDROGEN\_ALL, HYDROGEN\_TERMINAL, HYDROGEN\_TERMINAL\_AND\_HETERO

See error 2051.

2056 Invalid value for BackgroundColor (%s)

See error 2051.

2057 Invalid value for ForegroundColor (%s)

See error 2051.

2058 Invalid value for PolAtomDisplayMode (%s), allowed values are POL\_STYLE\_BEAD, POL\_STYLE\_TEXT

See error 2051.

2059 Invalid value for DisplayAtomMappings (%s), allowed values are TRUE, FALSE

See error 2051.

2060 Invalid value for ReactingCenterDisplay (%s), allowed values are NONE, HASHES, COLOR, THICKNESS, ALL

See error 2051.

2061 Invalid MOLIMAGE/RXNIMAGE option: %s

**Explanation:** An invalid parameter for MOLIMAGE or RXNIMAGE was specified.

**Action:** Correct the parameter and try again.

2062 WARNING: Ignoring previous unpack errors during reaction delete

**Explanation:** The reaction being deleted at the specified ROWID cannot be unpacked, and will not be removed from the FASTSEARCH index. This should not result in incorrect RSS search results.

**Action:** The reaction is corrupted in some way, and should be re-registered.

2063 Molecule failed query check: %s

**Explanation:** The molecule search query is invalid. The reason why it is invalid is included with the error message.

**Action:** Correct the query and try again.

2064 Molecule query has warnings: %s

**Explanation:** The molecule search query is valid, but generated one or more warnings. The warnings are included with the error message.

**Action:** If warranted, correct the query and try again.

2065 Molecule query check failed: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2066 Reaction failed query check: %s

**Explanation:** The reaction search query is invalid. The reason why it is invalid is included with the error message.

**Action:** Correct the query and try again.

2067 Reaction query has warnings: %s

**Explanation:** The reaction search query is valid, but generated one or more warnings. The warnings are included with the error message.

**Action:** If warranted, correct the query and try again.

2068 Reaction query check failed: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2069 Error dropping sequence, SQL=%s

**Explanation:** An error occurred while dropping the domain index sequence.

**Action:** Use the accompanying error messages to help diagnose the problem.

2070 Unable to create sequence, SQL=%s

**Explanation:** An error occurred while creating the domain index sequence.

**Action:** Check the SQL command and Oracle error messages that are included to help diagnose the problem.

2071 Unable to create sequence, SQL=%s

**Explanation:** An error occurred while creating the domain index sequence.

**Action:** Check the SQL command and Oracle error messages that are included to help diagnose the problem.

2072 Unable to load global templates: %s

**Explanation:** An error occurred loading the global template definitions.

**Action:** If this occurs during MDLAUX.SETENVFILE it probably indicates an error in the format of the definitions, correct the file and try again.

2073 Could not find template %s/%s in local or global templates

**Explanation:** The molecule contains a sequence template which does not exist in the global template definitions, and which does not have any local template definition in the molfile. This occurs if a molfile is written that does not include any sequence template definitions.

**Action:** Correct the molfile by adding the local sequence template definition and try again.

2074 unable to set global templates in molecule: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2075 unable to set expand local templates in molecule: %s

**Explanation:** An error occurred while expanding sequence template atoms into their full chemistry.

2076 Mismatched parentheses in formula at %s

**Explanation:** A formula search query does not contain matching open and close parentheses characters.

**Action:** Correct the query and try again.

2077 No atom symbol(s) present

**Explanation:** No atom symbol was found in a formula search query where one was expected.

**Action:** Correct the query and try again.

2078 Quoted atom symbol is empty at %s

**Explanation:** No atom symbol was found in a formula search query where one was expected.

**Action:** Correct the query and try again.

2079 No closing quote found for atom symbol at %s

**Explanation:** A formula search query does not contain matching start and end quote characters.

**Action:** Correct the query and try again.

2080 Illegal atom symbol: %s

**Explanation:** A formula search query contains an invalid atom symbol.

**Action:** Correct the query and try again.

2081 No atom symbol found at %s

**Explanation:** No atom symbol was found in a formula search query where one was expected.

**Action:** Correct the query and try again.

2082 Illegal atom symbol: %s

**Explanation:** A formula search query contains an invalid atom symbol.

**Action:** Correct the query and try again.

2083 Invalid atom range in formula starting at %s

**Explanation:** A formula search query does not contain a valid range of atom counts.

**Action:** Correct the query and try again.

2084 No closing parenthesis found in formula starting at %s

**Explanation:** A formula search query does not contain matching open and close parentheses characters.

**Action:** Correct the query and try again.

2085 Error generating keys for molecule: %s

**Explanation:** An error occurred while generating substructure keys for a molecule.

2086 Error generating keys for reaction: %s

**Explanation:** An error occurred while generating substructure keys for a reaction.

2087 Error generating fragment hash: %s

**Explanation:** An error occurred generating the FLEXMATCH hash screen for a molecule.

2088 Homology group abbreviation star atom cannot be connected to another homology group star atom

**Explanation:** A star atom with a homology group abbreviation (such as Alkyl) cannot be connected to another star atom which has a homology group abbreviation.

**Action:** Correct the molecule and try again.

2089 Error getting homology group information: %s

**Explanation:** An error occurred while getting information about homology group star atoms in the molecule.

2090 Error getting homology group information: %s

See error 2089.

2091 Error generating molecule structure keys

**Explanation:** An error occurred while generating molecule substructure search registration keys.

**Action:** There should be a more specific error that can be used to help diagnose the problem.

2092 Error generating molecule query keys

**Explanation:** An error occurred generating molecule substructure search query keys.

**Action:** There should be a more specific error that can be used to help diagnose the problem.

2093 Error preparing molecule for query operation: %s

**Explanation:** An error occurred while preparing a molecule for use as a substructure query.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2094 Error generating molecule flexmatch query keys

**Explanation:** An error occurred while generating molecule FLEXMATCH search query keys.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2095 Unable to parse formula string: %s

**Explanation:** An error occurred while processing a formula query string.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2096 Unable to process formula counts for formula: %s

See error 2095.

2097 Error generating structure fragment hash

**Explanation:** An error occurred while generating molecule FLEXMATCH search screens for registration.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2098 Error generating query fragment hash

**Explanation:** An error occurred while generating molecule FLEXMATCH query search screens.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2099 Error generating query fragment hash: %s

See error 2097 or 2098.

2100 Unable to calculate formula: %s

**Explanation:** An error occurred computing the molecular formula for a molecule.

2101 Unable to calculate enumerated specific information

**Explanation:** An error occurred while computing information about enumerated specific structures for a markush molecule.

2102 Unable to calculate enumerated specific information: %s

See error 2101.

2103 Error generating reaction structure keys

**Explanation:** An error occurred while generating reaction substructure search registration keys.

**Action:** There should be a more specific error that can be used to help diagnose the problem.

2104 Error generating reaction query keys

**Explanation:** An error occurred while generating reaction substructure search query keys.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2105 Error preparing reaction for query operation: %s

**Explanation:** An error occurred while preparing a reaction for use as a substructure query.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2106 Error creating reaction from molecule: %s

**Explanation:** An error occurred while creating a reaction from a single reactant or product molecule.

2107 Unable to get highlight sequence IDs: %s

**Explanation:** An error occurred calculating the sequence ID numbers for the sequence atoms mapped by a substructure query.

2109 Unable to parse formula query string: %s

**Explanation:** An error occurred while parsing a formula query string.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2110 Unable to parse target formula string: %s

**Explanation:** An error occurred while parsing a target formula string.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2111 Unable to calculate target formula: %s

**Explanation:** An error occurred computing a formula for a search target.

2112 Unable to process formula counts

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2113 Error preparing markush search query: %s

**Explanation:** An error occurred while preparing a molecule search query.

2114 Error preparing reaction substructure search query: %s

**Explanation:** An error occurred while preparing a reaction search query.

2115 Error preparing substructure search query: %s

**Explanation:** An error occurred while preparing a molecule search query.

2116 Invalid substructure search query: %s

**Explanation:** An error occurred processing a substructure search query.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2117 Invalid substructure search query

See error 2116.

2118 Invalid substructure search query: %s

See error 2116.

2119 Invalid flexmatch map mode

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2120 Invalid flexmatch/overlap search query

**Explanation:** An error occurred processing a FLEXMATCH or OVERLAP search query.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2121 Invalid flexmatch/overlap search query: %s

See error 2120.

2122 Entire query consists of salt fragments, nothing left to search

**Explanation:** A FLEXMATCH query which does have the /SAL flag set consists entirely of salt fragments. Without the /SAL flag, all salt fragments are removed from the query; if the query is just one or more salts then nothing is left and no search can be performed.

**Action:** Correct the query and try again.

2123 Invalid reaction substructure search query

**Explanation:** An error occurred processing a reaction substructure search query.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2124 Invalid reaction substructure search query: %s

See error 2123.

2125 Target mapping preparation failed: %s

**Explanation:** An error occurred while preparing a target for substructure or flexmatch mapping.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2126 Target mapping preparation failed: %s

See error 2126.

2127 Target mapping preparation failed: %s

See error 2126.

2128 Invalid initialization

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2129 warning: Flattening 3D molecule to 2D

**Explanation:** This message is informational, not an error. It indicates that during registration of a 3D model or a reaction containing 3D models, the model was flattened to 2D by setting the Z coordinates of all atoms to zero and adding wedge marks to stereocenters.

**Action:** To preserve the original molecule or reaction, add a new column and store the original molfile, rxnfile, or Chimestring in it.

2131 Error generating reaction SMILES

**Explanation:** An error occurred generating the SMILES string for a reaction.

2132 Error generating reaction SMILES: %s

See error 2131.

2133 Reaction SMILES missing ">>" characters

**Explanation:** The input SMILES string to MDLAUX.SMILESTORXNFILE does not contain the required two '>' characters. The input string is not a reaction SMILES string and cannot be converted.

2134 warning: Removed wedge from atom that is not a stereo center

**Explanation:** This message is informational, not an error. It indicates that during registration one or more up or down (tetrahedral stereo center) bond marks was removed from the molecule or reaction at an atom that is not a stereo center, for example a trivalent nitrogen.

**Action:** To preserve the original molecule or reaction, add a new column and store the original molfile, rxnfile, or Chimestring in it.

2135 MOLSKEYDEFS contains invalid header

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2136 MOLSKEYDEFS contains invalid key number at line %d

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2137 MOLSKEYDEFS does not contain enough entries

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2138 molecule key definitions cannot be empty

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2139 reacting center key definitions cannot be empty

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2140 Reaction SMILES cannot be converted to molecule

**Explanation:** A SMILES string containing the ">" character cannot be converted to a molecule.

**Action:** Use SMILESTORXNFILE to convert a reaction SMILES string to a reaction.

2141 warning: Removed invalid double-either bond(s)

**Explanation:** This message is informational, not an error. It indicates that during registration one or more double-either bond marks were removed because the double bond could not actually be cis or trans.

**Action:** To preserve the original molecule or reaction, add a new column and store the original molfile, rxnfile, or Chimestring in it.

2144 molecule query was modified

**Explanation:** The molecule substructure search query was modified during query processing. For example, hydrogen was removed from a NOT atom list containing hydrogen.

**Action:** Use the Pipeline Pilot Client Query Check Filter component to get detailed information about the change made to the query.

2145 reaction query was modified

**Explanation:** The reaction substructure search query was modified during query processing. For example, hydrogen was removed from a NOT atom list containing hydrogen.

**Action:** Use the Pipeline Pilot Client Query Check Filter component to get detailed information about the change made to the query.

2146 Unable to uncompress binary molecule

See error 1933.

2147 Unable to compress binary molecule

See error 25.

2148 Unable to uncompress binary reaction

See error 1936.

2149 Unable to compress binary reaction

See error 25.

2150 warning: Removed stereogroup from atom that is not a stereo center

**Explanation:** This message is informational, not an error. It indicates that during registration one or more atoms with enhanced stereo information but no wedge bonds had the enhanced stereo information removed from the molecule or reaction at an atom which is not a stereo center, for example at a trivalent nitrogen.

2151 Unable to prepare duplicate REGNO search, SQL=%s

**Explanation:** An error occurred while attempting to fetch value from the indexname\_CONV table. This error occurs when inserting a new record if Direct is unable to determine if a duplicate value for REGNO exists.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

2152 Corruption detected in index: Duplicate REGNO value %s

**Explanation:** This is a serious error indicating corruption in the domain index. The error occurs when inserting a new molecule or reaction and the domain index' sequence specifies a REGNO value which already exists in the index.

**Action:** To correct the error you must drop and recreate the index, rebuilding the index is not sufficient. Contact Dassault Systèmes Customer Support.

2153 warning: Removed invalid inversion/retention flag

**Explanation:** This message is informational, not an error. It indicates that during reaction registration one or more atoms with the inversion/retention flag were not stereo centers and had the flag removed.

2154 REPORTFIELD column name is too long: %s

**Explanation:** The REPORTFIELD argument to MDLAUX.SCANINDEX is not correct. It must be REPORTFIELD=columnname where columnname cannot exceed 30 characters.

**Action:** Correct the argument and try again.

2155 Invalid property name argument

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2156 Error compressing LOB

**Explanation:** An error occurred compressing data to be stored in a LOB.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2157 Error decompressing LOB

**Explanation:** An error occurred decompressing data stored in a LOB.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2158 Error compressing data: %s

**Explanation:** An error occurred in the gzip compression routine.

**Action:** Additional information is provided in the message, please contact FNORD

2159 Error decompressing data: %s

**Explanation:** An error occurred in the gzip decompression routine.

**Action:** Additional information is provided in the message, please contact Dassault Systèmes Customer Support.

2160 Unable to fetch first partition name for partitioned index

**Explanation:** An error occurred fetching the name of the first partition for a partitioned molecule or reaction index.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2161 Partition name must be specified in GETINDEXENVFILE

**Explanation:** When using MDLAUX.GETINDEXENVFILE with a partitioned molecule or reaction index the index partition name must be specified.

**Action:** Use syntax 'index-name PARTITION index-partition-name' or 'table-name PARTITION table-partition-name', for example:

```
SELECT MDLAUX.GETINDEXENVFILE('MOLTABLE PARTITION USER10', 'PTABLE') FROM DUAL;
```

2162 Partition name must be specified in SGROUPFIELDS

**Explanation:** When using MDLAUX.SGROUPFIELDS with a partitioned molecule or reaction index the index partition name must be specified.

**Action:** Use syntax 'index-name PARTITION index-partition-name' or 'table-name PARTITION table-partition-name', for example:

```
SELECT MDLAUX.SGROUPFIELDS('MOLTABLE PARTITION USER10') FROM DUAL;
```

2163 ALTER INDEX without REBUILD is not supported for a partitioned reaction index

**Explanation:** Direct does not support use of ALTER INDEX with a partitioned index unless the REBUILD option is present.

**Action:** Re-enter the command using the REBUILD option.

2164 Error executing %s partition loop SQL: %s

**Explanation:** An error occurred while executing SQL to loop over all partitions of a partitioned domain index.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2165 Error setting environment in %s partition loop

**Explanation:** An error occurred while setting up the chemical environment for a specific index partition during a loop over all index partitions.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2166 Local index partitions cannot be dropped

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2167 Unable to move partition, SQL=%s

**Explanation:** An ALTER TABLE MOVE PARTITION command failed.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2168 Unable to rebuild index partition, SQL=%s

**Explanation:** An ALTER INDEX REBUILD PARTITION command failed.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2169 Unable to add table partition, SQL=%s

**Explanation:** An ALTER TABLE ADD PARTITION command failed.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2170 Unable to merge table partitions, SQL=%s

**Explanation:** An ALTER TABLE MERGE PARTITIONS command failed.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2171 Unable to exchange table partition, SQL=%s

**Explanation:** An ALTER TABLE EXCHANGE PARTITION command failed.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2172 Error locking classcode (insert)

**Explanation:** See error 651.

2173 Error locking classcode (update)

**Explanation:** See error 652.

2174 Unable to select partition data, SQL=%s

**Explanation:** An error occurred while selecting table partition data.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2175 Unable to select partition data, SQL=%s

**Explanation:** An error occurred while selecting table partition data.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2176 CRCV table has too many partitions, SQL=%s

**Explanation:** The indexname\_CRCV table, read from an import dump file, contains more partitions than does the index being imported.

**Action:** Contact Dassault Systèmes Customer Support.

2177 CRCV table has too few partitions, SQL=%s

**Explanation:** The indexname\_CRCV table, read from an import dump file, contains fewer partitions than does the index being imported.

**Action:** Contact Dassault Systèmes Customer Support.

2178 Cannot get creation parameters for adding partition

**Explanation:** See error 1918.

2179 Unable to get UNIQUE setting for partition

**Explanation:** See error 1043.

2180 UNIQUE constraint cannot be applied, there would be duplicates

**Explanation:** This indicates that the UNIQUE constraint cannot be applied to the domain index partition because there are duplicate molecules or reactions.

**Action:** You must remove all duplicates from the partition before using the UNIQUE parameter.

2181 FS index can only be initialized at partition level

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2182 FS index can only be opened at partition level

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2183 FS index can only be closed at partition level

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2184 unable to determine number of partitions for index

**Explanation:** An error occurred in the SQL statement which fetches partition information.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2185 Number of partitions is zero for index %s

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2186 Number of partitions does not match import CRPRM data for index %s

**Explanation:** The indexname\_CRPRM table, read from an import dump file, contains a different number of partitions than does the index being imported.

**Action:** Contact Dassault Systèmes Customer Support.

2187 Unable to select index partition data, SQL=%s

**Explanation:** An error occurred in the SQL statement which fetches partition information.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2188 Unable to select index partition data, SQL=%s

**Explanation:** See error 2187.

2189 Table has too many partitions, SQL=%s

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2190 Import CRPRM parameter table does not contain partition parameters for index partition %s

**Explanation:** The indexname\_CRPRM table, read from an import dump file, is missing information for one of the index partitions.

**Action:** Contact Dassault Systèmes Customer Support.

2191 Number of index partitions does not match number of table partitions, SQL=%s

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2192 Index is partitioned but import property table does not contain partition data

**Explanation:** The indexname\_CRPRM table, read from an import dump file, is missing information for all partitions.

**Action:** Contact Dassault Systèmes Customer Support.

2193 Index is not partitioned but import property table contains partition data

**Explanation:** The indexname\_CRPRM table, read from an import dump file, has partition information but the index is not partitioned.

**Action:** Contact Dassault Systèmes Customer Support.

2194 Unable to prepare or execute partition position select, SQL=%s

**Explanation:** An error occurred in the SQL statement which fetches partition information.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2195 Unable to prepare or execute partition select, SQL=%s

**Explanation:** See error 2194.

2196 Molecule index partition exchange failed

**Explanation:** This is the general exception which is posted when an ALTER INDEX EXCHANGE PARTITION operation fails.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2197 Molecule index partition merge failed

**Explanation:** This is the general exception which is posted when an ALTER INDEX MERGE PARTITIONS operation fails.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2198 Molecule index partition split failed

**Explanation:** This is the general exception which is posted when an ALTER INDEX SPLIT PARTITION operation fails.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2199 Error exchanging index partition, unable to get creation parameters

**Explanation:** An error occurred fetching information from one of the two domain indexes being exchanged.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2200 Error exchanging index partition, unable to get sequence start value

**Explanation:** See error 2199.

2201 Error exchanging index partition, unable to get index partition version information

**Explanation:** See error 2199.

2202 Error exchanging index partition, unable to get index version information

**Explanation:** See error 2199.

2203 Error exchanging index partition, unable to exchange secondary partition"

**Explanation:** An error occurred executing SQL to exchange two domain indexes.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2204 Error exchanging index partition, unable to install properties for partition

**Explanation:** See error 2203.

2205 Error exchanging index partition, unable to install properties for table

**Explanation:** See error 2203.

2206 Error exchanging index partition, unable to recreate sequence

**Explanation:** See error 2203.

2207 Cannot exchange index partition unless index types are the same

**Explanation:** A non-partitioned domain index and a partitioned domain index partition cannot be exchanged unless both have the same index type, for example if one was created with parameters 'GENERIC' then the other must have been created the same way.

**Action:** The index partition and index cannot be exchanged.

2208 Cannot exchange indexpartition: unable to get version of partitioned index

**Explanation:** An error occurred fetching the version of one of the domain indexes being exchanged.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2209 Cannot exchange indexpartition: unable to get version of non-partitioned index

**Explanation:** See error 2208.

2210 Cannot exchange indexpartition, partitioned and non-partitioned index versions are different: %s and %s

**Explanation:** A non-partitioned domain index and a partitioned domain index partition cannot be exchanged unless both have the same index major and minor version. A Direct 2021 partitioned index partition can only be exchanged with a Direct 2021 non-partitioned index, not with a Direct 9.0 index or a Direct 9.0 non-partitioned index.

**Action:** The index partition and index cannot be exchanged.

2211 Cannot merge partitions unless UNIQUE settings are the same

**Explanation:** Two partitioned domain index partitions can only be merged if they have the same settings for their UNIQUE parameter; this ensures that duplicate checking is consistent between the two partitions.

**Action:** Use ALTER INDEX PARTITION REBUILD PARAMETERS ('UNIQUE=flexmatch-switches') to change one of the partition's definition to match the other one; then they can be merged.

2212 Cannot merge partitions unless UNIQUE settings are the same

**Explanation:** See error 2211.

2213 Cannot merge partitions unless UNIQUE settings are the same

**Explanation:** See error 2211.

2214 Cannot merge partitions unless environments are the same

**Explanation:** Two partitioned domain index partitions can only be merged if they have the same chemical environments.

**Action:** You can alter each of the two environments so it is up to date with the current global environment by using ALTER INDEX PARTITION REBUILD PARAMETERS ('ENVIRONMENT') on each of the two partitions first; then they can be merged.

2215 Unable to update property table, SQL=%s

**Explanation:** An error occurred while updating a row in the indexname\_PROP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

2216 Unable to commit property table change

**Explanation:** See error 2215.

2217 Unable to delete from table, SQL=%s

**Explanation:** An error occurred while deleting a row from the indexname\_PROP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

2218 Unable to truncate table, SQL=%s

**Explanation:** An error occurred while truncating the indexname\_PROP table.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

2219 Unable to locate partition %d

**Explanation:** The property table containing information about the domain index is missing an entry for one of the partitions.

**Action:** Contact Dassault Systèmes Customer Support.

2220 Unable to locate partition index for partition %s

**Explanation:** See error 2219.

2221 Unable to update table, SQL=%s

**Explanation:** See error 2215.

2222 Unable to locate partition index for partition %s

**Explanation:** See error 2219.

2223 Unable to locate partition index for partition %s

**Explanation:** See error 2219.

2224 Partitions %s and %s must be adjacent

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2225 Unable to update table, SQL=%s

**Explanation:** See error 2215.

2226 Unable to locate partition index for partition %s

**Explanation:** See error 2219.

2227 Unable to update table, SQL=%s

**Explanation:** See error 2215.

2228 Reaction index partition exchange failed

**Explanation:** This is the general exception which is posted when an ALTER INDEX EXCHANGE PARTITION operation fails.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2229 Reaction index partition merge failed

**Explanation:** This is the general exception which is posted when an ALTER INDEX MERGE PARTITIONS operation fails.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2230 Reaction index partition split failed

**Explanation:** This is the general exception which is posted when an ALTER INDEX SPLIT PARTITION operation fails.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2231 Unable to get table partition, SQL=%s

**Explanation:** An error occurred fetching the table partition name for a specified index partition.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2232 Unable to get table partition, SQL=%s

**Explanation:** See error 2231.

2233 Unable to create sequence, SQL=%s

**Explanation:** An error occurred while creating a sequence for a partitioned domain index.

**Action:** Check the SQL command and Oracle error message that are included to help diagnose the problem.

2234 Unable to insert sequence name into PROP table

**Explanation:** An error occurred while inserting a partitioned index sequence name into the indexname\_PROP table.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2235 Unable to generate partition sequence name

**Explanation:** A new name for the sequence to be used with a partitioned domain index partition cannot be created.

**Action:** Contact Dassault Systèmes Customer Support.

2236 Unable to create sequence, SQL=%s

**Explanation:** See error 2233.

2237 Unable to insert sequence name into PROP table

**Explanation:** See error 2234.

2238 Unable to fetch sequence name for index partition %s

**Explanation:** An error occurred while fetching a partitioned index sequence name from the indexname\_PROP table.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2239 Sequence name is missing for index partition %s

**Explanation:** The partitioned index sequence name is missing from the indexname\_PROP table.

**Action:** Contact Dassault Systèmes Customer Support.

2240 Invalid call to MDLSqncName

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

2241 Molecule will not be indexed at ROWID=%s

**Explanation:** This message is output when a chemical structure error occurs during an index build or rebuild operation. Indexing will not terminate, however the molecule will not be indexed. The molecule table ROWID of the molecule is provided in the error message.

**Action:** The reason for the chemical structure failure will appear in the error log and in the indexname\_LOG table (see MDLAUX.LOGTABLE). Searches which use the index will not find the molecule, searches which do not use the index may or may not find the molecule and may generate errors. The molecule should be corrected or removed from the table.

2242 Reaction will not be indexed at ROWID=%s

**Explanation:** This message is output when a chemical structure error occurs during an index build or rebuild operation. Indexing will not terminate, however the reaction will not be indexed. The reaction table ROWID of the reaction is provided in the error message.

**Action:** The reason for the chemical structure failure will appear in the error log and in the indexname\_LOG table (see MDLAUX.LOGTABLE). Searches which use the index will not find the reaction, searches which do not use the index may or may not find the reaction and may generate errors. The reaction should be corrected or removed from the table.

2243 Error in molecule stereoresolution: %s

**Explanation:** An error occurred while perceiving information about a molecule.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

2244 Invalid value for DisplayRS (%s), allowed values are TRUE, FALSE

**Explanation:** See error 2051.

2245 Invalid value for DisplayEZ (%s), allowed values are TRUE, FALSE

**Explanation:** See error 2051.

2246 Invalid value for ChiralityLabels (%s), must be string  
"ANDtext,ABStext,ORtext,MIXEDtext"

**Explanation:** See error 2051.

2247 BOOSTDIR parameter "%s" is invalid, cannot create test file: %s

**Explanation:** The BOOSTDIR=<dirname> parameter specifies an invalid directory name. The operating system error message is included in the error text.

**Action:** Either the directory does not exist, or the Oracle external procedure process does not have rights to create a file in the directory. Specify a directory exists and which is writable by the extproc process. Note that on Windows, the extproc process is probably not logged in to any domain, and may not be able to access network drives.

2248 Error setting isotope data: %s

**Explanation:** An error occurred while setting up information about atom isotopes.

**Action:** Contact Dassault Systèmes Customer Support.

2249 Invalid thread count in SSS for multi-threaded search

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2250 Invalid thread count in RSS for multi-threaded search

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2251 Invalid thread count in Markush SSS for multi-threaded search

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

2252 Invalid thread count in FLEXFS for multi-threaded search

**Explanation:** This is an internal error and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

# Chapter 3:

## Direct Upgrade Errors

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### Introduction to Upgrade Errors

Using `directupgrade.exe` might generate the following errors.

- In the messages, %s is replaced with text by the program, and %d is replaced by a number.
- Most of the errors are fatal errors. Warning messages are indicated in the descriptions.
- Upgrade error numbers start at 5001.

### Upgrade Error Messages

5001 unable to open log file %s: %s

**Explanation:** The log file cannot be opened.

**Action:** Check for an operating system error is given to help diagnose the problem. Correct the LOGFILE parameter and rerun the command.

5002 Invalid argument: %s

**Explanation:** The command line argument is too long.

**Action:** See errors 5005 and 5006 for more details.

5004 Missing mandatory parameter: %s

**Explanation:** The command line or parameter file has certain mandatory entries. This error indicates that one of these mandatory entries is missing.

**Action:** Correct the parameters and rerun the command.

5005 keyword is too long: %s

**Explanation:** Keywords in the parameter file and on the command line are limited to 63 characters.

**Action:** Correct the entry in the parameter file or on the command line and rerun the command.

5006 value is too long: %s

**Explanation:** Values in the parameter file or on the command line are limited to 511 characters.

**Action:** Correct the entry in the parameter file or on the command line and rerun the command.

5007 Parameter must have a value: %s

**Explanation:** Some parameters take the form <keyword> = <value>. This error indicates that the <keyword> was found, but that its value was not present.

**Action:** Correct the parameter and value and rerun the command.

5011 Invalid parameter: %s

**Explanation:** This error indicates that an unknown parameter was found in the parameter file or on the command line. The unknown (invalid) entry is printed.

**Action:** Correct the parameter and rerun the command.

5013 Unable to open parameter file %s: %s

**Explanation:** The parameter file cannot be opened.

**Action:** Check for an operating system to help diagnose the problem (generally misspelled name.) Correct the parameter file and rerun the command.

5014 Line %d in parameter file is too long, exceeds 606 characters

**Explanation:** A line in the parameter file is too long.

**Action:** The %d value is replaced with the line number to help you location the problem. Correct the parameter file and rerun the command.

5015 Invalid parameter at line %d: %s

**Explanation:** An argument in the parameter file or on the command line is too long

**Action:** See errors 5005 and 5006 for more information.

5016 Parameter may not occur more than once: %s

**Explanation:** A parameter in the parameter file or on the command line occurs more than once.

**Action:** Remove the extra parameter and rerun the command.

5020 OUTPUTFILE parameter can only be used with PTABLE or SALTS parameter

**Explanation:** Invalid input.

**Action:** See the *BIOVIA Direct Administration Guide* for more information.

5021 OUTPUTFILE parameter cannot be combined with CONNSTR, TABLE or INDEX parameters

**Explanation:** Invalid input.

**Action:** See the *BIOVIA Direct Administration Guide* for more information.

5022 R atom replacement symbol is too long, cannot exceed 3 characters

**Explanation:** The value for the RATOMSYMBOL parameter must be an atom symbol from one to three characters.

**Action:** Change the atom symbol and rerun the command.

5023 Z atom replacement symbol is too long, cannot exceed 3 characters

**Explanation:** The value for the ZATOMSYMBOL parameter must be an atom symbol from one to three characters.

**Action:** Change the atom symbol and rerun the command.

5024 R atom replacement symbol cannot be %s, symbol already exists

**Explanation:** The value for the RATOMSYMBOL parameter must be an atom symbol that does not already exist among natural or man-made elements or in the custom element section of the PTABLE.

**Action:** Change the atom symbol and rerun the command.

5025 Z atom replacement symbol cannot be %s, symbol already exists",

**Explanation:** The value for the ZATOMSYMBOL parameter must be an atom symbol that does not already exist among natural or man-made elements or in the custom element section of the PTABLE.

**Action:** Change the atom symbol and rerun the command.

5026 Error verifying R or Z atom symbol replacement: %s

**Explanation:** This is an internal error and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5028 unable to connect to Oracle, invalid CONNSTR parameter: %s

**Explanation:** The CONNSTR parameter does not specify a valid Oracle connection string.

**Action:** Correct the parameter and rerun the command.

5029 unable to establish second connection to Oracle

**Explanation:** directupgrade was able to establish one connection to Oracle, but not a second connection.

**Action:** Check for a more specific error that can be used to help diagnose the problem.

5032 Table does not exist: %s

**Explanation:** The table name specified by the TABLE parameter does not exist.

**Action:** Specify only a table name (no schema). If the table name includes lower-case letters, enclose it in double quotes. Rerun the command using the correct table name.

5033 Column %s does not exist in table %s

**Explanation:** The column name specified by the CTAB parameter does not exist in the table.

**Action:** Rerun the command using the correct column name.

5034 Error installing PTABLE into environment

**Explanation:** An internal error occurred while reading the PTABLE environment. This error should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5035 Error installing PTABLE into environment: %s

See error 5034.

5036 An index with this name already exists: %s

**Explanation:** The index name specified by the INDEX parameter already exists.

**Note:** Note: there must not be any index on the molecule or reaction column when running directupgrade.

**Action:** Specify an index name that does not exist.

5037 Primary key or unique index required

**Explanation:** There must be a single-column primary key constraint or unique index on the molecule or reaction table, this is needed so that structure conversion can be restarted after a failure.

**Action:** Add a primary key constraint or unique index to the table and rerun the command.

5038 Unable to create output file "%s": %s

**Explanation:** The program is unable to create the output file specified in the OUTPUTFILE parameter.

**Action:** Check for an operating system error to help diagnose the problem.

5039 Error writing to output file "%s": %s

**Explanation:** The program is unable to write new PTABLE lines to the output file specified in the OUTPUTFILE parameter.

**Action:** Check for an operating system error to help diagnose the problem.

5040 Error writing to output file "%s": %s

**Explanation:** The program is unable to write new SALTS lines to the output file specified in the OUTPUTFILE parameter.

**Action:** Check for an operating system error to help diagnose the problem.

5041 Table %s does not contain a BLOB molecule or reaction column

**Explanation:** The table specified in the TABLE parameter does not contain any BLOB columns. The table must be a molecule or reaction table.

**Action:** Specify a molecule or reaction table in the TABLE parameter.

5042 Table %s contains more than one BLOB column, specify molecule or reaction column with CTAB parameter

**Explanation:** The table specified in the TABLE parameter contains more than one BLOB column. directupgrade cannot determine which column contains molecules or reactions.

**Action:** Rerun the command and add the CTAB parameter to specify which column contains molecules or reactions.

5043 Column %s already has an index

**Explanation:** The molecule or reaction column already has an index on it.

**Note:** Note: There must not be any index on the molecule or reaction column when running directupgrade.

**Action:** Drop the index and rerun the command.

5044 Unable to select from existing temporary environment table, SQL=%s

**Explanation:** directupgrade reads and writes progress and environment information in a temporary table named DIRUPG\_tablename (where tablename is the first 23 characters of the molecule or reaction table).

An error has occurred while accessing this table.

**Action:** Check for an Oracle error message with additional information to help diagnose the problem.

5045 Temporary environment table is empty, drop table and try again, SQL=%s

See error 5044.

5046 Unable to create temporary environment table, SQL=%s

See error 5044.

5047 Unable to insert row into environment table, SQL=%s

See error 5044.

5048 Unable to commit insert of row into environment table, SQL=%s

See error 5044.

5049 Unable to insert environment lobbs, SQL=%s

See error 5044.

5050 Error inserting progress data, SQL=%s

See error 5044.

5051 Invalid progress string: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5052 warning: Unable to drop table %s

**Explanation:** An error occurred while dropping the progress/environment information temporary table.

**Action:** Drop the table manually. The table is named DIRUPG\_tablename, where tablename is the first 23 characters of the molecule or reaction table name being upgraded.

5053 warning:Unable to drop index %s

**Explanation:** An error occurred dropping the molecule or reaction domain index after a failure that occurred while trying to create the index.

**Action:** Drop the index manually, you might also need to drop all of the secondary objects associated with the index.

5054 Unable to prepare structure select, SQL=%s

**Explanation:** An error occurred preparing the SELECT statement that fetches rows from the molecule or reaction table.

**Action:** Check for an Oracle error message with additional information to help diagnose the problem.

5055 Unable to prepare structure select, SQL=%s

See error 5054.

5056 Unable to fetch from structure select, SQL=%s

**Explanation:** At least two errors occurred while fetching rows from the molecule or reaction table. directupgrade will retry the select and fetch once in case the error is "snapshot too old". If the fetch fails again immediately, this error occurs.

**Action:** Check for an Oracle error message with additional information to help diagnose the problem.

5057 Unable to update progress table

See error 5044.

5058 Unable to COMMIT

**Explanation:** An error occurred committing updates to the molecule or reaction table.

**Action:** Check for an Oracle error message with additional information to help diagnose the problem.

5059 Unable to COMMIT

See error 5058.

5060 Unable to update structure, SQL=%s

**Explanation:** An error occurred updating a structure in the molecule or reaction table.

**Action:** Check for an Oracle error message with additional information to help diagnose the problem.

5061 Error processing structure at ROWID=%s, primary key value=%s

**Explanation:** This error indicates the row that has a structure which cannot be upgraded. The failure to upgrade the structure might be due to an Oracle problem (for example, insufficient table space) or it might be due to a structure that has features that prevent it from being upgraded, such as atom symbols not in the periodic table (error 5088).

**Action:** Check for a more specific error message indicating the reason for the failure.

5062 Error processing structure at ROWID=%s

See error 5062.

5063 unable to get structure lob length

**Explanation:** An error occurred reading the molecule or reaction LOB.

**Action:** Check for an Oracle error message with additional information to help diagnose the problem.

5064 unable to read structure lob

See error 5063.

5065 unable to unpack structure lob to reaction

**Explanation:** An error occurred while trying to unpack the Direct 6, 7, or 8 binary reaction connection table.

**Action:** Contact Dassault Systèmes Customer Support.

5066 unable to unpack structure lob to molecule

**Explanation:** An error occurred while trying to unpack the Direct 6, 7, or 8 binary molecule connection table.

**Action:** Contact Dassault Systèmes Customer Support.

5067 unable to unpack structure lob to molecule or reaction

**Explanation:** The binary molecule or reaction connection table in the first row of the structure column could not be unpacked to either a molecule or a reaction.

This error could indicate that the table is not a Direct 6, 7, or 8 structure table. For example, the table might already have been upgraded to Direct 2021.

5068 unable to convert internal handle to molfile string

**Explanation:** An error occurred writing a molecule to a molfile.

**Action:** Contact Dassault Systèmes Customer Support.

5069 unable to convert internal handle to rxnfile string

**Explanation:** An error occurred writing a reaction to an rxnfile.

**Action:** Contact Dassault Systèmes Customer Support.

5070 unable to write rxnfile, error=%d

See error 5068.

5071 unable to write molfile, error=%d

See error 5069.

5072 unable to open %s file %s: %s

**Explanation:** The program is unable to open the input file specified in the PTABLE or SALTS parameter. The operating system error is included to help diagnose the problem.

**Action:** Specify the correct file name and rerun the command.

5073 unable to open %s file %s: %s

See error 5072.

5074 Line in %s file %s is too long: %s

**Explanation:** A line in the input PTABLE or SALTS file exceeds 4000 characters. This indicates that the file does not contain valid data and it is probably the wrong file.

**Action:** Specify the correct file and rerun the command.

5075 unable to allocate memory for %s file

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5076 Expecting H atom in PTABLE file: %s

**Explanation:** The input PTABLE file does not contain an entry for hydrogen. This indicates that the file does not contain valid data, and it is probably the wrong file.

**Action:** Specify the correct file and rerun the command.

5077 Invalid atom symbol in PTABLE file: %s

**Explanation:** The input PTABLE file does not contain a valid atom symbol. This indicates that the file does not contain valid data, and it is probably the wrong file.

**Action:** Specify the correct file and rerun the command.

5078 Invalid atom symbol in PTABLE file: %s

See error 5077.

5079 Invalid symbol in PTABLE, expected %s but found %s

See error 5077.

5080 Error processing PTABLE file: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5081 First character in SALTS file must be blank, E, or F: %s

**Explanation:** The input SALTS file does not contain valid data, and it is probably the wrong file.

**Action:** Specify the correct file and rerun the command.

5082 Salt name in SALTS file is too long, exceeds 80 characters: %s

See error 5081.

5083 No salt definition in SALTS file: %s

See error 5081.

5084 Unable to read salt definition in SALTS file (error %d): %s

**Explanation:** An error occurred while reading the chemical line notation entry in the SALTS file. This probably indicates that the wrong file was used.

**Action:** Specify the correct file and rerun the command.

5085 Error converting salt definition to molfile: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5086 Unable to create index, SQL=%s

**Explanation:** An error occurred while creating the Direct 2021 molecule or reaction domain index on the upgraded table. The output from MDLAUX.ERRORS is included to help diagnose the problem.

**Action:** You can try to correct the problem (which might be insufficient table space), drop the index and rerun directupgrade with the same parameters. The program will start up where it failed, and try to create the domain index again.

Or you can drop the index, drop the DIRUPG\_tablename temporary table, and create the index manually. If you create the index manually you might need to modify your global PTABLE environment.

5087 WARNING: MDLAUX.RECREATEFASTSEARCH failed

**Explanation:** After successfully creating the molecule or reaction domain index with Fastsearch disabled, the MDLAUX.RECREATEFASTSEARCH command failed. The output from MDLAUX.ERRORS is included to help diagnose the problem.

The domain index should be in a valid state and can be used for searching and registration, however, substructure searches will not use Fastsearch technology and will be slower than usual.

**Action:** Correct the problem (for example insufficient tablespace) and run MDLAUX.RECREATEFASTSEARCH manually to add Fastsearch data to the domain index.

5088 Periodic table does not contain atom symbol %s

**Explanation:** This error indicates that a molecule or reaction being upgraded contains an atom symbol that is not in the periodic table (PTABLE) being used in the upgrade.

**Action:** Either use the original Direct 6.x, 7.0, or 8.0 domain index PTABLE (with the PTABLE parameter to directupgrade) or modify your Direct 2021 global PTABLE to include the new atom symbol.

5089 Error processing atoms in molecule: %s

**Explanation:** This is an internal error, and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

5090 Error processing atoms in molecule: %s

**Explanation:** This is an internal error, and should never occur.

**Action:** Contact Dassault Systèmes Customer Support.

5091 Error processing atoms in reaction: %s

**Explanation:** This is an internal error, and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

5092 warning: Added implicit hydrogens to metal atom

**Explanation:** This message is informational, not an error.

It indicates that during the upgrade process one or more metal atoms had an implicit hydrogen count added to it so that its valence in Direct 9.0 would match its valence in the previous version of Direct.

5093 Error removing homology data Sgroups in molecule: %s

**Explanation:** This is an internal error, and should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

5094 Unable to update structure with NULL, remove any NOT NULL constraint before running directupgrade

**Explanation:** An error occurred updating a structure in the molecule or reaction table with a NULL value (because of use of SKIPBAD parameter).

**Action:** Typically the problem is that there is a NOT NULL constraint on the molecule or reaction column; if this is the case remove the constraint and rerun directupgrade. If this is not the case there should be an Oracle error message with additional information to help diagnose the problem.

5095 Cartridge version in schema containing table to upgrade must be 9.0 or higher

**Explanation:** Direct upgrade requires that the schema containing the table to be upgraded must be set up for Direct 9 or higher

**Action:** Either the schema has not been set up at all or the version is 8 or lower. To set up the schema for Direct 2021 execute the following statements from SQL\*Plus:

```
EXECUTE MDLAUX.UNSETUP;
```

```
EXECUTE C$DIRECT2021.MDLAUXOP.SETUP;
```

5096 Temporary directory %s does not exist or is not writable: %s

**Explanation:** The directory argument to the TEMPDIR parameter is not valid.

**Action:** Replace the parameter value with a valid directory name.

5097 Missing closing quote in TEMPDIR argument

**Explanation:** When enclosing TEMPDIR value in double quote characters, there must be a double quote character at the end.

**Action:** Add a double quote character at the end of the parameter value.

5098 Quote inside quoted TEMPDIR argument must be doubled

**Explanation:** When enclosing TEMPDIR value in double quote characters, any double quote inside the value must be doubled.

**Action:** Double any double quote characters inside the parameter value.

5099 TEMPDIR argument cannot be empty

**Explanation:** When enclosing TEMPDIR value in double quote characters, the value may not be empty.

**Action:** Replace the parameter value with a valid directory name.

5100 unable to create error table, be sure table does not already exist

**Explanation:** Table name specified by ERRORTABLE argument can not be created.

**Action:** If table already exists, drop it and the rerun directupgrade. If table does not exist there will be additional error messages providing more information about why it could not be created.

5101 Periodic table does not contain R atom replacement symbol %s

**Explanation:** The value for the RATOMSYMBOL parameter does not exist in the periodic table (ptable).

**Action:** Specify the name of a symbol which already exists in the custom element section of the ptable, or specify a PTABLE argument for a Direct 8 ptable which contains the R symbol.

5102 Periodic table does not contain Z atom replacement symbol %s

**Explanation:** The value for the ZATOMSYMBOL parameter does not exist in the periodic table (ptable).

**Action:** Specify the name of a symbol which already exists in the custom element section of the ptable, or specify a PTABLE argument for a Direct 8 ptable which contains the Z symbol.

5103 Error validating RATOMSYMBOL or ZATOMSYMBOL: %s

**Explanation:** This is an internal error which should not occur.

**Action:** Contact Dassault Systèmes Customer Support.

5104 warning: Changed atom symbol of R atom

**Explanation:** This message is informational, not an error. It indicates that during the upgrade process an R atom was converted to its replacement atom symbol.

5105 warning: Changed atom symbol of Z atom

**Explanation:** This message is informational, not an error. It indicates that during the upgrade process a Z atom was converted to its replacement atom symbol.

# Chapter 4:

## Oracle Error Messages

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### Common Oracle Error Messages

ORA-00005 bindinfo:invalid date

**Explanation:** A date value is out of the range that can be stored in an Oracle database.

**Action:** Reissue the command with a valid date.

ORA-00009 bindinfo:conversion error

**Explanation:** A data value could not be converted to text, or its text representations is longer than 4000 bytes.

**Action:** Check input data for errors.

ORA-00012 bindinfo:scalar value expected

**Explanation:** This is an internal error message.

**Action:** Contact Dassault Systèmes Customer Support.

ORA-00057 maximum number of temporary table locks exceeded

**Explanation:** The number of temporary tables has reached or exceeded the number of temporary table locks allowed by Oracle. This error is most commonly caused by an SQL statement that has performed a very large sort. The sort has created a number of temporary tables that has exceeded the limit specified in Oracle.

**Action:** To correct this problem, increase the TEMPORARY\_TABLE\_LOCKS parameter in Oracle and perform a restart in Oracle.

ORA-000439: feature not enabled: [feature\_name]

**Explanation:** The database or product being used needs an Oracle feature not present in your Oracle installation. This can happen if you try to install a chemical database that needs Oracle Enterprise Edition features into an Oracle Standard Edition instance.

**Action:** Install the version of Oracle required to use this chemical database or product.

ORA-00600: internal error code, arguments:[17090]

**Explanation:**

1. A resource such as shared pool, memory, temporary tablespace or open cursors has been exhausted.
2. There is an Oracle bug in the management of parsed SQL statements in the SGA that can result in this error. The error code might appear in a trace file (where ORA-03113 end of file on communications channel is seen by the client). It is also possible that the Direct error message Molstructure parameter must not be NULL will result from this bug, and that there will be no trace file.

To check to see if this is the cause of the problem, log in to SQL\*Plus as a DBA, and count the number of active SQL statements:

```
SQL> select count(*) from sys.v_$sqltext;
```

If the result value is in the tens of thousands, then you might have encountered this bug. You can examine the SQL statements to see if they are similar, and to identify what part of your application is generating the SQL statements:

```
SQL> select sql_text from sys.v_$sqltext;
```

**Action:**

1. Check the trace file and examine your Oracle parameters to see if any resource is set too low.
2. To remedy this problem, alter your application to generate fewer unique SQL statements. One method that might help is the binding of variables in places where your application currently inserts constants into the SQL statements.

Increasing the SHARED\_POOL\_SIZE init.ora parameter might reduce the frequency of this error condition.

ORA-00955 [name] is already used by an existing object

**Explanation:** DBCONVERT makes assumptions about the object names it can use. This message might appear during the database creation phase of the database conversion if a name collision occurs or if the creation process has been repeated.

**Action:** If the object should not exist, drop it and retry the operation. Whenever the database creation phase of DBCONVERT has been run and needs to be rerun, you must first run the DELETE.SQLscript to remove the objects that the database creation scripts will try to recreate.

ORA-01000 maximum open cursors exceeded

**Explanation:** The tablespace is too fragmented, the default storage parameter values are set too low, or the open\_cursors parameter value is set too low for the operation.

**Action:** Increase the init.ora parameter open\_cursors. Increase this value in increments of 64 cursors.

ORA-01502: index [s] or partition of such index is in unusable state

**Explanation:** An IMPORT operation was incomplete, or an index CREATE or ALTER failed, or Direct was uninstalled and re-installed.

**Action:** If the index is a domain index and is invalid because Direct was reinstalled, use the MDLAUX.RECREATEINDEXES function to repair the index. For all other cases, to rebuild the specified index, either drop and then create the table or use the ALTER INDEX...REBUILD command.

For more information, see the *Direct Administration Guide*.

ORA-01630 max # of extents [i] reached in temp segment in tablespace [name]

**Explanation:** The tablespace is too fragmented or the object being created needs to be created with higher INITIAL and/or NEXT parameter values.

**Action:** Add new space to the tablespace or try to create the object with different storage parameter values for INITIAL and NEXT.

ORA-01631 max # of extents [i] reached in table [name]

**Explanation:** The table cannot be created from the available extents of disk storage in the tablespace. This condition can be caused by fragmentation or by INITIAL and NEXT storage parameter values that are too low.

**Action:** Determine whether the STORAGE parameter values used to create the table are adequate. Look in the user\_free\_space view to see if the tablespace is too fragmented to create the table. If the

tablespace is too fragmented, either add new, contiguous space to the tablespace, or export the data in the tablespace, recreate the tablespace, and then import the data back into the tablespace.

ORA-01632 max # of extents [i] reached in index [name]

**Explanation:** The STORAGE parameter values for the index are inadequate or the tablespace is fragmented.

**Action:** Create the index using STORAGE parameter values that will enable the index to be created in fewer extents.

ORA-01652 unable to extend temp segment

**Explanation:** This error message is caused by an accumulation of LOB values. Oracle does not provide an record-level duration for LOB values (the smallest duration is that of the cursor).

**Action:** Increase the size of your temporary tablespace until you can reliably perform normal operations.

ORA-01658 unable to create INITIAL extent for segment in tablespace name

**Explanation:** The tablespace does not contain a contiguous extent large enough to create the object.

**Action:** Coalesce the tablespace, or add space to the tablespace.

ORA-2085: database link <database\_link\_name> connects to <global\_database\_name>.

**Explanation:** In an Oracle database with GLOBAL\_NAMES=TRUE, the service name in the TNSNAMES file does not match the global database name, or it lacks a domain in the database alias. Replication requires GLOBAL\_NAMES to be TRUE.

**Action:** Set the database alias equal to the database global name, or rename all instances that are involved in communications with GLOBAL\_NAMES=TRUE instances so that they have a domain in their name.

ORA-03001:unimplemented feature

**Explanation:** This message occurs when attempting to create a table in a tablespace whose features do not support LOB data types. Oracle does not support SEGMENT SPACE MANAGEMENT AUTO with LOB or LONG data types.

**Action:** Use a tablespace that was created with SEGMENT SPACE MANAGEMENT MANUAL.

ORA-03106: fatal two-task communication protocol error

**Explanation:** This message can arise when accessing a column of type ROWID in a table that was created with Oracle 7.x. The rowidformat changed with Oracle version 8.

**Action:** Drop this column from the table.

ORA-04030 out of process memory when trying to allocate [i] bytes

**Explanation:** The user process is out of virtual memory quota. BIOVIA programs use as much as 100 MB of virtual memory under ordinary conditions, and when handling very large chemical structures, the memory demands can be much higher.

**Action:** Make sure that the user account can allocate at least 100 MB of virtual memory. If structures that contain more than 2,000 atoms are being processed, set the quota to 200 MB or higher, as needed. Extreme memory exhaustion might indicate an BIOVIA program defect.

ORA-04031 unable to allocate [i] bytes of shared memory

**Explanation:** The Oracle shared memory pool is exhausted or corrupted.

**Action:** Increase the `init.ora` parameter `shared_pool_size`.

ORA-12560: TNS:protocol adapter error

**Explanation:** The Oracle server process has run out of virtual memory.

**Action:** Restart the Oracle server.

ORA-12701: Invalid or unknown NLS parameter specified

**Explanation:** The files in the `$ORACLE_HOME/ocommon/nls` folder (Linux) or the `%ORACLE_HOME%\ocommon\nls` folder (Microsoft Windows) are not accessible.

**Action:** Ensure that all users have execute rights to all the folders in the path down to the `nls` folder, and read access to the files in that folder.

ORA-12704: character set mismatch

**Explanation:** An attempt was made to store data into a column of type `NCLOB`, `NCHAR`, or `NVARCHAR`.

**Action:** Do not use tables that contain these types with `Direct`.

ORA-12154 TNS:could not resolve service name

**Explanation:** The user process does not have sufficient access to read the Oracle `tnsnames.ora` file.

**Action:** Grant the user appropriate file access.

ORA-22292 Cannot open a LOB in read-write mode without a transaction

**Explanation:** This might be caused by Oracle bug 1219226.

**Action:** Contact Oracle to request the patch for bug 1219226, or upgrade to an Oracle version where this bug is fixed.

ORA-22866: default character set is of varying width

**Explanation:** The `inti.ora` parameter `COMPATIBLE` is set too low, which blocks the creation of tables with columns of type `CLOB`. This affects sites with multibyte character sets.

**Action:** Edit the `inti.ora` parameters to set `COMPATIBLE` to 8.1.0 or higher.

ORA-22992: cannot use LOB locators selected from remote tables

**Explanation:** An attempt was made to retrieve a LOB value through a `DBLINK`.

**Action:** A workaround is to create a separate Oracle session on the remote Oracle database and use that session to retrieve data.

ORA-24805: LOB type mismatch

**Explanation:** This might be caused by an Oracle bug.

**Action:** Check the BIOVIA software requirements for the specific Oracle version to run with the product that you are using. Ensure that you are running the supported version.

SP2-0642 SQL\*Plus internal error state 2147, context 0:0:0 Unsafe to proceed

**Explanation:** When you terminate a Direct operation by pressing Ctrl-C, SQL\*Plus might lose state. This condition might also be seen with LOBhandling.

**Action:** Exit SQL\*Plus and start a new session.

the dynamic link library OCI.dll could not be found in the specified path

**Explanation:** The user process does not have access to the run Oracle executables, or the Oracle BIN folder is not on the user's PATH.

**Action:** Correct the user's PATH or grant the user appropriate permissions.

### Oracle Runtime Error Messages

The following ORA-20100 error message apply to any of the PL/SQL functions in Direct which take as an argument the name of a molecule or reaction index or table, or the name of a molecule or reaction index or table partition.

ORA-20100: <name-of-function>: Index or table name is NULL

**Explanation:** This error occurs if the index or table name argument is a NULL or an empty string.

**Action:** Correct the argument to include a valid table or index name.

ORA-20100: <name-of-function>: Invalid format for domain index or table name: <argument-to-function>

**Explanation:** This error occurs if the index or table name starts or ends with a period.

**Action:** Ensure that the schema, table or index is present and the name does not start or end with a period.

ORA-20100: <name-of-function>: Table contains more than one molecule or reaction index, you must specify the index name: <argument-to-function>

**Explanation:** This error occurs if the argument specifies a molecule or reaction table name which contains more than one domain index.

**Action:** Correct the argument to include the name of the desired domain index, do not use the table name.

ORA-20100: <name-of-function>: No molecule or reaction index or table which has a molecule or reaction index exists with this name: <argument-to-function>

**Explanation:** This error occurs if the argument does not specify a molecule or reaction domain index or a table containing exactly one molecule or reaction domain index.

**Action:** Correct the argument to include a molecule or reaction domain index or a table that contains exactly one molecule or reaction domain index.

ORA-20100: <name-of-function>: Domain index cartridge owner <owner-name-of-index-indextype> does not match current cartridge owner <owner-name-of-cartridge-schema>

**Explanation:** This error indicates that the domain index was created by a version of Direct which is not the same as the version included in the synonyms defined in the schema.

**Action:** To upgrade the domain index to the new version of Direct use MDLAUX.UPGRADEINDEXES\_PREPARE/UPGRADE. To continue using the old version of the index, either use MDLAUX.UNSETUP followed by <old-direct-schema>.MDLAUX.SETUP to reset synonyms to the old version of Direct, or prefix your function or operator with the name of the old version of Direct, for example:

```
SELECT C$DIRECT2021.MDLAUXOP.INDEXPARAMETERS('indexname') FROM DUAL;
```

ORA-20100: <name-of-function>: Molecule index is either invalid or undergoing maintenance: <index-schema>.<index-name>

**Explanation:** This error indicates that even though the argument includes a molecule domain index it is not marked as VALID in the Oracle data dictionary. The cartridge cannot operate on an invalid index.

**Action:** Either the index is undergoing maintenance (for example, another user is using the ALTER INDEX command on it) or you must rebuild the index using ALTER INDEX REBUILD. If you find that you must drop and recreate the index please contact BIOVIA Customer Support.

ORA-20100: <name-of-function>: Reaction index is either invalid or undergoing maintenance: <index-schema>.<index-name>

**Explanation:** This error indicates that even though the argument includes a reaction domain index it is not marked as VALID in the Oracle data dictionary. The cartridge cannot operate on an invalid index.

**Action:** Either the index is undergoing maintenance (for example, another user is using the ALTER INDEX command on it) or you must rebuild the index using ALTER INDEX REBUILD. If you find that you must drop and recreate the index please contact BIOVIA Customer Support.

ORA-20100: <name-of-function>: Missing partition name: <argument-to-function>

**Explanation:** This error indicates that a table or index partition name included the PARTITION keyword but the partition name was missing.

**Action:** Correct the argument to include a partition name.

ORA-20100: <name-of-function>: Invalid format for partition name: <partition-name>

**Explanation:** This error indicates that the partition name following the PARTITION keyword was invalid, for example it starts with a period.

**Action:** Correct the argument to include a valid partition name.

ORA-20100: <name-of-function>: Index partition does not exist: <partition-name>

**Explanation:** This error indicates that the index partition name specified in the argument does not exist.

**Action:** Correct the argument to include a valid index partition name.

ORA-20100: <name-of-function>: Table partition does not exist: <partition-name>

**Explanation:** This error indicates that the table partition name specified in the argument does not exist.

**Action:** Correct the argument to include a valid table partition name.

ORA-20100: PrepareIndexExport: Partitioned domain index cannot be exported

**Explanation:** This error indicates that a partitioned domain index cannot have its secondary table data included in the export dump file.

**Action:** Do not use MDLAUX.PREPAREINDEXEXPORT before exporting a table containing a partitioned domain index.

ORA-20100: PrepareIndexExport: There is no single primary key column for the table: <table-schema>.<table-name>

**Explanation:** This error indicates that MDLAUX.PREPAREINDEXEXPORT is unable to create a table containing ROWID information because there is no single-column primary key.

**Action:** Create a single-column primary key on the table containing the domain index to be exported, then rerun MDLAUX.PREPAREINDEXEXPORT.

ORA-20100: PrepareIndexExport: Error executing SQL statement: <sql-string>

**Explanation:** This error indicates that MDLAUX.PREPAREINDEXEXPORT is unable to create a table containing ROWID information.

**Action:** Contact BIOVIA Customer Support.

ORA-20100: CREATE SYNONYM privilege required (granted directly, not via role)

**Explanation:** This error indicates that the user account does not have the CREATE SYNONYM privilege.

**Action:** The Oracle DBA must grant the CREATE SYNONYM privilege to this account in order for it to create the synonyms needed to access the cartridge.

ORA-20100: Object name in use: <name>

**Explanation:** The synonym name specified is already used to name another object (for example, a table).

**Action:** Rename the object currently using the specified name.

ORA-20100: Error defining synonym: <name>

**Explanation:** The procedure was unable to create the synonym.

**Action:** Contact BIOVIA Customer Support.

ORA-20100: RegenAAMaps: Reaction table, reaction column, and status table names must be specified

**Explanation:** The reaction table, reaction column, and/or status table name was not specified.

**Action:** Specify the missing name, or specify a non-NULL argument for the missing name.

ORA-20100: RegenAAMaps: Invalid atom-atom mapping mode: <mode-argument>

**Explanation:** The atom-atom mapping argument is invalid.

**Action:** Specify a valid atom-atom mapping mode. One of the following modes:

NULL (defaults to 'REGENALTER')

'REGENALTER'

'REGENAUTO'

'DEFAULT'

ORA-20100: RegenAAMaps: The reaction table must exist: <table-name-argument>

**Explanation:** The reaction table argument specifies a table name that does not exist.

**Action:** Specify the name of an existing reaction table.

ORA-20100: RegenAAMaps: The reaction column must exist: <column-name-argument>

**Explanation:** The reaction table argument specifies a column name that does not exist.

**Action:** Specify the name of a reaction column in the reaction table.

ORA-20100: RegenAAMaps: The status-table must exist: <status-table-name-argument>

**Explanation:** The status table argument specifies a table name that does not exist.

**Action:** Specify the name of an existing status table.

ORA-20100: RegenAAMaps: The status-table must contain columns named RID, STATUS, and CHANGES

**Explanation:** The status table exists, but it does not contain the correct columns.

**Action:** Create a status table with the following three columns:

```
CREATE TABLE <status-table-name> (RID ROWID, STATUS NUMBER, CHANGES NUMBER );
```

## Chapter 5:

# Registration Errors

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There are two errors for the registration check, one for molecules and one for reactions:

MDL-1919 Molecule failed registration check: <text>

MDL-1921 Reaction failed registration check: <text>

The value for <text> can any of the following. Reactions have one additional message which is reaction-specific:

Error: Reaction must contain both reactants and products

**Explanation:** A reaction must have at least one component (reactant or product) molecule.

Most of the following errors arise from molfiles that were not created with BIOVIA tools and indicate some kind of corruption in the molecule.

The Rgroup errors include the offending Rgroup number (shown as "R%d" in the message) if it is known, e.g. "R2".

The Sgroup errors include the offending Sgroup number (shown as "%d"). This would be its index number in the molfile.

Error: (%s) No query features allowed for registration

Error: No 3D features are allowed for registration

Error: Non-MDL structure, no registration checking available

**Explanation:** Substructure search query features (for example an "A" atom) are not allowed in a registered structure. If possible the offending feature is included in the message.

Error: Rgroup: R%d definition present without Rgroup usage(s)

**Explanation:** Rgroup members for an Rgroup are present in the structure but that particular R# atom never appears in the connection table.

Error: Rgroup: R%d atom neighbor count must match Rgroup member attachment point definition

**Explanation:** The number of connection to an R# atom in the connection table does not match the number of attachment points for its defined members.

Error: (%s) Unknown atom symbols:

**Explanation:** Only atom symbols present in the Direct global environment are allowed in a registered structure. The offending atom symbol is included in the message.

Error: Rgroup: R%d missing definition.

**Explanation:** An R# atom is present in the connection table but there is no definition of its members.

Error: Rgroup: R%d definition must have a fixed number of attachment points

**Explanation:** The Rgroup members for the specified Rgroup do not all have the same number of attachment points.

Error: Rgroup: R%d definition has more than 250 members

**Explanation:** The number of Rgroup members for the specified Rgroup exceeds 250.

Error: Rgroup: R%d atoms must have a fixed number of attachments

**Explanation:** There are more than one R# atoms in the connection table with differing numbers of attachment points.

Error: Rgroup: R%d atoms cannot be bonded to more than one of the same Rgroup atoms

**Explanation:** A substructure query cannot have an Rn bonded to more than one Rm, for example R2-R1-R2 is illegal.

Error: Rgroup: R%d atoms cannot be bonded to >2 attachments

**Explanation:** Rgroup atoms can only be bonded to zero, one or two neighbors.

Error: Rgroup: R%d atoms cannot have 0 attachments

**Explanation:** A substructure query cannot have an rgroup which is not bonded to any other atoms.

Error: Sgroup: %d (%s) invalid SRU Sgroup, internal error

Error: Sgroup: %d (%s) invalid multiple group, internal error

Error: Sgroup: %d (%s) invalid polymer Sgroup, internal error

**Explanation:** The Sgroup has invalid data for crossing bonds or basis atoms.

Error: Sgroup: %d (%s) invalid polymer Sgroup, unconnected backbone

Error: Sgroup: %d (%s) invalid SRU Sgroup, unconnected backbone

Error: Sgroup: %d (%s) invalid multiple group, unconnected backbone

**Explanation:** A crossing bond is illegal, it either crosses back into the Sgroup or does not originate within the Sgroup.

Error: Sgroup: %d (%s) invalid multiple group, no stereo bonds allowed on crossing bond(s)

Error: Sgroup: %d (%s) invalid SRU Sgroup, no stereo bonds allowed on crossing bond(s)

Error: Sgroup: %d (%s) invalid polymer Sgroup, no stereo bonds allowed on crossing bond(s)

**Explanation:** Crossing bonds cannot have stereochemistry (i.e. be up or down wedge bonds).

Error: Sgroup: %d (%s) invalid polymer Sgroup, crossing bond type mismatch

Error: Sgroup: %d (%s) invalid SRU Sgroup, crossing bond type mismatch

Error: Sgroup: %d (%s) invalid multiple group, crossing bond type mismatch

**Explanation:** The crossing bonds must all be the same type (e.g. if one is a double bond the others must be also).

Error: Sgroup: %d (%s) invalid multiple group, only multiple group, abbreviation, data and generic Sgroup(s) allowed as children

**Explanation:** A multiple Sgroup can only have child (enclosed) Sgroups which are superatom (abbreviation), data or generic Sgroups. No other type of child Sgroup is allowed.

Error: Sgroup: %d (%s) invalid multiple group, only 0 or 2 crossing bonds allowed

**Explanation:** A multiple Sgroup can only have zero or two crossing bonds, not one or more than two.

Error: Sgroup: %d (%s) invalid multiple group, repeat count must be >=1

**Explanation:** A multiple Sgroup repeat count cannot be zero.

Error: Sgroup: %d (%s) invalid multiple group, crossing bond mismatch between parent atom basis and atom basis

Error: Sgroup: %d (%s) invalid multiple group, missing parent basis definition

Error: Sgroup: %d (%s) invalid multiple group, parent basis mismatch to repeat count

Error: Sgroup: %d (%s) invalid multiple group, parent basis must be a subset of Sgroup basis

Error: Sgroup: %d (%s) invalid multiple group, illegal parent basis

**Explanation:** The list of atoms defining the multiple group is invalid, possibly caused by invalid crossing bond connections.

Error: Sgroup: %d (%s) invalid monomer, no crossing bond(s) allowed

**Explanation:** A monomer Sgroup cannot have any crossing bonds.

Error: Sgroup: %d (%s) invalid data Sgroup, Sgroup basis cannot be empty

**Explanation:** A data Sgroup must be associated with one or more atoms or bonds.

Error: Sgroup: %d (%s) invalid data Sgroup, Sgroup basis must contain atom(s) other than H,Lp

**Explanation:** A data Sgroup must be associated with atoms other than H and Lp.

Error: Sgroup: %d (%s) invalid data Sgroup, no fieldname present

**Explanation:** A data Sgroup must have a fieldname.

Error: Sgroup: %d (%s) invalid data Sgroup, fieldname exceeds 30 characters

**Explanation:** The fieldname of a data Sgroup cannot be more than 30 characters long.

Error: Sgroup: %d (%s) invalid data Sgroup, no fielddata present

**Explanation:** A data Sgroup must have associated data.

Error: Sgroup: %d (%s) invalid data Sgroup, fielddata exceeds 4000 characters

**Explanation:** The data for a data Sgroup cannot be more than 4000 characters long.

Error: Sgroup: %d (%s) invalid SRU Sgroup, 0 or 2-4 crossing bonds required

**Explanation:** An SRU Sgroup cannot have one or more than four crossing bonds.

Error: Sgroup: %d (%s) invalid SRU Sgroup, [ [ ]n...[ ]n ]n is disallowed

**Explanation:** An SRU Sgroup cannot have a child (enclosed) SRU Sgroup comprised of the same atoms as the parent.

Error: Sgroup: %d (%s) invalid SRU Sgroup, SRU children must have >0 crossing bonds

**Explanation:** When an SRU Sgroup has a child (enclosed) SRU Sgroup, the child Sgroup must have two, three or four crossing bonds.

Error: Sgroup: %d (%s) invalid SRU Sgroup, 0 crossing bond SRU requires 1 or more modification Sgroup children

**Explanation:** An SRU Sgroup with no crossing bonds must have at least one child (enclosed) modification (MOD) Sgroup.

Error: Sgroup: %d (%s) invalid SRU Sgroup, only EU polymer configuration allowed for 3 or >4 crossing bonds

**Explanation:** An SRU Sgroup with three or more than four crossing bonds must have an EU polymer configuration.

Error: Sgroup: %d (%s) invalid SRU Sgroup correspondence information

**Explanation:** The SRU Sgroup has invalid information about crossing bond correspondence.

Error: Sgroup: %d (%s) invalid copolymer Sgroup, must have at least 2 polymer children

**Explanation:** A copolymer Sgroup must enclose at least two polymer children in order to be a copolymer.

Error: Sgroup: %d (%s) invalid copolymer Sgroup, 0 or 2-4 crossing bonds required

**Explanation:** A copolymer Sgroup can only have zero or two crossing bonds, not one or more than two.

Error: Sgroup: %d (%s) invalid graft or modification Sgroup, 0 or 2-4 crossing bonds required

**Explanation:** A graft or modification polymer Sgroup can only have zero or two crossing bonds, not one or more than two.

Error: Sgroup: %d (%s) invalid crosslink Sgroup, 1-8 crossing bonds are required

**Explanation:** A crosslink polymer Sgroup must have one to eight crossing bonds.

Error: Sgroup: %d (%s) invalid polymer Sgroup, only EU polymer configuration allowed for 3 or >4 crossing bonds

**Explanation:** A polymer Sgroup with three or more than four crossing bonds must have an EU polymer configuration.

Error: Sgroup: %d (%s) invalid polymer Sgroup correspondence information

**Explanation:** The polymer Sgroup has invalid information about crossing bond correspondence.

Error: Sgroup: %d (%s) invalid mixture or formulation Sgroup, child Sgroup is not a component

Error: Sgroup: %d (%s) invalid mixture or formulation Sgroup, 2 or more component Sgroup children required

Error: Sgroup: %d (%s) invalid mixture or formulation Sgroup, non-component fragment in Sgroup basis

**Explanation:** A mixture or formulation Sgroup must have two or more child (enclosed) component Sgroups, no other type of child Sgroup is allowed.

Error: Sgroup: %d (%s) invalid mixture Sgroup, illegal ordered component

**Explanation:** A mixture Sgroup cannot have a number indicating component ordering.

Error: Sgroup: %d (%s) invalid formulation Sgroup, illegal unordered component

**Explanation:** A formulation Sgroup must have a number indicating component ordering.

Error: Sgroup: %d (%s) invalid component Sgroup, missing required mixture or formulation parent

**Explanation:** A component Sgroup must be a child of (i.e. enclosed by) a parent mixture or formulation Sgroup.

Error: Sgroup: %d (%s) invalid formulation Sgroup, invalid child component order

**Explanation:** Each component Sgroup enclosed by a formulation Sgroup must have a unique component ordering number.

Error: Sgroup: %d (%s) invalid abbreviation, multiple crossing bonds to the same exterior atom(s)

**Explanation:** A superatom (abbreviation) Sgroup cannot have more than one crossing bond to the same atom outside of the superatom.