Program Flow in readJDX

Bryan A. Hanson^a

^aDept. of Chemistry & Biochemistry, DePauw University; hanson@depauw.edu

This version was compiled on July 19, 2020

This vignette is based on readJDX version 0.5.1.

Program Flow

readJDX is coded in such a way that it should be easy to add features. Contributions to improve or expand the package, including pull requests, are always welcome! Table 1 shows the overall flow of the function calls. Only a couple of these functions are exported, so take a look at the source code for documentation. Be sure to check out the *MiniDIFDUP_1* and *MiniDIFDUP_2* vignettes for additional information about the JCAMP-DX file structure and how readJDX functions extract the data.

Table 1. Program Flow.

function	input
readJDX	file name
- findVariableLists	character vector: all lines from original file
- extractParams	character vector: just the metadata lines
 processVariableList 	character vector: a single VL
processXYY	character vector: a single VL
decompLines	character vector: a single VL
getComp	character vector: a single VL
unSQZ	character vector: named with the ASDF mode, called via lapply
insertDUPs	character vector: named with the ASDF mode, called via lapply
repDUPs	a string of length one
deDIF	*list* of character vectors from a single VL; the character vectors are named with the ASDF mode, the list is named with line numbers
unDIF	character vector: one line from VL, entries named by ASDF code
yValueCheck	*list* of character vectors from a single VL; the character vectors are named with the ASDF mode, the list is named with line numbers
processPT	character vector: a single VL

Note:

VL stands for variable list, as defined in the JCAMP-DX standard. For examples see the *MiniDIFDUP_1* vignette.