RTOF PDS L2-TO-L3 DATA PROCESS

Documentation

Abstract

This document contains the description of the software converting the RTOF PDS CODMAC L2 to L3

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1. SOFTWARE DEVELOPMENT

This software was first developed by Brian Magee in 2012 but not usable in state. Thierry Sémon and Sébastien Gasc have completed the software and updated the algorithms to be fully compatible with the Reflectron-type Time-Of-Flight (RTOF) science data.

2. METHOD OVERVIEW

2.1. Method Description

For each PDS level 2 data product we wish to create a respective PDS level 3 data product which will include a calibrated mass scale and corrected signal calibrated to counts (ions) per second. The data products fall into two major categories: GCU (Gas Calibration Unit) measurements and non-GCU measurements. The GCU measurements are meant for calibration purposes only, supporting the non-GCU measurements which actually sample the target environment. RTOF has been operated in various instrument modes, each specific to GCU or non-GCU measurements. For each non-GCU mode there is a suitably paired GCU mode (same resolution, such that the TOF-to-mass calibration variables would be the same in ideal circumstances).

The location of measured mass peaks (in bins) are expected to be fairly consistent over long periods of time (for each mode), changing only slightly due to temperature/environmental effects during the mission. Re-optimization of the instrument modes for the flight model in space (FS) have been performed for few times during the course of the mission. Given these circumstances, PDS-compliant data files have been created for each optimization phase of each instrument mode in order to aid calibration. These files describe the expected locations (in bins) of known mass peaks (e.g. CH_4 at 15.9943… amu) expected to be present for the respective instrument mode, and are to be called “Mass Peak Search Tables”. Additionally, these tables may be updated each time a GCU mode L2 spectra is analyzed and converted to a calibrated L3 spectra, with the expected peak locations modified to reflect the most recent GCU mass scale calibration factors.

GCU measurements have an advantage in accurate mass-scale calibration as the measured signal represents a known gas mixture with sufficient amplitude peaks that cover a wide mass range.

The non-GCU modes are expected to typically produce higher uncertainties when self-calibrating to fewer known species which will provide sufficient signal. Given the afore-mentioned expected consistency of mass peak locations, the non-GCU measurements thus reference recent GCU measurements (at the paired instrument mode) in order to use their mass-scale calibration information - if it can be verified with the available peaks. If the GCU reference mass scale is found to deviate by a certain threshold (500 ppm is the current standard), then the self-calibrated mass scale will be used instead.

2.2. Method Process

Below is the step-by-step overview of conversion from one PDS level 2 data file to its corresponding PDS level 3 output data file:

1. Set up necessary values and variables
2. Retrieve the L2 source file data
3. Process corrections of the raw L2 data signal
4. Initiate the output L3 data based on corrected L2 source data
5. Locate and retrieve the appropriate “Mass Peak Search Table” data file
6. Perform peak-finding and fitting of the peaks described in the “Mass Peak Search Table” data
7. Determine the mass calibration factors based self-calibration
8. (if a GCU spectra) Complete the L3 output Housekeeping Data, generate new “Mass Peak Search Table” files if update option is chosen
9. (if a non-GCU spectra) Locate and retrieve the appropriate processed L3 GCU spectra file to aid calibration
10. Choose between GCU or Self-determined mass calibration factors, determine the data quality id, and calculate the mass scale
11. Write the completed output L3 spectra data to file
12. Cleanup

Although the L2 to L3 conversion is handled one spectra file at a time, the conversion software has been developed to process multiple spectra (all L2 files in a single directory) during the execution of the program.

1. Read the specified COPS data file containing measurements corresponding to the time range of the L2 spectra files to convert
2. Read the specified RTOF Mode ID table
3. Retrieve the list of all L2 spectra files in the specified L2 directory, sorted in the order in which they should be processed (chronological order with all GCU spectra before all non-GCU spectra)
4. Initiate the L3 converter data quality log file and write the header line
5. Loop through each L2 spectra file (in the ordered list) and convert to L3 spectra files (see above stepwise conversion overview above)
6. Cleanup

2.3. Dummy GCU files

To account for the large changes in mass scale that occurred due to various change of settings, optimizations, or warming up of the instrument during the mission, the software needs to be "assisted", i.e. some "dummy" GCU spectra are needed to provide the software accurate mass scale parameters, thus improving greatly the quality of the conversion.

There are two kinds of dummy GCU:
- The software processes the files in a chronological order; a change in the mass scale will be acknowledged by the software only when the first GCU spectrum following the change will be converted. Nevertheless, to let the instrument warm up, the GCU spectra were usually acquired after a few non-GCU spectra were recorded; to apply the mass scale correctly on the latter non-GCU spectra, a **dummy L2 GCU** (based on a real GCU acquired later in time) had to be copied and renamed right before the first non-GCU spectrum.
- The **dummy L3 GCU** spectra were manually created when no "real" GCU existed, with the same purpose as the dummy L2 GCU spectra.

The tables below list the dummy L2 & **dummy L3** GCU spectra for each phase, along with the reference spectra used for the creation of each dummy spectrum.

PRL – Ref Spectrum	Dummy GCU spectra	C	t0
OS_20140513_143027539_M0183	OS_20140424_071527157_M0173.TAB	3092.4879	29.0694
OS_20140513_143027539_M0183	OS_20140424_071627157_M0183.TAB	3092.4879	29.0694
OS_20140513_081039_3_M0515	**OS_20140513_080939_3_M0173.TAB**	3180.7958	63.3393
OS_20141017_114656_3_M0523	**OS_20141017_114556_3_M0183.TAB**	3131.3314	-86.9516
no dummy - DO NOT DELETE	OS_20141017_124757496_M0183.TAB	3056.3400	27.9957
OS_20141103_125555_3_M0524	**OS_20141103_125455_3_M0183.TAB**	3053.9500	25.4397
OS_20141105_160732_3_M0524	**OS_20141105_155255_3_M0183.TAB**	3052.6800	32.3826
SS_20140424_163825_3_M0511	**SS_20140424_163725_3_M0171.TAB**	3170.4100	15.2075
SS_20140725_061242393_M0181	SS_20140424_055503519_M0171.TAB	3165.7752	26.9347
SS_20140725_061242393_M0181	SS_20140424_055603519_M0181.TAB	3165.7752	26.9347
SS_20140529_101700157_M0171	SS_20140526_150401603_M0171.TAB	3210.6632	25.9849
SS_20140725_061242393_M0181	SS_20140726_084842141_M0171.TAB	3165.7752	26.9347
SS_20140903_121457648_M0181	SS_20140903_110136382_M0171.TAB	3104.1533	29.1291
SS_20140903_121457648_M0181	SS_20140903_110236382_M0181.TAB	3104.1533	29.1291
SS_20140803_060902247_M0181	SS_20140904_111908048_M0171.TAB	3166.3673	27.9253
SS_20140907_110121_3_M0511	**SS_20140907_110021_3_M0171.TAB**	3178.3700	22.6131
SS_20140915_085935568_M0181	SS_20140908_112910117_M0181.TAB	3111.7700	29.9123
SS_20140910_110555_3_M0521	**SS_20140910_110455_3_M0181.TAB**	3106.5000	30.5000
SS_20140910_113702_3_M0521	**SS_20140910_113602_3_M0181.TAB**	3108.7000	24.0000
SS_20140910_123815_3_M0521	**SS_20140910_123715_3_M0181.TAB**	3110.0000	23.0000

SS_20140915_091011_3_M0181	SS_20140910_134100_3_M0181.TAB	3111.9600	22.0268
no dummy - DO NOT DELETE	SS_20140915_085935568_M0181.TAB	3112.1129	27.5929
SS_20140917_123358_3_M0521	SS_20140917_123258_3_M0181.TAB	3106.5000	30.5000
SS_20140917_130158_3_M0521	SS_20140917_130058_3_M0181.TAB	3108.7000	24.0000
SS_20140917_140313_3_M0521	SS_20140917_140213_3_M0181.TAB	3110.0000	23.0000
SS_20140917_150335_3_M0521	SS_20140917_150235_3_M0181.TAB	3111.9600	22.0268
SS_20140921_123400_3_M0521	SS_20140921_123300_3_M0181.TAB	3110.3200	13.6335
SS_20140529_101700157_M0171	SS_20141003_145949551_M0171.TAB	3210.6632	25.9849
SS_20141024_203546224_M0181	SS_20141003_150049551_M0181.TAB	3126.7500	27.3758
SS_20141005_124024_3_M0521	SS_20141005_123556_3_M0181.TAB	3125.3700	21.6061
SS_20141019_130435_3_M0521	SS_20141019_123556_3_M0181.TAB	3124.7700	13.4115
SS_20141019_143825_3_M0521	SS_20141019_143725_3_M0181.TAB	3125.6700	27.5000
SS_20141025_125555_3_M0521	SS_20141025_125455_3_M0181.TAB	3125.6500	30.5000
SS_20141025_145723_3_M0521	SS_20141025_145623_3_M0181.TAB	3127.5500	30.5000
SS_20141028_145654_3_M0521	SS_20141028_145554_3_M0181.TAB	3123.5900	30.0000
SS_20141028_165824_3_M0521	SS_20141028_165724_3_M0181.TAB	3125.6900	30.0000
SS_20141028_194217_3_M0511	SS_20141028_194117_3_M0171.TAB	3181.2500	21.7000
SS_20141031_035756_3_M0522	SS_20141031_035656_3_M0181.TAB	3123.3800	31.8000
SS_20141031_055821_3_M0522	SS_20141031_055721_3_M0181.TAB	3126.5400	31.8000
SS_20141113_193926_3_M0181	SS_20141113_152136_3_M0181.TAB	3122.0800	45.3415
SS_20141113_194737_3_M0511	SS_20141113_194637_3_M0171.TAB	3179.8472	25.6498

ESC1 – Ref Spectrum	Dummy GCU spectra	C	t0
from PRL	OS_20141114_135558452_M0183.TAB	3053.6400	29.3426
from PRL	SS_20141113_194253506_M0181.TAB	3126.8200	26.2257

ESC2 – Ref Spectrum	Dummy GCU spectra	C	t0
dummy from ESC1	OS_20150119_002317411_M0173.TAB	3053.4700	29.4751
from ESC1	OS_20150119_002317411_M0183.TAB	3053.4700	29.4751
dummy from ESC1	SS_20150217_230321503_M0171.TAB	3122.7200	27.1679
from ESC1	SS_20150217_230321503_M0181.TAB	3122.7200	27.1679
SS_20150319_125800_3_M0511	SS_20150319_092752_3_M0171.TAB	3225.7800	-588.2060
SS_20150328_051956_3_M0521	SS_20150328_024958_3_M0181.TAB	3122.8700	23.0102
SS_20150510_152136061_M0181	SS_20150412_165059282_M0171.TAB	3116.2918	37.6121
SS_20150510_152136061_M0181	SS_20150412_165159282_M0181.TAB	3116.2918	37.6121
SS_20150513_091216124_M0181	SS_20150513_061158003_M0171.TAB	3124.5517	28.0060
SS_20150513_091216124_M0181	SS_20150513_061258003_M0181.TAB	3124.5517	28.0060
SS_20150527_110226384_M0181	SS_20150523_061416309_M0181.TAB	3124.6400	27.6602

ESC3 – Ref Spectrum	Dummy GCU spectra	C	t0
from ESC1	OS_20150119_002317411_M0183.TAB	3053.4700	29.4677
dummy from ESC2	SS_20150527_110226384_M0171.TAB	3124.6400	27.6602
from ESC2	SS_20150527_110226384_M0181.TAB	3124.6400	27.6602
SS_20150715_071735070_M0181	SS_20150715_061051187_M0181.TAB	3119.5900	23.1956

ESC4 – Ref Spectrum	Dummy GCU spectra	C	t0
from ESC1	OS_20150119_002317411_M0183.TAB	3053.4700	29.4677
dummy from ESC3	SS_20150911_043141329_M0171.TAB	3120.6800	21.6441
from ESC3	SS_20150911_043241329_M0181.TAB	3120.6800	21.6441
SS_20151216_105748_3_M0521	**SS_20151216_105648_3_M0181.TAB**	3114.7700	29.7597
SS_20151216_120233_3_M0521	**SS_20151216_120133_3_M0181.TAB**	3120.2200	26.2967
SS_20151217_114321_3_M0521	**SS_20151217_114221_3_M0181.TAB**	3125.6600	22.8336

EXT1 – Ref Spectrum	Dummy GCU spectra	C	t0
from ESC1	OS_20150119_002317411_M0183.TAB	3053.4700	29.4677
from ESC4	SS_20151222_071228077_M0181.TAB	3127.0800	23.6828
SS_20151230_211913_3_M0521	**SS_20151230_211813_3_M0181.TAB**	3114.3300	26.0000
SS_20151230_222205_3_M0521	**SS_20151230_222105_3_M0181.TAB**	3116.5357	35.1026
SS_20151231_030227_3_M0521	**SS_20151231_030127_3_M0181.TAB**	3121.1800	26.0000
SS_20151231_072922_3_M0521	**SS_20151231_072822_3_M0181.TAB**	3121.4777	33.6357
SS_20151231_173855_3_M0521	**SS_20151231_173755_3_M0181.TAB**	3124.5500	26.0000
SS_20160109_105456_3_M0521	**SS_20160109_105356_3_M0181.TAB**	3109.5235	52.9286
SS_20160115_224502_3_M0181	**SS_20160101_140825_3_M0181.TAB**	3125.8600	26.0000
SS_20160118_030352_3_M0521	**SS_20160118_030252_3_M0181.TAB**	3118.7800	26.0000
SS_20160126_221551_3_M0181	**SS_20160123_190051_3_M0181.TAB**	3122.5600	26.0000
SS_20160127_071447_3_M0521	**SS_20160127_071347_3_M0181.TAB**	3114.1100	26.0000
SS_20160128_000731_3_M0521	**SS_20160128_000631_3_M0181.TAB**	3117.4000	26.0000
SS_20160128_200117_3_M0521	**SS_20160128_200017_3_M0181.TAB**	3118.6800	26.0000
SS_20160208_130451_3_M0521	**SS_20160208_130351_3_M0181.TAB**	3118.5000	30.2868
SS_20160208_140551_3_M0521	**SS_20160208_140451_3_M0181.TAB**	3121.5000	28.1434
SS_20160208_150611_3_M0521	**SS_20160208_150511_3_M0181.TAB**	3123.3200	26.0000
SS_20160213_105457_3_M0521	**SS_20160213_105357_3_M0181.TAB**	3112.4100	26.0000
SS_20160213_135649_3_M0521	**SS_20160213_135549_3_M0181.TAB**	3115.8100	26.0000
SS_20160214_080247_3_M0521	**SS_20160214_080147_3_M0181.TAB**	3117.1900	26.0000
SS_20160215_010201_3_M0521	**SS_20160215_010101_3_M0181.TAB**	3118.4600	26.0000
SS_20160220_104812_3_M0521	**SS_20160220_104712_3_M0181.TAB**	3118.5700	26.0000
SS_20160220_150135_3_M0521	**SS_20160220_150035_3_M0181.TAB**	3119.7400	26.0000
SS_20160220_230127_3_M0521	**SS_20160220_230027_3_M0181.TAB**	3120.7900	26.0000

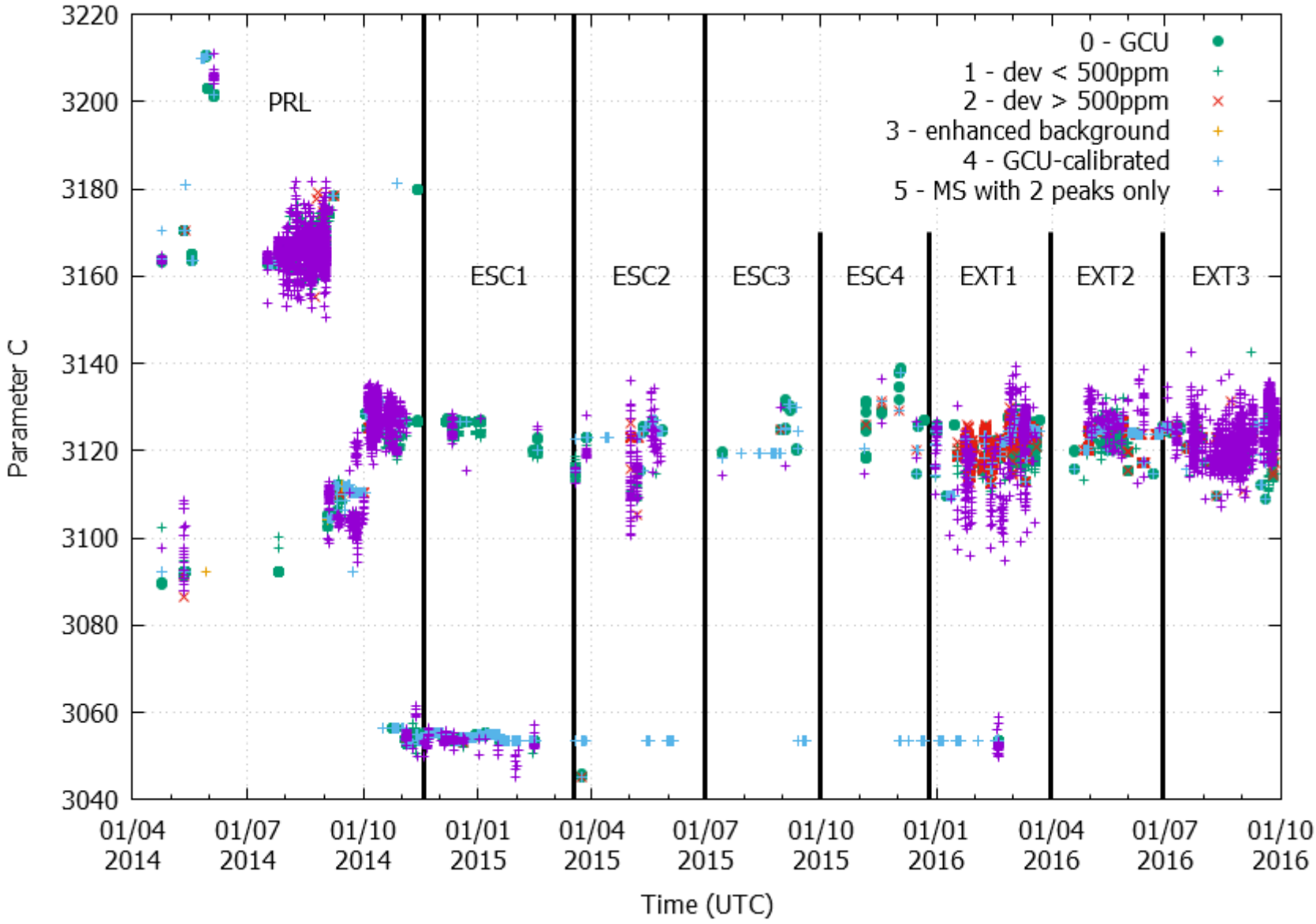
SS_20160221_090107_3_M0521	SS_20160221_090007_3_M0181.TAB	3121.7900	26.0000
SS_20160227_071453_3_M0521	SS_20160227_071353_3_M0181.TAB	3124.5200	26.0000
SS_20160302_230126_3_M0521	SS_20160302_230026_3_M0181.TAB	3124.3100	26.0000
SS_20160303_040402_3_M0521	SS_20160303_040302_3_M0181.TAB	3126.0100	26.0000
SS_20160303_190241_3_M0521	SS_20160303_190141_3_M0181.TAB	3127.4900	26.0000
SS_20160304_170107_3_M0521	SS_20160304_170007_3_M0181.TAB	3124.4100	26.0000
SS_20160312_104853_3_M0181	SS_20160312_104753_3_M0181.TAB	3112.9700	43.0797
SS_20160312_114850_3_M0181	SS_20160312_114950_3_M0181.TAB	3118.4100	20.7412
SS_20160312_205536_3_M0521	SS_20160312_205436_3_M0181.TAB	3122.7600	22.9047
SS_20160313_165829_3_M0521	SS_20160313_165729_3_M0181.TAB	3125.6700	29.1008
SS_20160317_020321_3_M0521	SS_20160317_020221_3_M0181.TAB	3124.7300	26.0000
SS_20160320_010104_3_M0521	SS_20160320_010004_3_M0181.TAB	3124.4100	26.0000

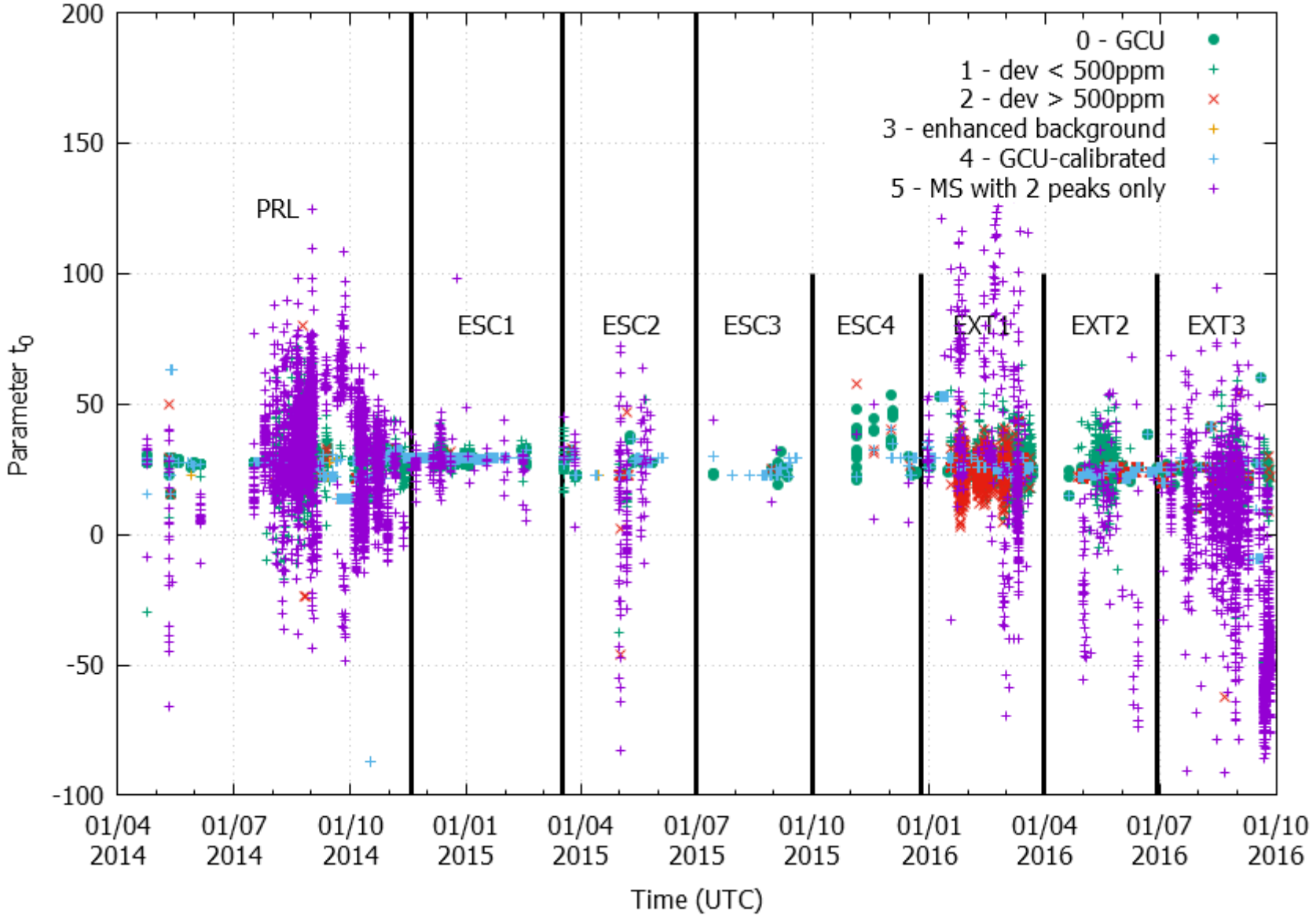
EXT2 – Ref Spectrum	Dummy GCU spectra	C	t0
from EXT1	SS_20160322_174132183_M0181.TAB	3127.1839	27.1101
SS_20160420_072224_3_M0521	SS_20160420_071354_3_M0181.TAB	3115.9500	14.8520
SS_20160501_081511_3_M0521	SS_20160501_074949_3_M0181.TAB	3120.8100	21.5488
SS_20160501_091341_3_M0521	SS_20160501_085147_3_M0181.TAB	3122.6700	22.5195
SS_20160430_230543_3_M0181	SS_20160501_101300_3_M0181.TAB	3124.5300	23.4902
SS_20160515_155543_3_M0521	SS_20160515_155443_3_M0181.TAB	3120.0000	25.0000
SS_20160515_164056_3_M0521	SS_20160515_163956_3_M0181.TAB	3124.0000	24.0000
SS_20160514_230114_3_M0181	SS_20160515_180533_3_M0181.TAB	3125.9800	23.0057
SS_20160601_060558_3_M0521	SS_20160601_060458_3_M0181.TAB	3115.4100	26.0622
SS_20160601_072147_3_M0521	SS_20160601_070655_3_M0181.TAB	3119.7300	23.8804
SS_20160607_225709_3_M0181	SS_20160601_073807_3_M0181.TAB	3124.0400	21.6985
SS_20160613_030046_3_M0521	SS_20160613_025946_3_M0181.TAB	3117.1400	25.6303
SS_20160622_070841_3_M0181	SS_20160622_070741_3_M0181.TAB	3114.5400	38.2331
SS_20160607_230223_3_M0181	SS_20160622_073515_3_M0521.TAB	3123.7300	23.9394

EXT3 – Ref Spectrum	Dummy GCU spectra	C	t0
from EXT2	SS_20160628_230846518_M0181.TAB	3125.4800	25.6686
SS_20160717_143518_3_M0181	SS_20160717_105737104_M0181.TAB	3120.6100	26.3517
SS_20160717_120822_3_M0521	SS_20160717_120722_3_M0181.TAB	3115.8100	29.6241
SS_20160717_143518_3_M0181	SS_20160717_130729_3_M0181.TAB	3120.6100	26.3517
SS_20160720_211021_3_M0521	SS_20160720_211021_3_M0181.TAB	3115.8100	29.6241
SS_20160717_143518_3_M0181	SS_20160720_221034_3_M0181.TAB	3120.6100	26.3517
SS_20160730_040431_3_M0521	SS_20160730_040331_3_M0181.TAB	3123.1300	10.1168
SS_20160809_172756_3_M0181	SS_20160802_091038_3_M0181.TAB	3117.4300	25.9041
SS_20160810_223712_3_M0521	SS_20160810_223612_3_M0181.TAB	3109.4800	41.3475
SS_20160813_004159_3_M0181	SS_20160811_040007_3_M0181.TAB	3123.0800	19.8220

SS_20160814_172917_3_M0521	SS_20160814_172817_3_M0181.TAB	3117.0000	23.0000
SS_20160813_004853_3_M0181	SS_20160815_145242_3_M0181.TAB	3122.6100	22.9876
SS_20160821_145341_3_M0521	SS_20160821_145241_3_M0181.TAB	3117.5000	16.7000
SS_20160820_034038_3_M0181	SS_20160823_170843_3_M0181.TAB	3121.2300	26.4124
SS_20160902_054330_3_M0181	SS_20160901_195054_3_M0181.TAB	3117.5900	26.7519
SS_20160902_212544_3_M0521	SS_20160902_181650_3_M0181.TAB	3122.4900	28.3998
SS_20160908_222642_3_M0181	SS_20160908_133110_3_M0181.TAB	3124.1900	22.4668
SS_20160909_111915_3_M0521	SS_20160909_111815_3_M0181.TAB	3125.8200	-9.0153
SS_20160915_134344_3_M0521	SS_20160915_134244_3_M0181.TAB	3112.0300	27.5851
SS_20160915_144351_3_M0521	SS_20160915_144251_3_M0181.TAB	3118.9250	9.2849
SS_20160915_154409_3_M0521	SS_20160915_154309_3_M0181.TAB	3125.8200	-9.0153
SS_20160916_071343_3_M0521	SS_20160916_071243_3_M0181.TAB	3112.0300	27.5851
SS_20160916_081352_3_M0521	SS_20160916_081252_3_M0181.TAB	3125.8200	-9.0153
SS_20160918_113348_3_M0521	SS_20160918_113248_3_M0181.TAB	3108.9900	60.0992
SS_20160918_123357_3_M0521	SS_20160918_123257_3_M0181.TAB	3117.4050	25.5420
SS_20160918_133416_3_M0521	SS_20160918_133316_3_M0181.TAB	3125.8200	-9.0153
SS_20160921_143331_3_M0521	SS_20160921_131350_3_M0181.TAB	3127.9300	-49.7342
SS_20160921_162710_3_M0521	SS_20160921_161542_3_M0181.TAB	3129.8400	-59.1871
SS_20160923_202820_3_M0521	SS_20160923_202349_3_M0181.TAB	3119.5400	8.8649

With the help of the files above, the changes in mass scales can be handled and the variations of C and t_0 computed on the converted L3 spectra are shown below; the different colors correspond to the different quality flags defined in section 5.5.


0 - GCU
1 - dev < 500ppm
2 - dev > 500ppm
3 - enhanced background
4 - GCU-calibrated
5 - MS with 2 peaks only
PRL
ESC1
ESC2
ESC3
ESC4
EXT1
EXT2
EXT3
Parameter C
Time (UTC)
3220
3200
3180
3160
3140
3120
3100
3080
3060
3040
01/04 2014
01/07 2014
01/10 2014
01/01 2015
01/04 2015
01/07 2015
01/10 2015
01/01 2016
01/04 2016
01/07 2016
01/10 2016


0 - GCU
1 - dev < 500ppm
2 - dev > 500ppm
3 - enhanced background
4 - GCU-calibrated
5 - MS with 2 peaks only
PRL
ESC1
ESC2
ESC3
ESC4
EXT1
EXT2
EXT3
Parameter t_0
Time (UTC)
200
150
100
50
0
-50
-100
01/04 2014
01/07 2014
01/10 2014
01/01 2015
01/04 2015
01/07 2015
01/10 2015
01/01 2016
01/04 2016
01/07 2016
01/10 2016

2.4. Software code source

The code source is located in the **SOFT_L3_RTOF_[MISSION_PHASE].ZIP** file, where **[MISSION_PHASE]** corresponds to the mission phase (i.e. **PRL**, **ESC1**, **ESC2**, **ESC3**, **ESC4**, **EXT1**, **EXT2**, or **EXT3**).

The software was built using **Eclipse IDE for C/C++ Developers**, version Luna service Release 1 (4.4.1).

The **main.c** file contains the following set up variables (values below are the default values for the processing of non-GCU RTOF spectra):

nProcess_GCU_only = 0; // determines whether all files (1) or only the GCU files (1) will be processed
nAllow_nonGCU_cal = 1; // allows (1) or disallows (0) non-GCU files to be self-calibrated (if possible)
nUpdate_MPS_file = 1; // updates (1) or not (0) the MPS tables
nPreliminary_Output_file = 1; // determines the number of digits for the mass value (1 = 2 digits, 0 =8 digits)

The executables used to generate the PDS L3 output files are located in the SOFTWARE/RTOF directory of the **SOFT_L3_RTOF_[MISSION_PHASE].ZIP** file.

- **1_ROSINA_RTOF_PDS_L2_to_L3_GCU.exe** (**nProcess_GCU_only** set to 1)
- **2_ROSINA_RTOF_PDS_L2_to_L3_non_GCU.exe** (**nProcess_GCU_only** set to 0)
- **3_ROSINA_RTOF_PDS_L2_to_L3_manual.exe** (**nAllow_nonGCU_cal** set to 0)
- **4_ROSINA_RTOF_PDS_L2_to_L3_OS_M515.exe** (**MODE_ID_TABLE** changed to define M0515 as an OS mode)

The table below lists the characteristics of all the executables as well as their use in each mission phase.

Executable	1_..._GCU.exe	2_..._non_GCU.exe	3_..._manual.exe	4_..._OS_M515.exe
L2 path	L2/ [MISSION_PHASE]	L2/ [MISSION_PHASE]	L2/ [MISSION_PHASE]_man	L2/ [MISSION_PHASE]_OS_M0515
L3 path	RESOURCES/ GCU_reference	L3	L3	L3
nProcess_GCU_only	1	0	0	0
nAllow_nonGCU_cal	1	1	0	1
PRL	Yes	Yes	Yes	Yes
ESC1	Yes	Yes	No	No
ESC2	Yes	Yes	Yes	No
ESC3	Yes	Yes	Yes	No
ESC4	Yes	Yes	Yes	No
EXT1	Yes	Yes	Yes	No
EXT2	Yes	Yes	Yes	No
EXT3	Yes	Yes	Yes	No

2.5. Running the Software

Structure of the directories:

- All following `paths` are given relative to executable files (`SOFTWARE/RTOF/*.exe`)
- `L2/[MISSION_PHASE]` is the folder containing the RTOF L2 spectra to be converted to L3
- `L2/[MISSION_PHASE]_man` is the folder containing the RTOF L2 spectra to be *manually* converted to L3, i.e. without self-calibration (**nAllow_nonGCU_cal** = 0)
- `L2/[MISSION_PHASE]_corrected` is the folder containing some RTOF L2 spectra which were flagged with a QUALITY_FLAG = 0 in the CODMAC level 2 version of the dataset, and which have been corrected (e.g. for byte shifts).
- `L2/[MISSION_PHASE]_OS_M0515` is the folder containing the RTOF L2 OS M0515 spectra to be converted to L3 (PRELANDING mission phase only)
- `L3` is the folder in which the RTOF L3 spectra will be created
- `RESOURCES/ADC_TDC_CORR_TABLE` is the folder containing the ADC-TDC correction table, where all the factors have been set to 1 (see section 4.2)
- `RESOURCES/COPS/CSV` is the folder containing the COPS density values
- `RESOURCES/DUMMY/DUMMY_L2_GCU` contains the dummy L2 GCU needed to handle a change of mass scale
- `RESOURCES/DUMMY/DUMMY_L2_MPS` contains the MPS associated to the dummy L2 GCU
- `RESOURCES/DUMMY/DUMMY_L3_GCU` contains the dummy L3 GCU needed to handle a change of mass scale
- `RESOURCES/DUMMY/DUMMY_L3_MPS` contains the MPS associated to the dummy L3 GCU
- `RESOURCES/GCU_reference` is the folder containing the L3 GCU (reference)
- `RESOURCES/MASS_PEAK_SEARCH_TABLE` is the folder containing the mass peak search tables created by the conversion software, to be used for the application of the mass scale
- `RESOURCES/MODE_ID_TABLE` is the folder containing the mode ID table, listing all the RTOF modes used during the mission

Steps:

Launching the conversion requires two actions from the user:

a. Copy the corrected L2 files from `L2/[MISSION_PHASE]_corrected` to `L2/[MISSION_PHASE]` (+ copy as well `L2/EXT1_man_corrected` in `L2/EXT1_man`).
b. Run the executable file **1_ROSINA_RTOF_PDS_L2_to_L3_GCU.exe**.

The executable will automatically proceed with the following steps:

1. As soon as the executable **1_ROSINA_RTOF_PDS_L2_to_L3_GCU.exe** is launched, the following folders are emptied:
   - `L3`
   - `RESOURCES/GCU_reference`
   - `RESOURCES/MASS_PEAK_SEARCH_TABLE`

Additionally, the following files are copied:

- from RESOURCES/DUMMY/DUMMY_L2_GCU to L2/[MISSION_PHASE]
- from RESOURCES/DUMMY/DUMMY_L2_MPS to RESOURCES/MASS_PEAK_SEARCH_TABLE

2. The software then proceeds to convert the GCU spectra found in the L2/[MISSION_PHASE] folder. The L3 files are written in RESOURCES/GCU_reference.

3. After conversion of the GCU spectra, **1_ROSINA_RTOF_PDS_L2_to_L3_GCU.exe** deletes the dummy L2 GCU from the L2/[MISSION_PHASE] folder, and launches the second executable: **2_ROSINA_RTOF_PDS_L2_to_L3_non_GCU.exe**.

4. As soon as the executable **2_ROSINA_RTOF_PDS_L2_to_L3_non_GCU.exe** is launched, the following files are copied:
   1. from RESOURCES/DUMMY/DUMMY_L3_GCU to RESOURCES/GCU_reference
   2. from RESOURCES/DUMMY/DUMMY_L3_MPS to RESOURCES/MASS_PEAK_SEARCH_TABLE

5. The software then proceeds to convert the non-GCU spectra found in the L2/[MISSION_PHASE] folder. The L3 files are written in RESOURCES/L3.

6. After conversion of the non GCU spectra (and except in the case of the ESCORT1 mission phase), **2_ROSINA_RTOF_PDS_L2_to_L3_non_GCU.exe** launches the third executable: **3_ROSINA_RTOF_PDS_L2_to_L3_manual.exe**.

7. **3_ROSINA_RTOF_PDS_L2_to_L3_manual.exe** processes the L2 spectra located in L2/[MISSION_PHASE]_man with the variable nAllow_nonGCU_cal set to 0, i.e. without self-calibration. . The L3 files are written in RESOURCES/L3.

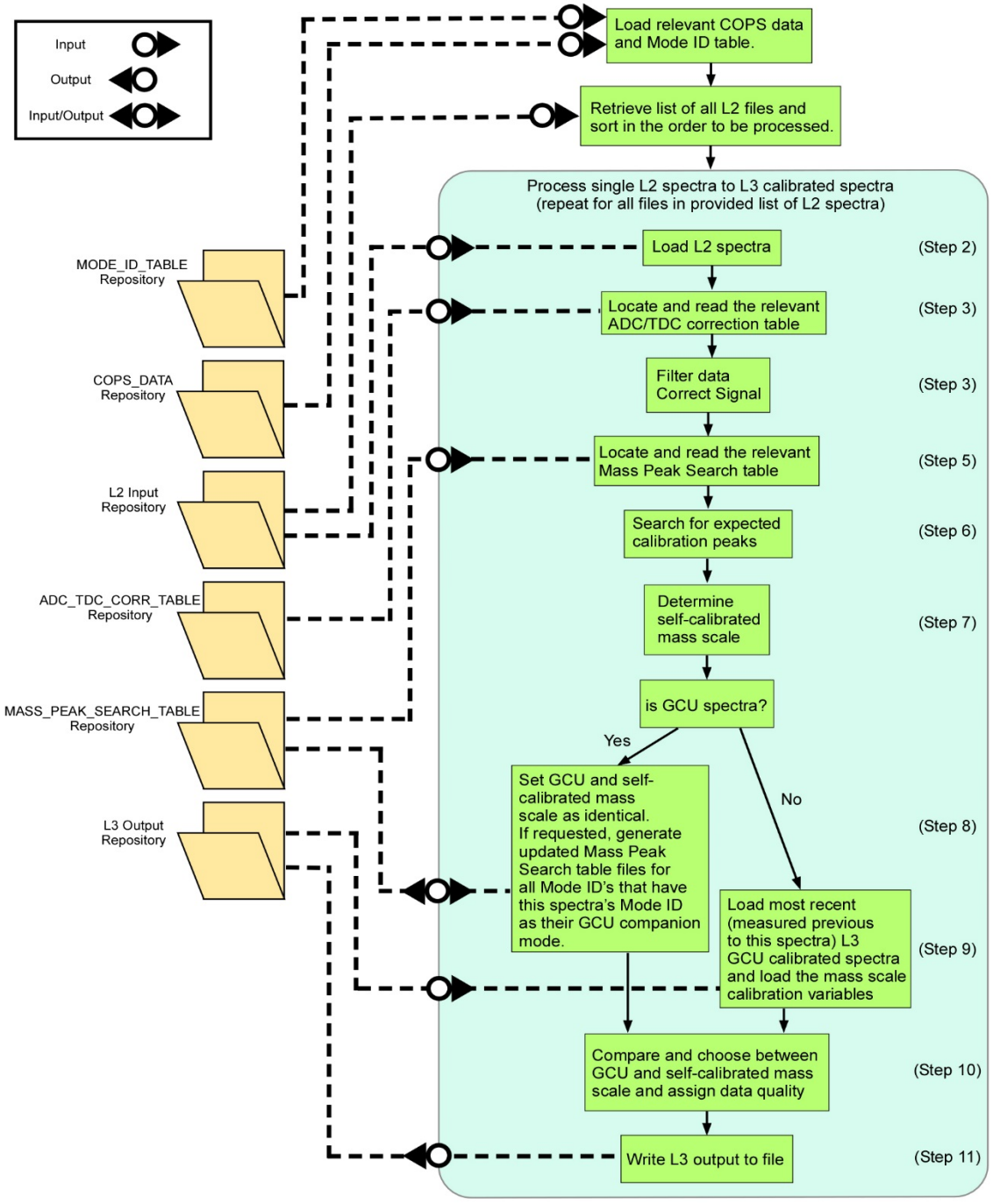
8. After conversion of the "manual" spectra the conversion is finished, except in the case of the PRELANDING mission phase (see "Dataset dependent remarks" below). For PRL only, after conversion of the "manual" spectra, **4_ROSINA_RTOF_PDS_L2_to_L3_OS_M515.exe** is started. It processes the L2 files located in L2/[MISSION_PHASE]_OS_M0515 (with [MISSION_PHASE] = PRL here) and saves the L3 outputs in RESOURCES/L3.

Remark:

In the **PRL** dataset, as M0515 is common to both SS and OS, the M0515 files need to be processed separately. The file **MODE_ID_TABLE.TAB** located in the folder MODE_ID_TABLE needs to be chosen accordingly, and the mass peak search tables associated to SS-M0515 have to be replaced by the ones associated to OS-M0515 (all located in DUMMY/DUMMY_L2_GCU).

3. DATA MANAGEMENT – PDS FILES ORGANIZATION AND WORKFLOW

The below diagram shows the organization of all RTOF PDS files and the L2-to-L3 conversion process with file access/modification/creation chronology. Collections of each file type are separated into their own repository (directory) where all files of that type are to be stored. It is advised that the repositories should exist in directories that split up the RTOF data into logistically planned segments (e.g. one week increments between GCU measurements).



4. CORRECTING THE "RAW" INPUT L2 DATA SIGNAL

4.1. Electronic noise

A pattern due to an electronic noise is visible in many spectra and is corrected by settings all the points around specific bin values to a negative intensity (i.e. a central bin + the previous 48 bins + the following 48 bins are set to -1). This electronic pattern may be seen in the figure at the end of section 4.2. Several configurations exist, depending on the time period to be converted. The lists of the central bins are given below:

10kHz spectra – configuration 1 (MTP2 & MTP4):

3865, 4310, 4986, 5428, 10455, 12248, 13366, 14491, 15208, 21758, 22877, 24717, 25840, 26511, 27639, 34232

10kHz spectra – configuration 2 (MTP3 & MTP5):

3262, 3892, 4409, 5052, 5565, 6206, 6725, 7365, 7882, 8525, 9055, 9685, 10235, 10455, 10992, 11621, 12248, 12767, 13404, 13930, 14565, 15208, 15720, 16358, 16868, 17513, 18024, 18663, 19184, 19822, 20342, 20930, 21758, 22140, 22640, 22925, 24060, 24717, 25210, 25888, 26511, 27021, 27677, 28168, 28829, 29329, 29971, 30484, 31126, 31643, 32277, 32789, 33440, 33960, 34232, 34600

10kHz spectra – configuration 3 (MTP19 to MTP24):

3310, 3923, 4484, 5107, 5650, 6266, 6805, 7434, 7972, 8603, 9136, 9773, 10308, 10455, 11017, 11621, 12248, 12812, 13414, 13980, 14606, 15208, 15772, 16398, 16948, 17568, 18109, 18733, 19289, 19905, 20467, 21075, 21758, 22235, 22785, 22925, 24115, 24717, 25285, 25888, 26511, 27076, 27677, 28243, 28874, 29414, 30046, 30584, 31211, 31748, 32377, 32914, 33545, 34095, 34232, 34725

10kHz spectra – configuration 4 (all other MTPs):

3285, 3913, 4454, 5082, 5620, 6241, 6780, 7409, 7947, 8575, 9111, 9748, 10283, 10455, 10992, 11621, 12248, 12787, 13414, 13955, 14581, 15208, 15747, 16373, 16923, 17543, 18084, 18708, 19264, 19880, 20442, 21050, 21758, 22210, 22760, 22925, 24090, 24717, 25260, 25888, 26511, 27051, 27677, 28218, 28849, 29389, 30021, 30559, 31186, 31723, 32352, 32889, 33520, 34070, 34232, 34700

5kHz spectra:

6480, 7359, 7651, 7943, 12248, 12540, 12832, 17429, 17721, 18013, 18600, 18892, 19184, 23492, 23784, 24076, 28379, 28671, 28963, 29844, 30136, 30428, 33854, 34733, 35025, 35317, 39625, 39917, 40209, 44806, 45098, 45390, 45982, 46274, 46566, 50871, 51163, 51455, 55756, 56048, 56340, 57224, 57516, 57808, 61231, 62110, 62402, 62694, 67001, 67293, 67585

4.2. ADC/TDC corrections

The RTOF ADCs and TDCs suffer from gain differences which add unwanted noise to the spectra and thus must be corrected to obtain a more accurate signal from the raw data.

The signal correction algorithm for the histogram and event data utilizes a set of re-calibration adjustment values for the 16 ADC (resp. TDC) channels. For each record of the event and histogram data, the raw signal is multiplied by the appropriate adjustment value (using the bin number to determine the channel) to obtain the corrected value.

These adjustment values (or correction factors) are calculated by summing the contribution in a spectrum of each ADC / TDC individually, and then normalizing these sums to obtain a correction factor to apply on each ADC / TDC. The code used for the calculation of the correction factors is given below:

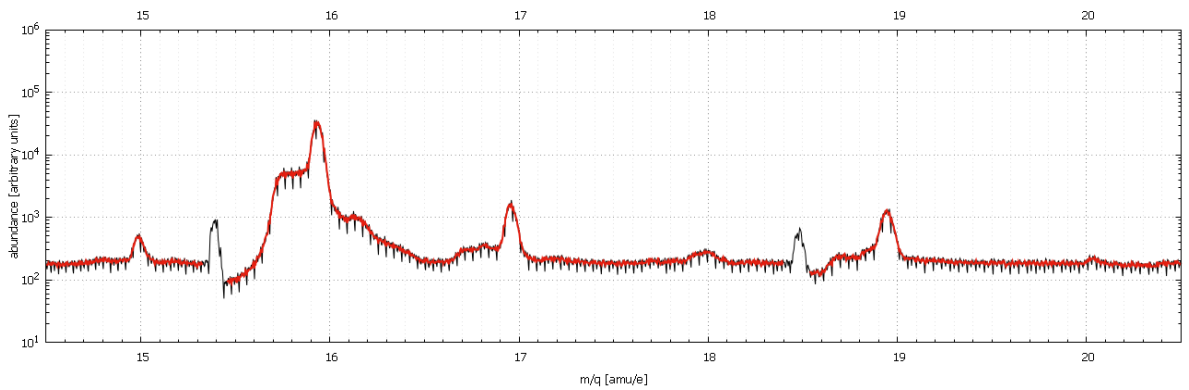
```
// calculate the ADC factors for each spectrum
for (i=3392; i<xThis_PDS_RTOF_DATA_TABLE_L2->records-16; i=i+16)
{
    // calculate the mean ADC values for the 16 ADC
    for (k=0; k<16; k=k+1)
    {
        anADC_mean[k] += xThis_PDS_RTOF_DATA_TABLE_L2->record[i+k].histogram_counts;
    }
}

// calculate the mean of the 16 mean ADC values previously calculated, to be used for normalization
for (k=0; k<16; k=k+1)
{
    anADC_norm += anADC_mean[k]/16.;
}

// calculate the correction factor for each ADC
for (k=0; k<16; k=k+1)
{
    anADC_correction[k] = anADC_mean[k]/anADC_norm;
}

// adjust data according to the ADC (histogram counts) correction factors
for (i=0; i<xThis_PDS_RTOF_DATA_TABLE_L2->records; i=i+1)
{
    nCorrectedData = xThis_PDS_RTOF_DATA_TABLE_L2->record[i].histogram_counts /
        anADC_correction[(xThis_PDS_RTOF_DATA_TABLE_L2->record[i].bin - 1) % 16];
    xThis_PDS_RTOF_DATA_TABLE_L2->record[i].histogram_counts = nCorrectedData;
}
```

Below is an example of the ADC/TDC correction technique on FM Storage Source data (histogram / ADC counts), where the raw signal is in black and the corrected spectrum (for the electronic noise + ADC/TDC pattern) is in red.



4.3. Limiting the data range

The RTOF L2 data files are quite large and contain an excessive number of bins in most cases. In order to reduce the size of RTOF L3 data files, the limited range of bins to retain in the L3 data are listed for each mode ID in the PDS RTOF Mode ID table files. This is defined by all bins occurring between a minimum and maximum bin number (i.e. the bin values of fields '`.retain_bin_start`' and '`.retain_bin_stop`').

4.4. Convert signal to counts (ions) per second

A "signal factor" (as stored in the L3 product RTOF_HK_TABLE) is calculated from the L2 data in order to convert input L2 data into the resultant L3 signal representing counts (ions) per second.

For Storage Source (SS) spectra, the "signal factor" is defined as the inverse of the ratio of total histogram counts (with ADC corrections) to total event counts (with TDC corrections) across the entire spectrum multiplied by the integration time in seconds.

SS_signal_factor = 1 / ((total histogram counts / total event counts) * integration time)

This factor is then multiplied by the ADC corrected L2 histogram data to obtain the resultant signal in counts (ions) per second.

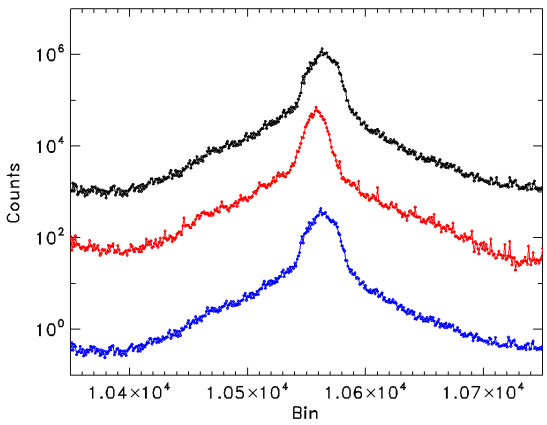
For Orthogonal Source (OS) spectra only event data is available, so the "signal factor" is simply the inverse of the integration time in seconds.

OS_signal_factor = 1 / (integration time)

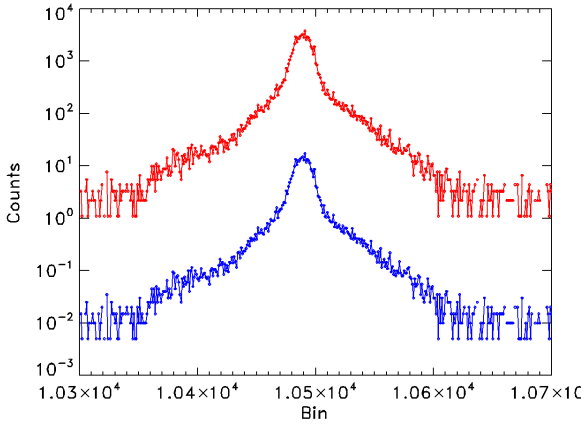
This factor is then multiplied by the TDC corrected L2 event data to obtain the resultant signal in counts (ions) per second.

Below are examples of the signal calibration to ions per second (blue) from Histogram counts (black) and Event counts (red). Both spectra were measured with a 200-second integration time.

SS spectra



OS spectra



5. MASS SCALE CALIBRATION

The mass scale calibration for each spectra is calculated using the factors C and t_0 in the equation below.

mass = ((time-of-flight – t_0) / C)^2

These factors are derived by matching the known masses of species in the collected gas sample with the location of their peaks in the data. As described in section 1, the location of these mass peaks is expected to be fairly consistent. However their location will depend upon the instrument settings. Thus for each instrument Mode ID there will exist a RTOF Mass Peak Search Table file (dated for reference) which describes the expected location (in bins) of the peak of several key species expected to be present in the measured sample, i.e. H_2O, CO, and CO_2 for the non-GCU spectra and He, C, CO, CO2, and ^{84}Kr for the GCU spectra. A bin "window" is defined where this peak alone is meant to be located, allowing for slight fluctuations in the peak locations.

Each spectra locates the most appropriate RTOF Mass Peak Search Table file, i.e. the most recently produced file with the same listed Mode ID via a subroutine. All mass peaks listed in this RTOF Mass Peak Search Table file are sent through the Peak Finder (see below) and then used as needed to determine the factors C and t_0 as well as the resultant mass scale precision (from the average PPM deviance).

5.1. Peak Finding / Fitting

Mass peaks are first located in the corrected L3 data within their "bin search window" (from the RTOF Mass Peak Search table) by a simple peak finder. Found peaks are then fit to a simple Gaussian to produce a more accurate determination of the peak center (which is then related to the known mass).

The peak finder first locates the bin with the maximum signal within the "bin search window" of the desired peak and this value is adopted as the potential peak height (amplitude). A minimum height threshold is set to 2 times the L3 signal factor. If this potential peak height is greater than the minimum height threshold and four or more bins contain signal within 50% of this potential peak height then the peak is considered to be found. If not enough peaks are within 50% of the potential peak height then the bin with the next greatest signal is considered as the potential peak height. This process is repeated until the criteria is either met or the potential maximum signal is lower than the minimum height threshold. If the criteria is met then the peak height is set to the mean signal amplitude of the bins within 50% of the potential peak height and the peak center is set to the mean of the bin numbers that meet the same criteria. Otherwise these values are all set to zero.

For peaks found with the simple peak finder the Marquardt non-linear curve fitting algorithm is used to fit the peaks (as described in P.R. Bevington, "Data Reduction and Error Analysis for the Physical Sciences," McGraw-Hill, 1969). The expected peak shape is a pseudo-voigt form; however a simple Gaussian is used as the proxy fitting shape as the Gaussian portion of the peak shape comprises the majority of the signal. The peak center and height from the simple peak finder are used as initial estimates for the Gaussian function center and amplitude. Additionally the initial estimate of the Gaussian function width is set to 100 (found as the most reliable in achieving valid results from the curvefit algorithm). Data points with signal equal to or greater than 2% of the initial estimate peak height are given equal weighting (equal to 1). Data points with signal below this threshold are given much smaller weights (10^{-4}) as the wider Lorentzian portion of the pseudo-voigt peak shape becomes significant at that point and will skew results of fitting to a simple Gaussian.

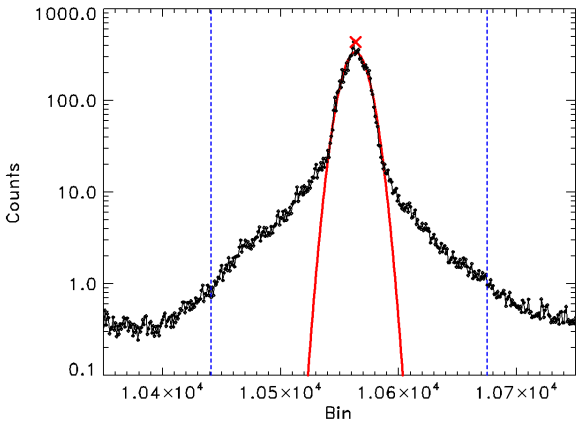
The results of the curvefit are tested to ensure their validity by checking against the following criteria:

- the returned Gaussian function height is within 0.25 and 4 times the initial estimated peak height
- the returned Gaussian function center is within the “bin search window”

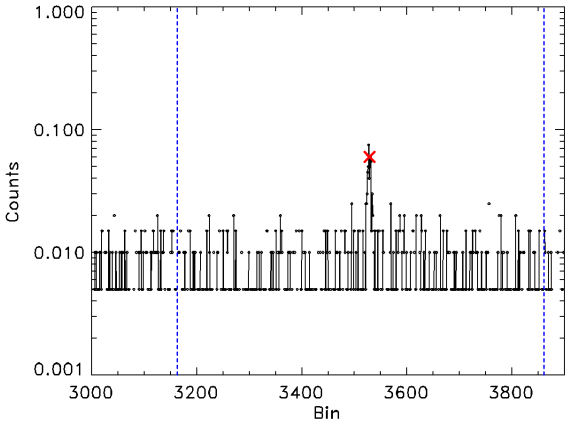
If the following requirements are met then the peak’s entry in the L3 spectra file’s RTOF Mass Calibration table will reflect the results of the curvefit results. If the curvefit results do not meet the criteria then the peak’s entry in the RTOF Mass Calibration table will instead reflect the results from the simple peak finder. The determined peak centers are then used as the peak locations (proxy for time-of-flight) to match to the known mass in the calibration process.

Below are two examples of the results from the peak finding and fitting process. The edges of the “bin search window” are marked by vertical blue dashed lines, the peak center and amplitude found by the simple peak finder is shown by a red X, and the fitted peak is shown by a thick red line.

Found Peak with Successful Curvefit



Found Peak with Unsuccessful Curvefit



5.2. Calibration/Verification peaks

The mass peaks listed in the "Mass Peak Search Table" files for mass scale calibration fall into two categories: 'calibration' peaks, and 'verification' peaks. 'Calibration' peaks are used to determine the calibration factors C and t_0. Therefore these mass peaks should only be the most prominent and reliable for the specific Mode. 'Verification' peaks are then used along with the 'calibration' peaks, to determine the average PPM deviance of all known peaks to the mass scale assumed by the factors C and t_0.

5.3. GCU-aided calibration

As mentioned above, GCU measurements will have an advantage in accurate mass-scale calibration as the measured signal represents a known gas mixture with sufficient amplitude peaks that cover a wide mass range. In order to take advantage of these GCU measurements, all non-GCU modes will have an accompanying GCU mode such that the mass peaks will be expected in the same locations (and thus C and t_0 will ideally be the same). The GCU companion Mode ID is found from the supplied PDS RTOF Mode ID table file.

After performing self-calibration of C and t_0, non-GCU spectra will then locate the most recent L3 GCU spectra file through a subroutine, and load its values for the mass calibration factors C and t_0. The PPM accuracy of all the found 'verification' mass peaks of the non-GCU spectra are calculated using the C and t_0 of the most recent L3 GCU spectra file. If the average PPM deviance of all 'verification' mass peaks using the GCU-reference C and t_0 is greater than a given threshold (current standard is 500 ppm) then the self-calibrated values will be adopted to calculate the mass scale. Otherwise the GCU-reference values will be adopted. Additionally, a flag may be set in the software to force the GCU values to be used (logged in the field "`ROSINA_RTOF_SCI_ALLOW_NONGCU_CAL`" in the RTOF_HK_TABLE). This information is logged appropriately in the RTOF_HK_TABLE where the "`GCU_*`" and "`SELF_*`" values are labeled with "`OFF`" or "`ON`" status as appropriate.

5.4. Mass Scale Precision

The mass scale precision has been fixed to a value of 0.005 u/e due to the known uncertainty of the instrument.

5.5. Choosing the Mass-Scale and Data Quality

GCU spectra will by default always use their self-calibrated mass scale. Non-GCU spectra will adopt the mass scale of their reference GCU spectra so long as the average PPM deviance of the verification peaks is less than 500 ppm when using the GCU mass calibration factors. Non-GCU spectra which do not meet this threshold will adopt their self-calibrated mass scale instead.

The data quality ID is determined from the decision to use non-GCU mass scale in favor of the (reference) GCU mass scale, the average PPM deviance of the adopted mass scale, the spectra background level, and the number of peaks from the Mass Peak Search Table that were found/fit during processing. Spectra whose average PPM deviance is less than 500 when using the reference GCU mass scale are assigned a data quality ID of "0" which is the highest quality. For non-GCU spectra which adopt self-calibrated mass scales with an average PPM deviance less than 500 ppm are assigned a data quality ID of "1" (GCU spectra cannot have this data quality ID as their GCU and self-calibrated mass scales are the same). When a spectra's adopted mass scale has an average PPM deviance greater than 500 ppm, the data quality ID of "2" is assigned. Spectra with a background signal level (average signal within the background determination region specified in the Mode ID table) that is greater than a set "enhanced noise threshold" (currently 0.5 ions/s) have a data quality ID set to "3". If less than two peaks from the Mass Peak Search Table were able to be found/fit then mass scale calibration/verification cannot be performed and the data quality ID is set to "4". If only two peaks from the Mass Peak Search Table were able to be found/fit then the data quality ID is set to "5".

Below is the list of data quality IDs and their descriptions, as listed in the L3 PDS Header.

```
0 means 'Nominal quality, avg. PPM deviance < 500'
1 means 'Self-calibrated, GCU avg. PPM deviance >= 500, SELF < 500'
2 means 'Adopted mass scale avg. PPM deviance >= 500'
3 means 'Enhanced Noise'
4 means 'Not enough peaks found for accurate calibration/verification'
5 means 'Self-calibrated from only two peaks, uncertain PPM deviance'
```

NOTE - If the background signal is greater than the "enhanced noise threshold", then the data quality will be set to 3 regardless of the applicability of any other data quality levels (e.g. not enough peaks were found, self-calibrated, etc.).

5.6. Automated Updating of Mass Peak Search Table files

An option is available to automate the production of updated RTOF Mass Peak Search Table files every time an L2 GCU spectra is processed by the L2-to-L3 conversion software. This provides a helpful way to take into account any changes to the expected mass scale and therefore the expected peak locations of the desired calibration/verification mass peaks. This is controlled by a flag set in the '`main`' routine where all other variables are to be set by the user (for the paths of PDS file repositories, etc.).

If this option is chosen, then the following is performed every time a L2 GCU spectrum is processed. First all mode IDs are found that are linked to the mode ID of this GCU spectra (i.e. is the same as their "GCU companion mode ID"). For each linked mode ID the most recent (in the past relative to the date/time of the GCU spectra being processed) RTOF Mass Peak Search table file corresponding to that mode ID is loaded. For each file the expected bin locations in the RTOF Mass Peak Search Table are re-calculated using the C and t_0 values found from this GCU spectra. The left and right edges of the "bin search window" are calculated such that they correspond to 0.07*sqrt(m) + 0.3 amu from the expected bin center (i.e. ≈ 0.5 amu for masses around 10 amu and ≈ 0.8 amu for masses around 50). Once the modifications have been made then it is written to file as a new PDS RTOF Mass Peak Search Table file, dated according to the date/time of the GCU spectra being processed. These files are deposited into the same repository as those that were referenced, thereby ensuring that they can be accessed when processing subsequent L2 spectra in the same execution of the conversion software.

6. DATA MANAGEMENT – PDS COMPONENTS

The RTOF PDS level 2 and level 3 files are divided into different components, as described below, which are all handled separately for ease of operation and data management purposes. Each instance of a component will have the same structure but not the same number of records or contents.

Components of files…

- PDS Header
- PDS Object Descriptions (essentially part of the header).
- PDS Objects – data tables (italics denote new tables for processing to PDS level 3)
    - RTOF housekeeping data
    - RTOF data table (L2)
    - *RTOF mass peak search table*
    - *RTOF mass-scale calibration table*
    - *RTOF data table (L3)*
    - *RTOF mode ID table*
    - *RTOF ADC/TDC correction table*

Types of files and their components (as they are written in the file)…

- RTOF Level 2 data files
    - PDS Header
    - PDS Object Description of the RTOF housekeeping table
    - PDS Object Description of the RTOF data table (L2)
    - RTOF housekeeping table
    - RTOF data table (L2)

- RTOF Mass Peak Search table files
    - PDS Header
    - PDS Object Description of the RTOF mass peak search table
    - RTOF mass peak search table

- RTOF Mode ID table files
    - PDS Header
    - PDS Object Description of the RTOF mode ID table
    - RTOF mode ID table

- RTOF ADC/TDC correction table files
    - PDS Header
    - PDS Object Description of the RTOF ADC/TDC correction table
    - RTOF ADC/TDC correction table

- RTOF Level 3 data files
    - PDS Header
    - PDS Object Description of the RTOF housekeeping table
    - PDS Object Description of the RTOF mass-scale calibration table
    - PDS Object Description of the RTOF data table (L3)
    - RTOF housekeeping table
    - RTOF mass-scale calibration table
    - RTOF data table (L3)

Every type of component has a related data structure in the software...

	Component	**Data Structure**
-	PDS Header	xPDS_Header
-	PDS Object Description	xPDS_OBJECT_DESC
-	RTOF housekeeping table	xPDS_RTOF_HK_TABLE
-	RTOF data table (L2)	xPDS_RTOF_DATA_L2_TABLERTOF
-	mass peak search table	xPDS_RTOF_MASS_PEAK_SEARCH_TABLE
-	RTOF mass-scale calibration table	xPDS_RTOF_MASS_CAL_TABLE
-	RTOF data table (L3)	xPDS_RTOF_DATA_L3_TABLE
-	RTOF mode ID table	xPDS_RTOF_MODE_ID_TABLE
-	RTOF ADC/TDC correction table	xPDS_RTOF_ADC_TDC_CORR_TABLE

(Additionally there are data structures for COPS data…).

NOTE - All components (aside from the PDS Object Description) store the majority of their data in a sub-structure which represents a single record (line of data) of that component. This sub-structure is used as an array within the main structure (listed above) for organizational purposes.

Each PDS component type has its own associated routines to “read” and “write” the data structure, as well as “initialization” routines that support creation and proper field information. Additionally each PDS file type has its own associated routines to “read” and “write” which covers all PDS components contained in the PDS file type.

7. FILE LINE FORMATS OF ALL TABLES

This section describes how data tables are read and written by the routines in the RTOF PDS processing software Two example records are provided for each data table, followed by the line format (explained below) by character, and then a description of each field and the values that the formatting supports. This information is also described in the ".FMT" files corresponding to each RTOF PDS data tables.

b = blank space
C = character (including possible blank space)
x = possible numerical digit (or blank space)
x = possible numerical digit but allowing for a negative sign replacing the first used digit
X = definite numerical digit
E+ = the "E+" or "E-" characters used for displaying scientific notation
, = the comma character
" = the double apostrophe character

PDS_Header

```
PDS_VERSION_ID                  =     PDS3
LABEL_REVISION_NOTE             =     "2007-09-27,Thierry Semon(UoB),
                                       version2.1 release;"
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC?CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

1 - name	The PDS header keyword name (33 character length string)
2 - value	The value assigned to the PDS header keyword (78 character length string)

NOTE- PDS Header records are read in a special way. Each record is first checked to see if it contains an "=" at character 34, in which case it is assumed to represent the first (perhaps only) line of a new unique keyword entry. As entire lines can be used for the keyword value, the value string for each record has the full 78 character length. The keyword value will be blank until the 40th character space, unless it relates to a multi-line keyword entry.

RTOF_HK_TABLE

```
"ROSINA_RTOF_SCI_HM_PW           ","     ","-3.8360E-001   ","V    "
"ROSINA_RTOF_SCI_GCU_C           ","ON   ","3.09234E+003   ","     "
"CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC","CCCCC","CCCCCCCCCCCCCCC","CCCCC"b(10)
                                  1,      2,               3,      4    5
```

1 - field name — The name of the housekeeping data for which the record's information applies.
(supports 32-character strings)

2 - field status — Indicates the status, interpreted value, or discrete value of the housekeeping data (e.g. "ON", "OFF", "HIGH").
(supports 5-character strings)

3 - field value — Exact value of the housekeeping data (e.g. "67", "0X62", "2.345E+003").
(supports 15-character strings)

4 - field units — Indicates the unit of the exact housekeeping data value (e.g. "V", "mA", "DegC", "ppm").
(supports 5-character strings)

5 - blank spaces to end of line

RTOF_MODE_ID_TABLE:

```
"M0181", "SS", "FS", 1, 1, "M0181", 0, 1,   2950,  35000,   6500,   8000,
200, 10, 200, "FRAG00", "SENS00",

"M0521", "SS", "FS", 1, 0, "M0181", 0, 1,   2950,  35000,   6500,   8000,
200, 10, 200, "FRAG00", "SENS00",

"CCCCC",b"CC",b"CC",bX,bX,b"CCCCC",bX,bX,bxxxxxX,bxxxxxX,bxxxxxX,bxxxxxX,b
      1,    2,    3, 4, 5,       6, 7, 8,      9,     10,     11,     12,
xxX,bxX,bxxX,b"CCCCCC",b"CCCCCC",b(2)
 13, 14,  15,       16,       17, 18
```

1 - mode ID	The mode ID to which the following info applies (supports 5-character strings)
2 - instrument source	The instrument source, "SS" for Storage Source, "OS" for Orthogonal Source (supports 2-character strings)
3 - instrument model	The instrument model, "FM" for Flight Model *à la maison*, "FS" for Flight Spare model (supports 2-character strings)
4 - filament mode	Indicates whether the mode is using filament ("1") or not using filament ("0") (supports single-digit integer values)
5 - GCU mode	Indicates whether the mode is a GCU mode ("1") or non-GCU mode ("0") (supports single-digit integer values)
6 - companion GCU mode ID	The companion GCU mode ID for this mode (supports 5-character strings)
7 - hi-res mode	Indicates whether the mode is a high resolution mode ("1") or nominal resolution mode ("0") (supports single-digit integer values)
8 - reflection mode	Indicates whether the mode is run in triple reflection mode ("3") or single reflection mode ("1") (supports single-digit integer values)
9 - retain bin start	Indicates the first bin of the L2 spectra data to retain in the L3 spectra data files with this mode. (supports 6-digit integer values)
10 - retain bin stop	Indicates the final bin of the L2 spectra data to retain in the L3 spectra data files with this mode. (supports 6-digit integer values)

11 - background bin start	Indicates the first bin of the L2 spectra data to use to determine the background signal level in this mode. (supports 6-digit integer values)
12 - background bin stop	Indicates the final bin of the L2 spectra data to use to determine the background signal level in this mode. (supports 6-digit integer values)
13 - integration time	Indicates the integration time (in seconds) of spectra taken in this mode (supports 5-digit integer values)
14 - extraction rate	Indicates the extraction rate, in kHz, for this Instrument Mode (supports 2- digit integer values)
15 - filament emission	Indicates the filament emission current, in micro-amps (supports 2- digit integer values)
16 - fragmentation id	Indicates the fragmentation file ID applicable for this Instrument Mode (supports 6-character strings)
17 - sensitivity id	Indicates the sensitivity file ID applicable for this Instrument Mode (supports 6-character strings)
18 - (blank spaces to end of line)	

RTOF_ADC_TDC_CORR_TABLE:

```
"ADC", "FS",  "ETS ",  1,  1.00000000E+000,
"TDC", "FM",  "ETSL", 15,  1.00000000E+000,
"CCC",b"CC",bc"CCCC",bxX,bbX.XXXXXXXXE+XXX,b(35)
    1,    2,       3,  4,                5,    6
```

1 - component	Indicates whether the correction value of this record is a TDC adjustment value or an ADC offset value. (supports 3-character strings)
2 - instrument model	Indicates whether the correction value of this record applies to the FM (lab) or FS (flight) instrument. (supports 2-character strings)
3 - data type	Indicates whether the correction value of this record applies to ETS (Storage Source) or ETSL (Orthogonal Source) spectra data. (supports 4-character strings)
4 - channel number	The channel number for which the correction value of this record applies. (supports 2-digit integer values)
5 - value	The correction value to apply to the type of data as indicated by the other fields of this record. (supports values to 10^{-8} precision)
6 - blank spaces to end of line	

RTOF_MASS_PEAK_SEARCH_TABLE:

```
"^4He           ",    4.00205466,  1,    6355,    6031,    6664,     4,
"^12C           ",   11.99945142,  1,   10985,   10801,   11166,     9,
"CCCCCCCCCCCCCCC",bbxxX.XXXXXXXX,bbX,bbxxxxxX,bbxxxxxX,bbxxxxxX,bbxxxX,b(7)
                1,             2,  3,       4,       5,       6,     7,   8
```

1 - peak name	The name of the mass peak to search for in the spectrum. (supports 15-character strings)
2 - peak mass	The exact mass of the peak. (supports values between 0 and 999.99999999)
3 - peak calibration type	Indicates whether the peak is a ‘calibration’ peak (`0`) or verification peak (`1`). (supports single-digit integer values)
4 - expected bin center	The expected center of the peak in bins. (supports 6-digit integer values; bins are always 1-131099)
5 - expected bin left bracket	The left side (minimum) of the range of bins in which the peak is expected. (supports 6-digit integer values; (bins are always 1-131099)
6 - expected bin right bracket	The right side (maximum) of the range of bins in which the peak is expected. (supports 6-digit integer values; bins are always 1-131099)
7 - peak min width	The minimum width (in bins) to use for peak finding. (supports 4-digit integer values)
8 - blank spaces to end of line	

RTOF_DATA_L2_TABLE

```
     1,                92,               562,
115042,                 0,                 0,
xxxxxX,xxxxxxxxxxxxxxxX,xxxxxxxxxxxxxxxX,b(35)
     1,                 2,                 3,    4
```

1 - bin	The bin number of the data record. (supports 6-digit integer values; bins are always 1-131099)
2 - histogram counts	The histogram counts (ADC signal) of the data record. (supports 17-digit integer values)
3 - event counts	The event counts (TDC signal) of the data record. (supports 17-digit integer values)
4 - blank spaces to end of line	

RTOF_DATA_L3_TABLE

```
  2950,           0.87,          0.005,  8.58346512E-002,
  5001,           2.53,          0.005,  7.22288534E-002,
xxxxxX,bbbbbbbxxxX.XX,bbbbbbxxxX.XXX,bbX.XXXXXXXXE+XXX,b(23)
     1,              2,              3,                 4,    5
```

1 - bin	The bin number of the data record. (supports 6-digit integer values; bins are always 1-131099)
2 - mass	The calibrated mass of the data record. (supports values from 0 to 9999.99999999)
3 - mass uncertainty	The uncertainty in the calibrated mass of the data record. (supports values from 0 to 9999.99999999)
4 - signal	The calibrated signal intensity in ions/second. (scientific notation allows for all values to 10^{-8} precision)
5 - blank spaces to end of line	

RTOF_MASS_CAL_TABLE:

```
"H2O       ", 1, 0,    0.000,  0.000, 0.000E+000,  0.000E+000,
"CO        ", 1, 1,  16390.842,  40.418, 2.480E-002,  2.977E+001,
"CCCCCCCCCCCCCCC",bbX,bbX,bbxxxxxX.XXX,bbxxX.XXX,bbX.XXXE+XXX,bbbX.XXXE+XXX,b(2)
        1, 2, 3,      4,    5,      6,      7, 8
```

1 - peak name	The name of the mass peak used for mass-scale calibration. (supports 15-character strings)
2 - peak calibration type	Indicates whether the peak is a 'calibration' peak (0) or verification peak (1). (supports single-digit integer values)
3 - peak found	Indicates whether the peak was found in the spectrum (1) or not (0). (supports single-digit integer values)
4 - peak center	The center of the mass peak, if found (0 if not) (supports values between 0 and to 10^{-3} precision)
5 - peak width	The Gaussian width of the mass peak, if the curvefit was performed successfully (0 if not). (supports values to 10^{-3} precision)
6 - peak height	The height of the mass peak, if found (0 if not). (scientific notation allows for all values to 10^{-3} precision)
7 - ppm deviance	The deviation of the calculated mass of the peak from its known mass, in parts per million. (scientific notation allows for all values to 10^{-3} precision)
8 - blank space to end of line	

8. DESCRIPTIONS OF PDS HEADER KEYWORDS NEW FOR L3 DATA PRODUCTS

The following PDS Header keywords in the L3 data products are added from those in the L2 data products and are described here for reference.

SOFTWARE_NAME	The name of the software used to produce this L3 data file from L2 data.
SOFTWARE_VERSION_ID	The version id of the software used to produce this L3 data file from L2 data.
SOURCE_FILE_NAME	The filename of the source L2 data file from which this L3 data file was produced.
ROSETTA:ROSINA_CAL_ID1	The filename of the reference L3 GCU data file which served as a mass-scale calibration aid for this L3 data file (in the case that this L3 file is itself a GCU spectra, it will reference itself).
ROSETTA:ROSINA_CAL_ID2	The filename of the RTOF Mass Peak Search Table file used to locate the peaks in this spectrum which were used in the mass-scale calibration of this L3 data file (listed in the files RTOF Mass-Scale Calibration Table).

9. DESCRIPTIONS OF HK DATA NEWLY DEFINED FOR THE L3 DATA PRODUCTS

The following HK data fields were newly defined for the L3 data products and are described here for reference.

ROSINA_COPS_PRESSURE_NG	The average COPS NG pressure sensor reading during the time of this spectra measurement.
ROSINA_COPS_PRESSURE_RG	The average COPS NG pressure sensor reading during the time of this spectra measurement.
ROSINA_RTOF_SCI_SIGNAL_FACTOR	The signal calibration factor used to convert the L2 data signal into ions/second.

ROSINA_RTOF_SCI_BG_LEVEL	The RTOF signal background level (in ions/second) determined from the background determination region.
ROSINA_RTOF_SCI_BG_STDEV	The standard deviation of the RTOF background signal level (in ions/second) determined from the background determination region.
ROSINA_RTOF_SCI_BG_STARTBIN	The first bin of the RTOF background signal level determination region.
ROSINA_RTOF_SCI_BG_STOPBIN	The final bin of the RTOF background signal level determination region.
ROSINA_RTOF_SCI_UPDATE_MPS_FILE	Indicates whether automatic updating of RTOF_MASS_PEAK_SEARCH_TABLE files was performed (“ON”) or not (“OFF”) during the execution of the RTOF PDS L2-to-L3 conversion software which produced this L3 data product.
ROSINA_RTOF_SCI_ALLOW_NONGCU_CAL	Indicates whether non-GCU self-calibration was allowed (“ON”) or not (“OFF”) during the execution of the RTOF PDS L2-to-L3 conversion software which produced this L3 data product.
ROSINA_RTOF_SCI_GCU_C	The value of the GCU reference spectra’s C mass-scale calibration factor.
ROSINA_RTOF_SCI_GCU_C_UNC	The uncertainty of the GCU reference spectra’s C mass-scale calibration factor.
ROSINA_RTOF_SCI_GCU_T0	The value of the GCU reference spectra’s t_0 mass-scale calibration factor.
ROSINA_RTOF_SCI_GCU_T0_UNC	The uncertainty of the GCU reference spectra’s t_0 mass-scale calibration factor.
ROSINA_RTOF_SCI_SELF_C	The value of the spectra’s self-determined C mass-scale calibration factor.
ROSINA_RTOF_SCI_SELF_C_UNC	The uncertainty of the spectra’s self-determined C mass-scale calibration factor.

ROSINA_RTOF_SCI_SELF_T0	The value of the spectra's self-determined t_0 mass-scale calibration factor.
ROSINA_RTOF_SCI_SELF_T0_UNC	The uncertainty of the spectra's self-determined t_0 mass-scale calibration factor.
ROSINA_RTOF_SCI_AVG_PPM_DEV	The average deviation of the calculated masses of all mass peaks listed in this spectra's RTOF_MASS_CAL_TABLE from their known mass, in parts per million.

10. L3 PRODUCT DATA QUALITY LOG FILE

For each execution of the software, a L3 product data quality log file is created to log the determined data quality of all successfully processed L3 spectra files. This is a simple comma separated value file (".csv") which consists of two columns – L3 spectra filename, and the data quality ID.

Below is an example of the text in an L3 product data quality log file.

```
L3 spectra filename, Data Quality ID
SS_20140424_062449_3_M0171, 0
SS_20140424_062815_3_M0171, 0
OS_20140424_074503_3_M0173, 0
```

11. PROCESS LOG FILE/ ERROR HANDLING

A log file is produced for each execution of the software, listing the L2 spectra files to convert to L3 spectra files and then logging the procedure's progress of each spectra file. Any errors or warnings found and handled by the software will also be logged. Handled errors during setup of the processing queue will terminate the software and no L3 data products will be produced. Handled errors during the processing of a single L2 spectra file into an L3 spectra file will terminate the conversion process of that L2 file and not produce its L3 product. However the software will proceed to process the rest of the L2 files in the processing queue. Warnings are also logged for errors that may not harm the processing, and the software will continue as normal after they have been logged. After each of the 12 steps in the L2-to-L3 conversion, the step number is written as having been completed. This can then be examined to help diagnose where and why any errors occurred, thus aiding any debugging or investigation into faulty data files, etc. Not all potential errors will be caught by the software's error handling, however the process log file provides a helpful way to investigate runtime difficulties.

The following text is an example of the output text in a process log file where two L2 spectra files were processed. The first spectra was processed successfully. Processing of the second spectra first found a warning during Step 2, and later a (terminating) error during Step 6.3. In this example, the software would not have created an L3 product file for the second spectra due to the processing error.

```
  L2 spectra files to convert to L3 calibrated spectra
================================================================================
    (filename)         (date and time)    (Mode ID) (Source) (GCU)
SS_20120101_010000000_M0171   2012-01-01 01:00:00.000  M0171   SS   1
SS_20120101_020000000_M0511   2012-01-01 02:00:00.000  M0511   SS   0

 Number L2 files to convert = 2


L2 spectra file 1: SS_20120101_010000000_M0171
 *** RTOF PDS L2 to L3 conversion ***
  -- processing file: C:\RTOF_L2_to_L3\data\L2\SS_20120101_010000000_M0171.TAB
  -- Completed Step 1
  -- Completed Step 2
  -- Completed Step 3
  -- Completed Step 4
  -- Completed Step 5
  -- Completed Step 6
  -- Completed Step 7
  -- Completed Step 8
  -- Completed Step 9
  -- Completed Step 10
  -- Completed Step 11
  -- Completed Step 12
  -- L3 output file:  C:\RTOF_L2_to_L3\data\L3\SS_20120101_010000000_3_M0171.TAB
  -- complete and successful


L2 spectra file 2: SS_20120101_020000000_M0511
 *** RTOF PDS L2 to L3 conversion ***
  -- processing file: C:\RTOF_L2_to_L3\data\L2\SS_20120101_020000000_M0511.TAB
  -- Completed Step 1
  WARNING in 'BAM_read_RTOF_DATA_L2_TABLE': at least one invalid RTOF Data Table (L2)
                       record found; first invalid record found
                       at RTOF Data Table (L2) record 150 on
                       file line 525 of file...
             "C:\RTOF_L2_to_L3\dataL2\SS_20120101_020000000_M0511.TAB"
  -- Completed Step 2
  -- Completed Step 3
  -- Completed Step 4
  -- Completed Step 5
  ERROR in 'BAM_process_L2_to_L3_spectra': error at STEP 6.3, returning -1
                      malloc for L3 output RTOF_MASS_CAL_TABLE
                      records failed


 **********************
 **********************
  Process Complete
 **********************
 **********************
```