

# *TROPESS Peroxyacetyl Nitrate*

## *Level 2 Standard Data Product User Guide*

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## 1 Introduction

### 1.1 Overview and Document Scope

This document is to be used as a Quick start user guide for using the TROPESS CrIS PAN Level 2 Standard product files. This document is intended to be used with the README, which describes the variables included in the data products.

### 1.2 Dataset Description

This user guide describes the TROPESS CrIS Level 2 Standard product files for peroxyacetyl nitrate (PAN).

Product Information	Description
Parameters	PAN
Data Product Provenance	TROPESS Program Version 1.11
Approximate file size	~15 MB for this special collection
Spatial coverage	Regular collections have global coverage: Nominal latitude range: 70 N to 50 S Nominal longitude range: -180 to 180  Special collections: Spatial coverage varies by collection
Temporal coverage	Each L2 nominal Standard file contains 1 day of data
File format	netcdf
Vertical sensitivity	PAN has sensitivity between approximately 800 hPa and the tropopause. Only a vertically integrated quantity should be used, as values at individual pressures do not contain independent information.
Data quality	The data have undergone a pre-quality check, which involves checks for retrieval convergence. There are no checks for clouds or land versus ocean as we do not find these to substantively affect the quality of the retrieval as long as the retrieval has converged. Note that retrievals over thick clouds will not be sensitive to PAN below the clouds.
Uncertainty	Uncertainties on vertically-averaged PAN values between 825.4 and 215.4 hPa are estimated at 0.17 ppb for a single sounding.
Validation Stage	Stage 2 according to NASA guidelines <a href="https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels">https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels</a>
Retrieval Levels	16 levels: from surface to top-of-atmosphere
FillValues	-999

### 1.3 Filename

The Standard Products adhere to the following filename convention:

```
[ProjectID]_[Instrument-Platform]_[ProductLevel]_[ProductType]_[ProductName]_[DateStamp]_[AlgorithmName]_[AlgorithmVersion]_[ProcessingStrategy]_[FormatVersion].nc
```

#### Example:

```
TROPES_CrIS-SNPP_L2_Standard_PAN_20200912_MUSES_R1p11_FS_F0p1.nc
```

## 2 Product File Contents and Parameter Description

### 2.1 Variables listed in the Standard Product

Please see the README for a list of variables included in the L2 Standard product files.

## 3 References

### 3.1 Citing these data

Please cite the following references if you intend to use these data:

1. Payne, V. H. et al., Satellite measurements of peroxyacetyl nitrate from the Cross-track Infrared Sounder: Comparison with ATom aircraft measurements, in preparation for submission to *Atmos. Meas. Techniques*, 2021
2. Juncosa Calahorrano, J. et al., Evolution of PAN in wildfire smoke plumes detected by the Cross-track Infrared Sounder (CrIS) over the western US during summer 2018, *Geophys. Res. Lett.*, in review, 2021

### 3.2 Additional references

The following references were also used in the development of this documentation:

1. **Payne, V. H. et al**, Satellite observations of peroxyacetyl nitrate from the Tropospheric Emission Spectrometer, *Atmos. Meas. Tech.*, 7, 3737-3749 (2014)

2. Bowman, K.W. et al., Tropospheric Emission Spectrometer: Retrieval Method and Error Analysis, *IEEE Trans. Geosci. Remote Sensing*, 44, 1297- 1307, May 2006.
3. Rodgers, C. D., and B. J. Connor (2003), Intercomparisons of remote sounding instruments, *J. Geophys. Res.*, 108(D3), 4116, doi:[10.1029/2002JD002299](https://doi.org/10.1029/2002JD002299)

#### 4 *Extended User Guide: How to compare the L2 Standard Product to reference profiles*

This extended user guide shows how to compare these fields to aircraft or model fields.

##### 4.1 **How to compare to aircraft or model fields and test**

All comparisons between remotely sensed data and *in situ* measurements or high resolution model fields must account for the sensitivity of the remotely sensed measurement and any regularization used with the remotely sensed measurements. Otherwise large errors will be incurred with the comparisons.

Here is the general approach for comparison of the TROPES data to model fields or vertical profile measurements such as from aircraft:

We first construct an observation operator that is used for comparison of the TROPES PAN data to models or vertical profile measurements such as from aircraft.

- 1) Construct the PAN profile using the model or aircraft fields (for the purpose of this demonstration we will call this  $x_{true}$ ).
- 2) Construct the observation operator as the following :

$$H(\cdot) = \ln(x_a) + A(\ln(\cdot) - \ln(x_a))$$

- 3) Apply observation operator to the PAN profile:

$$\hat{x} = \exp[H(x_{true})]$$

In the netcdf product file and in the equation,  $x_a$  is the constraint vector used to regularize the retrieval.  $H(\cdot)$  is the observation operator, where the  $(\cdot)$  represents a model or *in situ* profile.  $A$  is the averaging kernel matrix and must be matrix multiplied by  $\ln(x_{true}) - \ln(x_a)$ . After this

operation one can compare the modified PAN profile ( $\hat{x}$ ) to the retrieved “x” profile in the netcdf product file. Note that the averaging kernel matrix ( $A$ ) is not symmetric, so getting the row/column order of  $A$  correct is critical. You can check your work by using the above equation

with the zeroth entries for the averaging kernel,  $\mathbf{x}_a$  and using the zero<sup>th</sup> entry for  $\mathbf{x}$  as  $\mathbf{x}_{\text{true}}$ . If your test operation (steps 1-3) matches the variable  $x_{\text{test}}$  then the operation is correct.

Important: For PAN, the retrievals do not provide information on the vertical distribution of PAN. Therefore, we recommend to look at a vertically averaged quantity (the average volume mixing ratio between 825.4 and 215.4 hPa) rather than individual pressure levels.

## 4.2 Validation summary

Summary Statement: Based on the NASA Validation Guidelines (see link in Table 1), we determined that the TROPES L2 Standard PAN products are at Validation Stage 2.

Our rationale is that the CrIS PAN has been evaluated by comparing retrievals with reference in situ aircraft profiles in the tropics, mid-latitudes, and high-latitudes. CrIS PAN retrievals have been validated using in situ aircraft profile measurements from the ATom campaigns. Profile measurements from two different aircraft instruments (PANTHER and GTCIMS) were used in this work. Further details can be found in Payne et al. (2021). Note that this validation has been performed using vertically-averaged PAN (the average volume mixing ratio between 825.4 and 215.4 hPa).

Figure 1 shows differences between vertically averaged (825.4-215.4 hPa) PAN values from CrIS and from the PANTHER aircraft instrument, for the four ATom campaign periods. CrIS PAN values here have been bias-corrected (see Appendix). The table shows the mean and standard deviation of CrIS-aircraft differences, by instrument and campaign. For further details, see Payne et al. (2021).

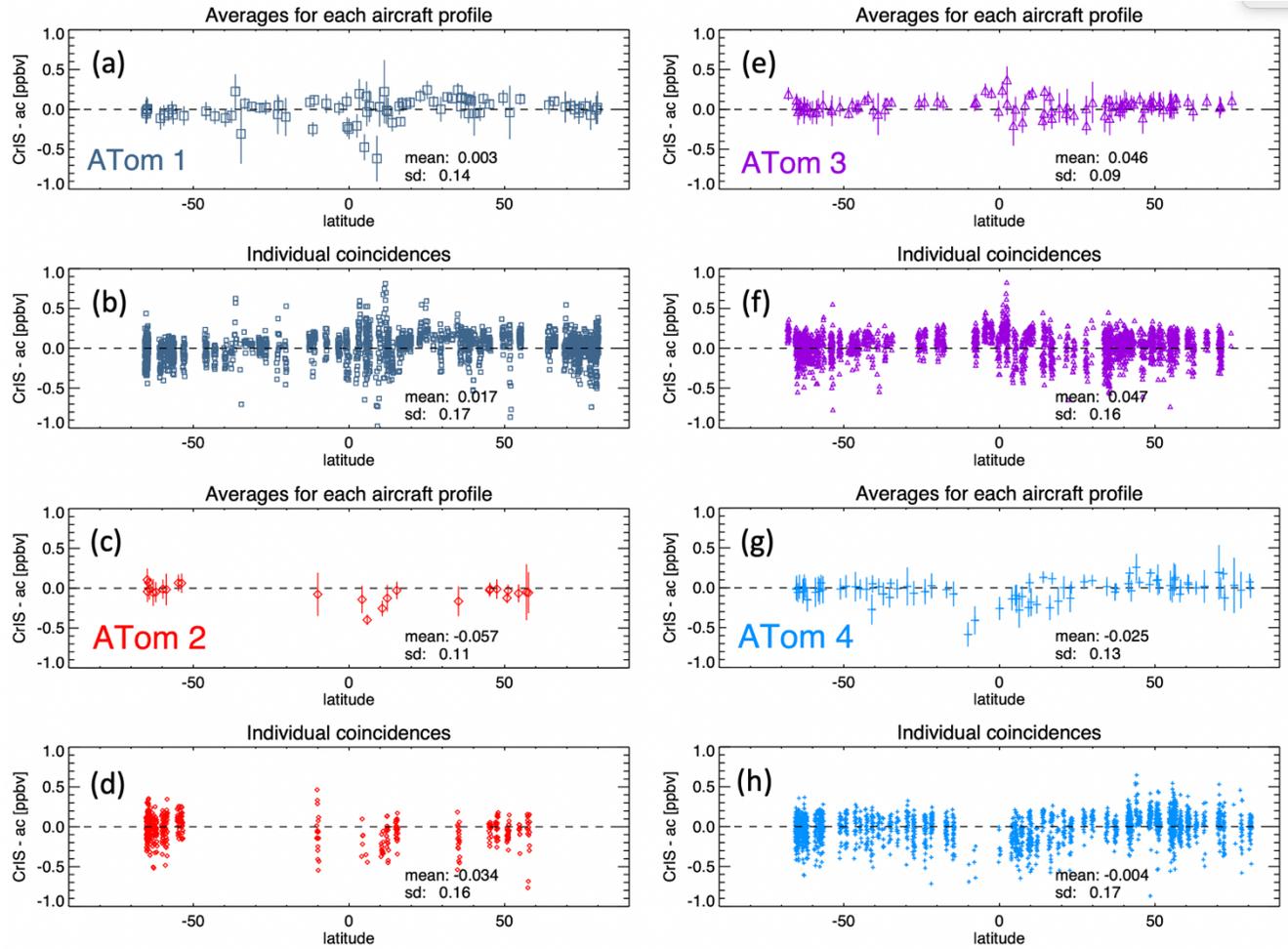


Figure 1. CrIS-PANTHER PAN differences against latitude for the four ATom aircraft campaigns. PAN values compared here are vertical average VMRs over the range 825.4 to 215.4 hPa. Results from ATom 1 are shown in panels (a) and (b), ATom 2 in (c) and (d), ATom 3 in (e) and (f) and ATom 4 in (g) and (h). Panels (a), (c), (e) and (g) show the results after averaging all the CrIS co-incidences for each aircraft profile. Vertical bars on the points in these panels show the standard deviation of the averaged CrIS result for each aircraft profile. Panels (b), (d), (f) and (h) show the results for individual CrIS soundings (multiple CrIS co-incidences with each aircraft profile).

ATom campaign (dates)	CrIS-PANTHER PAN [ppbv]				CrIS-GTCIMS PAN [ppbv]			
	Individual CrIS		Averaged CrIS		Individual CrIS		Averaged CrIS	
	Mean	Std. dev.	Mean	Std. dev.	Mean	Std. dev.	Mean	Std. dev.

<b>ATom 1</b> <b>July-August 2016</b>	0.017	0.17	0.003	0.14	n/a	n/a	n/a	n/a
<b>ATom 2</b> <b>January-February 2017</b>	0.034	0.16	0.057	0.11	0.033	0.18	0.062	0.11
<b>ATom 3</b> <b>September-October 2017</b>	0.047	0.16	0.046	0.09	0.045	0.16	0.043	0.10
<b>ATom 4</b> <b>April-May 2018</b>	0.004	0.17	0.025	0.13	0.013	0.18	0.008	0.14
<b>All</b>	0.017	0.17	0.004	0.12	0.024	0.17	0.010	0.12

### Appendix A. Bias Correction

In analysis of spectral residuals, we found a water vapor dependent systematic bias in modeled radiances in the region of the PAN spectral feature. This bias in the modeled radiances leads to a water vapor dependent bias in the retrieved PAN. This is corrected with the following formula:

$$x\_800\_bias = -0.07 - 0.10 * 1.0e-23 * h2o\_column$$

$$x\_800 = x\_800\_original - x\_800\_bias$$

$x\_800$  is the PAN partial column between 825.4 hPa and 215.4 hPa, divided by the air partial column for the same pressure range (weighted vertical average volume mixing ratio).

H2O column is `data[ii].column[0]` from the MUSES water product.

Note that the values in the PAN Standard product files are **not** bias corrected.

### Appendix B. Retrieval levels

The table below contains the nominal retrieval levels. For each sounding, the surface pressure level is inserted into the retrieval levels set. Any retrieval levels below the surface pressure level are omitted.

<b>Index</b>	<b>Pressure [hPa]</b>
1	1040.00
2	1000.00
3	825.402
4	681.291
5	562.342
6	464.16
7	383.117
8	316.227
9	261.016
10	215.444
11	161.561
12	121.152
13	90.8518
14	51.0896
15	28.7299

16	0.10000
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