# PACE Level 1C Users Guide

James G. Allen, GESTAR II/University of Baltimore County, Baltimore, Maryland Kirk D. Knobelspiesse, NASA Goddard Space Flight Center, Greenbelt, Maryland

1. Overview2
Introduction2
Scope
Reference documentation and data sources3
2. Why have a L1C format?
3. Geometric considerations5
4. Radiometric and polarimetric considerations7
Polarimetry7
Radiometry9
OCI considerations9
HARP2 considerations9
SPEXone considerations9
5. Instrument and Data Characteristics9
Data groups9
Data dimensions10
Ocean Color Instrument (OCI)10
Hyper-Angular Rainbow Polarimeter 2 (HARP2)11
Spectro-Polarimeter for Exploration (SPEXone)14
Ancillary Files
6. Appendices
Glossary of Terms
Technical Specs of instruments17
Links to software tools for data analysis17
7. References

## 1. Overview

#### Introduction

NASA's Plankton, Aerosol, Cloud, ocean Ecosystem (<u>PACE</u>) mission makes global ocean color and atmospheric measurements to provide extended data records on ocean ecology and global biogeochemistry, along with polarimetry measurements to provide advanced systematic observations of aerosols, clouds, and the ocean. Its core objectives are to:

- 1) Extend key systematic ocean biological, ecological, and biogeochemical climate data records and cloud and aerosol climate records,
- 2) Make new global measurements of ocean color to improve our understanding of the carbon cycle and ocean ecosystem responses to a changing climate,
- 3) Collect global observations of aerosol and cloud properties, focusing on reducing the largest uncertainties in climate and radiative forcing models of the Earth system, and
- 4) Improve our understanding of how aerosols influence ocean biogeochemical cycles and ecosystems and how ocean biological and photochemical processes affect the atmosphere.

The PACE observatory has three sensors: the Ocean Color Instrument (OCI), the Hyper-Angular Rainbow Polarimeter 2 (HARP2), and the Spectro-Polarimeter for Exploration (SPEXone). OCI is a hyperspectral imaging radiometer whose continuous coverage extends from 340 nm in the ultraviolet to 890 nm in the near infrared spectrum at 2.5 nm resolution (with bandwidths of 5 nm). HARP2 is a wide angle imaging polarimeter that combines data from four spectral bands in the visible and near infrared ranges, multiple along-track (in the direction of the orbit of the observatory) viewing angles (60 in the red, and 10 for the other three wavelengths, all  $\pm$ 57°), and three components of the state of linear polarization of incoming light. SPEXone is a hyperspectral polarimeter that also provides observations of three linear polarization components, but for continuous wavelength coverage from 385 nm to 770 nm at 2-5 nm spectral resolution at five along-track viewing angles (0°,  $\pm$ 20°,  $\pm$ 58°) (Werdell et al., 2019).

NASA's Earth Observing System Data and Information System (EOSDIS) data products are processed at various levels ranging from Level 0 (raw payload data at full instrument resolution) to Level 4 (model outputs or results from analysis of lower-level data)<sup>1</sup>. The PACE Science Data Processing System produces Level 1B data (geolocated radiances with calibration applied) individually for each instrument. There is also a strong desire to produce data in a format that merges the disparate spatial resolutions, viewing geometry and sampling nature of the three instruments. This data file format, termed Level 1C (L1C), eases data synergy by representing radiometric data observed by all PACE instruments at

<sup>&</sup>lt;sup>1</sup> https://www.earthdata.nasa.gov/engage/open-data-services-and-software/data-information-policy/data-levels

all wavelengths and viewing angles on a swath-based common equal area sampling grid. The data are reoriented to represent the multi-angle views about the observation location (default is the surface), while also managing the extra dimensionality of polarization information, facilitating their merged usage in higher level algorithms. Additionally, ancillary data useful for L1 to L2 data processing is created on the L1C grid.

#### Scope

The purpose of this document is to serve as a User Guide as a supplement to the full PACE L1C Technical Report. It is intended to get a new PACE data user quickly up to speed in the data organization and file structure and explain the reasoning behind the structure of this file. Full specification for the format is available in <u>NASA/TM – 2024-219027/Vol. 12</u>. Section 2 describes in more detail the reasoning behind the L1C format. In Section 3, the framework and parameters for the L1C geometry is given, while Section 4 gives an introductory overview of the radiometry and polarization variables in the dataset. Section 5 describes the NetCDF data groups and dimensions for the L1C products details the data organization for each of the three PACE instruments, as well as the ancillary data used in processing.

#### Reference documentation and data sources

- The full technical specifications for the PACE Level-1C can be found in the Technical Report (NASA/TM – 2024-219027/ Vol. 12) <u>https://oceancolor.gsfc.nasa.gov/files/NASA\_TM2024219027v12\_Level1C.pdf</u>
- PACE data can be found using one of the options listed in the GSFC Ocean Color webpage: <a href="https://oceancolor.gsfc.nasa.gov/data/find-data/">https://oceancolor.gsfc.nasa.gov/data/find-data/</a>
- Have a question or want to give us feedback? Feel free to ask us in the NASA Earthdata Forums: <u>https://forum.earthdata.nasa.gov/</u>
- For more details about specific algorithms, check out the Algorithm Theoretical Basis Documents: <u>https://oceancolor.gsfc.nasa.gov/resources/atbd/</u>
- Tutorials and basic scripts to download and visualize some Level-2 and Level 3 products can be found here: <u>https://oceancolor.gsfc.nasa.gov/resources/docs/tutorials/</u>

## 2. Why have a L1C format?

The overall philosophy of the L1C format is to provide a means to represent all three PACE instruments in a uniform manner that eases subsequent use in an algorithm generating L2 data. In some situations, this means the format can appear complex or less appropriate for an individual dataset. It also means that redundant data are contained within a file – ease of use has priority over compactness. The L1B format may be the most appropriate input to a L2 algorithm in some situations, and this format is available for all instruments. To help a data user determine the best format for their use, this section describes the guiding principles of the L1C format. We should also note that other L1C formats exist but may have different characteristics because of varying needs. An example is the format designed

for the forthcoming EUMETSAT Multi-viewing, Multi-channel and Multi-polarisation Imager (3MI) to be launched on Metop-SG (Lang et al., 2019).

#### Reason 1: Organize multi-angle views for L2 algorithms

The L1C format evolved from the experience of airborne multi-angle polarimeters such as the Research Scanning Polarimeter (RSP, e.g. <u>Chowdhary et al. 2002</u>). RSP (and also HARP2 and SPEXone) observes from multiple viewing geometries in the along-track direction as the instrument passes over the imaged scene. These multi-angle observations provide useful information utilized by L2 algorithms that determine geophysical parameters. However, L1B files are organized as multi-angle views at the point of observation, each pointing to a different location on the surface or in the atmosphere. Thus, the multi-angle observations must be reorganized, or 'aggregated' so that they represent the multi-angle scattering about a location. This is accomplished by binning geographically projected observations onto a uniform grid. The result are non-simultaneous observations representing the angular scattering about the point of observation. The time difference for HARP2 and SPEXone between the most extreme angle views is roughly between six and seven minutes, described exactly in the bin\_attributes/view\_time\_offsets field. By default, the altitude about which this aggregation occurs is the surface, whose height is noted in the geolocation\_data/height field. Figure 1, originally in the L1C Technical Report, graphically illustrates aggregation.





#### Reason 2: Facilitate multi-sensor data fusion

The three PACE instruments have disparate characteristics, including differences in spatial resolution and swath, spectral sampling, and observation geometry. However, all three observe simultaneously, and there is great potential benefit in easing data fusion as has been demonstrated by the Terra Fusion Project (Zhao et al, 2019). Radiometric and polarimetric comparison between instruments is valuable for confirming calibration

fidelity, and can potentially be used for cross-calibration. Level 2 products can inherit the L1C grid and provide for the product comparison for different instruments. Furthermore, Level 2 algorithms can be created that utilize observations from multiple PACE instruments.

The L1C format uses a spacecraft swath based projection called Spacecraft Oblique Cylindrical Equal Area (SOCEA) (see Snyder, <u>1978</u> and <u>1987</u> for a description of the Oblique Cylindrical Equal Area projection). A swath based projection was chosen so that there is a straightforward reconstruction of imagery from a L1C file, and SOCEA was selected for its equal area properties. A 5.2x5.2km grid was selected to encompass the spatial resolution of the SPEXone and HARP2 polarimeters, which are inherently coarser than that of OCI. Projection is a process of binning, meaning that depending on sensor characteristics and location within a granule, a variable number of pixels were averaged for that bin. This information is contained in the observation\_data/number\_of\_observations field.

#### Reason 3: Enable the use of ancillary datasets

While it was not the original purpose of the L1C format, we found it to be a convenient means to provide ancillary and cloud mask information that is co-registered with OCI, HARP2 and SPEXone. This means that L2 algorithms do not need to regrid ancillary data independently.

#### Reason 4: Provide accurate geometric and polarimetric parameters

Use and interpretation of multi-angle polarimetric data in some cases requires geometric and polarimetric transformations, such as rotation of Stokes vector elements from the default meridional plane to the scattering plane (see subsequent sections). Rather than requiring a L2 algorithm to calculate parameters like the rotation angle (geolocation\_data/rotation\_angle), these parameters are included in the L1C format. This has the additional benefit of ensuring that these parameters are correctly computed.

### 3. Geometric considerations

Understanding the geometric framework of satellite remote sensing data is fundamental to interpreting how sunlight interacts with Earth's surface and atmosphere. The multi-angle polarimeters are designed to capture the angular dependence of scattering for a surface or volume of the atmosphere, so the L1C data are organized to represent this scattering about a single point, defined at the center of each grid bin. Solar zenith and azimuth, coupled with their sensor counterparts, define a satellite's "viewpoint" of each of these bins and offer a structured way to interpret surface and atmospheric conditions. **Figure 2** describes the geometry conventions of the L1C format.



**Figure 2** Observation and geometry illustration. The sun illuminates a point at location **O** along the vector **AO**. The associated *solar zenith angle* ( $\theta_s$ ) is the angle **ZOA** from the zenith direction (normal to surface plane) from **O** to the vector in the direction of illumination, **OA**. The *solar azimuth angle* ( $\phi_s$ ) is the angle **YOS** due North from **O** to the projection of the Sun vector on the surface plane. The *solar meridional plane* contains vectors **OA** and **OZ** and is illustrated in red in the figure. The sensor observes scattered radiation from a point at location **O** along the vector **OB**. The associated *sensor zenith angle* ( $\theta$ ) is the angle **ZOB** from the zenith direction (normal to surface plane) from **O** to the scattered vector **OB**. The *sensor azimuth angle* ( $\theta$ ) is the angle **ZOB** from the zenith direction (normal to surface plane) from **O** to the scattered vector **OB**. The *sensor azimuth angle* ( $\phi$ ) is the angle **YOE** due North from **O** to the projection of the sensor observation vector on the surface plane. The *sensor meridional plane* contains vectors **OB** and **OZ** and is illustrated in sensor *azimuth angle* ( $\phi$ ) is the angle **YOE** due North from **O** to the projection of the sensor observation vector on the surface plane. The *sensor meridional plane* contains vectors **OB** and **OZ** and is illustrated in blue in the figure. Items labeled in green indicate properties relating these two planes. The *scattering angle* ( $\alpha$ ) is the angle from the solar illumination vector **AOP** to the scattered vector **OB**. The *rotation angle* ( $\sigma$ ) is the angle from the *sensor meridional plane* to the scattering plane containing the vectors **OB** and **OA**. Finally, the *relative azimuth angle* is the  $\phi - \phi_s$  difference between the *sensor azimuth angle* and the *solar azimuth angle*. After Hovenier and van der Mee (1983) and Xu and Wang (2019).

The solar zenith angle,  $\theta_s$  (geolocation\_data/solar\_zenith\_angle), is the angle between the direction directly upwards (zenith, **OZ**) from the observation point and the sun (**OA**). A solar zenith angle of 0° means the sun is directly overhead of the observation point, while an angle of 90° means the sun is currently setting (or rising) over the horizon. The solar azimuth angle,  $\phi_s$  (geolocation\_data/solar\_azimuth\_angle), is the angle between a point due North of the observation point (**OY**) and the position of the sun (**OA**). This angle increases in the clockwise direction from North, so if the sun is due East, the solar azimuth angle would be 90°, while an azimuth angle of 270° means the sun is due West.

The sensor viewing angles follows the same pattern. The sensor zenith angle,  $\theta$  (geolocation\_data/sensor\_zenith\_angle), is the angle between the zenith direction from the observed point (**OZ**) and PACE (**OB**), while the sensor azimuth angle,  $\phi$  (geolocation\_data/sensor\_azimuth\_angle), is the angle between a point due North (**OY**) and PACE's position (**OB**). We can also now define a relative azimuth angle,  $\phi - \phi_s$ , the difference between the sensor azimuth angle and the solar azimuth angle.

Another geometry parameter that may be of interest is the scattering angle,  $\alpha$  (geolocation\_data/scattering\_angle equations for which are provided in the L1C Technical Report. The scattering angle is the angle between the solar illumination vector (**OP**) and the vector from the observed location to the sensor (**OB**). A scattering angle of 180° represents the backscattering direction. The scattering angle helps directly connect the observation geometry to the underlying scattering optics. While it could be calculated by a data user from the sensor and solar zenith and azimuth angles, we include it in the L1C format both for convenience and to ensure standardization of definition conventions.

Polarization units are expressed with respect to a reference plane. The the rotation angle,  $\sigma$  (geolocation\_data/rotation\_angle), is used to convert polarization parameters from the sensor meridional plane (containing vectors **OZ** and **OB**) and the solar scattering plane (containing vectors **OA** and **OB**). Polarimetric units are expressed in L1C files in the sensor meridional plane, so this angle is used to convert polarimetric units to the scattering plane for application that require this form. See equations 4-6 in the L1C Technical Report for more details. Like the scattering angle, this parameter could be calculated from sensor and solar zenith and azimuth angles, but we include it in the L1C format both for convenience and to ensure standardization of definition conventions.

All geometry parameters are stored in three dimensions in the L1C format: two for the along and cross track bin location, and another corresponding to the view angle of the observation. This dimensionality even exists for the solar azimuth and zenith angles because the sun position changes slightly during the time required (see *bin\_attributes/view\_time\_offsets*) to make all angle measurements. While the impact solar azimuth and zenith angles may only be a few degrees, this is still relevant for most uses.

## 4. Radiometric and polarimetric considerations

### Polarimetry

The L1C Technical Report and many overview publications (e.g. <u>Hansen and Travis, 1974</u>) provide complete descriptions of polarimetric units, so here we will give only a brief introductory overview.

While there are several ways to represent light polarization, we use the Stokes vector:

$$\boldsymbol{I} = \begin{bmatrix} \boldsymbol{I} \\ \boldsymbol{Q} \\ \boldsymbol{U} \\ \boldsymbol{V} \end{bmatrix}$$

The first Stokes vector element, *I*, represents the total amount of electromagnetic radiation, represented either as an intensity, irradiance, radiance or reflectance. All three instruments are sensitive to *I*, and it is contained within the *observation\_data/i* field as the Top of Atmosphere (TOA) radiance, with units of W sr<sup>1</sup> m<sup>-2</sup> µm<sup>-1</sup>. OCI is *only* sensitive to this element of the vector, so L1C files from that instrument to not contain subsequently described polarimetric units. *Q* and *U* describe the angle and magnitude of linear polarization. The reference frame in L1C files is the meridional plane mentioned in the previous section. Linear polarization is the component that is constant with phase, meaning that it stays the same regardless of where in the wave one assesses polarization state. *Q* and *U* are contained in the *observation\_data/q* and *observation\_data/u* fields and are present for HARP2 and SPEXone. Circular polarization capability of any PACE instrument, and therefore not included in L1C files.

We should also note that some Stokes vector notation uses case to differentiate between Q and U (W sr<sup>-1</sup> m<sup>-2</sup> per  $\mu$ m) and Q/I and U/I (unitless), the latter represented as a lower case 'little q and u'. Since our CF-compliant field naming convention does not recognize case, we use the fields *observation\_data/q\_over\_i* and *observation\_data/u\_over\_i* to denote these normalized fields. *q* and *u* are only contained in SPEXone files since that is the form of the inherent polarimetric measurement made by that instrument, and Q and U are derived. HARP2 inherently observes Q and U, so, the normalized fields are not contained in HARP2 files.

Another common polarimetric parameter is the Degree of Linear Polarization (*DoLP*, unitless) which describes the fraction of electromagnetic radiation that is linearly polarized:

$$DoLP = \frac{\sqrt{Q^2 + U^2}}{I}$$

*DoLP* is independent of reference frame, which has some advantages in interpretation and use. For some instruments *DoLP* is an inherently more accurate measurement than *Q* and *U*, since calibration coefficients cancel. In any case, it represents a reduction in information from *Q* and *U* alone, which is addressed by calculating the Angle of Linear Polarization (*AoLP*, degrees):

$$AoLP = \frac{1}{2}\tan^{-1}\frac{U}{Q}$$

where we adopt the common convention (<u>Hansen and Travis</u>, <u>1974</u>) to select the value in the interval  $0 \le AoLP \le \pi$  for which cos(2AoLP) has the same sign as Q. AoLP is defined in

the meridional plane. These parameters are contained in the *observation\_data/dolp* and *observation\_data/aolp* fields. Since they can be calculated from Q and U, they are redundant, but included in the L1C file to ease use and ensure consistent calculation.

#### Radiometry

I, Q and U have units of radiance (W sr<sup>-1</sup> m<sup>-2</sup>  $\mu$ m<sup>-1</sup>). Conversion to reflectance (unitless) is performed by calculating

$$R_{[I,Q,U]} = \frac{[I,Q,U]\pi r^2}{F_0 \cos \theta_s}$$

Where *r* (unitless) is the sun earth distance relative to the distance at which  $F_0$  is defined (in *sun\_earth\_distance* global attribute),  $F_0$  is the mean solar flux in W m<sup>-2</sup> µm<sup>-1</sup>, spectrally resolved values for which are in *sensor\_views\_bands/intensity\_f0* and *sensor\_views\_bands/polarization\_f0* fields. The solar zenith angle,  $\theta_s$  (degrees), is in the *geolocation\_data/solar\_zenith\_angle* field.

To summarize, the following radiometric and polarimetric parameters are included in the L1C file for each instrument:

OCI: I

HARP2: I, Q, U, DoLP (derived), AoLP (derived)

**SPEXone**: i; i\_polsample; q\_over\_i; u\_over\_i, Q (derived), U (derived), DoLP (derived), AoLP (derived)

## 5. Instrument and Data Characteristics

### Data groups

The data fields for the L1C format are common for all instruments, although the dimensions may vary. Data are to be organized into four groups:

- 1. *sensor\_views\_bands*: which contains common bin information such as viewing geometry and band center wavelengths,
- 2. *bin\_attributes*: which contains information specific to each bin,
- 3. *geolocation\_data*: which contains latitude, longitude, altitude, observation and solar geometry, and
- 4. *observation\_data*: which contains the data observed by the instrument.

Each file also has associated global attributes, which lists important metadata such as the file creation date, the processing history, geospatial boundaries, and pointers to documentation about the spectral response functions and uncertainty models.

#### Data dimensions

Data from all three instruments are binned to a 5.2 km x 5.2 km spatial resolution at the surface. As each instrument has a different "footprint" of observations along the orbit, this means that the number of bins in the across track dimension (*bins\_across\_track*) in the L1C file for each instrument varies. SPEXone has a narrow swath so the number of bins is 29. Both HARP2 and OCI have wider swaths so this dimension has 519 bins. In the case of HARP2, the swath varies with view angle but the bin size is held constant and unobserved bins use fill values. To make it easier to align the different instrument files, the *nadir\_bin* attribute is included in the global attributes of each file. This is the across track pixel (using 0-based indexing) that has the western bin edge aligned with the subsatellite nadir track.

The number of bins in the along track direction (*bins\_along\_track*) is typically about 396. The length of the granule is based upon a five minute spacecraft observation time, which occasionally corresponds to slightly more or less along track bins.

Each instrument also has dimensions corresponding to the number of viewing angles (*number\_of\_views*), the spectral resolution of the intensity measurements per viewing angle (*intensity\_bands\_per\_view*), and the spectral resolution of the linear polarization components per viewing angle (*polarization\_bands\_per\_view*). Details about the dimensional organization specific to each instrument are given below.

Dimension	OCI	HARP2	SPEXone
number_of_views	2	90	5
intensity_bands_per_view	286	1	400
polarization_bands_per_view	-	1	50
bins_along_track	~396	~396	~396
bins_across_track	519	519	29

### Ocean Color Instrument (OCI)

PACE's primary sensor features a cross-track rotating telescope with a single science detector design to inhibit image striping. It has a tilt mechanism to minimize sun glint from the ocean surface. This is characterized in the *number\_of\_views* dimension, where in the Northern Hemisphere, all measurements are in the 20° forward viewing angle dimension, while in the Southern Hemisphere, all measurements are in the 20° aft viewing angle dimension. As PACE passes the Equator from the Southern Hemisphere to the Northern Hemisphere in the daytime, there is a period of time where the data are flagged as the tilt switches. The timing of this tilting is varied for every subsequent orbit to allow for patches of previously flagged regions to be retrieved in the following pass. This also means that in each Hemisphere, one entire dimension is NaN-filled.

As mentioned previously, OCI is *only* sensitive to the *I* element of the Stokes vector, so L1C files from that instrument to not contain polarimetric units. In other formats, these data are

often labeled as radiance, which is physically equivalent. Additionally, note that the *polarization\_bands\_per\_view* dimension is unused. **Table 1** lists the fields available in the *observation\_data* group, while Figure 3 is the *observation\_data/i* field for 664nm displayed with Panoply.

#### Table 1 OCI observation data

Name	bins_along_track	bins_across_track	number_of_views	intensity_bands_per_view	Unit	Description
number_of _observations	396	519	2	-	Unitless	Observations contributing to bin from each view
qc	396	519	2	286	Unitless	Quality indicator
i	396	519	2	286	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	I Stokes vector component
i_stdev	396	519	2	286	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Standard deviation of I in bin



Figure 3 OCI I(664.6nm) as displayed in Panoply from PACE\_OCI.20240321T173720.L1C.5km.nc

Note that OCI imagery has missing values at the swath edges, since spacing between pixels at swath edge grows such that there are no data to fill a bin.

### Hyper-Angular Rainbow Polarimeter 2 (HARP2)

HARP2 has 60 view angles for the channel centered at 669 nm and 10 view angles otherwise. Each channel accesses unique viewing angles across the full dynamic range of HARP2 viewing angles, and so all are indexed independently, i.e. the first 10 indices of the *number\_of\_views* dimension (from 56.3° fore to 53.3° aft) correspond to the blue waveband, then the following 60 indices (from 55.7° fore to 56.5° aft) correspond to the red waveband, etc. This also means the *intensity\_bands\_per\_view* and

*polarization\_bands\_per\_view* dimensions each of a length of one, as there is a single spectral channel for each unique view angle.

For data waveband dimensions, the quality indicator, the *I* Stokes vector element, and the associated uncertainty measurements have the dimension *intensity\_bands\_per\_view*, while the Q and U Stokes vector elements, the degree of linear polarization (DOLP), the angle of linear polarization (AOLP), and their associated uncertainties have the dimension *polarization\_bands\_per\_view*.

Table 2 contains the fields in the HARP2 *observation\_data* group, while Figure 4 and **Figure 5** show the *observation\_data/i* and *observation\_data/dolp* fields for 664nm.

Name	bins_	bins_	number_of_	intensity_bands	polarization_bands	Unit	Description
number_of _observations	396	519	90	per_view	per_view	Unitless	Observations contributing to bin from each view
qc	396	519	90	1	-	Unitless	Quality indicator
i	396	519	90	1	-	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	I Stokes vector component
i_stdev	396	519	90	1	-	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Standard deviation of I in bin
q	396	519	90	-	1	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Q Stokes vector component
q_stdev	396	519	90	-	1	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Standard deviation of Q in bin
u	396	519	90	-	1	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	U Stokes vector component
u_stdev	396	519	90	-	1	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Standard deviation of U in bin
dolp	396	519	90	-	1	Unitless	Degree of linear polarization (DOLP)
dolp_stdev	396	519	90	-	1	Unitless	Standard deviation of DOLP in bin
aolp	396	519	90	-	1	degrees	Angle of linear polarization (AOLP)
aolp_stdev	396	519	90	-	1	degrees	Standard deviation of AOLP in bin

#### Table 2 HARP2 observation data



Figure 4 HARP2 I(664.6nm) in Panoply from PACE\_HARP2.20240321T173720.L1C.5km.nc



Figure 5 HARP2 DoLP(664.6nm) in Panoply from PACE\_HARP2.20240321T173720.L1C.5km.nc

Note the fill values and narrower swath for this view angle (21.3°) than OCI. Due to pixel growth with view zenith angle, this swath is larger for more extreme angles and narrower for angles closer to nadir.

### Spectro-Polarimeter for Exploration (SPEXone)

SPEXone has the smallest spatial footprint of the three PACE instruments and thus has the fewest bins in the bins\_across\_track dimension, totaling 29. As with HARP2, it can be aligned with other PACE instrument data using the *nadir\_bin global attribute*, which designates the corresponding *bins\_across\_track* index just to the East of the nadir track line.

The SPEXone polarization data is normalized to the I Stokes vector intensity parameter and has "\_over\_i" incorporated into the variable name, as the field names require lowercase letters. Historically, the non-normalized Stokes vector components are uppercase (I, Q, U), while the normalized counterparts are in lowercase format (q and u).

Unlike HARP2, SPEXone has multiple wavebands associated with the 5 individual viewing angles. Additionally, the intensity variables are measured at higher (400 wavebands) resolution than the polarization measurements (50 wavebands) (<u>Rietjens et al., 2019</u>). This means that conversion of the polarization parameters ("lowercase q and u", i.e. *observation\_data/q\_over\_i* and *observation\_data/u\_over\_i*) to their forms found in HARP2 ("uppercase Q and U"), as well as the subsequent calculations of DOLP, requires using I that has been spectrally sampled like q and u, included in the file as *observation\_data/i\_polsample*, which has waveband dimensions of *polarization\_bands\_per\_view*.

Name	bins_ along_track	bins_ across_track	number_of_ views	intensity_bands _per_view	polarization_bands _per_view	Unit	Description
number_of _observations	396	29	5	-	-	Unitless	Observations contributing to bin from each view
qc	396	29	5	400	-	Unitless	Quality indicator
i	396	29	5	400	-	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	I Stokes vector component
i_stdev	396	29	5	400	-	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Standard deviation of I in bin
qc_polsample	396	29	5	-	50	Unitless	Quality indicator
i_polsample	396	29	5	-	50	$W m^{-2} sr^{-1} \mu m^{-1}$	I Stokes vector component at polarimeter spectral sampling
i_polsample _stdev	396	29	5	-	50	W m <sup>-2</sup> sr <sup>-1</sup> $\mu$ m <sup>-1</sup>	Standard deviation of I_POLSAMPLE in bin
q_over_i	396	29	5	-	50	Unitless	Q over I (little q) Stokes vector component
q_over_i _stdev	396	29	5	-	50	Unitless	Standard deviation of Q_OVER_I in bin
u_over_i	396	29	5	-	50	Unitless	U over I (little u) Stokes vector component
u_over_i _stdev	396	29	5	-	50	Unitless	Standard deviation of U_OVER_I in bin

#### Table 3 SPEXone observation data

dolp	396	29	5	-	50	Unitless	Degree of linear polarization (DOLP)
dolp_stdev	396	29	5	-	50	Unitless	Standard deviation of DOLP in bin
aolp	396	29	5	-	50	degrees	Angle of linear polarization (AOLP)
aolp_stdev	396	29	5	-	50	degrees	Standard deviation of AOLP in bin

Table 3 contains the fields in the SPEXone dataset, while **Error! Reference source not found.** and **Error! Reference source not found.** show *I* and *DoLP*, respectively.



Figure 6 SPEXone I(664nm) in Panoply from PACE\_SPEXONE.20240321T173720.L1C.5km.nc



Figure 7 SPEXone DoLP(668nm) in Panoply from PACE\_SPEXONE.20240321T173720.L1C.5km.nc

### Ancillary Files

https://oceancolor.gsfc.nasa.gov/resources/docs/ancillary/

## 6. Appendices

#### **Glossary of Terms**

3MI	Multi-viewing, Multi-channel and Multi-polarization Imager
AolP	Angle of Linear Polarization
DoLP	Degree of Linear Polarization
EOSDIS	Earth Observing System Data and Information System
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
HARP2	Hyper-Angular Rainbow Polarimeter-2
L1C	Level 1C
L2	Level 2
NetCDF	Network Common Data Form
OBPG	Ocean Biology Processing Group
OB.DAAC	Ocean Biology Distributed Active Archive Center
OCI	Ocean Color Instrument

OCSSW	Ocean Color Science Software
PACE	Plankton, Aerosol, Cloud, ocean Ecosystem
RSP	Research Scanning Polarimeter
SOCEA	Spacecraft Oblique Cylindrical Equal Area
SPEXone	Spectro-Polarimeter for Planetary Exploration-one
SWIR	Short Wave Infrared
ΤΟΑ	Top of Atmosphere
UV	Ultraviolet
VIS	Visible

#### Technical Specs of instruments

	Ocean Color Instrument (OCI)	Hyper-Angular Rainbow Polarimeter 2 (HARP2)	Spectro-Polarimeter for Planetary Exploration one (SPEXone)
UV-VIS radiance channels	<b>240</b> : continuous coverage in 340-890nm range at 2.5nm spectral resolution (5nm bandwidth)	4: 441, 549, 669, 873 nm	~400: continuous coverage in 385-770nm at 2-5nm spectral resolution
UV-VIS polarimetric channels	-	<b>4</b> : 441, 549, 669, 873 nm	~50: continuous coverage in 385-770nm at 10-40nm spectral resolution
SWIR radiance channels	<b>7:</b> 940, 1038, 1250, 1378, 1615, 2130, and 2260 nm	-	-
Viewing zenith angles in the satellite reference frame for swath center	1: 20° North in northern hemisphere, 20° South in southern hemisphere to avoid ocean surface glint	60 angles between ± 57° along track for 669 nm, 10 angles for the other bands*	<b>5</b> : 0°, ±20° and ±58°
Nadir view, at-ground swath width	2663km@	1,556 km	100km
Spatial Resolution	1x1km at nadir@	5.2km <sup>2</sup> , subject to modification	5.4 x 4.6 km <sup>#</sup> for all view angles

#### Links to software tools for data analysis

SeaDAS: a comprehensive software package for the processing, display, analysis, and quality control of ocean color data. <u>https://seadas.gsfc.nasa.gov/</u>

Panoply: plots geo-referenced and other arrays from netCDF, HDF, GRIB, and other datasets. <u>https://www.giss.nasa.gov/tools/panoply/</u>

OCSSW: science processing software used within the Ocean Biology Processing Group. <u>https://oceancolor.gsfc.nasa.gov/docs/ocssw/</u>

Jupyter Notebooks for downloading and plotting Ocean Color data: <u>https://oceancolor.gsfc.nasa.gov/resources/docs/tutorials/</u>

### 7. References

Chowdhary, J., Cairns, B., and Travis, L.: Case Studies of Aerosol Retrievals over the Ocean from Multiangle, Multispectral Photopolarimetric Remote Sensing Data, J. Atmos. Sci., 59(3), 383--397, 2002.

Hansen, J.E. and Travis, L.D., 1974. Light scattering in planetary atmospheres. *Space science reviews*, *16*(4), pp.527-610.

Hovenier, J.W. and Van der Mee, C.V.M., 1983. Fundamental relationships relevant to the transfer of polarized light in a scattering atmosphere. *Astronomy and Astrophysics*, *128*, pp.1-16.

Lang, R., Poli, G., Fougnie, B., Lacan, A., Marbach, T., Riedi, J., Schlüssel, P., Couto, A.B. and Munro, R., 2019. The 3MI Level-1C geoprojected product–definition and processing description. *Journal of Quantitative Spectroscopy and Radiative Transfer*, *225*, pp.91-109.

Rietjens, J., Campo, J., Chanumolu, A., Smit, M., Nalla, R., Fernandez, C., Dingjan, J., van Amerongen, A., and Hasekamp, O.: {Expected performance and error analysis for SPEXone, a multi-angle channeled spectropolarimeter for the NASA PACE mission}. in: Polarization Science and Remote Sensing IX 34 -- 47) SPIE., 2019.

Snyder, J. P. 1978: The space oblique Mercator projection, Photogramm. Eng. Remote Sensing, 44, 585-596, 140.

Snyder, J.P., 1987. Map projections--A working manual (Vol. 1395). US Government Printing Office.

Werdell, P. J., Behrenfeld, M. J., Bontempi, P. S., Boss, E., Cairns, B., Davis, G. T., Franz, B. A., Gliese, U. B., Gorman, E. T., Hasekamp, O., Knobelspiesse, K. D., Mannino, A., Martins, J. V., McClain, C. R., Meister, G., and Remer, L. A.: The Plankton, Aerosol, Cloud, Ocean Ecosystem Mission: Status, Science, Advances, B. Am. Meteorol. Soc., 100(9), 1775-1794, https://doi.org/10.1175/BAMS-D-18-0056.1, 2019.

Xu, X. and Wang, J.: UNL-VRTM, A Testbed for Aerosol Remote Sensing: Model Developments and Applications, in: Springer Series in Light Scattering: Volume 4: Light Scattering and Radiative Transfer, edited by: A. Kokhanovsky, Springer International Publishing, Cham, 1--69, https://doi.org/10.1007/978-3-030-20587-4\_1, 2019.

Zhao, G., Yang, M., Clipp, L., Gao, Y., and Lee, J. H.: Basic Terra fusion product algorithm theoretical basis and data specifications, University of Illinois at Urbana-Champaign, https://www.ideals.illinois.edu/items/112706, 2019.