**Appendix - t-SNE hyperparameters & sensitivity analysis**

*Convergence of PC(t-SNE)*

The variance partition given by the eigenvalues of the covariance matrix provide a metric by which to assess convergence for increasing numbers of t-SNE realizations. Figure S1 shows the expected increase in curvature of the eigenvalue distribution reflecting increasing redundancy for additional realizations. As the low order dimensions account for most variance, convergence of the variance partition for the low order dimensions implies convergence of the structure of the resulting feature space of t-SNE clusters. It also implies consistency of the cluster memberships as the redundancy of additional realizations would not be expected to increase if cluster membership of spectra were random or variable from one realization to another. As shown by the inset in Figure S1, the 1, 2 and 3 dimensional spaces of the low order PC(t-SNE) dimensions all converge to effectively constant variance by 16 realizations, suggesting little benefit to additional realizations. Nonetheless, the PC(t-SNE) of the composite feature space used in this analysis is based on 30 realizations because added redundancy does cause the resulting clusters in the PC(t-SNE) feature space to coalesce and separate further making distinction and labeling easier. The rate of convergence would be expected to depend on the topology of the space and number of manifolds t-SNE resolves, so the convergence of the cryospheric composite space should not be assumed representative of other types of spectra.

*Figure S1 Eigenvalue distributions of PC(t-SNE) for increasing 2D t-SNE realizations. Beyond 16 realizations increasing curvature exceeds decreasing slope suggesting convergence. By 30 realizations, more than half of the PC dimensions account for < 0.1% variance each. The variance accumulation for 1D, 2D and 3D projections of the low order PCs (inset) all converge by 16 realizations, suggesting little additional benefit for additional computational cost.*

*Sensitivity to Perplexity*

The perplexity parameter is generally considered to be the strongest determinant of t-SNE performance (Wattenberg, Viégas, and Johnson 2016). Increasing t-SNE perplexity generally decreases the number of clusters and increases their separability in 2D t-SNE space as larger perplexity values correspond to larger local neighborhoods over which manifolds are defined within the feature space. Incremental increases in perplexity across multiple t-SNE realizations illustrate the variation of local feature space topology as a function of perplexity, as shown by Figure S2. For perplexity > 20, the number of clusters stabilizes and separation increases. Therefore, consistency of cluster membership among t-SNE realizations with different perplexity values can be interpreted as an indication of stability and repeatability of the t-SNE feature space. Consistency of cluster membership can be demonstrated (or not) by back propagation of cluster labels from PC(t-SNE) to individual realizations of different perplexity. The 7 most distinct clusters (including dis-continua) are labeled in the three low order dimensions of PC(t-SNE) derived from all 60 (2D x 3 realizations x 10 perplexities) dimensions of 30 2D t-SNE realizations. The results in Figure S2 are clear. The consistency of the t-SNE cluster membership from the PC(t-SNE) feature space to the individual t-SNE realizations indicates that the cryospheric feature space of the AVIRIS-NG composite is not particularly sensitive to the perplexity parameter, although the number of clusters does not converge below a perplexity of ~20. As with convergence of PC(t-SNE) dimensionality, the rate of convergence of perplexity should be expected to depend on the topology of the feature space being rendered.

*Figure S2 Spectral feature space evolution for varying t-SNE perplexity values. Individual realizations of t-SNE with the same perplexity are distinct but share clear similarities in number and sometimes shape of clusters. As perplexity increases, cluster separation increases and numerous smaller clusters aggregate into fewer larger clusters (top panels). PC(t-SNE) for suites of 6 t-SNE shows a similar progression with increasing perplexity (middle panels). PC(t-SNE) for a single suite of 30 realizations spanning 10 perplexities shows similar continua and dis-continua topology (bottom panels) to the perplexity = 30 suite used in text. Contiguous clusters (color labeled) in PC(t-SNE) 1v2 and 1v3 spaces generally correspond to individual AVIRIS-NG lines. The notable exceptions are the ice clusters (greens) in which W-transect and SeaIceW comingle with western ends of both K and Q-transects. The contiguity of these clearly distinct clusters in 30x PC(t-SNE) space can also be seen by the contiguity of label colors in the 6x PC(t-SNE) spaces and the individual t-SNE realizations.*

**Appendix - Computational specifics**

All t-SNE computations were performed on Lenovo t460s hardware running Linux (Ubuntu 18.04.6 LTS) with Intel i7-6600U CPU @ 2.60Ghz x 4, 24 GB RAM, and Intel HD Graphics 520 GPU. Computations used scikit-learn v0.24.0 in a Python 3.7 environment with the call:

*Y = sklearn.manifold.TSNE(n\_components = 2, perplexity = p).fit\_transform(X)*

where X is the (n x l) data matrix with l wavelengths and n pixels, and Y is the (n x 2) t-SNE output matrix.

Perplexity variation experiments on the subsampled data cube (n = 17164 pixels with 373 channels) found runtime sensitivity to perplexity value to be sublinear (runtime approximately 75 seconds for perplexity = 10; 90 seconds for perplexity = 50; 130 seconds for perplexity = 100).