Supplemental Information: Solubility and Solution-phase Chemistry of Isocyanic Acid, Methyl Isocyanate, and Cyanogen Halides

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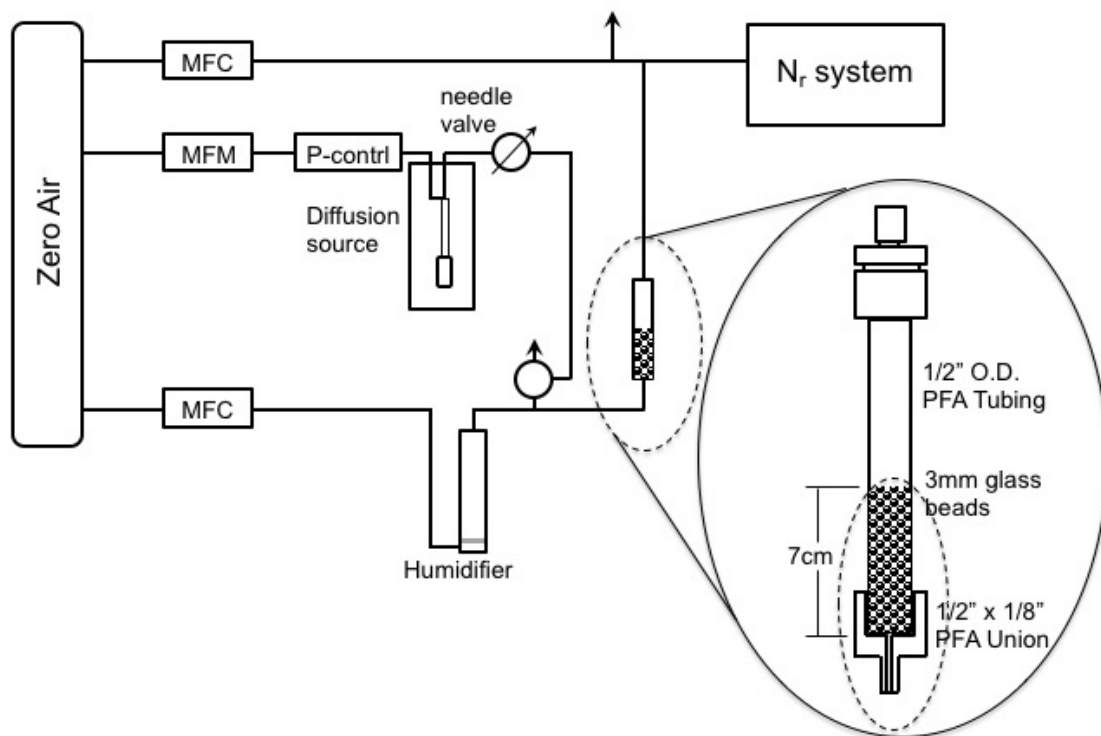
Figure S1., The small-scale Teflon PFA reactor used for ICN solubility measurements.

Unlike HNCO and CH₃NCO, the some of the XCN compounds have absorbances in the near UV-vis that could lead to photolysis in the lower atmosphere, Figure S2. The UV-vis spectra and photon fluxes estimated from the NCAR TUV model (NCAR, 2018) can be used to calculate photolysis rates, by integrating over the wavelength region where the absorption is significant, and assuming a quantum yield of 1. The absorption spectra are such that ClCN will not be photolyzed in the troposphere, BrCN has some slight absorption in the actinic region and ICN has substantial absorption. The lifetimes against photolysis at 0km altitude, 40°N, on June 30. 2015, were estimated to be 135 days for BrCN, and 9 hours for ICN.
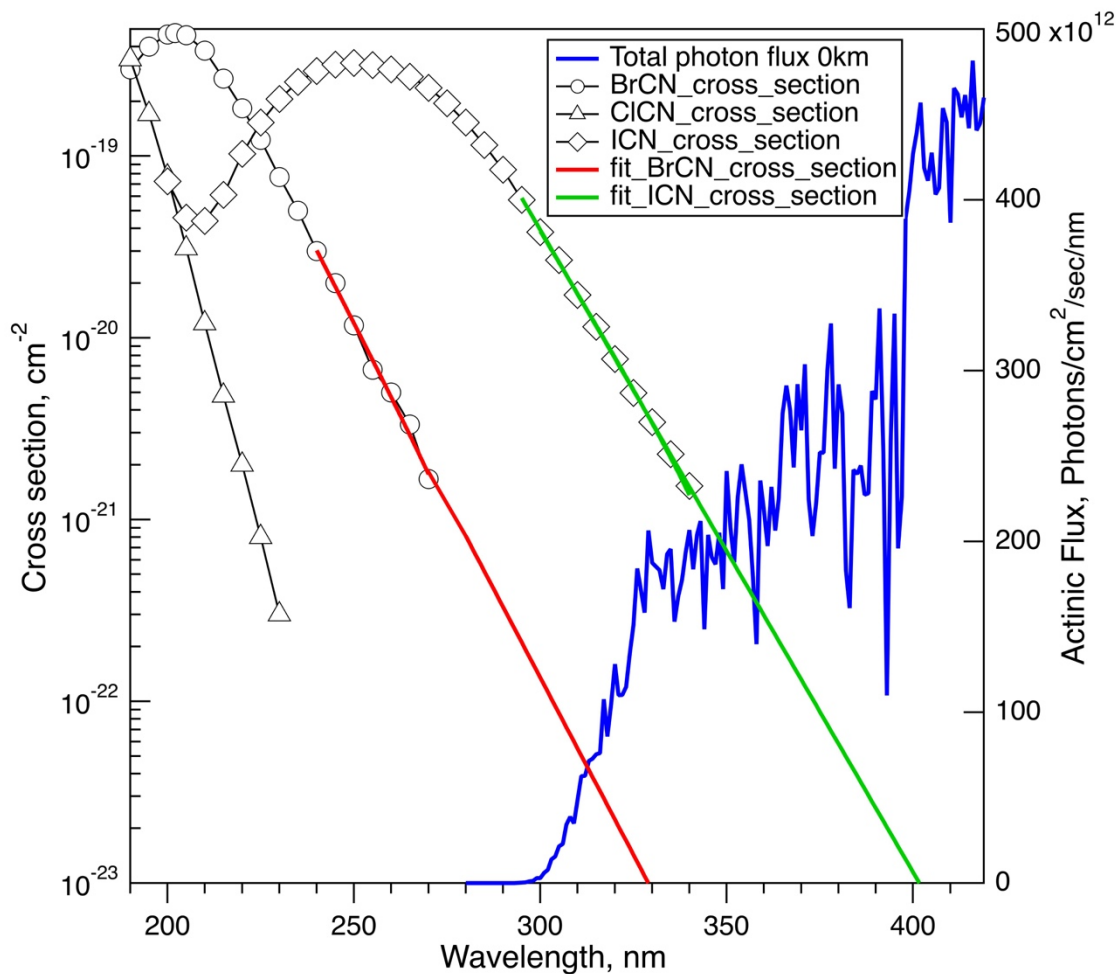
Figure S2. The UV-vis absorption spectra of ClCN, BrCN, ICN, (Barts and Halpern, 1989; Felps et al., 1991; Hess and Leone, 1987; Russell et al., 1987) and the photon flux spectrum estimated from the NCAR TUV model for 40° N, surface on June 30, 2015 (NCAR, 2018). The extrapolation assumes the cross-sections are ln-linear over the portions that tail into the actinic region.

References:

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Hess, W. P. and Leone, S. R.: Absolute I* quantum yields for the ICN Ã state by diode laser gain-vs-absorption spectroscopy, J. Chem. Phys., 86, 3773-3780, 1987.

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