Interactive comment on "Solubility and reactivity of HNCO in water: insights into HNCO's fate in the atmosphere" by N. Borduas et al.
Anonymous Referee #1
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Summary and General Comments: Borduas and coworkers report on a series of laboratory experiments designed to constrain the effective Henry's law coefficient for HNCO at a range of atmospherically relevant pH. Further, the authors determine the hydrolysis lifetime of HNCO as a function of pH and temperature for three known hydrolysis mechanisms. The paper is well written, systematic, and will have impact on the community. This paper should be published following the authors attention to a few comments.

Specific Comments:
Page 24218 Line 24: The study of isocyanates from an environmental perspective predates the work of Roberts. Some specific examples include the Bhopal Disaster in India. Perhaps a line on this in the introduction is worthwhile?

> This paper is based on the study of the HNCO molecule, whereas it was methyl isocyanate that was leaked out during the Bhopal, India disaster. We prefer not to include the discussion of the Bhopal Disaster in our introduction as it is not directly relevant to HNCO. No changes to the manuscript were made.

Page 24221 Line 6: Where are Reactions 1-3? They were listed in the abstract, but should be included in the main text.

> They are presented in Scheme 1.

Page 24221: It would be interesting to note what additional condensed phase reactions involving HNCO are potentially important. Is there any indication that NCO- reactions with condensed phase organics are important to atmospheric chemistry?

> We believe that the condensed phase reactive form of isocyanic acid is in its protonated from, i.e. HNCO. The conjugate base, NCO-, is a poor electrophile as well as a poor nucleophile and consequently is expected to be somewhat stable under ambient particle conditions. Page 24233 lines 13-15 addresses the reviewer's point on other potential reactions with HNCO and we added that these nucleophiles may be amines and alcohols.
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> The sentence now reads, "There is also the possibility that HNCO has other currently unknown sinks in cloud water that may be competitive with its hydrolysis and further work on HNCO's aqueous phase chemistry with nucleophiles such as amines and alcohols is currently underway in our laboratories."

Page 24222 Line 12: It is noted that 10 ions were tracked, although the manuscript discusses only NCO- (and indirectly acetate ion). What other ions were measured, and why? Were any other acids expected (or measured) in the system.

Other ions measured included m/z 59 (CH_3COO^-), m/z 119 ((CH_3COOH)CH_3COO^-)), m/z 51 (dark counts), m/z 35 (Cl^-), m/z 45 (HCOOH, as $HCOO^-$), m/z 46 (HONO, as NO_2^-), m/z 96 , m/z 102 and m/z 113. None of these ions was observed to change during the experiments and they were monitored to ensure the CIMS was operating correctly. This list of ions was added to the text after line 12.

The manuscript now reads, "Ions measured included m/z 59 (AcO-), m/z 119 ((AcOH)AcO-), m/z 51 (black counts), m/z 35 (Cl-), m/z 42 (NCO-), m/z 45 (HCOO-), m/z 46 (ONO-), m/z 96, m/z 102 and m/z 113. For the exception of m/z 42, none of the ions were observed to change during the experiments."

Page 24222: Is there an absolute humidity dependence on the sensitivity to NCO- that needs to be accounted for when changing the flow rate over the water solutions? Or is the NCO- sensitivity not dependent on absolute water concentration (or the analysis independent of this effect if it existed).

The reviewer raises a good point. Previous work suggests that there is no significant role of water vapour in HNCO's detection by acetate CIMS (Roberts et al. 2010), and so we did not investigate the RH dependence of HNCO. In addition, we had a N2 dilution flow for the inlet of the CIMS and thus was detecting HNCO under conditions of < 20% RH.

We added these clarifications in the text, "Previous work suggests there is no significant role of water vapour in HNCO's detection by acetate CIMS (Roberts et al. 2010). With the CIMS's inlet dilution, the RH within the ion molecule region was < 20%.

Page 24223 Line 12: Perhaps provide reference to one of the earlier Roberts papers (or perhaps even earlier in the literature) that first sublimed cyanuric acid as a HNCO calibration source.

Agreed. We have added the Belson and Strachan 1982 and Roberts et al. 2010 references to line 12.

References:

Roberts, J. M., Veres, P., Warneke, C., Neuman, J. A., Washenfelder, R. A., Brown, S. S., Baasandorj, M., Burkholder, J. B., Burling, I. R., Johnson, T. J., Yokelson, R. J. and de Gouw, J.: Measurement of HONO, HNCO, and other inorganic acids by negative-ion proton-transfer chemical-ionization mass spectrometry (NI-PT-CIMS): application to biomass burning emissions, Atmos. Meas. Tech., 3, 981-990, 2010.