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Supporting information for article:

Differences and similarities among hypoxanthinium nitrate hydrate structures

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Differences and similarities among hypoxanthinium nitrate hydrate structures - supplementary

Cell changes

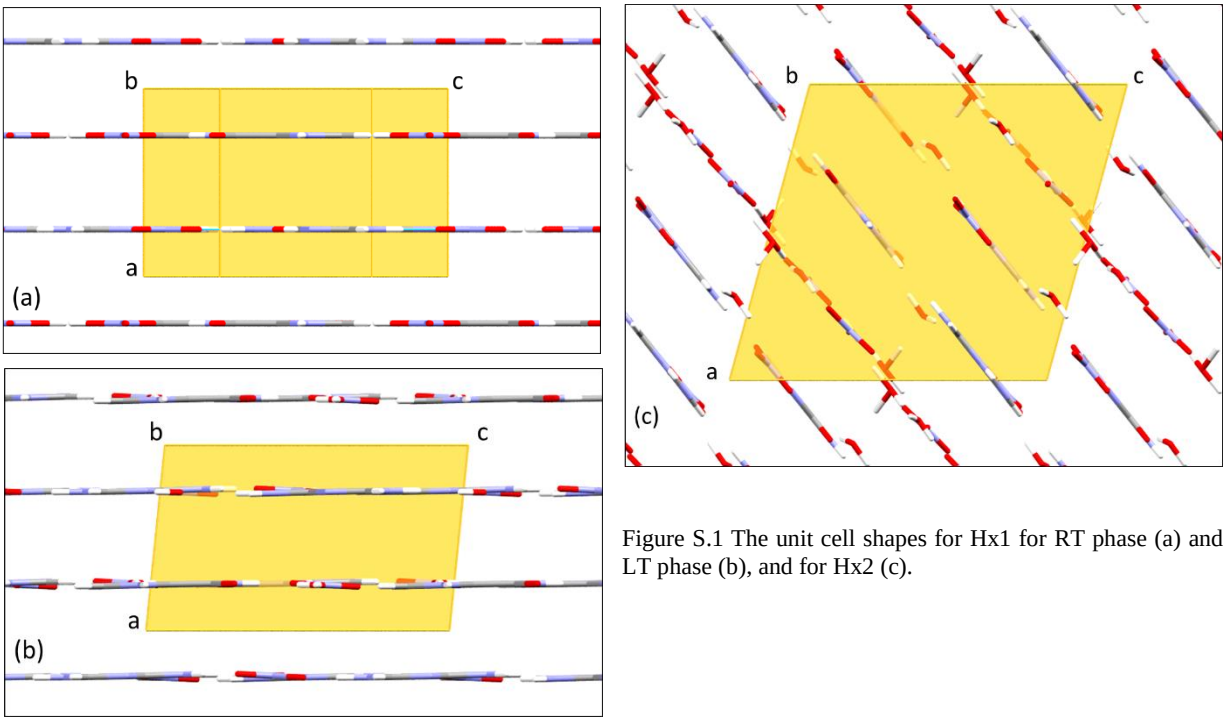

Figure S.1 The unit cell shapes for Hx1 for RT phase (a) and LT phase (b), and for Hx2 (c).

Fingerprint plots

As it was already pointed out in the main part of the publication the fingerprint plots for the corresponding molecules in both structures of hypoxanthinium nitrate hydrate are very similar (Figure S.2, Figure S.3) (Turner *et al.*, 2017).

Despite the phase transition in Hx1, the differences between the plots are almost nonexistent, and if there are any, they mainly show among the longest interactions.

For Hx2 it is noticeable that in higher temperature the fingerprint plots for nitrogen molecules are almost identical, whereas in the lower temperature the NO_3^- (N21) is visibly different and its left side is somehow slimmer. The H_3O^+ (O2) is the only cationic water molecule and its fingerprint plot differs from the rest of the water molecules mainly with the lack of elongated part representing the O…H interactions, and the shortest H…O interactions presented on the fingerprint plot as an elongated part on its left side. among the three water molecules presented in the structure the shortest O…H interactions belong to H_2O (O3).

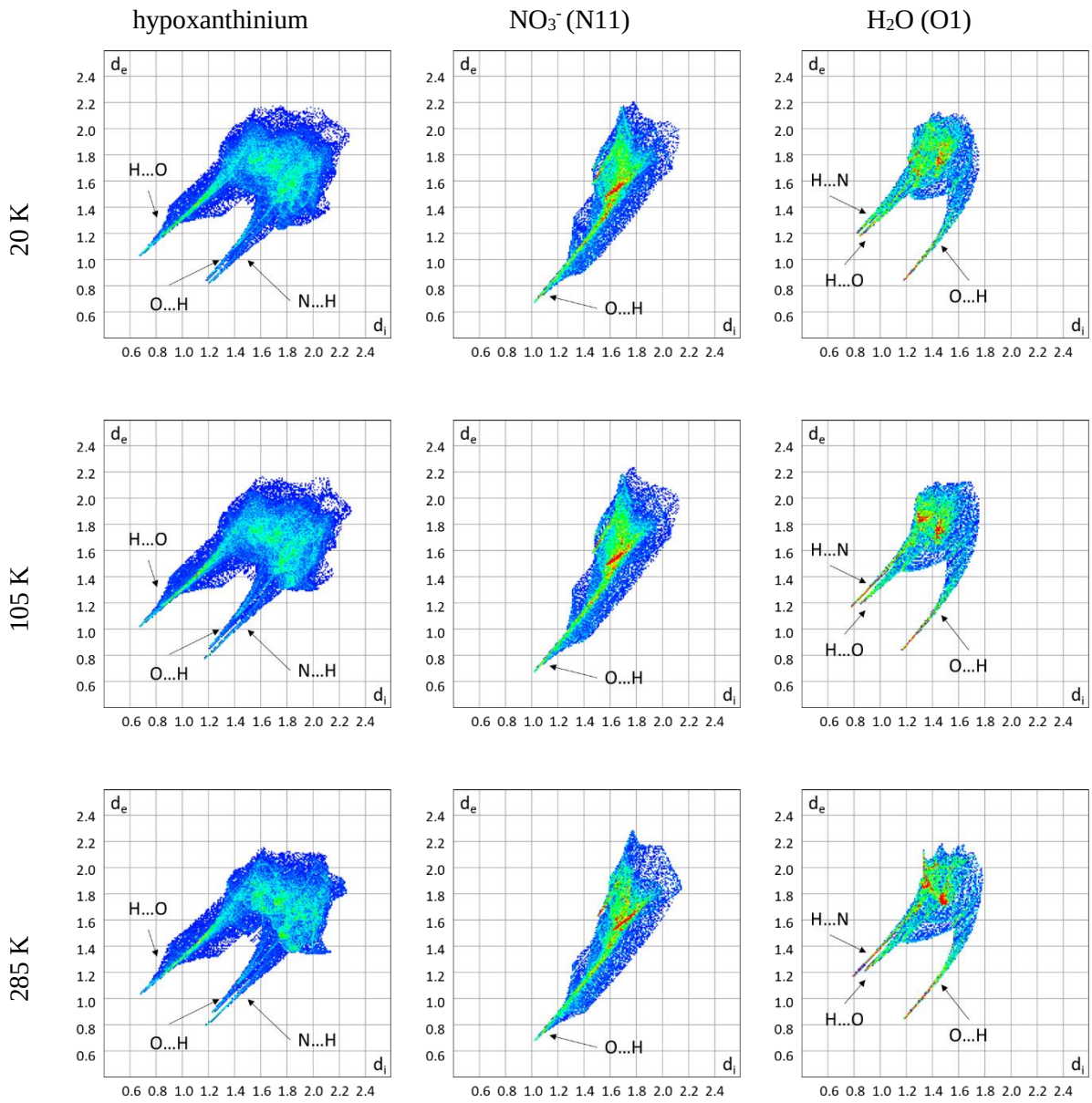

Figure S.2 Fingerprint plots for each independent molecule in Hx1.

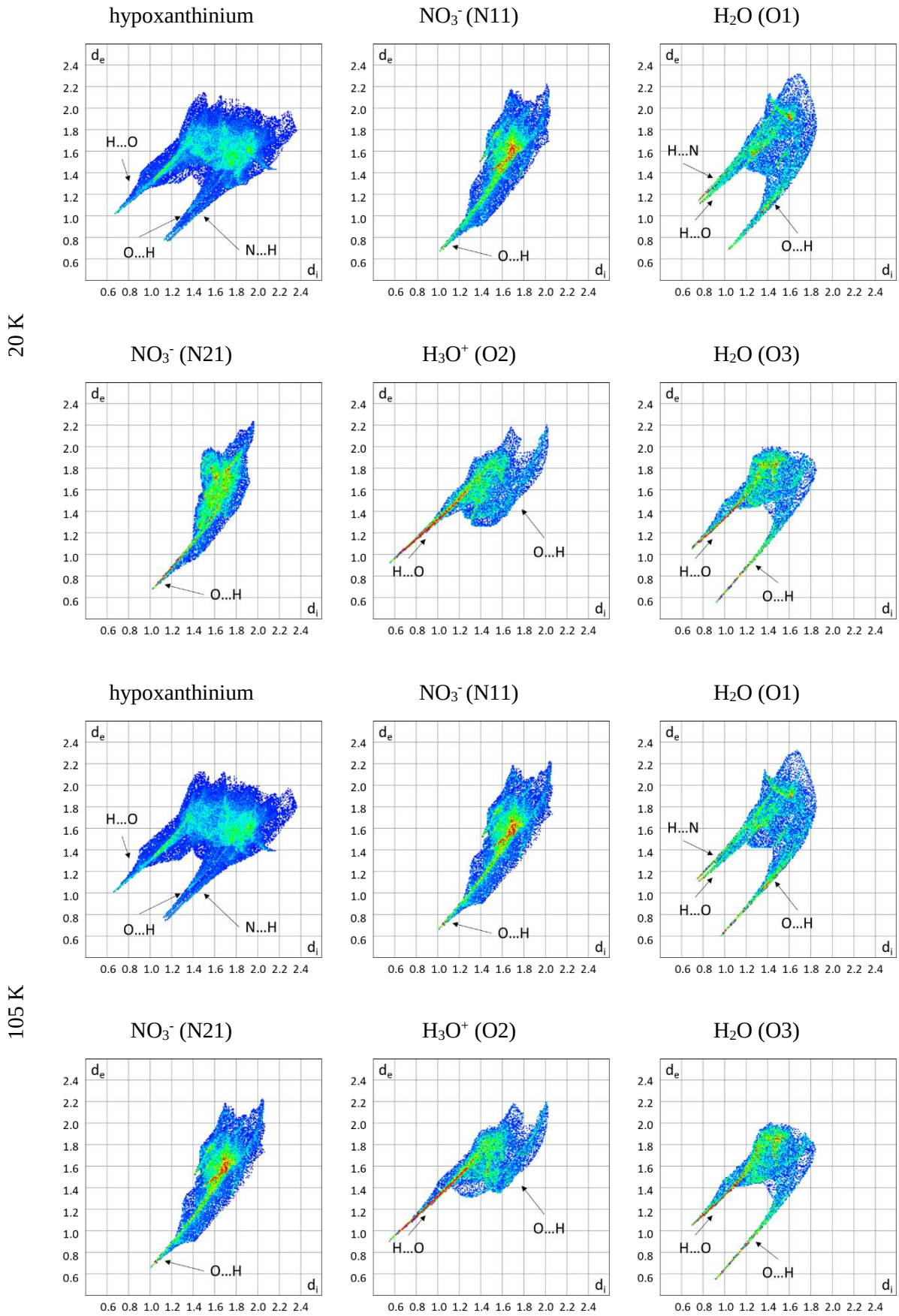

Figure S.3 Fingerprint plots for each independent molecule in Hx2.

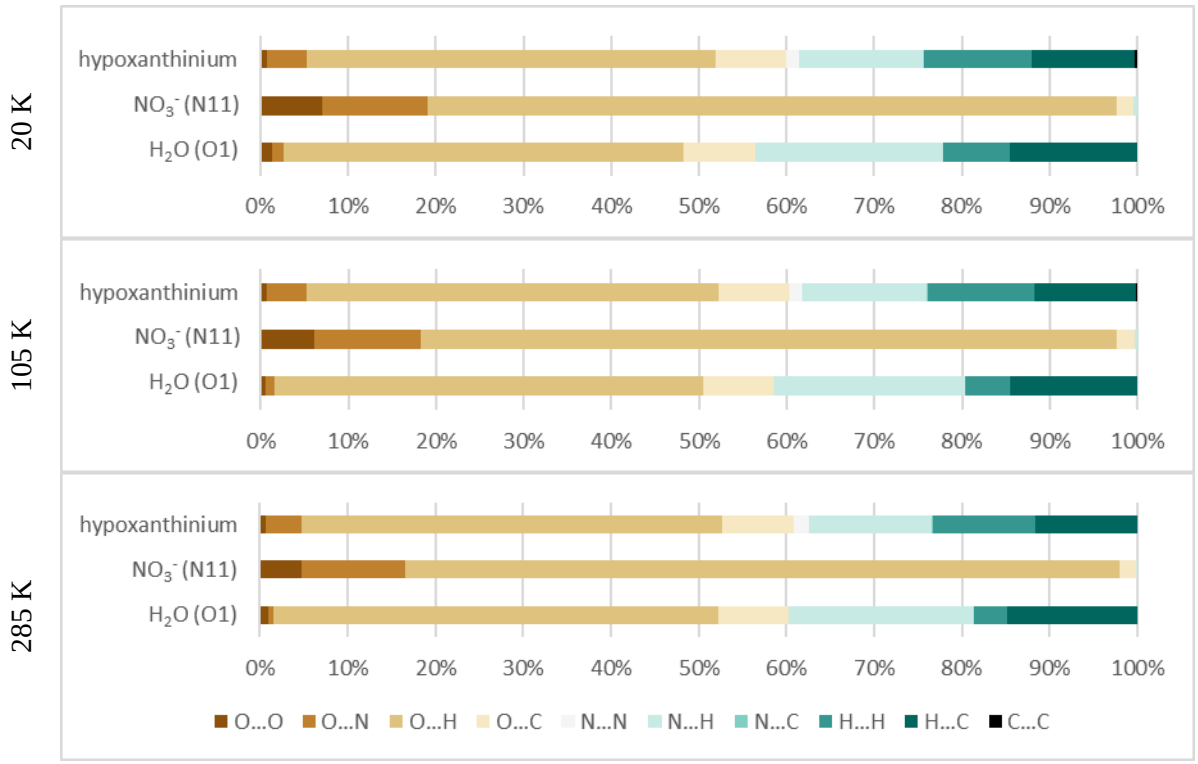

Figure S.4 Percent of interactions Hx1.

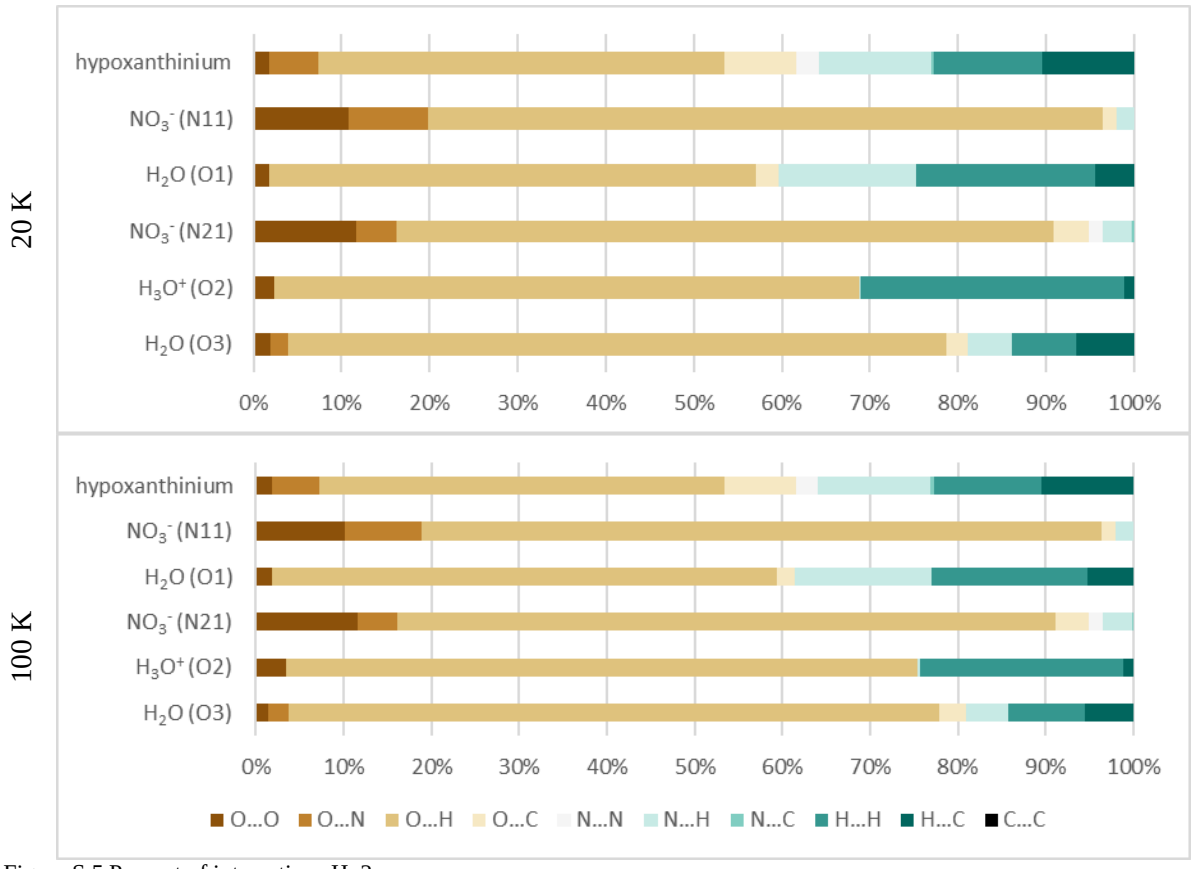

Figure S.5 Percent of interactions Hx2.

References

Turner, M. J. *et al.* (2017) ‘CrystalExplorer17’. University of Western Australia.