

Supplementary Materials

Taimin Yang ¹, Steve Waitschat ², Andrew Kentaro Inge ¹, Norbert Stock ², Xiaodong Zou ^{1,*} and Hongyi Xu ^{1,*}

¹ Department of Materials and Environmental Chemistry, Stockholm University, 106 91 Stockholm, Sweden;

² Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, 241 18 Kiel, Germany;

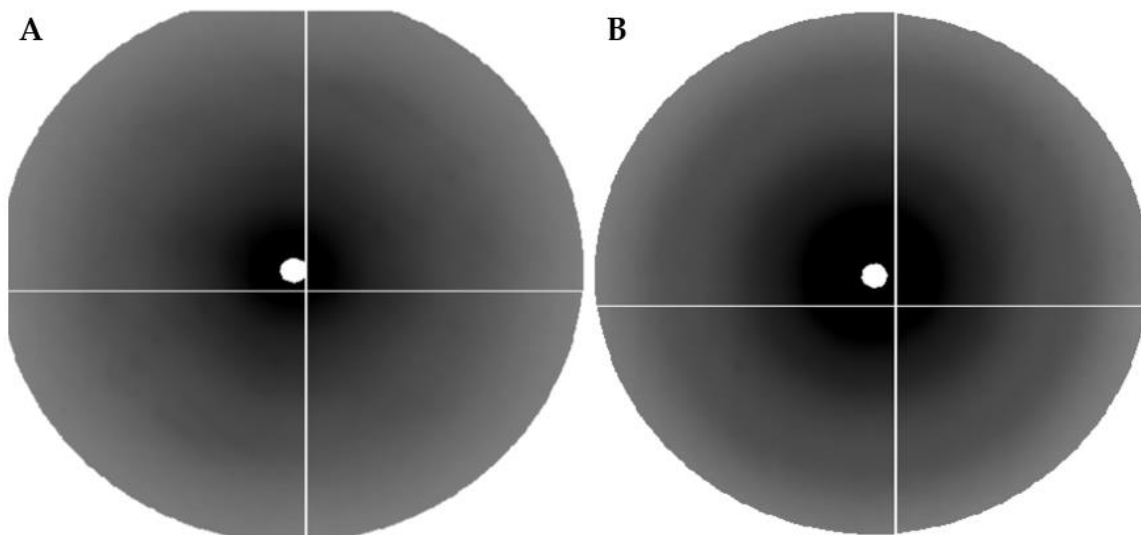


Figure S1. Estimated background by XDS of sucrose data collected at A) room temperature and B) cryogenic temperature.

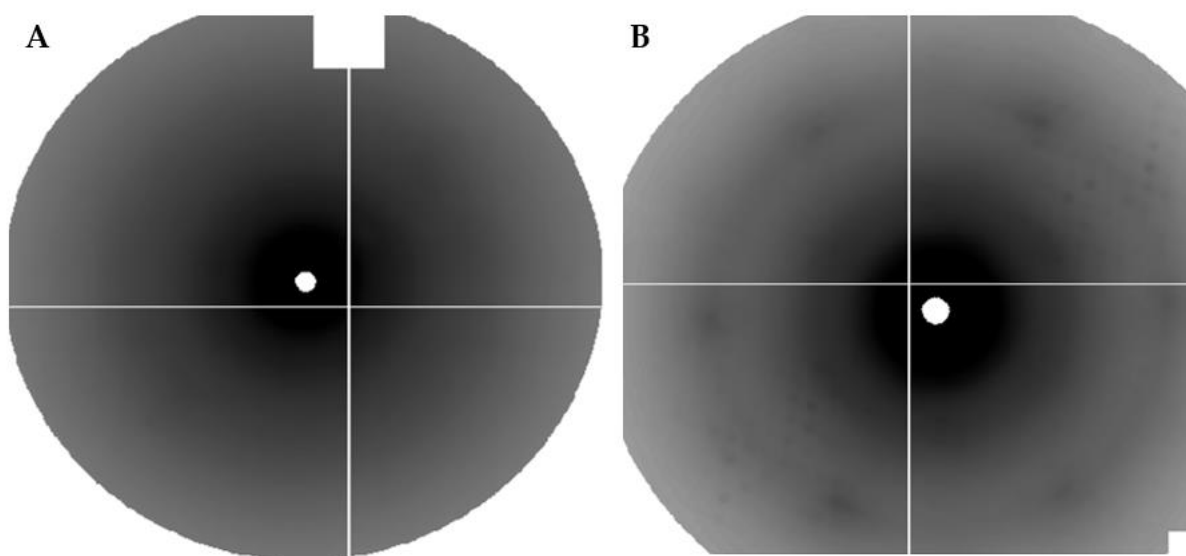


Figure S2. Estimated background by XDS of H₄ABTC data collected at A) room temperature and B) cryogenic temperature.

Table S1. ADRA of hydrogen atoms between the reference structure of sucrose [1] and structures determined from datasets obtained in both temperature conditions (2nd round of refinements for obtaining the best possible structure models).

Atom Label	ADRA (Å)	Atom Label	ADRA (Å)
~300 K		~100 K	
H1	0.146	H1	0.200
H2	0.177	H2	0.176
H3	0.072	H3	0.172
H4	0.177	H4	0.167
H5	0.199	H5	0.196
H6	0.110	H6	0.136
H7	0.317	H7	0.395
H10	0.088	H8	0.313
H11	0.077	H10	0.033
H12	0.156	H11	0.088
H13	0.366	H12	0.136
H14	0.138	H13	0.481
H15	0.229	H15	0.000
H16	0.088	H16	0.365
H17	0.143	H17	0.152
H18	0.152	H18	0.123
H19	0.203	H19	0.181
H20	0.142	H20	0.151
H21	0.192	H21	0.172
H22	0.185	H22	0.142
Average	0.17(9)	Average	0.20(11)

Table S2. Comparison between the ADPs of sucrose determined from merged datasets (refinement for obtaining better structure). ADPs close to 0.01 (the minimum ADP value set by “XNPD”) are marked in red.

Atom Label	ADP (Å ²)	Atom Label	ADP (Å ²)
~300 K		~100 K	
C1	0.038	C1	0.010
C2	0.038	C2	0.017
C3	0.051	C3	0.025
C4	0.034	C4	0.012
C5	0.062	C5	0.021
C6	0.038	C6	0.011
C7	0.055	C7	0.015
C8	0.041	C8	0.014
C9	0.056	C9	0.010
C10	0.043	C10	0.015
C11	0.071	C11	0.014
C12	0.060	C12	0.023
O1	0.031	O1	0.017
O2	0.052	O2	0.028
O3	0.061	O3	0.027
O4	0.046	O4	0.018
O5	0.092	O5	0.033
O6	0.046	O6	0.014
O7	0.119	O7	0.033
O8	0.058	O8	0.028
O9	0.045	O9	0.016
O10	0.077	O10	0.027
O11	0.064	O11	0.021
Average	0.056(20)	Average	0.019(7)

References

1. Brown, G.M.; Levy, H.A. Further Refinement of the Structure of Sucrose Based on Neutron-Diffraction Data. *Acta Cryst B* **1973**, *29*, 790–797, doi:10.1107/S0567740873003353.