Electronic Supplementary Material (ESI) for CrystEngComm.

COMMUNICATION

Supporting Information for Unusual Single Crystal to Single Crystal Phase Transition of a Nicotine Salt Monitored Using Temperature Dependent Single Crystal X-ray Diffraction

Devin J. Angevine, Travis B. Mitchell, Xiaotong Zhang, & Jason B. Benedict*

Department of Chemistry, University at Buffalo, Natural Sciences Complex, Buffalo, 14260-3000, USA

Supporting Information

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Methods & Materials

Materials

(S)-nicotine (>95%) and 2,6-dihydroxybenzoic acid (98%) were purchased from TCI and Alpha Aesar, respectively. Ethanol (USP grade; 190 proof) was purchased from Decon Laboratories Inc. n-Heptane (99%) was purchased from Fisher Scientific.

Salt Synthesis

2,6-dihydroxybenzoic acid (7.7060 g, 50.0 mmol) was added into a 200 mL beaker. Ethanol (50.0 mL) was added with vigorous agitation. (S)-Nicotine (8.00 mL, 50.0 mmol) was added via micropipette in the dark to avoid degradation. The resulting solution was stirred for 30 minutes at 1,000 rpm. The solution was then stored in the dark unsealed to allow for crystal formation while the solvent slowly evaporated. Once the solvent evaporated, the crystalline product was collected via vacuum filtration, washing (3x30 mL) with n-heptane (14.9112 g, 94.27%). The yield was computed based upon the formula weight of (S)-nicotinium 2,6-dihydroxybenzoate (F.W. 316.4 g/mol).

Single Crystal X-Ray Diffraction (SC-XRD)

X-ray diffraction data was collected using a Bruker SMART APEX-II CCD diffractometer installed at a rotating anode source (MoKα radiation, $\lambda = 0.71073$ Å) and equipped with an Oxford Cryosystems (Cryostream700) nitrogen gas-flow apparatus. Five sets of data (360 frames each) were collected by the rotation method with 0.5° frame-width (ω scans) with a 2.0 second exposure time for the single crystalline sample at $2\theta = -30°$. The sample was initially run at 293 K, then again at 90 K. Using Olex2, the structure was solved with intrinsic phasing via the ShelXT structure solution program and refined with the ShelXL software suite using least squares minimization.[25-27] A q-peak (0.33 e-/ Å3) was located 0.945 Å from N1 and was assigned as a proton consistent with charge transfer from the carboxylic acid of the salt former. The atomic coordinates of H atoms attached to heteroatoms were freely refined with thermal parameters constrained to be $U_{iso}(H) = 1.5U_{eq}(N)$ or $1.5U_{eq}(O)$. H atoms connected to carbon atoms were placed geometrically (C–H = 0.95 Å) and refined with thermal parameters constrained to be $U_{iso}(H) = 1.2U_{eq}(C)$. Images of the structures were created using Olex2 and the CSD: Mercury Visualization and Analysis of Crystal Structures software suite.[28] Absolute configuration was assigned based upon the stereochemistry of the API (S)-nicotine. The Flack parameter was removed in accordance with IUCr standards for reporting a structure in which the absolute configuration is assigned based upon a known reference molecule, which in this structure is (S)-nicotinium.

Stepwise Thermal Ramping X-Ray Diffraction Batch Indexing

X-ray diffraction data was collected using a Bruker SMART APEX-II CCD diffractometer installed at a rotating anode source (MoKα radiation, λ = 0.71073 Å) and equipped with an Oxford Cryosystems (Cryostream700) nitrogen gas-flow apparatus. Data was collected by the rotation method with 0.5° frame-width (ω scans) with a 2.0 second exposure time for the single crystalline sample at 2θ = −30°. The nature and reversibility of the phase transition between the low high temperature salt (**HT salt**) and its corresponding low temperature salt (**LT salt**) was determined using python scripts which automate routines within the APEX4 framework including all of the processes necessary to determine the unit cell for a set of frames: harvesting reflections, indexing using difference vectors and fast Fourier transform indexing methods, unit cell refinements, and assigning the unit cell to a Bravais lattice.[29] The Bravais lattice for this system was predetermined and set to monoclinic *P* since the **HT salt** and the **LT salt** were determined to have $P2_1$ symmetry. Unit cells obtained using this method enable the monitoring of changes in real time while utilizing temperature as an external stimulus. Each unit cell (or batch) was indexed using 20 frames per batch. The initial temperature was calibrated and set to 110 K. The temperature was decreased in a stepwise fashion by increments of 1 K every ten batches (200 frames) until 95 K was reached and similarly increased back to 110 K. The entire data collection yielded a total of 310 indexed batches. In the event of tied or very similar indexing scores, the corresponding batch was independently indexed.

Infrared (IR) Spectroscopy

Infrared spectral analysis was carried out on a Perkin Elmer Spectrum Two FTIR spectrometer equipped with an attenuated total reflectance (ATR) module. Eight scans were averaged for each spectrum.

Powder X-Ray Diffraction (PXRD)

Powder X-ray diffraction data was collected using a Rigaku Ultima IV X-ray Diffraction (XRD) System equipped with standard attachment (CuKα radiation, λ = 1.54 Å). Data collection was done over the 2θ range from 2° to 45° utilizing a 0.02° incremental step. A scanning speed of 5° per minute was utilized. Slit heights were set as follows: divergence slit: 2/3°; divergence height limiting slit: 10mm; scattering slit: 2/3°; receiving slit: 0.3mm. PXRD patterns were simulated using the Mercury 4.0 2021.2.0 visualization and analysis of crystal structures software suite.[26] A 0.02° step was utilized for the simulated PXRD pattern along with a full width half max of 0.1. All PXRD patterns were normalized to a maximum intensity of 10,000 counts.

Hirshfeld Surface Analysis

The Hirshfeld surfaces of the molecules in the **HT salt** structure and **LT salt** structure were generated using *Crystal Explorer 17.5*.[30] For all salts the d_{norm} surface was mapped using the color scale with the range −0.050 a.u. (red) to 0.600 a.u. (blue). In addition, 2-D fingerprint plots were generated as the outer nuclei (d_e) versus the inner nuclei (d_i) using an expanded interaction distance ranging from 0.6 Å to 2.8 Å.

Crystallographic Information

Structural Data Deposition

Deposition number 2233083 (**HT salt**) & 2233084 (**LT salt**) contains the supplementary crystallographic data for this paper. This data is provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.

(S)-Nicotinium 2,6-Dihydroxybenzoate 293 K (HT salt) Structure & Crystallographic Information

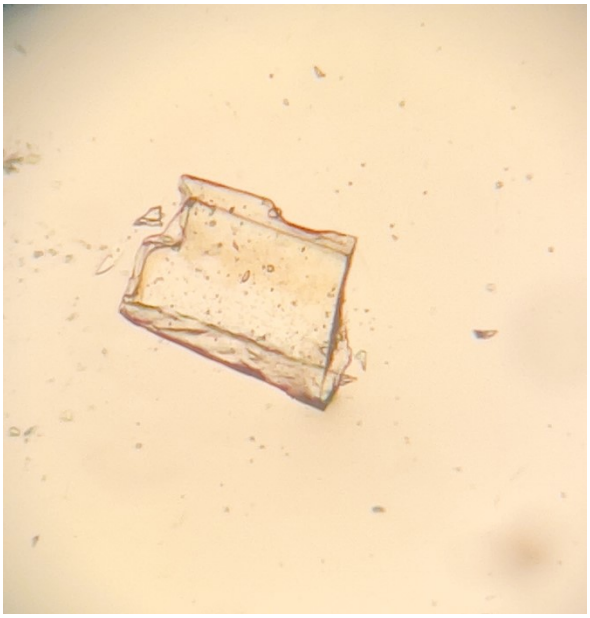


Figure S1: A crystal of **HT Salt**.

Figure S2: A vial of crystals of **HT Salt**.

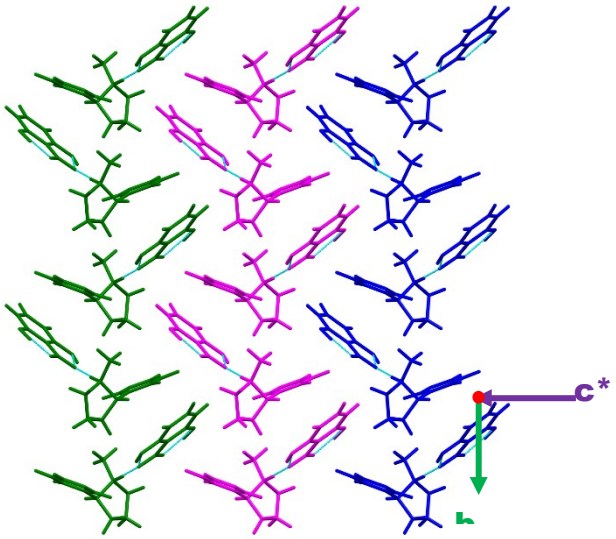


Figure S3: Packing diagram viewed along [100] of **HT salt** depicting columns parallel to [010] and stacking of these columns along [001].

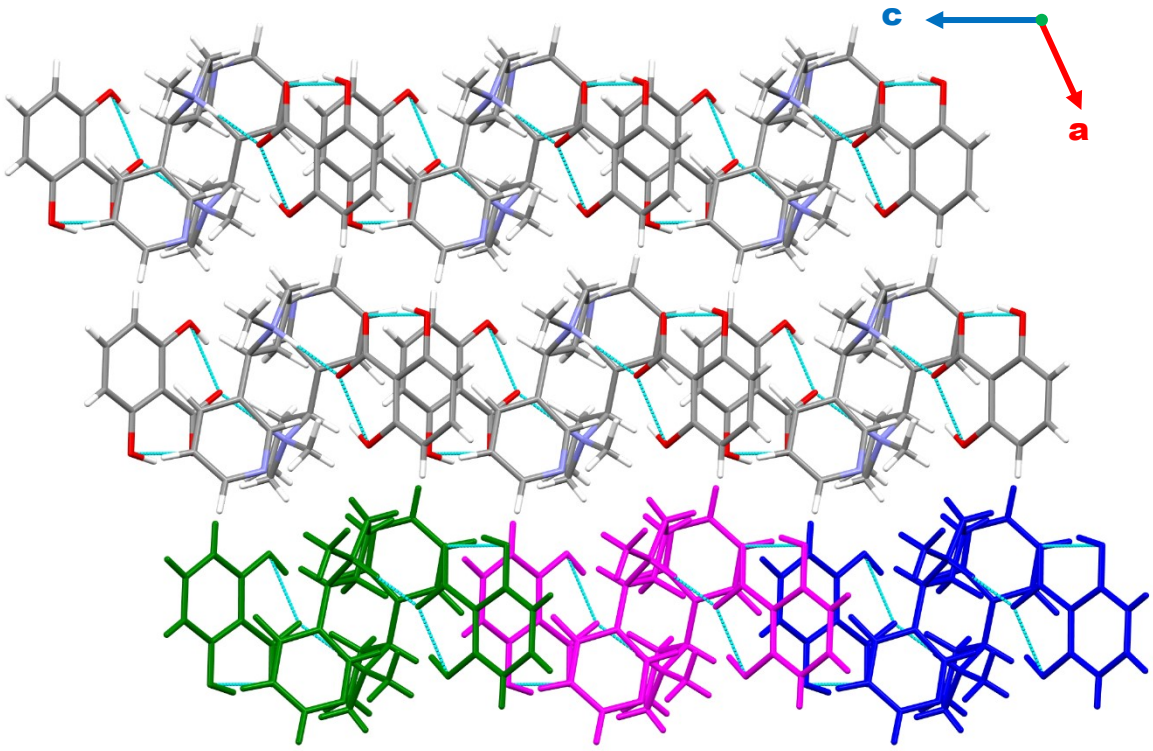


Figure S4: Packing diagram viewed down [010] of **HT salt** depicting intercalated sheets parallel to [001] and stacking of sheets along [100].

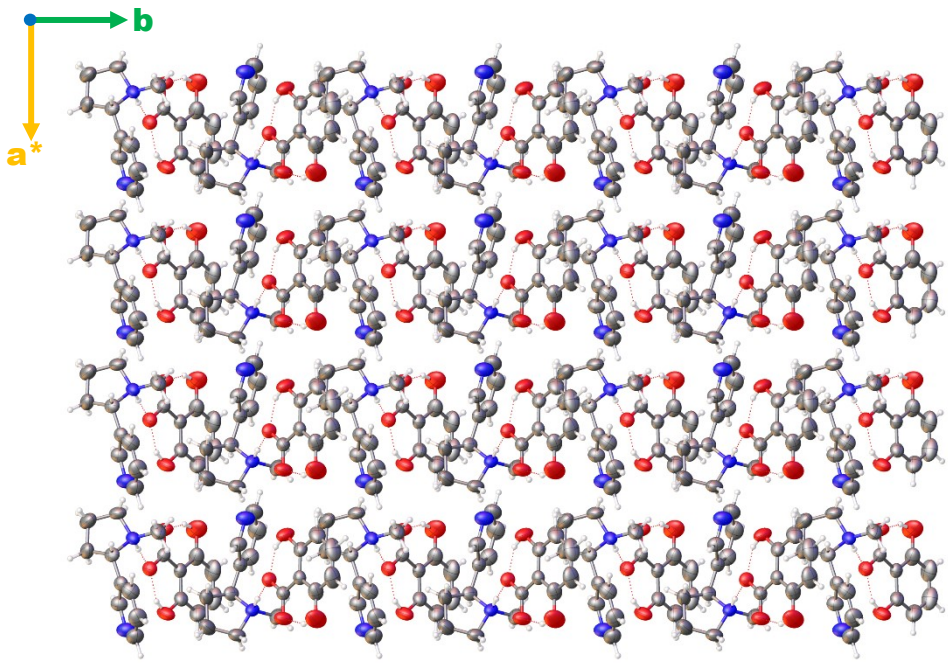


Figure S5: Packing diagram viewed down [001] of **HT salt** with the *b*-axis and *a**-axis normal to the plane. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

Table S1: Crystallographic details of (S)-nicotinium 2,6-dihydroxybenzoate at 293 K (**HT salt**).

Identification code	HT_Salt
Empirical formula	$C_{17}H_{20}N_2O_4$
Formula weight	316.35
Temperature/K	293.00
Crystal system	monoclinic
Space group	$P2_1$
a/Å	7.7196(5)
b/Å	11.7045(7)
c/Å	9.4241(6)
α/°	90
β/°	108.980(2)
γ/°	90
Volume/Å³	805.21(9)
Z	2
ρ_{calc}g/cm³	1.305
μ/mm⁻¹	0.094
F(000)	336.0
Crystal size/mm³	0.22 × 0.15 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.57 to 56.824
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 15, -12 ≤ l ≤ 12
Reflections collected	16130
Independent reflections	4019 [R_{int} = 0.0290, R_{sigma} = 0.0248]
Data/restraints/parameters	4019/1/218
Goodness-of-fit on F²	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1008
Final R indexes [all data]	R_1 = 0.0572, wR_2 = 0.1107
Largest diff. peak/hole / e Å⁻³	0.11/-0.13

(S)-Nicotinium 2,6-Dihydroxybenzoate 90 K (LT salt) Structure & Crystallographic Information

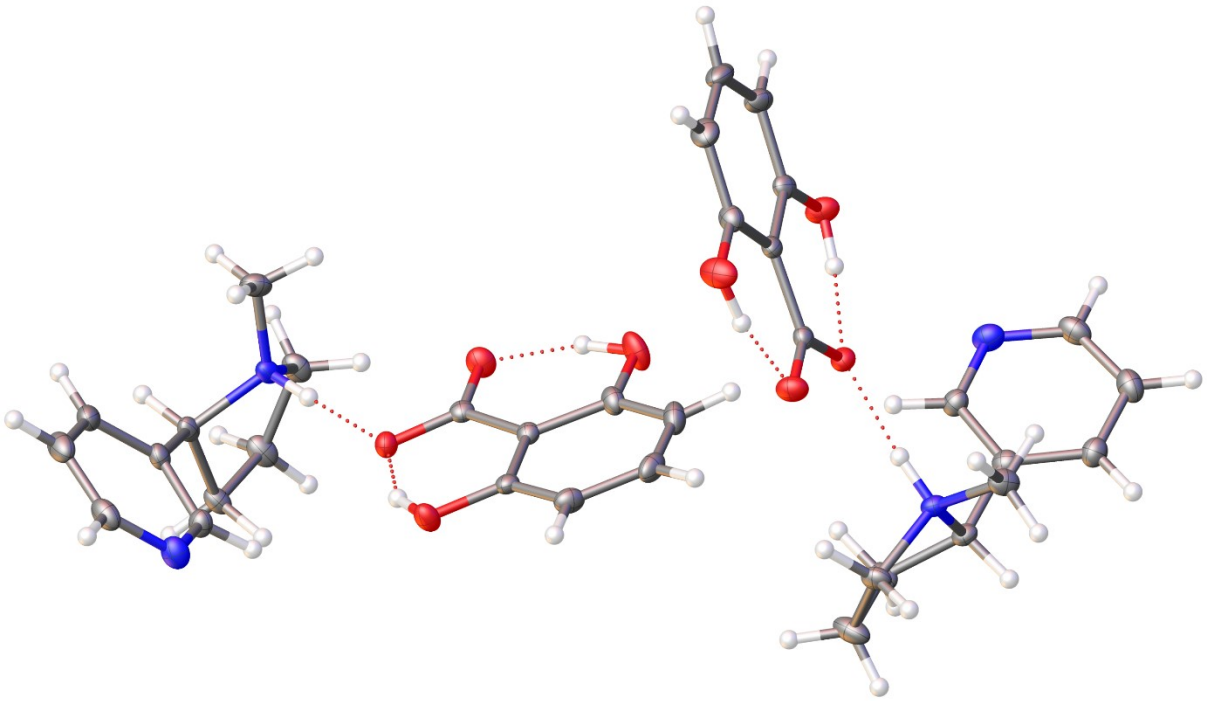


Figure S6: Asymmetric unit of **LT salt**. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

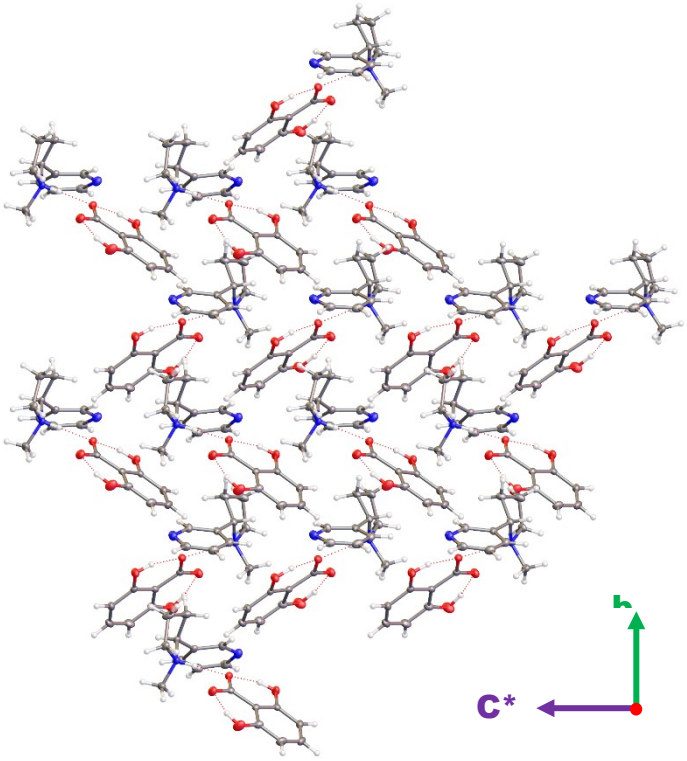


Figure S7: Packing diagram viewed down crystallographic *a*-axis of **LT salt** with *b* and *c** normal to the plane. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

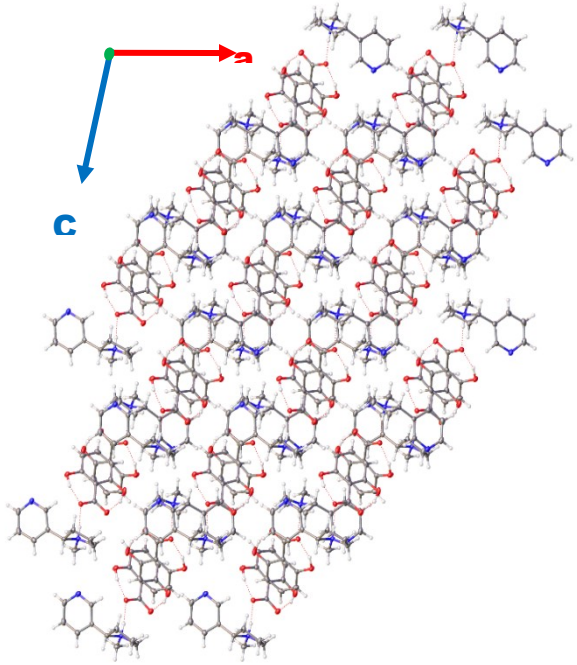


Figure S8: Packing diagram viewed down crystallographic *b*-axis of **LT salt** with *a* and *c* normal to the plane. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

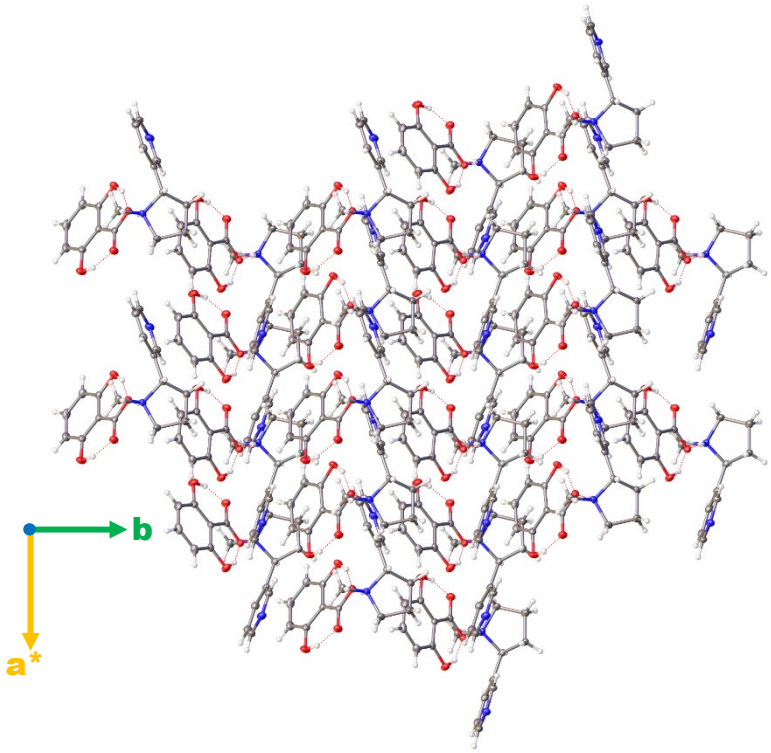


Figure S8: Packing diagram viewed down crystallographic *c*-axis of **LT salt** with the *b*-axis and *a**-axis normal to the plane. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

Table S2: Crystallographic details of (S)-nicotinium 2,6-dihydroxybenzoate at 90 K (**LT salt**).

Identification code	**LT_Salt**
Empirical formula	$C_{17}H_{20}N_2O_4$
Formula weight	316.35
Temperature/K	90
Crystal system	monoclinic
Space group	$P2_1$
a/Å	9.9691(4)
b/Å	11.5520(4)
c/Å	13.8196(5)
α/°	90
β/°	101.9950(10)
γ/°	90
Volume/Å^3	1556.76(10)
Z	4
ρ_{calc}g/cm^3	1.350
μ/mm^{-1}	0.097
F(000)	672.0
Crystal size/mm^3	0.22 × 0.15 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.176 to 56.732
Index ranges	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -18 ≤ l ≤ 18
Reflections collected	28199
Independent reflections	7777 [R_{int} = 0.0299, R_{sigma} = 0.0293]
Data/restraints/parameters	7777/1/435
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0335, wR_2 = 0.0844
Final R indexes [all data]	R_1 = 0.0379, wR_2 = 0.0874
Largest diff. peak/hole / e Å^{-3}	0.24/-0.22

Phase Transition Images & Contact Table

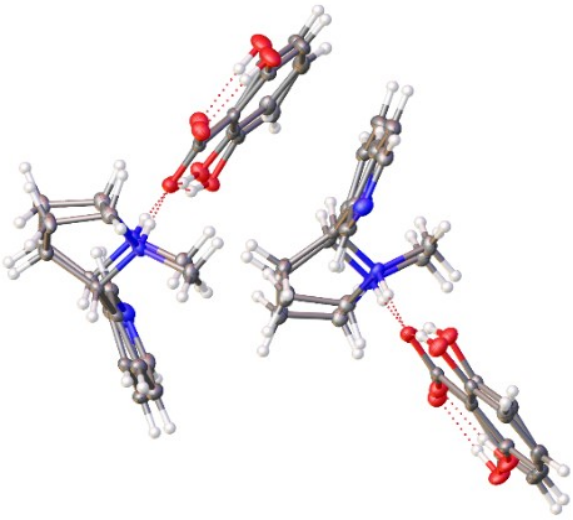


Figure S9: View of **LT salt** perturbation at 90 K. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

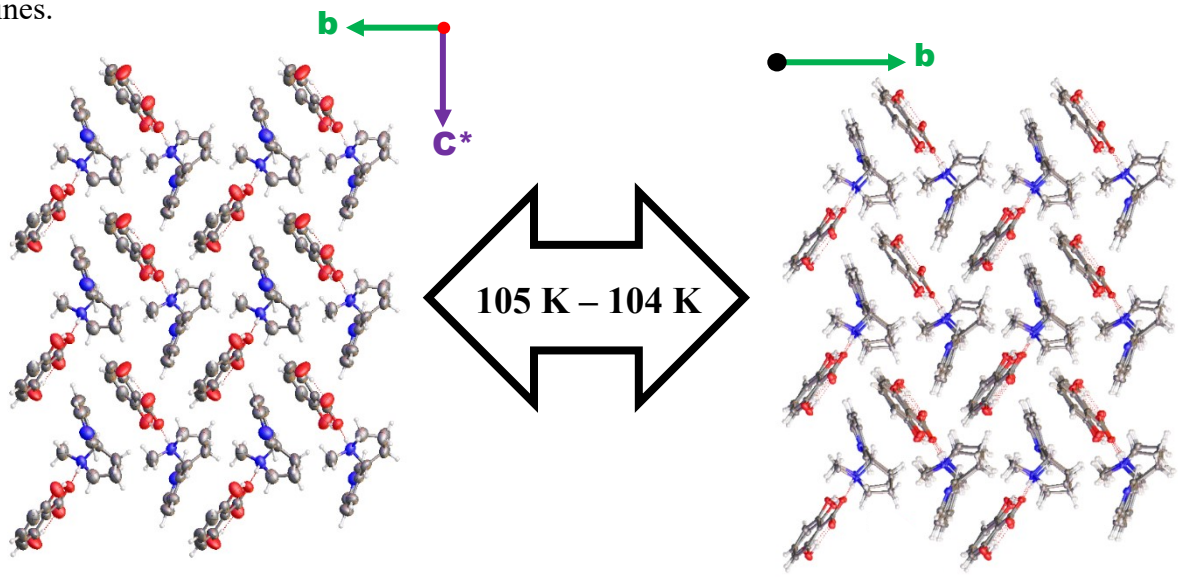


Figure S10: Packing diagram viewed down [100] of **HT salt** and viewed parallel to [101] of **LT salt** after undergoing a temperature induced phase transition at 105 K to 104 K. Atom colors: oxygen (red), nitrogen (blue), carbon (grey), hydrogen (white). Hydrogen bond interactions are highlighted in red dashed lines.

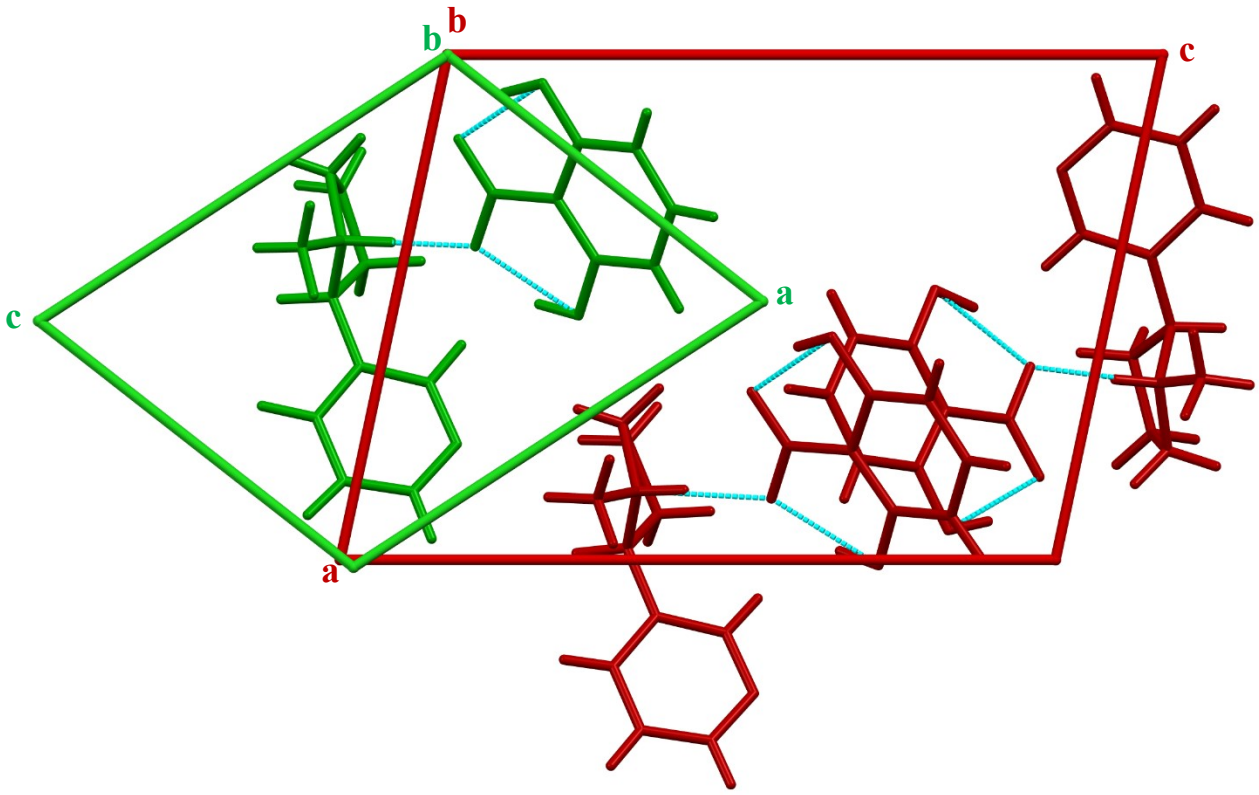


Figure S11: Diagram depicting the alignment of the unit cells of **HT salt** (green) and **LT salt** (red). [010], [101], and $[10\bar{1}]$ in **HT salt** correspond approximately to $[0\bar{1}0]$, [100], and [001] in **LT salt**, respectively**.** Hydrogen bonds highlighted in blue dashed lines.

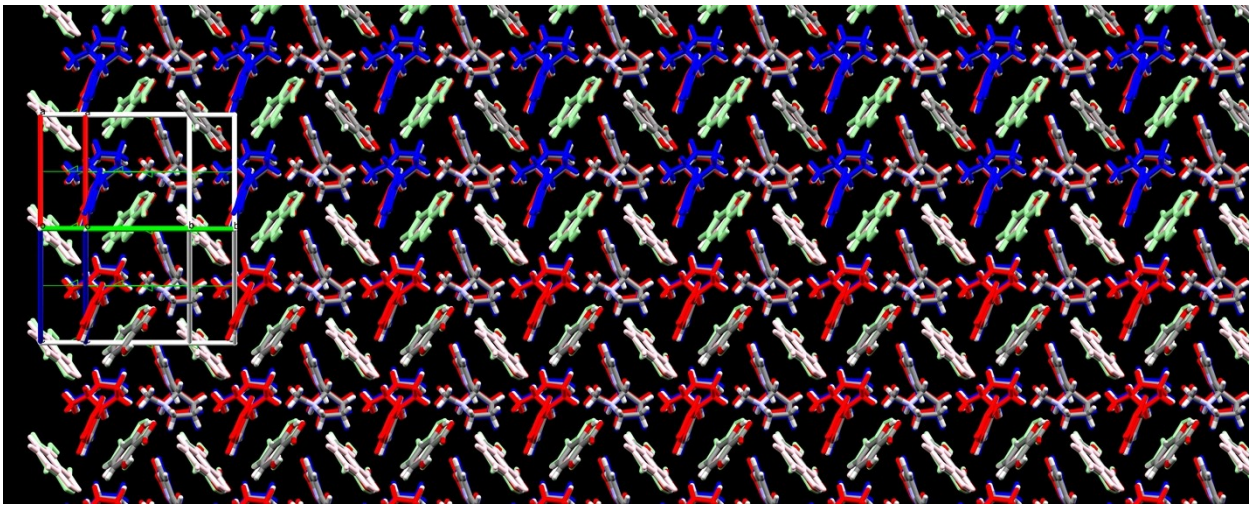


Figure S12: Overlayed view of the $P2_1$ and $B2_1$ structures showing the observable lattice shifts of the molecules in the low temperature phase transition $P2_1$. The vectors are aligned with [100], [010] and [001] being parallel between the structures and the screw axes are aligned along [010] between the structures. With respect to the $P2_1$ structure: nicotine #1 is shown in red; nicotine #2 is shown in blue; 2,6-DHB #1 is shown in pink; 2,6-DHB #2 is shown in green. With respect to the $B2_1$ structure: carbon atoms are shown in grey; hydrogen atoms are shown in white; oxygen atoms are shown in red; and nitrogen atoms are shown in blue. The molecule numbering scheme is found in Table S3.

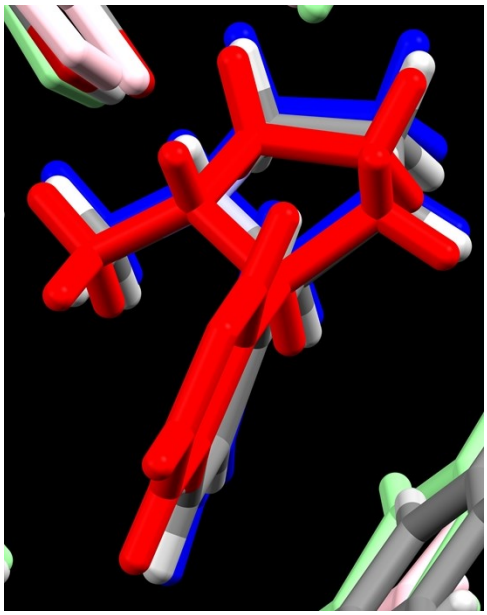


Figure S13: Overlayed view of the $P2_1$ and $B2_1$ nicotine molecules showing the observable lattice shifts of the nicotine moieties in the low temperature phase transition $P2_1$. With respect to the $P2_1$ structure: nicotine #1 is shown in red and nicotine #2 is shown in blue. With respect to the $B2_1$ structure: carbon atoms are shown in grey; hydrogen atoms are shown in white; oxygen atoms are shown in red; and nitrogen atoms are shown in blue. The molecule numbering scheme is found in Table S3.

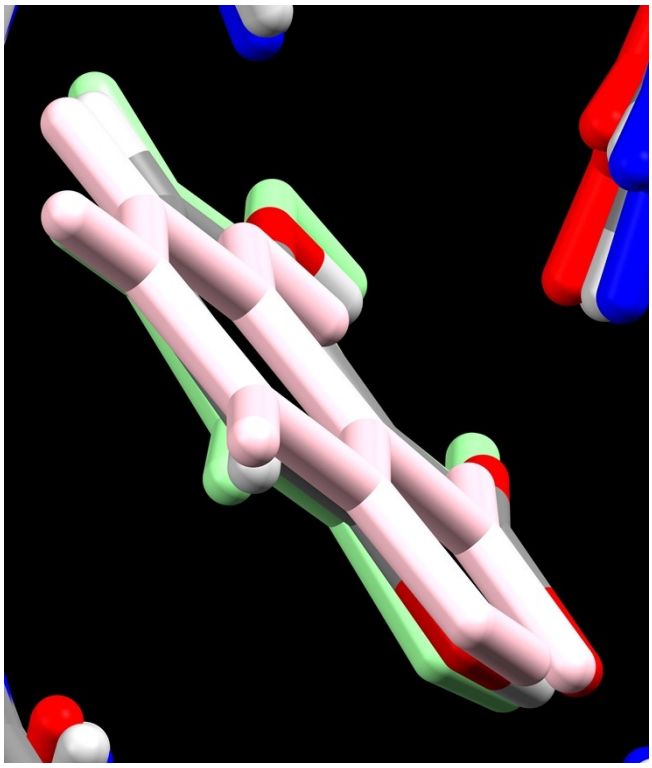


Figure S14: Overlayed view of the $P2_1$ and $B2_1$ nicotine molecules showing the observable lattice shifts of the nicotine moieties in the low temperature phase transition $P2_1$. With respect to the $P2_1$ structure: 2,6-DHB #1 is shown in pink and 2,6-DHB #2 is shown in green. With respect to the $B2_1$ structure: carbon atoms are shown in grey; hydrogen atoms are shown in white; oxygen atoms are shown in red; and nitrogen atoms are shown in blue. The molecule numbering scheme is found in Table S3.

Table S3: Heteroatoms and molecular numbering scheme for the **HT salt** and **LT salt** API nicotinium and salt former 2,6-DHB molecules.

Salt	**HT Salt**		**LT Salt**			
Molecule	Nicotinium	2,6-DHB	Nicotinium #1	Nicotinium #2	2,6-DHB #1	2,6-DHB #2
Heteroatoms	C1-C10 N1-N2	C11-C17 O1-O4	C1-C10 N1-N2	C11-C20 N3-N4	C21-C27 O5-O8	C28-C34 O1-O4

Crystal Images and Morphologies

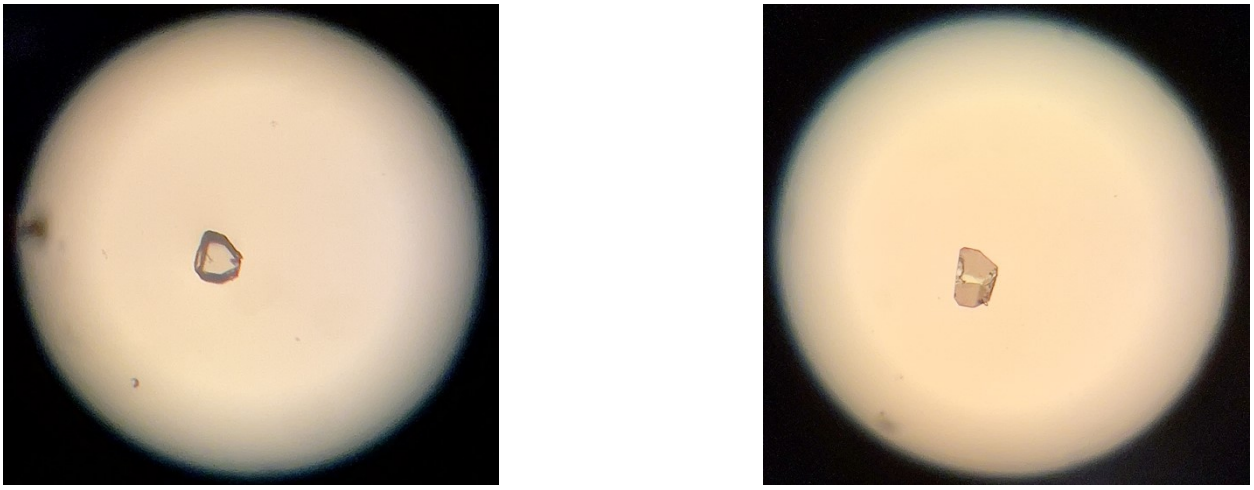


Figure S15: Optical microscopy images of a crystal of (S)-nicotinium 2,6-dihydroxybenzoate.

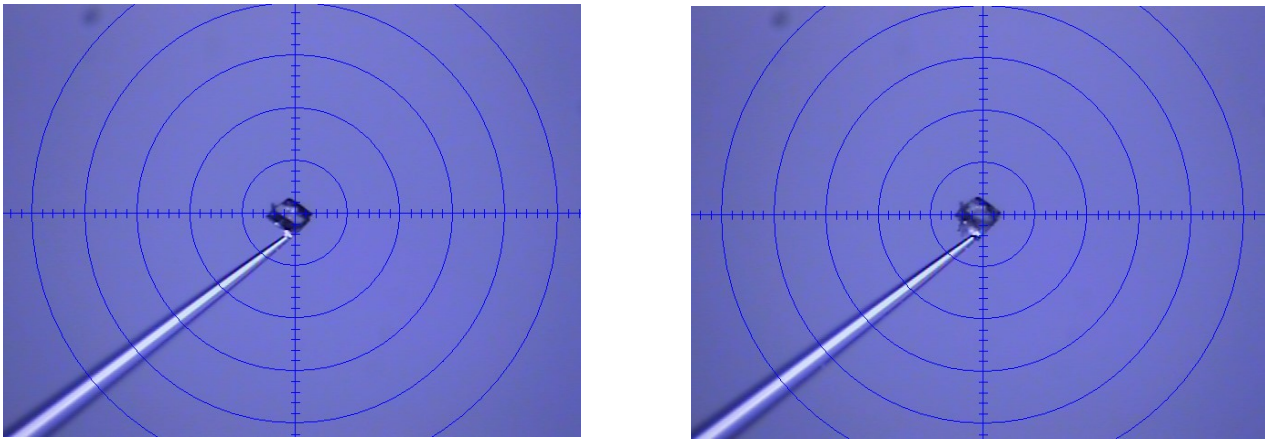


Figure S16: Images of a crystal mounted on the goniometer at 90 K (**LT salt**; left) and at 293 K (**HT salt**; right). No visible cracks or defects can be observed at the low temperature in comparison to the higher temperature.

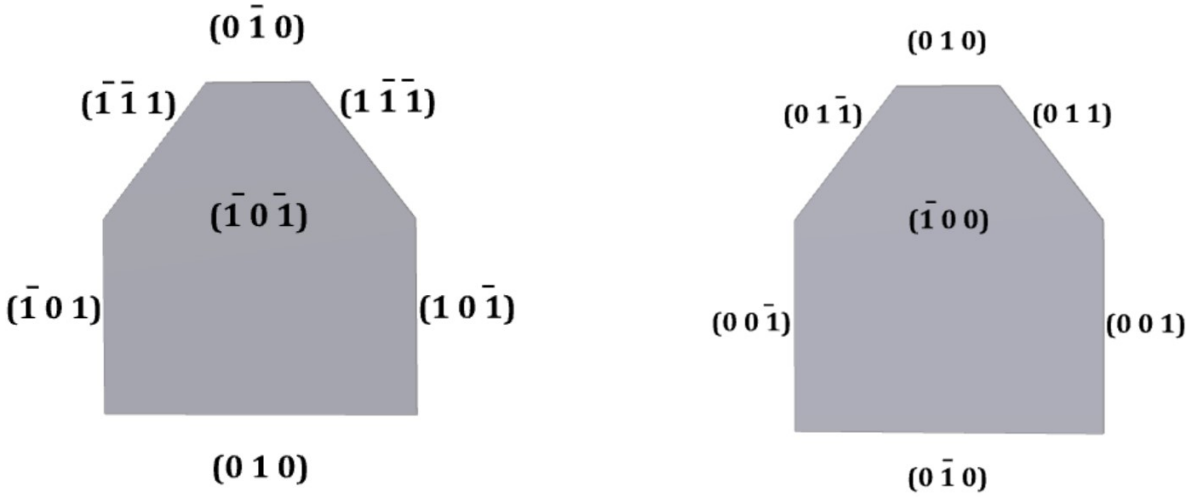


Figure S17: Simulated virtual morphology depictions of the crystallographic orientation of a crystal of (S)-nicotinium 2,6-dihydroxybenzoate at 90 K (**LT salt**; left) and at 293 K (**HT salt**; right) generated using WinXMorph.

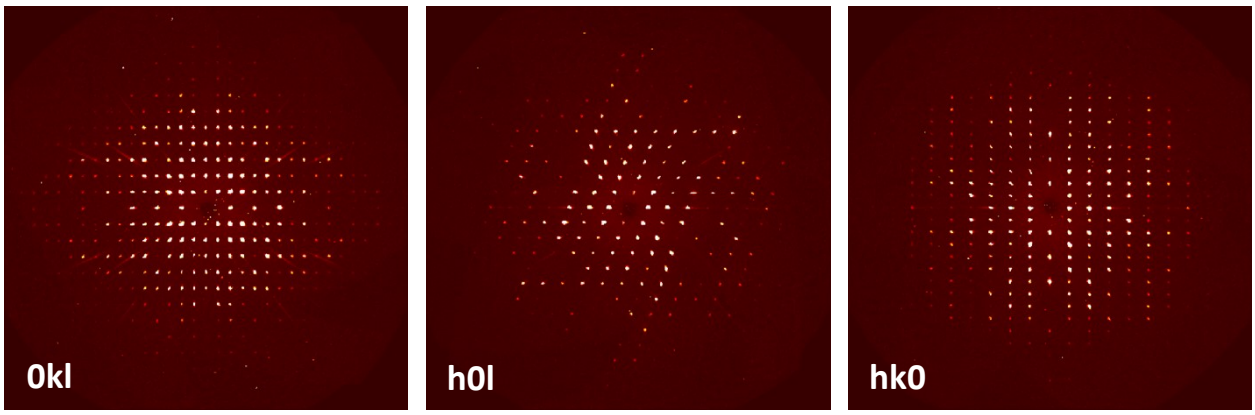
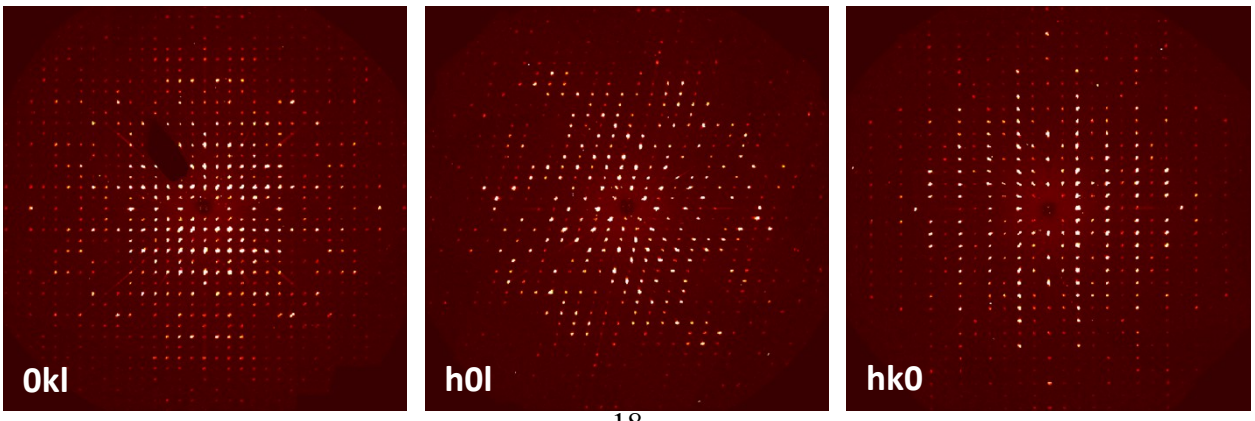


Figure S18: Calculated precision images for **HT salt** with miller planes indicated. Precession images were calculated using a resolution of 0.71 Å, the edge of the image. A layer thickness of 0.10 was utilized.

Calculated Precession Images



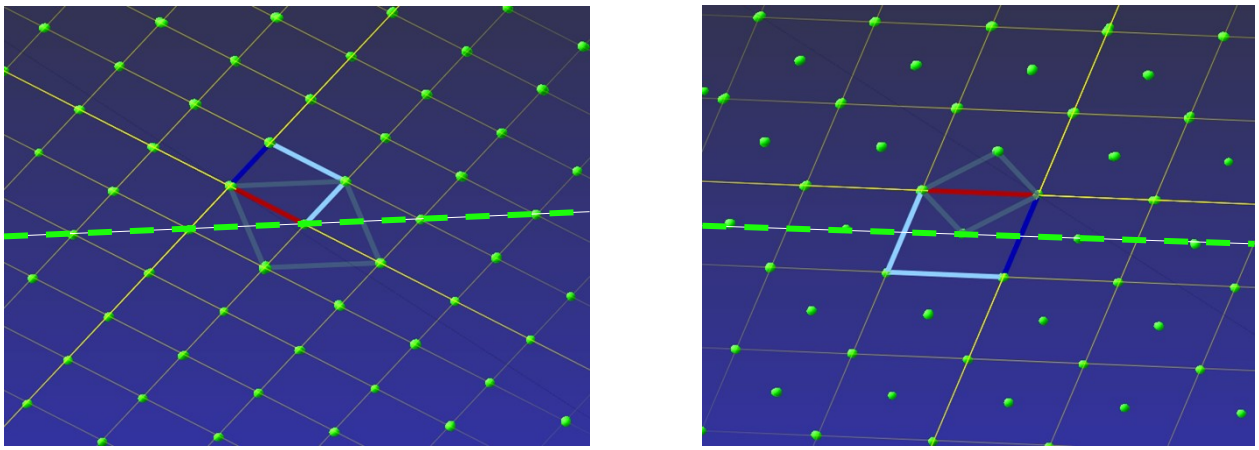


Figure S20: View of reciprocal lattice perpendicular to *ac* plane for data collected at 90 K in which larger $P2_1$ is highlighted (left) and reduced cell is highlighted (right). The dashed green line is (h k 0.5) in the reduced cell setting. *a**-axis (red), *c**-axis (dark blue).

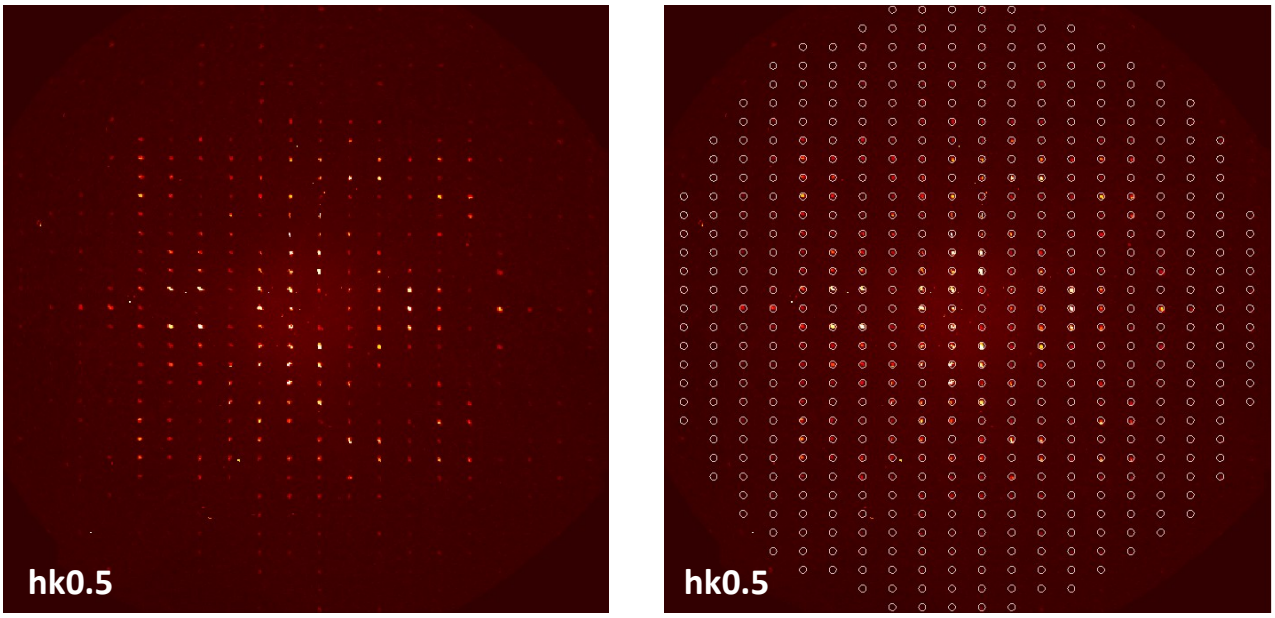
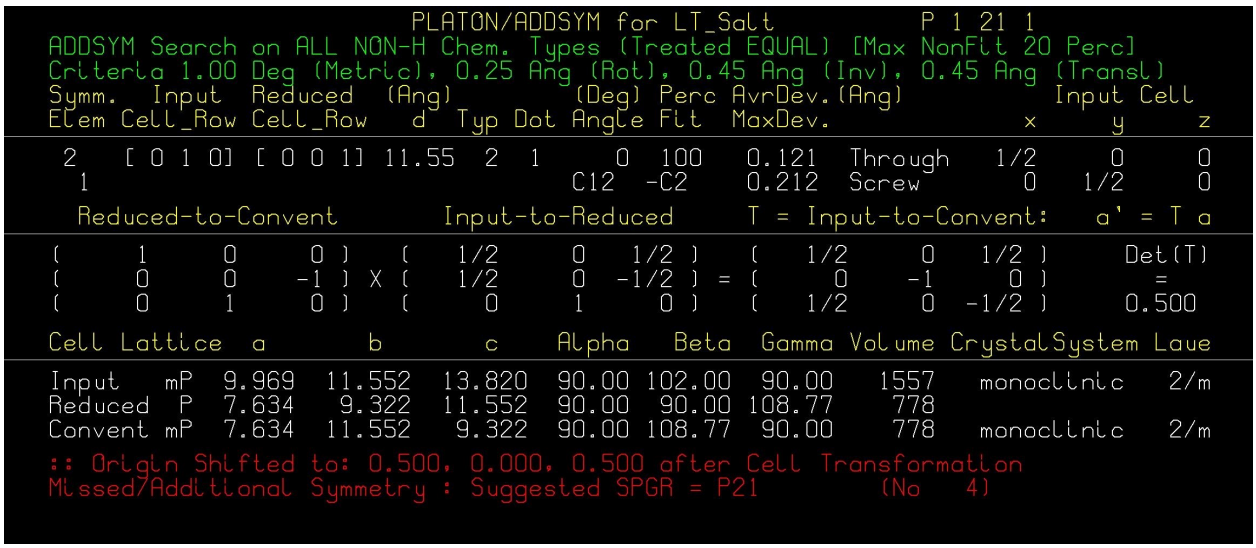


Figure S21: Calculated precession image for (*h k* 0.5) in the reduced cell setting for data collected at 90 K. Spot position overlays for reduced cell (left) and proposed larger primitive monoclinic cell (right). No spot overlays are visible for the reduced cell as this is a non-integer layer. Precession images were calculated using a resolution of 0.71 Å, the edge of the image.

PLATON/ADDSYM Images



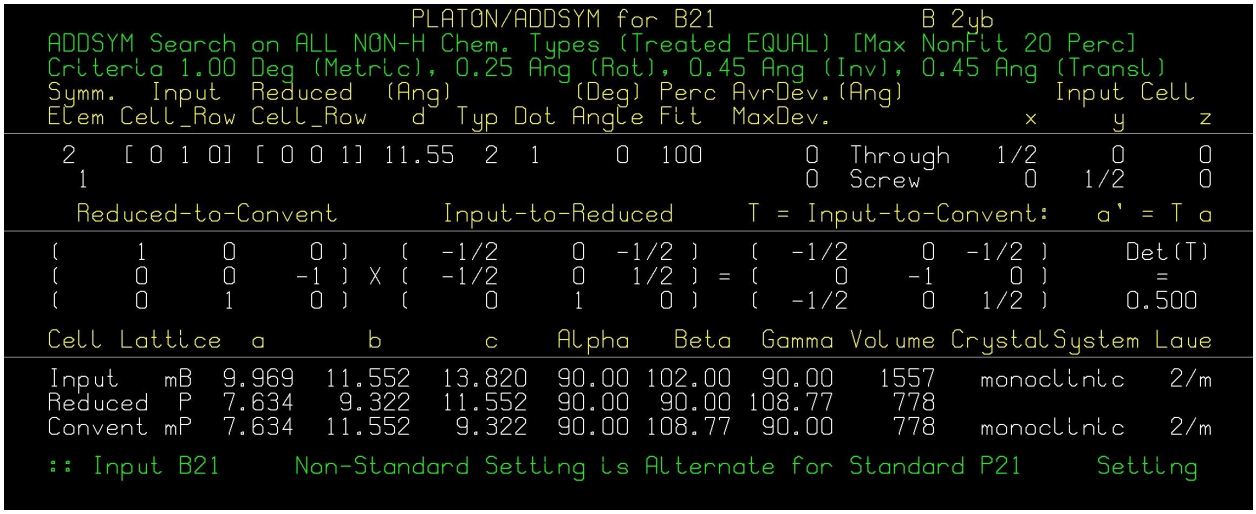


Figure S22: PLATON/ADDSYM readouts for the large cell $P2_1$ cell setting (**LT salt**; upper) and the $B2_1$ cell setting (lower) with both readouts indicating a reduction to a smaller $P2_1$ cell setting.

Table S4: Hydrogen bonding distances and geometries for **HT salt**.

Interacting Atoms (D—H···A)	D—H Distance (Å)	H···A Distance (Å)	D···A Distance (Å)	D—H···A Angle (°)
C7—H7*B*···O1^{i}	0.97	2.66	3.603 (3)	165
C8—H8*A*···O4^{ii}	0.97	2.58	3.192 (4)	121
N1—H1···O1	0.90 (3)	1.80 (3)	2.701 (3)	175 (3)
O3—H3*A*···O1	0.92 (5)	1.68 (5)	2.528 (3)	152 (4)
O4—H4···O2	0.101 (5)	1.60 (5)	2.521 (4)	149 (4)
Symmetry codes: (i) −x+1, y−1/2, −z+1; (ii) −x, y−1/2, −z.				

Hydrogen Bonding Interaction Tables

Table S5: Hydrogen bonding distances and geometries for **LT salt**.

Interacting Atoms (D—H···A)	D—H Distance (Å)	H···A Distance (Å)	D···A Distance (Å)	D—H···A Angle (°)
C11—H11···O2^{i}	0.93	2.60	3.367 (2)	140
C31—H31···O6	0.93	2.60	3.278 (2)	130
C17—H17A···O1	0.97	2.56	3.505 (2)	165
C7—H7A···O6^{ii}	0.97	2.56	3.513 (2)	168
C20—H20A···N2^{iii}	0.96	2.52	3.444 (2)	161
C8—H8A···O7^{iv}	0.97	2.54	3.283 (2)	134
N1—H1···O6^{v}	0.94 (3)	1.76 (3)	2.6981 (19)	175 (2)
N1—H1···O5^{v}	0.94 (3)	2.63 (3)	3.283 (2)	127 (2)
N3—H3···O1^{vi}	0.92 (3)	1.77 (3)	2.6825 (19)	176 (3)
O4—H4···O2	0.93 (3)	1.67 (3)	2.5408 (19)	154 (2)
O8—H8···O6	0.90 (3)	1.69 (3)	2.5454 (17)	157 (3)
O3—H3B···O1	0.95 (3)	1.64 (3)	2.5364 (17)	155 (2)
O7—H7···O5	0.90 (3)	1.68 (3)	2.531 (2)	157 (2)
Symmetry codes: (i) $-x+2, y-1/2, -z$; (ii) $-x+2, y+1/2, -z$; (iii) $x-1, y, z-1$; (iv) $-x+1, y+1/2, -z$; (v) $x, y, z+1$; (vi) $-x+1, y-1/2, -z$.				

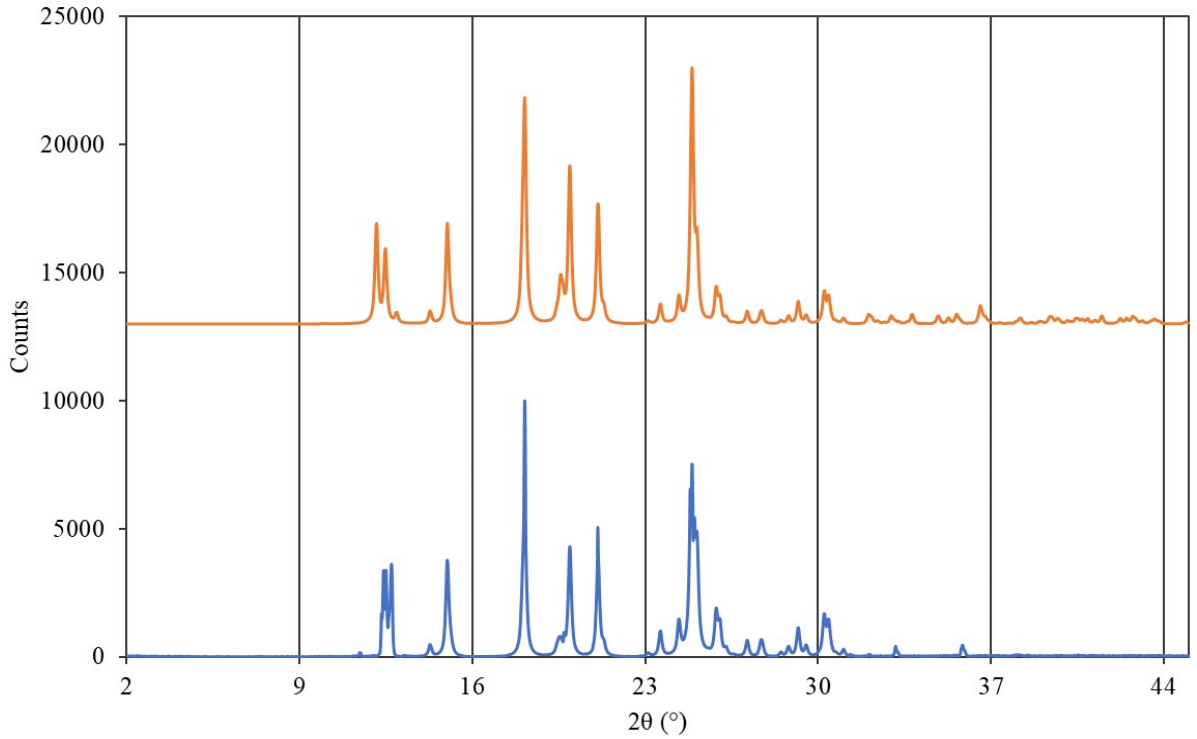


Figure S23: PXRD patterns of (S)-nicotinium 2,6-dihydrxoybenzoate at 293 K (**HT salt**) simulated from SC-XRD analysis (upper) and experimentally obtained (lower). The simulated pattern is offset by +13,000 counts.

Powder X-Ray Diffraction (PXRD) Pattern

LT Salt $P2_1$ vs $B2_1$ Symmetry

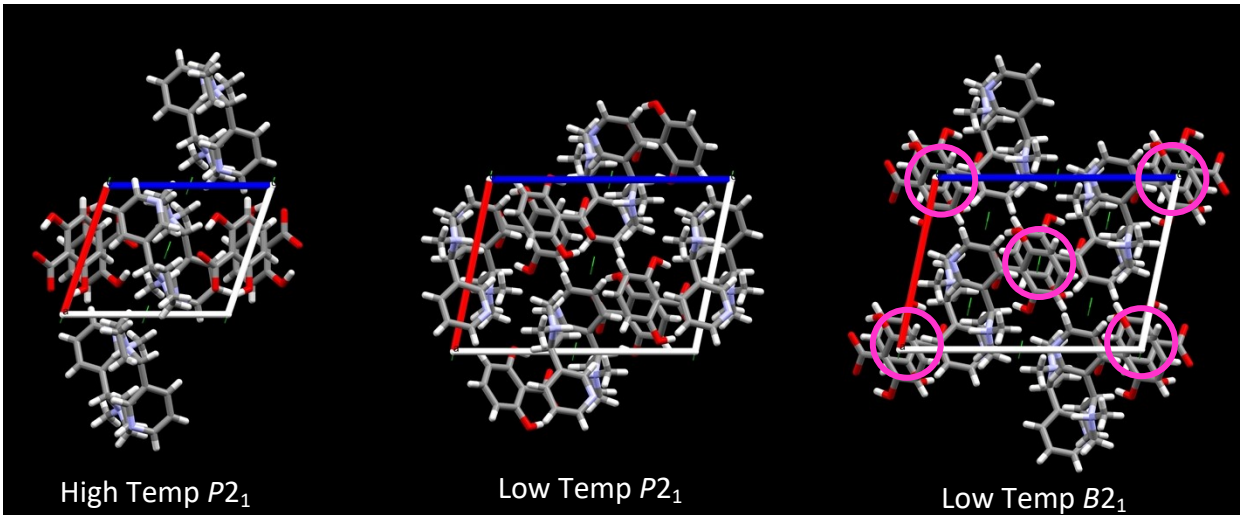


Figure S24: Views parallel to [010] showing the screw axes present in each structure. The screw axes that were analyzed to aid in confirmation of the $P2_1$ refinement are circled in pink in the $B2_1$ structure.

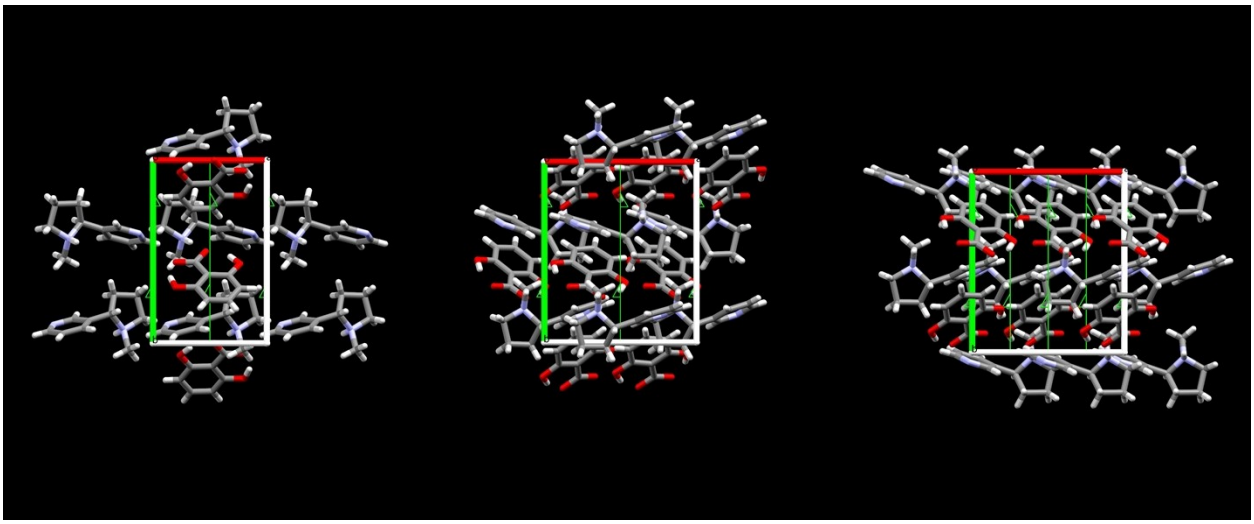


Figure S25: Views parallel to [001] further detailing the screw axes present in each structure.

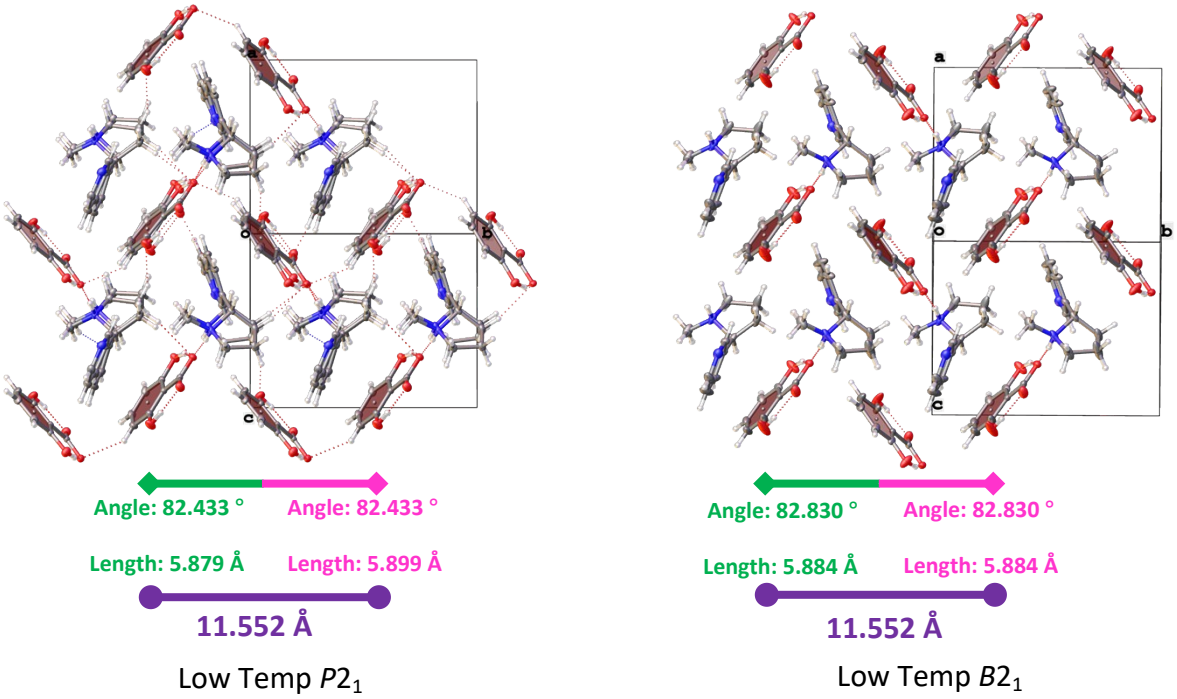


Figure S26: Calculated mean plane distances for the 2,6-DHB rings at 90 K showing the different distances between the planes for the $P2_1$ (left) versus what the distances would need to be for the system to be treated as $B2_1$ (right).

Table S6: Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the $B2_1$ structure. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

$B2_1$ Fractional Atomic Coordinates

Atom	*x*	*y*	*z*	U_{eq}
O	8696.0(14)	9565.5(12)	1613.6(10)	17.9(3)
O1	10841.4(16)	8960.1(15)	2138.4(13)	31.1(4)
O2	7270.0(18)	8849.1(17)	-14.2(11)	33.6(4)
C2	9608(2)	8261.6(18)	593.0(16)	19.1(4)
C3	9740.4(19)	8968.1(18)	1504.5(15)	18.8(4)
N1	6068.1(18)	5298.5(16)	1514.7(13)	24.2(4)
C5	8577(2)	5791.8(18)	2077.1(15)	19.5(4)
N	10185.6(19)	5543.8(17)	3625.7(14)	25.3(4)
C8	8955(2)	5857.8(18)	3101.0(14)	18.6(4)
O3	11916.2(18)	7578(2)	1093(2)	63.3(8)
C9	8372(2)	8212.3(18)	-115.9(14)	20.9(4)
C10	9347(3)	6838(2)	-1067.6(19)	33.3(6)
C11	10719(2)	7576(2)	434(2)	34.2(6)
C12	7189(2)	6189.9(19)	1519.5(15)	23.2(4)
C13	8240(3)	7499(2)	-944.9(16)	28.1(5)
C	6562(2)	7244(2)	1924(2)	32.3(6)
C14	10581(3)	6875(2)	-396(3)	41.8(7)
C15	9547(2)	5379(2)	1573.3(17)	33.0(6)
C16	11096(2)	5157(2)	3115(2)	34.9(6)
C1	6196(3)	4227(2)	952.2(16)	31.8(5)
C17	10826(2)	5055(3)	2102(2)	44.0(7)
C18	4734(2)	5940(2)	1144(2)	36.3(6)
C6	5071(3)	7227(2)	1353(3)	61.0(11)

Hirshfeld Surface Interaction Analysis

Table S7: Interaction types and percentages for each API in the **HT salt** and **LT salt** structures.

Interaction Type	LT Salt 2,6 DHB #2	LT Salt 2,6 DHB #1	HT Salt 2,6-DHB	LT Salt API #2	LT Salt API #1	HT Salt API
O-H/H-O	39.3	37.9	38.0	18.2	17.6	17.6
H-H	34.4	36.0	37.0	49.5	50.7	50.8
H-C/C-H	22.1	21.7	21.1	19.1	18.7	18.3
H-N/N-H	1.5	1.2	1.2	10.8	10.8	11.0
O-C/C-O	0.6	1.3	0.8	1.1	0.7	0.9
C-C	2.1	1.9	1.9	1.3	1.5	1.4

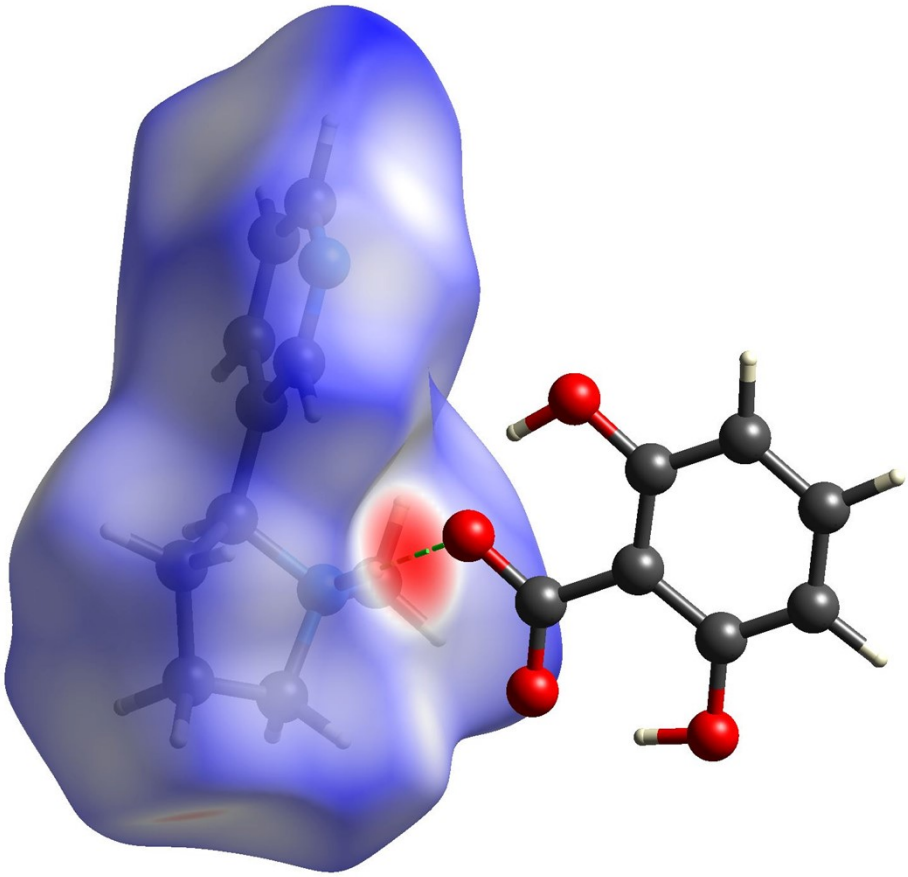


Figure S27: Image of the API Hirshfeld surface in the **HT salt**.

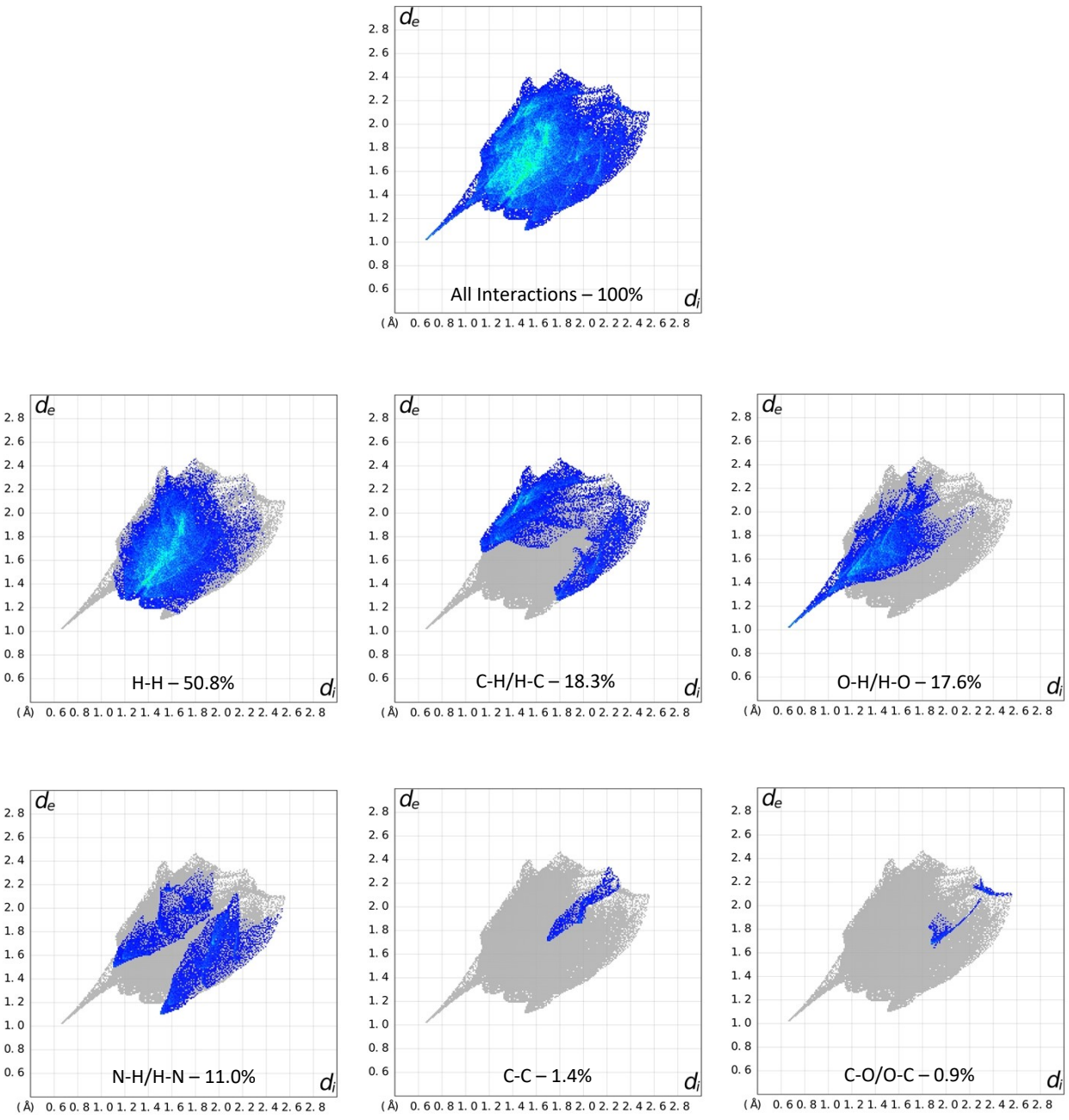


Figure S28: Hirshfeld surface fingerprint plots of the **HT salt**. The type of interaction and quantity is shown for each plot.

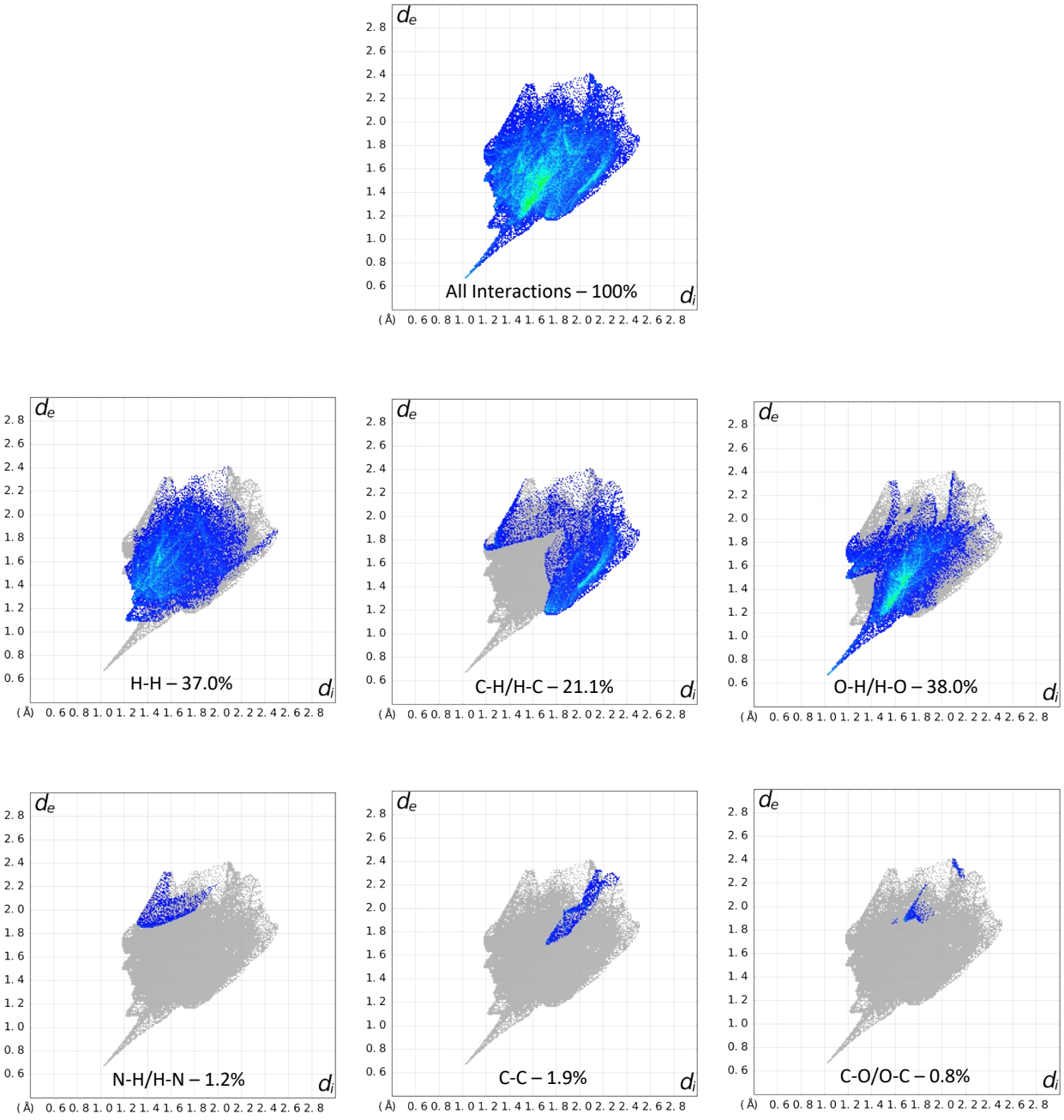


Figure S29: Hirshfeld surface fingerprint plots of the salt former 2,6-DHB in the **HT salt**. The type of interaction and quantity is shown for each plot.

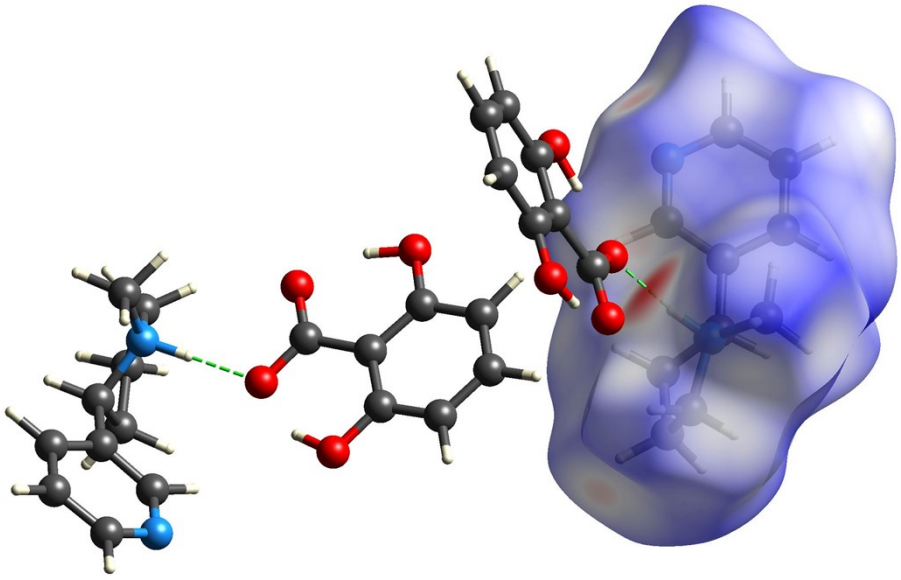


Figure S30: Image of the Hirshfeld surface of API #1 in the **LT salt**.

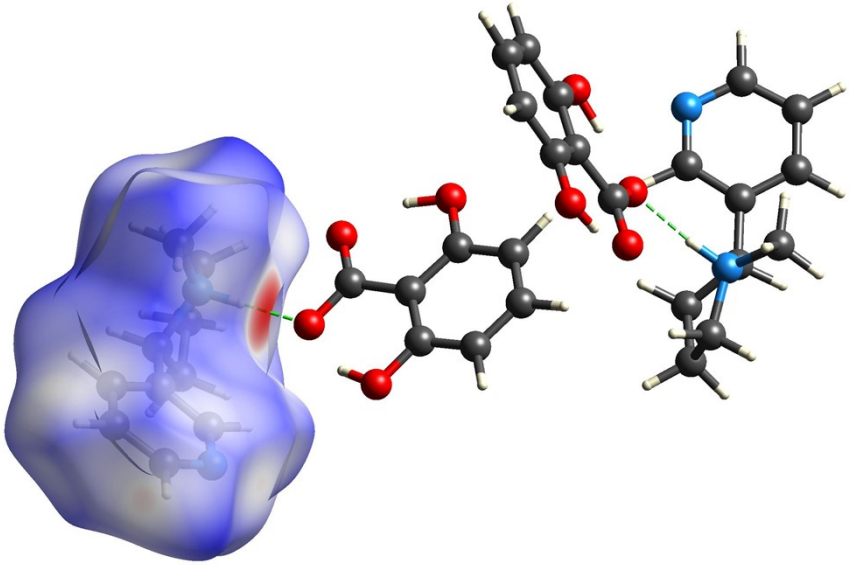


Figure S31: Image of the Hirshfeld surface of API #2 in the **LT salt**.

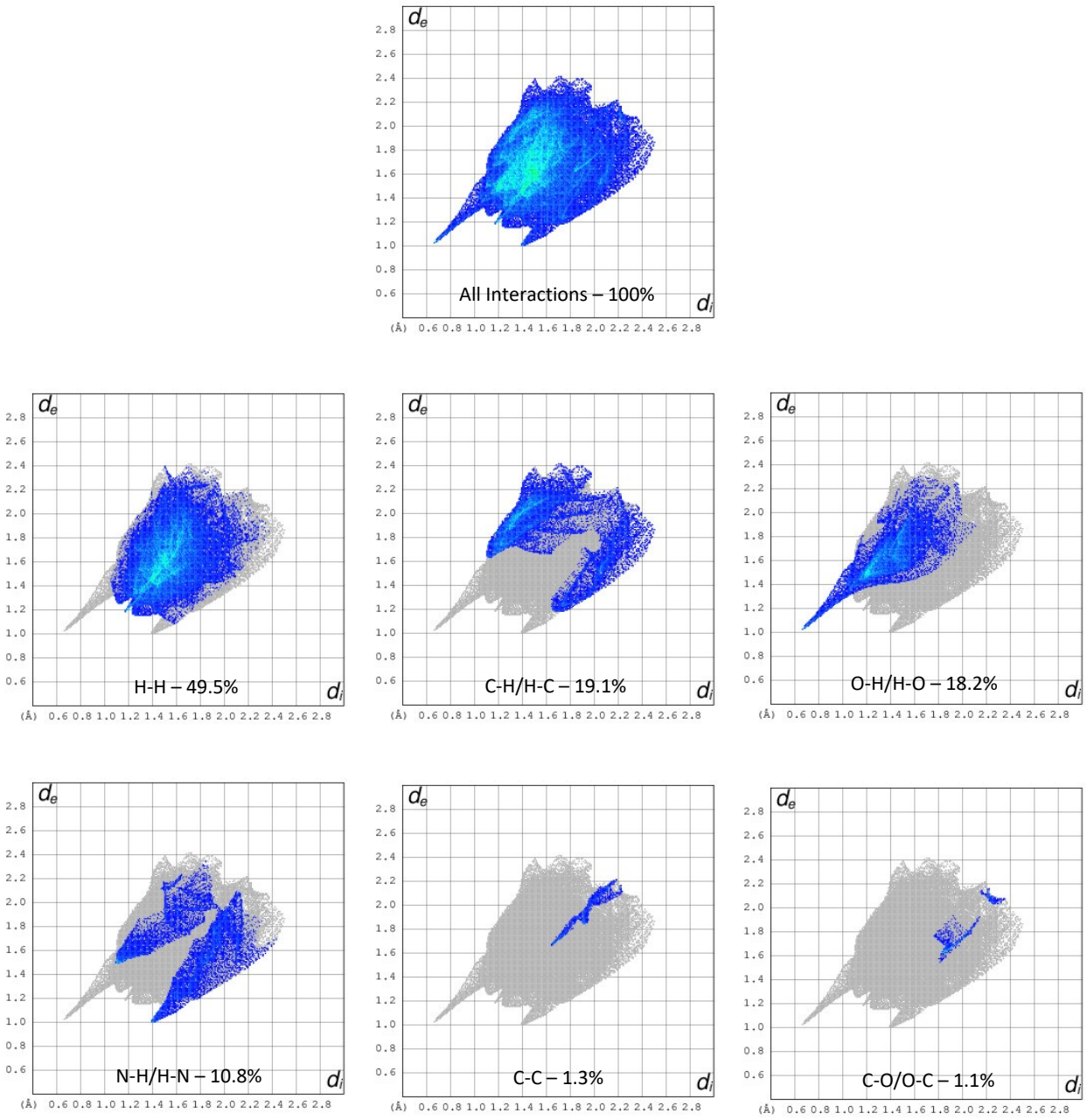


Figure S32: Hirshfeld surface fingerprint plots of API #1 in the **LT salt**. The type of interaction and quantity is shown for each plot.

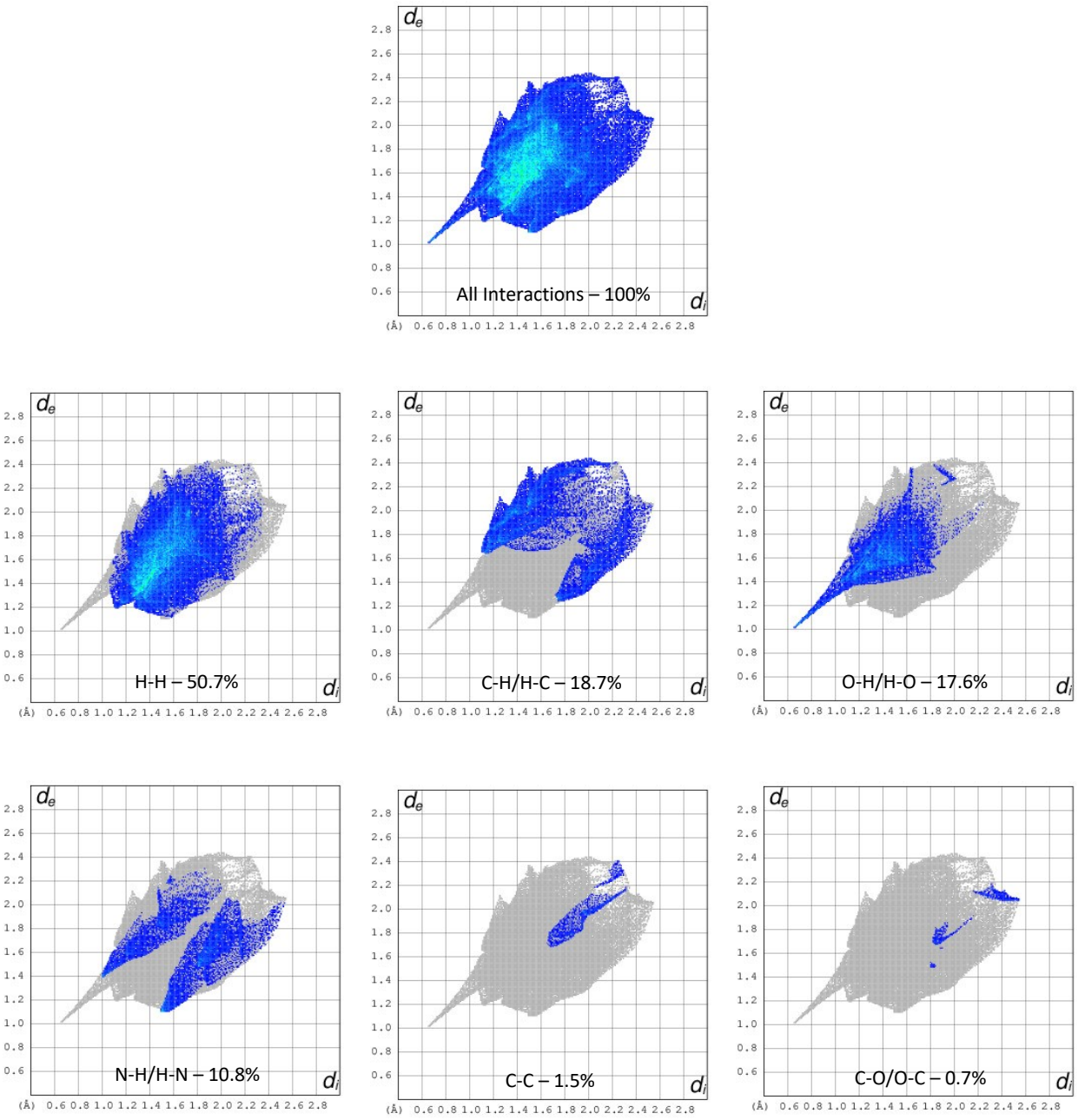


Figure S33: Hirshfeld surface fingerprint plots of API #2 in the **LT salt**. The type of interaction and quantity is shown for each plot.

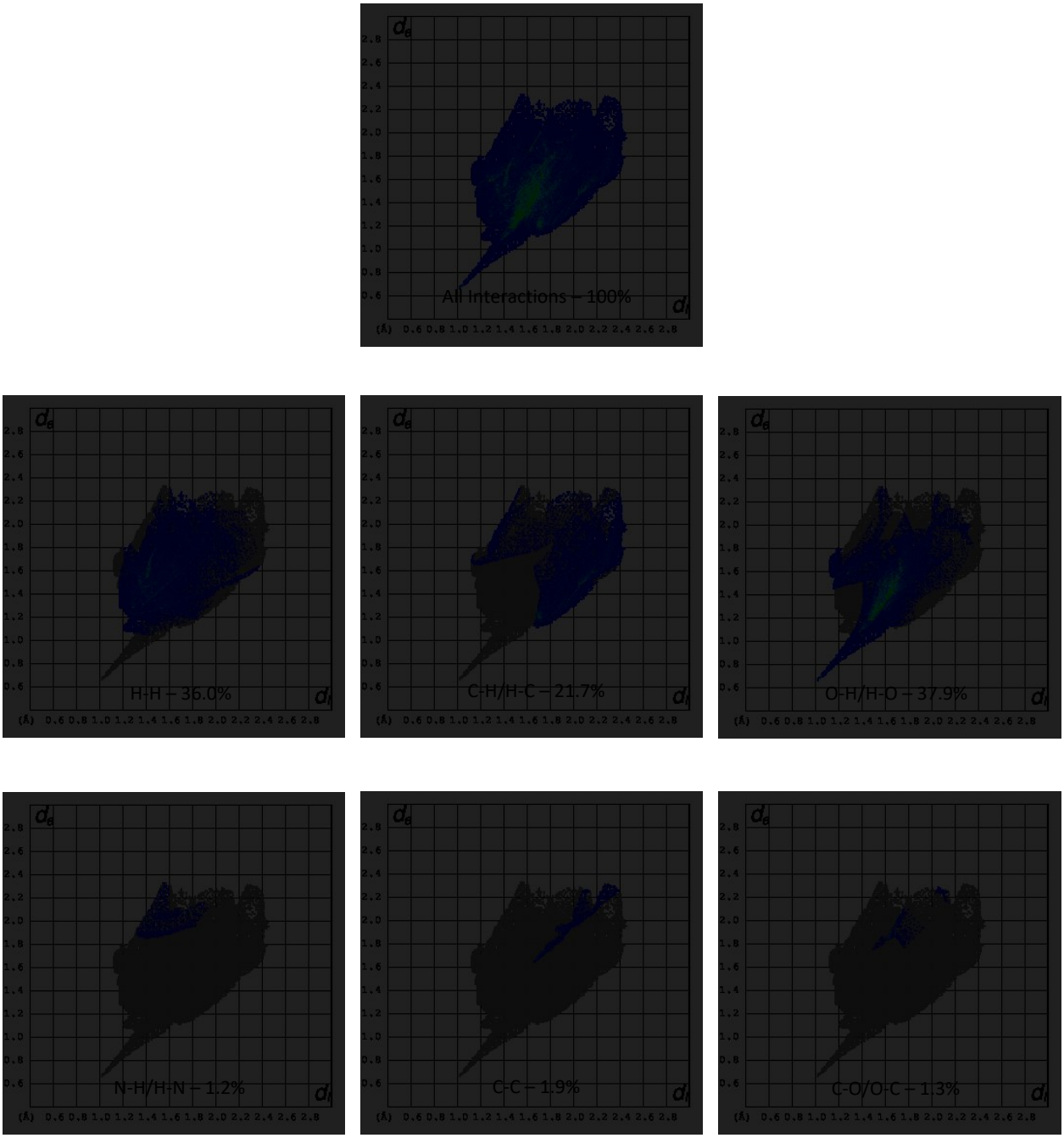


Figure S34: Hirshfeld surface fingerprint plots of the salt former 2,6-DHB #1 in the **LT salt**. The type of interaction and quantity is shown for each plot.

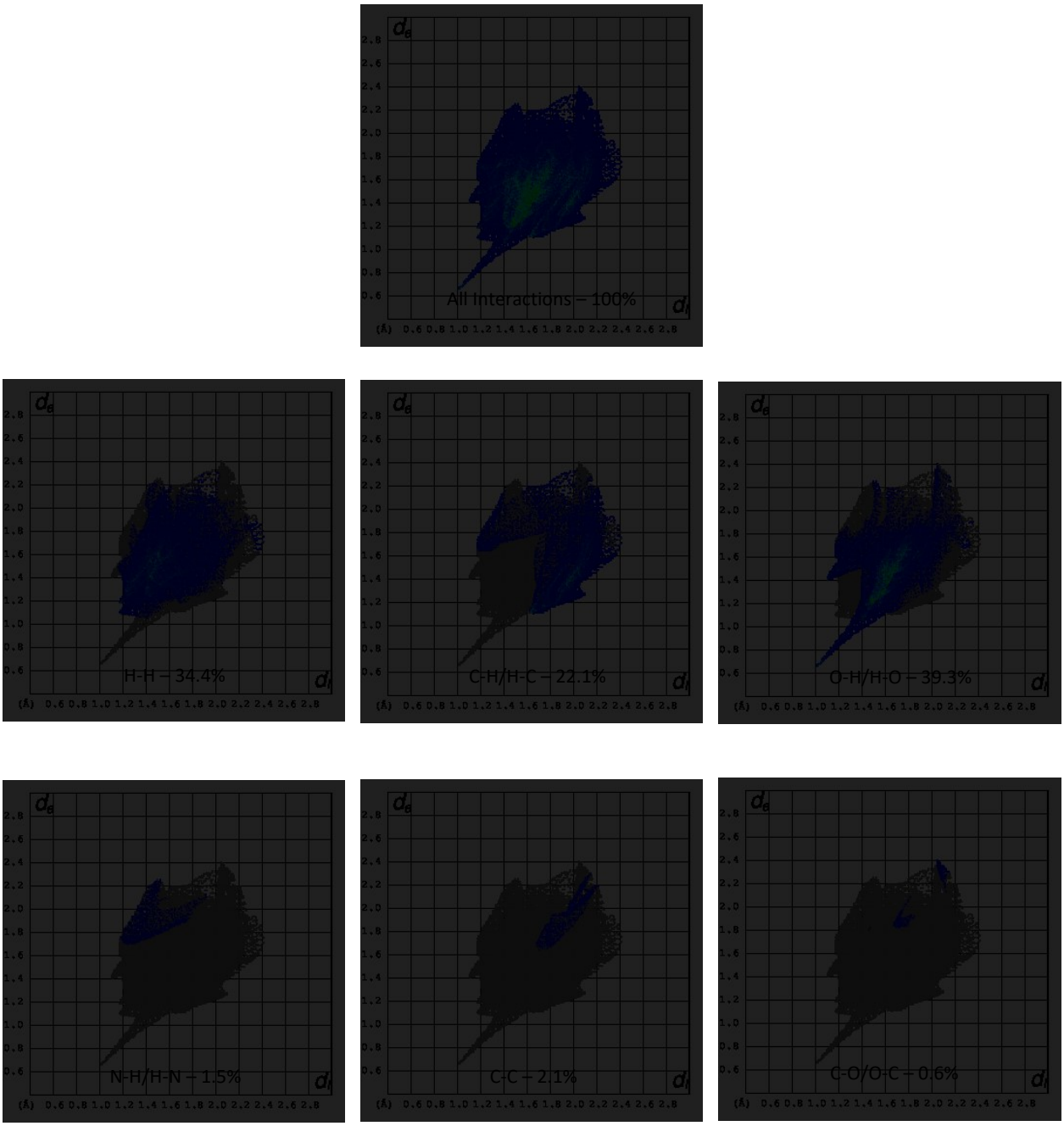


Figure S35: Hirshfeld surface fingerprint plots of the salt former 2,6-DHB #2 in the **LT salt**. The type of interaction and quantity is shown for each plot.

Infrared (IR) Spectroscopy

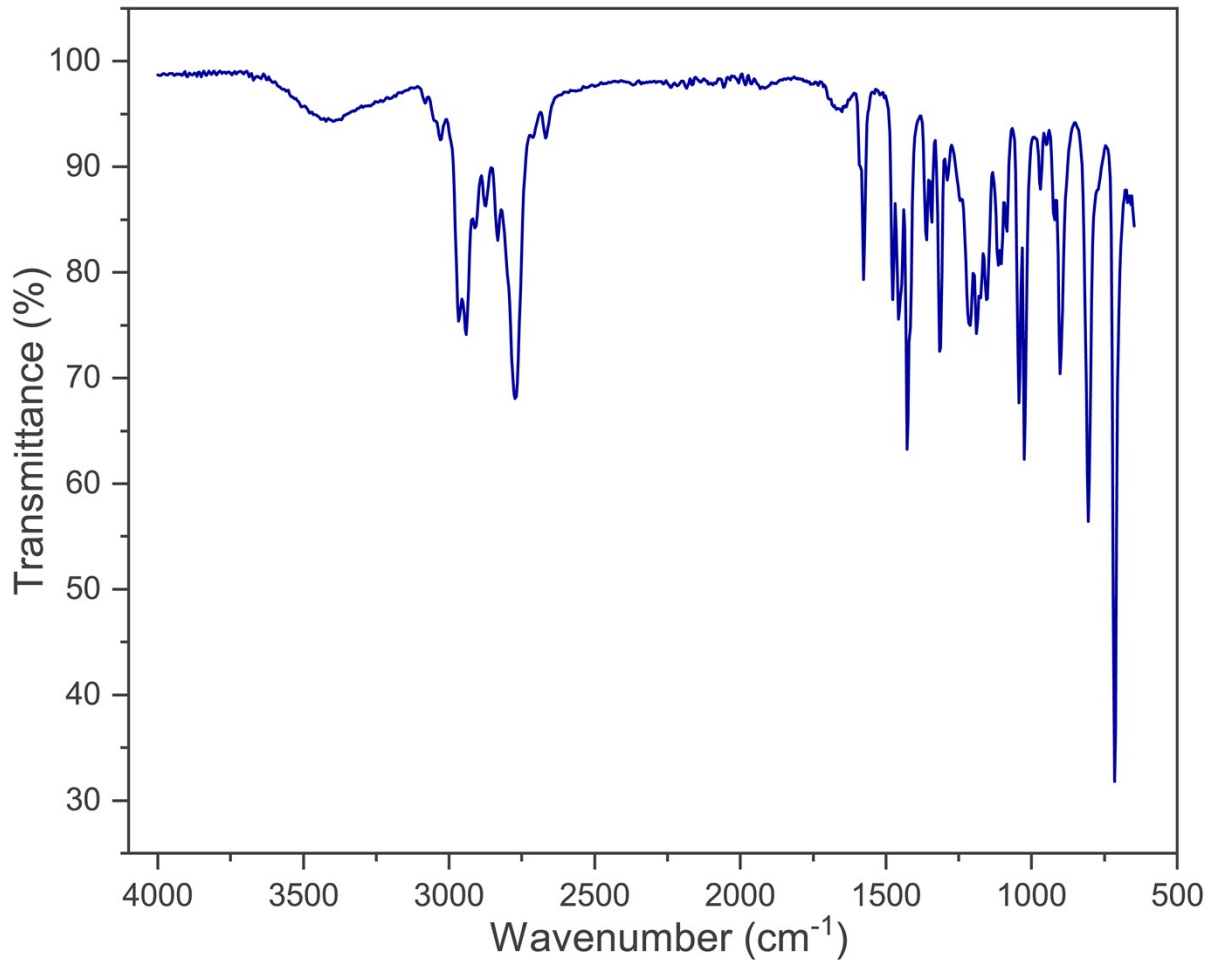


Figure S36: Infrared (IR) spectrum of (S)-nicotine.

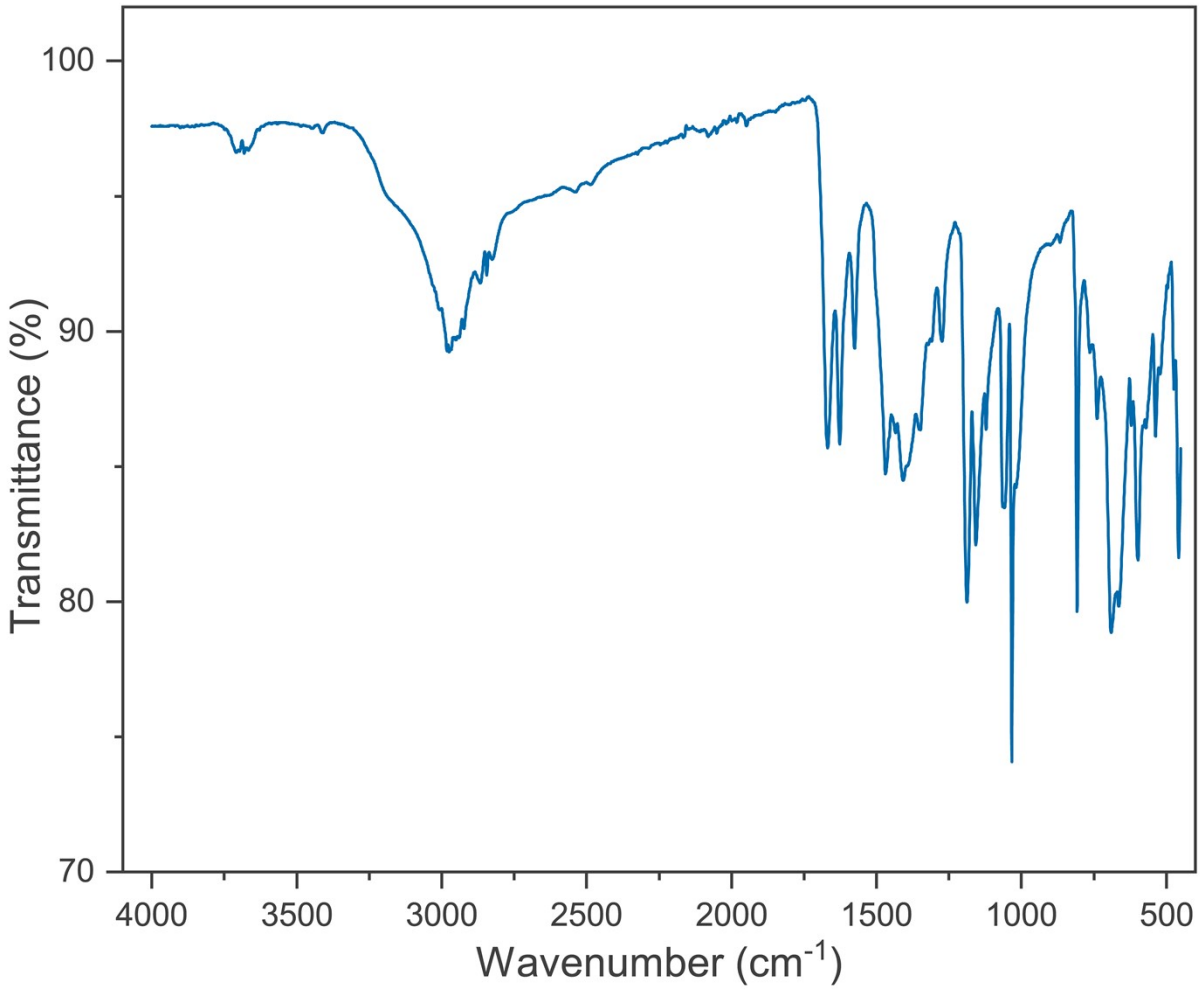


Figure S37: Infrared (IR) spectrum of 2,6-dihyrdoxybenzoic acid.

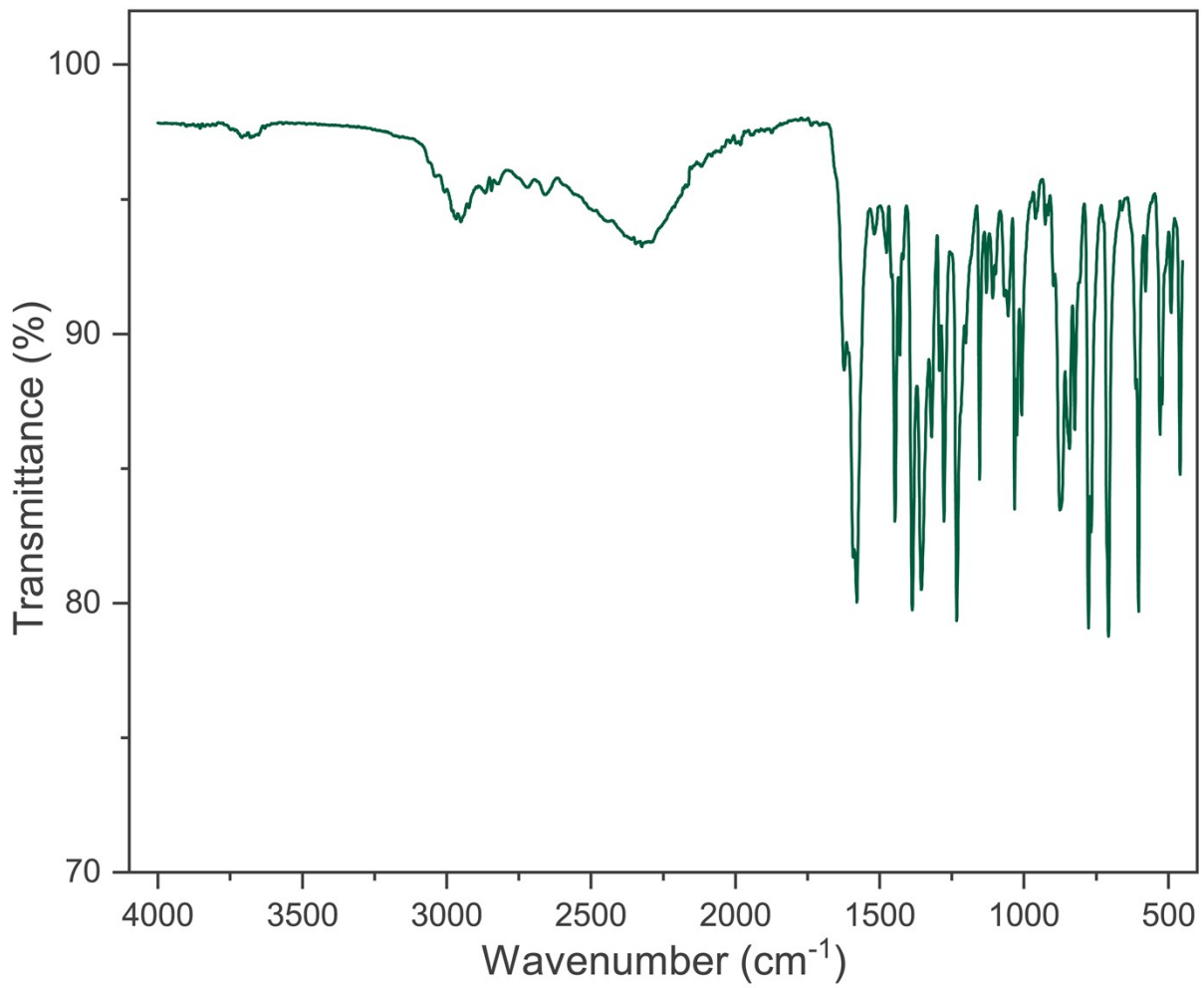


Figure S38: Infrared (IR) spectrum of (S)-nicotinium 2,6-dihyrdoxybenzoate (**HT salt**) at ambient conditions (293 K).

Table S8: Dynamic *in situ* X-ray diffraction data utilizing an in-house automated batch indexing program.

Dynamic In Situ X-Ray Diffraction Batch Indexing Data

Batch Number	a (Å)	Error a (Å)	b (Å)	Error b (Å)	c (Å)	Error c (Å)	α (°)	Error α (°)	β (°)	Error β (°)	γ (°)	Error γ (°)	Volume (Å³)	Error Volume (Å³)	Reflections Indexed	Total Number of Reflections
1	7.689	0.0118	11.6214	0.0072	9.3366	0.0061	90	0	108.6351	0.0548	90	0	790.549	2.117	126	145
2	7.6443	0.021	11.6243	0.0107	9.3392	0.0081	90	0	108.7384	0.0698	90	0	785.883	3.523	128	140
3	7.6361	0.0158	11.6087	0.0059	9.3308	0.005	90	0	108.682	0.037	90	0	783.552	2.151	125	134
4	7.6566	0.0105	11.6133	0.0059	9.3323	0.0053	90	0	108.6541	0.0308	90	0	786.219	1.818	125	144
5	7.6438	0.0078	11.6099	0.0046	9.3308	0.0042	90	0	108.5843	0.0264	90	0	784.879	1.247	132	156
6	7.6329	0.0058	11.5974	0.0036	9.314	0.0038	90	0	108.6338	0.0203	90	0	781.263	0.991	142	183
7	7.6285	0.0047	11.5945	0.0044	9.3112	0.0044	90	0	108.6318	0.02	90	0	780.398	0.986	131	168
8	7.6338	0.0034	11.5929	0.0038	9.3212	0.0031	90	0	108.6826	0.0175	90	0	781.443	0.723	136	177
9	7.6451	0.0041	11.5986	0.0046	9.3229	0.005	90	0	108.7049	0.0188	90	0	783.021	0.985	137	180
10	7.6456	0.0045	11.6119	0.0071	9.3187	0.0066	90	0	108.7232	0.0258	90	0	783.537	1.227	122	145
11	7.6638	0.0061	11.628	0.0121	9.3611	0.0092	90	0	108.7387	0.0268	90	0	789.988	1.852	118	128
12	7.6502	0.0053	11.5981	0.0114	9.3347	0.0075	90	0	108.6654	0.0219	90	0	784.69	1.631	118	128
13	7.6512	0.0074	11.6229	0.0108	9.3141	0.0097	90	0	108.7184	0.0324	90	0	784.473	2.085	115	126
14	7.6348	0.0068	11.5792	0.0105	9.319	0.009	90	0	108.6536	0.0331	90	0	780.57	2.019	114	124
15	7.6392	0.0055	11.5898	0.0093	9.3225	0.0076	90	0	108.5856	0.0401	90	0	782.335	1.621	117	131
16	7.6359	0.0094	11.6023	0.0154	9.3183	0.0111	90	0	108.7413	0.0734	90	0	781.776	2.639	106	113
17	7.665	0.0089	11.6175	0.0111	9.3284	0.0097	90	0	108.7297	0.0766	90	0	786.683	2.328	105	117
18	7.6579	0.0111	11.6055	0.0114	9.334	0.0101	90	0	108.7232	0.0805	90	0	785.644	2.655	108	118
19	7.6581	0.0081	11.6357	0.005	9.3904	0.0114	90	0	108.8788	0.0756	90	0	791.737	1.627	135	159
20	7.6392	0.0094	11.5998	0.0054	9.3672	0.0218	90	0	108.9196	0.1174	90	0	785.22	2.327	133	148

21	7.6678	0.0095	11.6454	0.0076	9.3654	0.0206	90	0	108.8593	0.0957	90	0	791.385	2.595	129	157
22	7.6387	0.0054	11.6069	0.0062	9.3251	0.0107	90	0	108.7473	0.0422	90	0	782.909	1.567	135	178
23	7.6428	0.0035	11.6229	0.0038	9.3236	0.0064	90	0	108.7118	0.0208	90	0	784.45	0.999	145	193
24	7.6519	0.0047	11.6286	0.0061	9.3517	0.0089	90	0	108.6808	0.0238	90	0	788.276	1.411	136	186
25	7.6302	0.0047	11.5979	0.007	9.3099	0.0077	90	0	108.7529	0.0173	90	0	780.14	1.363	130	161
26	7.6332	0.0043	11.5952	0.0077	9.3213	0.0065	90	0	108.7832	0.0147	90	0	781.077	1.254	150	174
27	7.6545	0.0051	11.6545	0.0125	9.3547	0.0073	90	0	108.7486	0.0204	90	0	790.251	1.654	135	162
28	7.6444	0.0053	11.6548	0.0181	9.334	0.0074	90	0	108.787	0.0214	90	0	787.297	1.882	124	142
29	7.6605	0.0035	11.6008	0.0119	9.3546	0.0044	90	0	108.7357	0.0139	90	0	787.272	1.271	132	153
30	7.6406	0.0035	11.5879	0.0117	9.3299	0.0049	90	0	108.7948	0.0121	90	0	782.015	1.394	133	144
31	7.6464	0.0057	11.5995	0.0149	9.3298	0.0072	90	0	108.7788	0.0181	90	0	783.45	1.917	126	149
32	7.6461	0.0044	11.5936	0.0101	9.3345	0.0056	90	0	108.819	0.0158	90	0	783.231	1.425	126	148
33	7.6635	0.0049	11.6189	0.0101	9.3603	0.0052	90	0	108.7991	0.0272	90	0	788.987	1.34	120	136
34	7.6715	0.0057	11.623	0.0111	9.3666	0.0066	90	0	108.8816	0.0402	90	0	790.237	1.59	119	133
35	7.6602	0.0044	11.6252	0.0047	9.369	0.0047	90	0	108.9175	0.0305	90	0	789.257	0.916	140	166
36	7.6495	0.0103	11.6043	0.0085	9.361	0.0121	90	0	108.9436	0.1039	90	0	785.947	1.783	118	138
37	7.6669	0.006	11.6358	0.0072	9.3651	0.0113	90	0	108.5387	0.0672	90	0	792.116	2.142	122	139
38	7.6558	0.0057	11.6463	0.0071	9.358	0.0096	90	0	108.8018	0.0613	90	0	789.853	1.886	125	145
39	7.6637	0.0059	11.6402	0.0069	9.3658	0.0083	90	0	108.6387	0.0465	90	0	791.675	1.754	132	147
40	7.6343	0.0032	11.5955	0.0039	9.323	0.0041	90	0	108.6885	0.022	90	0	781.791	0.876	143	172
41	7.6364	0.0058	11.5987	0.0071	9.3277	0.0065	90	0	108.694	0.0308	90	0	782.584	1.44	136	172
42	7.6323	0.0045	11.5735	0.0073	9.3136	0.0048	90	0	108.6735	0.021	90	0	779.383	1.052	135	203
43	7.6381	0.0029	11.6021	0.007	9.3303	0.0031	90	0	108.6947	0.0101	90	0	783.206	0.846	152	202
44	7.6585	0.0043	11.6618	0.0142	9.362	0.0047	90	0	108.6948	0.0124	90	0	792.021	1.408	139	176
45	7.6194	0.0034	11.5343	0.012	9.305	0.0041	90	0	108.7466	0.0105	90	0	774.381	1.245	136	177
46	7.6558	0.0024	11.638	0.0085	9.3513	0.0027	90	0	108.6618	0.0086	90	0	789.383	0.893	135	164
47	7.6467	0.0041	11.5976	0.0119	9.346	0.0045	90	0	108.6842	0.0133	90	0	785.152	1.437	137	157
48	7.6474	0.0043	11.6122	0.0114	9.3464	0.0053	90	0	108.6235	0.016	90	0	786.528	1.378	125	148
49	7.645	0.0034	11.6067	0.0076	9.3455	0.0046	90	0	108.6439	0.0135	90	0	785.735	1.067	122	139
50	7.6521	0.0044	11.612	0.0085	9.3613	0.0066	90	0	108.6278	0.0209	90	0	788.233	1.36	125	141

51	7.6403	0.0058	11.5875	0.0101	9.3545	0.0102	90	0	108.5378	0.0429	90	0	785.203	1.766	112	127
52	7.656	0.0045	11.6321	0.0078	9.3453	0.01	90	0	108.6002	0.0475	90	0	788.784	1.539	118	129
53	7.643	0.005	11.6038	0.0075	9.3537	0.013	90	0	108.5078	0.0788	90	0	786.658	2.123	110	128
54	7.6397	0.0042	11.601	0.0053	9.3172	0.0119	90	0	108.7702	0.0632	90	0	781.847	1.83	130	147
55	7.6588	0.0073	11.6197	0.0041	9.3356	0.0044	90	0	108.6534	0.0318	90	0	787.164	1.136	138	180
56	7.6383	0.0049	11.5842	0.0042	9.3184	0.0039	90	0	108.7315	0.0218	90	0	780.848	0.944	138	181
57	7.6445	0.0041	11.5973	0.0036	9.3237	0.0038	90	0	108.651	0.0186	90	0	783.189	0.821	143	175
58	7.6436	0.0033	11.5827	0.0033	9.3228	0.0035	90	0	108.7188	0.0155	90	0	781.721	0.702	141	184
59	7.6528	0.0032	11.5956	0.0044	9.336	0.0042	90	0	108.7622	0.0149	90	0	784.438	0.798	138	179
60	7.6428	0.0026	11.5859	0.0062	9.3234	0.0032	90	0	108.7329	0.0111	90	0	781.84	0.81	144	184
61	7.6687	0.0035	11.6542	0.0102	9.3527	0.0054	90	0	108.7408	0.0151	90	0	791.557	1.154	136	170
62	7.6443	0.0028	11.5805	0.0075	9.3262	0.0038	90	0	108.691	0.0103	90	0	782.059	0.913	136	164
63	7.6479	0.0033	11.5976	0.0075	9.3321	0.0039	90	0	108.743	0.0126	90	0	783.842	1.04	125	153
64	7.6643	0.0042	11.6195	0.0097	9.3484	0.0051	90	0	108.7375	0.0224	90	0	788.396	1.313	122	138
65	9.998	0.0054	11.6004	0.0076	13.8396	0.007	90	0	101.9114	0.0162	90	0	1570.564	2.284	125	146
66	9.9772	0.0061	11.5713	0.0069	13.8118	0.0071	90	0	102.0003	0.0222	90	0	1552.612	2.121	138	157
67	10.0149	0.0064	11.6071	0.007	13.8658	0.0061	90	0	101.7732	0.0363	90	0	1577.9	2.112	133	153
68	9.9768	0.0091	11.5723	0.0038	13.8369	0.0069	90	0	101.8903	0.0211	90	0	1572.372	2.132	137	169
69	9.9996	0.0102	11.5721	0.0059	13.8527	0.0054	90	0	101.8385	0.0298	90	0	1569.667	2.42	136	163
70	9.9981	0.0107	11.5923	0.0077	13.8144	0.0158	90	0	101.8387	0.0757	90	0	1567.049	4.321	118	141
71	9.9957	0.0042	11.5811	0.0063	13.8272	0.0088	90	0	101.8609	0.0159	90	0	1567.897	2.371	137	178
72	10.0101	0.0069	11.5852	0.0096	13.8724	0.0109	90	0	102.0223	0.0277	90	0	1574.264	2.936	123	156
73	9.9573	0.0059	11.5521	0.0069	13.8168	0.0072	90	0	102.007	0.0232	90	0	1554.632	2.301	137	154
74	9.9835	0.0067	11.5747	0.0059	13.8189	0.0067	90	0	101.9107	0.0187	90	0	1561.469	2.248	135	159
75	9.9833	0.0093	11.6161	0.0044	13.8411	0.0082	90	0	101.9669	0.0385	90	0	1572.46	2.544	133	152
84	9.9857	0.0072	11.5854	0.0089	13.8456	0.0136	90	0	102.0012	0.0329	90	0	1563.072	3.042	139	159
77	9.9728	0.0071	11.5823	0.0048	13.8269	0.0066	90	0	101.9903	0.0201	90	0	1562.272	2.222	136	170
78	9.9963	0.0057	11.5862	0.0039	13.8428	0.0052	90	0	102.0803	0.0132	90	0	1567.758	1.751	137	166
79	9.9901	0.0074	11.5773	0.0052	13.8193	0.007	90	0	102.0661	0.0205	90	0	1563.011	2.317	133	161
80	9.9811	0.0045	11.5893	0.005	13.8331	0.0056	90	0	102.0325	0.0176	90	0	1564.973	1.789	144	178

81	9.9726	0.0036	11.5718	0.0037	13.8167	0.005	90	0	102.0046	0.019	90	0	1559.589	1.423	129	151
82	10.0049	0.0064	11.6245	0.0088	13.8729	0.0094	90	0	102.0531	0.0357	90	0	1577.873	2.855	159	187
83	9.9856	0.0037	11.5788	0.0045	13.8482	0.0064	90	0	102.0052	0.0186	90	0	1566.129	1.66	147	179
84	9.9834	0.0068	11.5694	0.0087	13.8526	0.0132	90	0	102.0007	0.0339	90	0	1565.043	3.082	139	166
85	10.0045	0.0055	11.6057	0.0077	13.8422	0.0128	90	0	102.094	0.0235	90	0	1571.536	2.555	134	160
86	9.9986	0.0053	11.5835	0.0058	13.879	0.0147	90	0	102.1762	0.0244	90	0	1571.287	2.719	133	154
87	10.0009	0.0079	11.5825	0.0077	13.8416	0.0079	90	0	101.8892	0.0189	90	0	1568.992	2.765	133	154
88	9.9912	0.0089	11.5756	0.0083	13.8294	0.0088	90	0	101.8364	0.0212	90	0	1566.809	3.055	139	169
89	9.9997	0.0085	11.5674	0.0069	13.8523	0.0066	90	0	101.8731	0.0239	90	0	1567.157	2.715	127	139
90	9.9833	0.0092	11.5994	0.0081	13.8669	0.0202	90	0	101.9392	0.0799	90	0	1571.045	4.079	121	135
91	10.0045	0.0104	11.6061	0.006	13.868	0.009	90	0	101.7982	0.053	90	0	1576.246	3.424	134	161
92	9.9741	0.0096	11.5741	0.0048	13.8217	0.0094	90	0	101.8921	0.0696	90	0	1561.35	3.313	132	181
93	9.9859	0.0074	11.5832	0.0043	13.8295	0.0093	90	0	101.9869	0.0656	90	0	1564.759	2.827	137	167
94	9.9894	0.0071	11.5789	0.005	13.8162	0.01	90	0	101.9119	0.0383	90	0	1563.66	2.945	139	170
95	9.9702	0.004	11.5653	0.0035	13.8045	0.0075	90	0	101.9339	0.0311	90	0	1557.377	1.846	143	192
96	9.9794	0.0042	11.5724	0.0039	13.8155	0.0091	90	0	101.9521	0.0283	90	0	1560.903	2.108	115	219
97	9.9631	0.004	11.5615	0.0045	13.7935	0.0076	90	0	101.951	0.0166	90	0	1554.404	1.906	129	220
98	9.9785	0.003	11.5739	0.0033	13.8182	0.006	90	0	101.9404	0.0114	90	0	1561.338	1.406	149	218
99	9.973	0.0027	11.5672	0.0036	13.8241	0.0054	90	0	101.9304	0.01	90	0	1560.291	1.239	136	210
100	9.9755	0.0046	11.5809	0.0063	13.8252	0.0083	90	0	101.8909	0.0157	90	0	1562.895	2.171	137	180
101	10.0151	0.0066	11.5852	0.0096	13.8724	0.0109	90	0	102.0223	0.0277	90	0	1574.271	2.936	133	155
102	9.9583	0.0056	11.553	0.0069	13.8148	0.0076	90	0	102.0016	0.0231	90	0	1554.628	2.301	132	153
103	9.9735	0.0062	11.5745	0.0058	13.8239	0.007	90	0	101.9089	0.0186	90	0	1561.479	2.248	135	163
104	10.0014	0.0077	11.5725	0.007	13.8434	0.0078	90	0	101.8696	0.0188	90	0	1567.99	2.75	133	149
105	9.9911	0.009	11.5656	0.0082	13.8274	0.0089	90	0	101.8371	0.0213	90	0	1563.809	3.075	129	155
106	9.996	0.0088	11.5669	0.006	13.8416	0.0067	90	0	101.8711	0.0229	90	0	1566.184	2.615	126	139
107	9.9853	0.0112	11.5756	0.0061	13.8444	0.008	90	0	101.763	0.0289	90	0	1566.613	3.109	135	155
108	9.9896	0.0092	11.5691	0.0049	13.85	0.0054	90	0	101.8285	0.0308	90	0	1566.667	2.4	135	163
109	9.9832	0.003	11.579	0.0035	13.8583	0.0148	90	0	102.11	0.0223	90	0	1566.304	2.286	147	195
110	9.9971	0.005	11.5943	0.0041	13.8861	0.0302	90	0	102.1617	0.0745	90	0	1573.406	3.935	118	202

111	9.9818	0.0065	11.5949	0.005	13.8308	0.0229	90	0	101.8942	0.0634	90	0	1566.367	3.643	121	219
112	9.9799	0.0044	11.5885	0.0041	13.8343	0.0103	90	0	101.9467	0.0278	90	0	1565.327	2.116	151	228
113	9.9903	0.005	11.6011	0.0041	13.8574	0.0101	90	0	101.9905	0.024	90	0	1571.015	2.219	121	254
114	9.9628	0.0071	11.5731	0.0055	13.8229	0.0122	90	0	101.9534	0.0331	90	0	1559.226	2.827	104	233
115	9.965	0.0053	11.5719	0.0057	13.8158	0.0074	90	0	101.9993	0.0211	90	0	1558.352	2.087	118	233
116	9.9635	0.0051	11.5561	0.0077	13.8142	0.0073	90	0	102.0217	0.017	90	0	1555.671	2.318	101	234
117	9.9814	0.0042	11.5857	0.0068	13.8428	0.0051	90	0	102.0322	0.0126	90	0	1565.626	1.65	136	212
118	9.9868	0.0056	11.59	0.0088	13.8526	0.0062	90	0	102.0379	0.0104	90	0	1568.134	2.111	139	210
119	9.9575	0.0046	11.5553	0.0113	13.8107	0.0072	90	0	102.0059	0.0111	90	0	1554.326	2.764	100	210
120	9.9856	0.0036	11.5704	0.0081	13.848	0.005	90	0	102.0068	0.0102	90	0	1564.968	1.909	134	201
121	9.9688	0.004	11.5692	0.0088	13.8322	0.0061	90	0	102.0087	0.0138	90	0	1560.368	2.216	127	197
122	9.9724	0.0052	11.5531	0.0088	13.8381	0.0074	90	0	102.0115	0.017	90	0	1559.412	2.553	111	203
123	9.9634	0.0033	11.5434	0.0052	13.8231	0.0055	90	0	101.9681	0.0125	90	0	1555.255	1.579	138	184
124	9.9928	0.0038	11.5892	0.0054	13.8855	0.0064	90	0	102.0335	0.0132	90	0	1572.721	1.682	140	185
125	9.9721	0.0033	11.5628	0.0045	13.8385	0.0096	90	0	102.0391	0.0168	90	0	1560.552	1.925	128	188
126	9.9652	0.0039	11.5485	0.0054	13.7791	0.0155	90	0	101.9818	0.0235	90	0	1551.191	2.402	131	195
127	9.9891	0.0095	11.5859	0.0049	13.8328	0.0065	90	0	102.0168	0.0246	90	0	1565.812	2.681	144	178
128	9.9788	0.0121	11.5662	0.0069	13.8081	0.0089	90	0	101.9476	0.0278	90	0	1559.165	3.48	117	200
129	9.9832	0.0081	11.5995	0.0055	13.8397	0.0069	90	0	102.0139	0.0176	90	0	1567.542	2.505	152	222
130	9.994	0.0065	11.5721	0.0045	13.8249	0.0058	90	0	102.0526	0.0126	90	0	1563.627	1.986	123	237
131	9.9743	0.0094	11.5795	0.0062	13.816	0.0091	90	0	101.9978	0.0211	90	0	1560.863	2.827	118	226
132	9.968	0.0065	11.5703	0.0067	13.8068	0.0074	90	0	101.9935	0.0159	90	0	1557.618	2.202	127	268
133	9.9724	0.0037	11.5452	0.0073	13.812	0.0048	90	0	101.9817	0.0103	90	0	1555.577	1.722	154	283
134	10.0145	0.0041	11.603	0.0111	13.8642	0.0057	90	0	102.0539	0.0123	90	0	1575.471	2.231	128	247
135	9.9797	0.0042	11.5548	0.0098	13.8186	0.0054	90	0	101.9782	0.0083	90	0	1558.772	2.395	119	225
136	10.0015	0.0038	11.5514	0.0104	13.8501	0.0054	90	0	102.04	0.0088	90	0	1564.917	2.275	117	219
137	9.9813	0.0039	11.553	0.0077	13.8278	0.0049	90	0	102.0189	0.0115	90	0	1559.578	1.972	104	195
138	9.9846	0.0036	11.555	0.0078	13.8292	0.0057	90	0	102.0426	0.0146	90	0	1560.396	1.952	111	200
139	9.9743	0.0035	11.5436	0.0053	13.8176	0.0045	90	0	102.039	0.0145	90	0	1555.95	1.545	147	177
140	9.984	0.0042	11.5577	0.0046	13.8267	0.0045	90	0	102.0435	0.0165	90	0	1560.368	1.568	152	189

141	9.9801	0.0083	11.5492	0.0065	13.8194	0.008	90	0	102.0826	0.0338	90	0	1557.572	2.658	140	180
142	9.9811	0.0078	11.5629	0.0045	13.8277	0.0061	90	0	102.0619	0.0248	90	0	1560.618	2.265	151	179
143	10.0094	0.0109	11.5656	0.0051	13.8431	0.0077	90	0	102.1235	0.0372	90	0	1566.8	2.861	138	171
144	9.9504	0.0172	11.5485	0.0061	13.8095	0.0094	90	0	101.998	0.0562	90	0	1552.218	3.973	125	199
145	10.0023	0.0043	11.5888	0.0043	13.8569	0.0103	90	0	101.908	0.0336	90	0	1571.666	2.337	123	216
146	10.017	0.0034	11.6042	0.0036	13.8678	0.0078	90	0	101.8924	0.0218	90	0	1577.378	1.721	130	231
147	9.9669	0.0052	11.5589	0.0057	13.8137	0.0108	90	0	101.9386	0.0232	90	0	1557.005	2.434	114	241
148	9.9814	0.0039	11.5666	0.0052	13.8366	0.0075	90	0	101.9474	0.0119	90	0	1562.851	1.834	114	238
149	9.9976	0.0036	11.5969	0.0045	13.8567	0.0066	90	0	101.9172	0.0103	90	0	1571.936	1.656	141	238
150	9.9775	0.0032	11.5708	0.0057	13.8327	0.005	90	0	101.9454	0.0109	90	0	1562.366	1.575	146	235
151	9.9725	0.005	11.5495	0.0099	13.8231	0.0079	90	0	101.9833	0.0191	90	0	1557.409	2.479	117	205
152	9.9679	0.0032	11.5523	0.0075	13.8207	0.0049	90	0	101.9631	0.0145	90	0	1556.91	1.743	115	208
153	9.9682	0.0041	11.5414	0.0063	13.8184	0.0053	90	0	101.9699	0.0122	90	0	1555.199	1.868	121	208
154	9.9708	0.0044	11.5586	0.0063	13.8359	0.0052	90	0	101.9448	0.0117	90	0	1560.033	1.845	115	199
155	9.9738	0.0048	11.5568	0.0054	13.8253	0.0049	90	0	101.9057	0.0125	90	0	1559.301	1.763	141	177
156	9.989	0.0036	11.5584	0.0038	13.84	0.0046	90	0	101.8997	0.0128	90	0	1563.597	1.439	146	180
157	9.9659	0.0052	11.5525	0.0057	13.8226	0.0061	90	0	101.9412	0.0258	90	0	1556.982	1.951	122	185
158	9.9929	0.006	11.5628	0.0048	13.8568	0.0062	90	0	101.7539	0.0432	90	0	1567.519	2.024	125	200
159	9.9668	0.0072	11.5509	0.0046	13.8278	0.0079	90	0	101.9624	0.0543	90	0	1557.352	2.643	133	192
160	9.9994	0.0077	11.571	0.0055	13.8556	0.012	90	0	101.7837	0.0536	90	0	1569.35	3.347	128	193
161	9.9931	0.0062	11.5678	0.0045	13.8431	0.0111	90	0	101.8427	0.0471	90	0	1566.169	2.837	136	163
162	9.9806	0.0053	11.5593	0.005	13.8078	0.0106	90	0	101.9881	0.0378	90	0	1558.247	2.594	140	180
163	9.9698	0.0076	11.5597	0.0048	13.8275	0.0107	90	0	101.9428	0.0456	90	0	1559.092	2.626	124	184
164	9.9725	0.0082	11.5612	0.0046	13.8408	0.0088	90	0	102.0197	0.0359	90	0	1560.78	2.546	154	184
165	9.971	0.0078	11.5562	0.0042	13.8356	0.0072	90	0	102.0638	0.0334	90	0	1559.018	2.201	151	175
166	9.9675	0.0084	11.5606	0.0048	13.8395	0.0069	90	0	102.0638	0.0245	90	0	1559.496	2.394	117	205
167	9.9772	0.0079	11.5675	0.0058	13.8419	0.0074	90	0	102.0538	0.0198	90	0	1562.288	2.556	101	214
168	9.974	0.0052	11.5473	0.0037	13.8183	0.0052	90	0	102.0147	0.0129	90	0	1556.63	1.662	121	212
169	10.0042	0.0082	11.5544	0.0071	13.8489	0.0082	90	0	101.9661	0.0221	90	0	1566.04	2.806	107	200
170	9.9823	0.0045	11.5598	0.0045	13.8318	0.0056	90	0	101.9968	0.0159	90	0	1561.231	1.753	109	229

171	9.9895	0.0031	11.5618	0.0032	13.8462	0.0042	90	0	102.0097	0.0149	90	0	1564.193	1.227	128	199
172	9.957	0.0042	11.5371	0.0056	13.791	0.0057	90	0	102.0097	0.022	90	0	1549.575	1.8	144	223
173	9.9706	0.0037	11.5477	0.0048	13.8191	0.0062	90	0	101.9806	0.0202	90	0	1556.439	1.658	124	209
174	9.9767	0.0034	11.55	0.0041	13.8519	0.0067	90	0	102.0108	0.0153	90	0	1561.221	1.551	144	184
175	9.9723	0.0036	11.5527	0.0048	13.802	0.0078	90	0	101.9856	0.0151	90	0	1555.425	1.67	143	181
176	10.0054	0.0071	11.5806	0.0088	13.8656	0.0227	90	0	102.1477	0.036	90	0	1570.614	3.908	150	179
177	9.9952	0.0045	11.5645	0.0049	13.8553	0.0147	90	0	102.0926	0.0342	90	0	1565.998	2.458	143	164
178	9.9931	0.0051	11.5521	0.0047	13.8571	0.0142	90	0	102.2158	0.0485	90	0	1563.452	2.435	142	171
179	9.96	0.0059	11.5375	0.0041	13.8006	0.0119	90	0	101.9717	0.0441	90	0	1551.391	2.437	140	171
180	10.0005	0.01	11.5762	0.0071	13.8583	0.0184	90	0	102.0105	0.0704	90	0	1569.225	4.009	141	159
181	9.9734	0.0097	11.5683	0.0048	13.8422	0.0073	90	0	101.8484	0.0398	90	0	1563.031	2.953	128	190
182	10.0175	0.0132	11.5945	0.0059	13.8752	0.0115	90	0	101.7069	0.0846	90	0	1578.056	4.328	118	200
183	9.9667	0.0082	11.5677	0.0052	13.806	0.0103	90	0	102.0515	0.0686	90	0	1556.639	3.168	144	184
184	9.9907	0.0074	11.5693	0.0055	13.8289	0.0099	90	0	101.8948	0.041	90	0	1564.085	3.015	124	194
185	9.9828	0.0048	11.5699	0.0046	13.8146	0.009	90	0	101.9711	0.0389	90	0	1560.872	2.264	110	219
186	9.9628	0.0032	11.5531	0.0027	13.796	0.0068	90	0	101.988	0.0219	90	0	1553.312	1.549	132	237
187	9.9748	0.0035	11.5666	0.0041	13.8126	0.0072	90	0	101.9264	0.0173	90	0	1559.231	1.712	128	231
188	9.9677	0.0028	11.5479	0.0027	13.8178	0.0057	90	0	101.9429	0.0111	90	0	1556.076	1.236	149	233
189	9.9699	0.0033	11.5458	0.004	13.8296	0.0063	90	0	101.9326	0.0106	90	0	1557.549	1.502	135	240
190	9.9606	0.0031	11.5452	0.0045	13.7972	0.0058	90	0	101.9462	0.0116	90	0	1552.264	1.442	148	194
191	9.9916	0.0036	11.5662	0.0055	13.8546	0.0056	90	0	101.9665	0.0147	90	0	1566.308	1.635	140	169
192	9.9608	0.005	11.5419	0.0061	13.8025	0.0065	90	0	101.9839	0.019	90	0	1552.246	2.06	137	154
193	9.9852	0.0062	11.5667	0.006	13.8341	0.0072	90	0	101.8862	0.0189	90	0	1563.528	2.307	140	166
194	9.9683	0.007	11.5578	0.0064	13.8209	0.0072	90	0	101.9169	0.0174	90	0	1558.007	2.505	135	161
195	9.9624	0.0076	11.5517	0.007	13.8148	0.0076	90	0	101.8744	0.0185	90	0	1555.825	2.603	135	161
196	10.0147	0.0088	11.5742	0.0061	13.848	0.0073	90	0	101.8969	0.021	90	0	1570.678	2.769	127	150
197	10.0151	0.0103	11.582	0.0054	13.8669	0.0073	90	0	101.7127	0.028	90	0	1574.998	2.965	140	161
198	10.022	0.0091	11.5815	0.0048	13.8694	0.0052	90	0	101.7193	0.031	90	0	1576.276	2.402	132	171
199	9.9842	0.0042	11.5768	0.0051	13.832	0.0209	90	0	102.0978	0.0298	90	0	1563.264	3.231	105	197
200	9.9888	0.0051	11.5804	0.0041	13.8562	0.0273	90	0	102.1177	0.0636	90	0	1567.104	3.754	103	200

201	9.9604	0.0057	11.5552	0.0047	13.7866	0.0173	90	0	101.972	0.0468	90	0	1552.262	3.059	107	205
202	9.9711	0.0047	11.5917	0.0041	13.8108	0.0113	90	0	101.8753	0.0303	90	0	1562.108	2.286	130	226
203	9.9529	0.0056	11.5585	0.0046	13.7937	0.0114	90	0	101.9483	0.0271	90	0	1552.468	2.467	132	239
204	9.9678	0.0059	11.5788	0.0051	13.8305	0.0099	90	0	102.0067	0.0261	90	0	1561.344	2.382	120	223
205	9.9821	0.0053	11.6031	0.006	13.8598	0.0079	90	0	102.0261	0.0215	90	0	1570.052	2.214	151	217
206	9.9577	0.0066	11.5761	0.0067	13.8141	0.0088	90	0	101.9749	0.0214	90	0	1557.725	2.426	93	224
207	9.9621	0.0097	11.5739	0.0142	13.8265	0.0114	90	0	101.9737	0.0295	90	0	1559.521	3.588	142	200
208	9.9806	0.0052	11.5596	0.0108	13.8404	0.0062	90	0	102.0366	0.0111	90	0	1561.684	2.306	142	188
209	9.9931	0.0042	11.5836	0.0099	13.8594	0.0057	90	0	102.0322	0.0104	90	0	1569.062	2.246	121	213
210	9.9758	0.0046	11.5495	0.0087	13.8304	0.0067	90	0	102.012	0.0116	90	0	1558.589	2.313	135	182
211	9.9874	0.0039	11.5855	0.0077	13.8495	0.0056	90	0	102.0653	0.0134	90	0	1567.11	1.988	150	185
212	9.9626	0.0043	11.5499	0.0069	13.8064	0.0061	90	0	101.9988	0.0136	90	0	1553.962	2.027	143	178
213	9.9853	0.0042	11.5762	0.006	13.8618	0.0066	90	0	102.026	0.014	90	0	1567.143	1.959	138	165
214	9.9623	0.0049	11.5652	0.007	13.7963	0.0086	90	0	101.9923	0.0163	90	0	1554.87	2.28	135	163
215	9.9868	0.0027	11.5894	0.0037	13.8889	0.0076	90	0	102.0455	0.0138	90	0	1572.128	1.534	146	180
216	9.9972	0.0065	11.5867	0.0051	13.8978	0.0098	90	0	102.0435	0.0169	90	0	1569.157	1.597	149	179
217	10.0145	0.0087	11.5987	0.0041	13.8436	0.0056	90	0	102.0543	0.0249	90	0	1572.556	2.321	138	167
218	9.9972	0.0093	11.5939	0.0054	13.8346	0.0069	90	0	102.0161	0.0227	90	0	1568.386	2.676	146	175
219	9.9882	0.0083	11.6026	0.0053	13.8394	0.0068	90	0	102.0434	0.0185	90	0	1568.536	2.46	123	188
220	9.9731	0.0084	11.5768	0.0053	13.8134	0.0071	90	0	102.0072	0.0164	90	0	1559.957	2.466	154	227
221	9.9871	0.0068	11.5919	0.005	13.8238	0.0066	90	0	102.0326	0.0153	90	0	1565.21	2.1	121	212
222	9.9937	0.0067	11.5787	0.0073	13.8267	0.0075	90	0	101.9971	0.017	90	0	1564.994	2.231	151	243
223	9.9746	0.0037	11.5534	0.0074	13.8083	0.0047	90	0	101.9784	0.0105	90	0	1556.628	1.798	131	232
224	10.0034	0.0041	11.6055	0.0111	13.8387	0.0057	90	0	102.0032	0.0128	90	0	1571.473	2.142	163	198
225	9.9595	0.0047	11.5312	0.0108	13.7992	0.0058	90	0	101.9982	0.0104	90	0	1550.142	2.541	135	188
226	9.9723	0.0039	11.5462	0.0084	13.8047	0.0056	90	0	101.9964	0.0084	90	0	1554.789	2.027	144	199
227	9.9718	0.003	11.5599	0.0072	13.8105	0.004	90	0	102.0146	0.0097	90	0	1557.105	1.672	144	171
228	10.0006	0.0033	11.5933	0.0066	13.8351	0.0048	90	0	102.0326	0.0123	90	0	1568.806	1.733	142	170
229	10.0094	0.0032	11.599	0.0058	13.8474	0.0046	90	0	102.0481	0.0147	90	0	1572.247	1.577	132	151
230	9.9965	0.004	11.5812	0.0056	13.826	0.0049	90	0	102.0794	0.0193	90	0	1565.215	1.658	131	153

231	9.9845	0.0035	11.5666	0.0041	13.8319	0.0077	90	0	101.9164	0.0173	90	0	1558.231	1.912	158	172
232	9.9715	0.0029	11.5479	0.0027	13.8211	0.0057	90	0	101.9454	0.0112	90	0	1557.098	1.266	155	189
233	9.9688	0.0033	11.5475	0.0049	13.8307	0.0068	90	0	101.9333	0.0109	90	0	1556.649	1.576	135	167
234	9.9654	0.0037	11.5397	0.0046	13.7992	0.0061	90	0	101.9513	0.0118	90	0	1557.269	1.492	148	188
235	9.9967	0.0058	11.5721	0.0054	13.8107	0.0144	90	0	101.9296	0.0439	90	0	1559.836	3.155	167	201
236	9.9947	0.0049	11.6025	0.0054	13.8409	0.0103	90	0	101.8545	0.0267	90	0	1570.805	2.458	113	192
237	10.0107	0.0045	11.6101	0.0101	13.8323	0.0069	90	0	102.0009	0.0119	90	0	1571.713	2.113	163	193
238	9.9737	0.0037	11.5826	0.004	13.8165	0.0072	90	0	101.9412	0.0115	90	0	1561.564	1.682	107	196
239	9.992	0.0025	11.6038	0.0034	13.8388	0.005	90	0	101.9161	0.008	90	0	1569.966	1.174	149	179
240	9.9685	0.0027	11.5668	0.0052	13.8095	0.0044	90	0	101.9719	0.0095	90	0	1557.654	1.377	118	194
241	9.9849	0.0037	11.5727	0.0076	13.8344	0.0058	90	0	101.9909	0.0144	90	0	1563.713	1.872	141	172
242	7.653	0.0029	11.581	0.0077	9.3363	0.004	90	0	108.7384	0.0106	90	0	783.608	0.929	130	159
243	7.6578	0.0033	11.6029	0.0082	9.3447	0.004	90	0	108.7	0.0133	90	0	786.482	1.077	127	152
244	7.6423	0.0041	11.5728	0.0092	9.3223	0.005	90	0	108.6175	0.0217	90	0	781.342	1.274	121	137
245	7.6686	0.0036	11.6024	0.0085	9.3529	0.0047	90	0	108.6115	0.0267	90	0	788.651	1.139	120	136
246	7.6669	0.0045	11.6036	0.0066	9.3441	0.0047	90	0	108.7054	0.0234	90	0	787.378	1.182	115	127
247	7.6757	0.0049	11.6192	0.0073	9.3543	0.0049	90	0	108.7633	0.0311	90	0	789.931	1.131	118	144
248	7.6222	0.0081	11.5976	0.0074	9.3287	0.0053	90	0	108.9373	0.0402	90	0	780.019	1.348	120	138
249	7.6559	0.0119	11.5935	0.0061	9.3282	0.0046	90	0	108.7237	0.0353	90	0	784.144	1.789	126	144
250	7.6712	0.0131	11.5948	0.0075	9.3375	0.006	90	0	108.7923	0.0396	90	0	786.256	2.23	111	136
251	7.6641	0.0152	11.6167	0.0063	9.3435	0.0064	90	0	108.6848	0.0522	90	0	788.018	2.217	112	132
252	7.6394	0.0094	11.6176	0.0058	9.3341	0.0054	90	0	108.5824	0.0354	90	0	785.223	1.574	122	138
253	7.6541	0.0054	11.6059	0.0074	9.3467	0.018	90	0	108.8106	0.0376	90	0	785.943	2.298	123	136
254	7.656	0.0043	11.6118	0.0058	9.364	0.0127	90	0	108.813	0.0351	90	0	787.99	1.8	123	140
255	7.6656	0.0045	11.6306	0.0059	9.3624	0.011	90	0	108.8478	0.0411	90	0	789.96	1.674	119	139
256	7.647	0.0036	11.6063	0.0045	9.3459	0.0066	90	0	108.8148	0.029	90	0	785.16	1.18	129	148
257	7.6435	0.0036	11.6086	0.0051	9.3525	0.0056	90	0	108.7603	0.0273	90	0	785.763	1.134	131	146
258	7.6432	0.0026	11.5889	0.0045	9.337	0.0042	90	0	108.7072	0.0227	90	0	783.342	0.858	131	148
259	7.6563	0.0052	11.6228	0.006	9.3565	0.0052	90	0	108.7175	0.0306	90	0	788.577	1.242	128	147
260	7.6321	0.003	11.5929	0.005	9.3352	0.0036	90	0	108.72	0.0151	90	0	782.276	0.846	130	155

261	7.6347	0.0053	11.6061	0.0058	9.3317	0.0044	90	0	108.7002	0.0182	90	0	783.217	1.095	122	141
262	7.6439	0.0043	11.6181	0.0064	9.3495	0.004	90	0	108.723	0.014	90	0	786.366	0.993	129	154
263	7.6103	0.0051	11.581	0.0063	9.3081	0.0048	90	0	108.6454	0.021	90	0	777.316	1.12	125	149
264	7.673	0.0059	11.6092	0.007	9.373	0.0055	90	0	108.9314	0.0303	90	0	789.76	1.312	119	133
265	7.6488	0.0059	11.5912	0.0069	9.3545	0.0054	90	0	108.8838	0.043	90	0	784.715	1.166	121	144
266	7.6489	0.007	11.6041	0.0071	9.3528	0.0093	90	0	108.7746	0.0634	90	0	785.973	1.485	122	136
267	7.6464	0.0068	11.6023	0.0065	9.3614	0.0116	90	0	108.7445	0.0676	90	0	786.455	1.597	117	132
268	7.6499	0.0065	11.6167	0.0065	9.3857	0.0162	90	0	108.7421	0.0644	90	0	789.844	1.936	123	137
269	7.6325	0.0077	11.5876	0.0094	9.3268	0.0213	90	0	108.7579	0.0583	90	0	781.075	2.705	115	123
270	7.6575	0.0076	11.6246	0.0096	9.3751	0.0201	90	0	108.7448	0.0619	90	0	790.258	2.556	110	119
271	7.6721	0.008	11.6222	0.0052	9.3404	0.0044	90	0	108.7542	0.0329	90	0	788.632	1.517	127	139
272	7.6575	0.0191	11.6431	0.01	9.3487	0.0076	90	0	108.6953	0.0656	90	0	789.519	3.264	125	136
273	7.6367	0.0138	11.62	0.0053	9.344	0.0044	90	0	108.6486	0.0349	90	0	785.642	1.904	129	143
274	7.6734	0.0088	11.6192	0.0052	9.3471	0.0046	90	0	108.6355	0.0275	90	0	789.68	1.575	120	134
275	7.6586	0.008	11.6329	0.0048	9.3396	0.0038	90	0	108.5454	0.0285	90	0	788.872	1.231	127	155
276	7.6239	0.0057	11.5986	0.0035	9.3176	0.0035	90	0	108.6307	0.0203	90	0	780.746	0.932	147	188
277	7.6391	0.0056	11.6221	0.0049	9.3275	0.0051	90	0	108.5899	0.0243	90	0	784.907	1.14	138	180
278	7.6458	0.0035	11.6095	0.0038	9.3298	0.0034	90	0	108.6595	0.0175	90	0	784.621	0.747	138	179
279	7.6449	0.0042	11.5977	0.0048	9.3216	0.0055	90	0	108.6917	0.0194	90	0	782.891	1.056	135	181
280	7.6657	0.0044	11.6332	0.0068	9.3456	0.0064	90	0	108.6773	0.0259	90	0	789.527	1.164	124	153
281	7.6371	0.0043	11.5846	0.0082	9.3264	0.0063	90	0	108.661	0.0191	90	0	781.754	1.283	119	135
282	7.663	0.0051	11.6238	0.0098	9.3483	0.007	90	0	108.6992	0.0194	90	0	788.727	1.523	112	122
283	7.6442	0.006	11.6045	0.0094	9.3209	0.0081	90	0	108.6523	0.0257	90	0	783.403	1.737	118	132
284	7.6425	0.0066	11.5902	0.0099	9.3246	0.0087	90	0	108.7002	0.0317	90	0	782.355	1.944	116	129
285	7.661	0.0072	11.6197	0.0118	9.3484	0.0094	90	0	108.6013	0.045	90	0	788.709	2.105	112	124
286	7.653	0.01	11.5874	0.016	9.3432	0.0114	90	0	108.4786	0.0854	90	0	785.824	2.759	109	123
287	7.6573	0.0118	11.593	0.0143	9.3052	0.0119	90	0	108.6969	0.1058	90	0	782.437	2.951	107	120
288	7.65	0.0103	11.6164	0.0115	9.3263	0.0102	90	0	108.7815	0.0902	90	0	784.65	2.526	108	119
289	7.6484	0.0075	11.6187	0.0046	9.3707	0.0104	90	0	108.8343	0.0695	90	0	788.141	1.497	136	156
290	7.653	0.01	11.6134	0.0061	9.3885	0.0221	90	0	109.0236	0.1178	90	0	788.858	2.467	128	142

291	7.6333	0.0072	11.6084	0.0059	9.3182	0.0151	90	0	108.6122	0.0707	90	0	782.505	1.924	130	155
292	7.6404	0.0048	11.6192	0.0052	9.3027	0.0098	90	0	108.6622	0.0393	90	0	782.435	1.392	137	174
293	7.6378	0.0043	11.6099	0.0046	9.3142	0.0078	90	0	108.7099	0.0258	90	0	782.288	1.209	146	190
294	7.6725	0.0044	11.6397	0.0054	9.3788	0.0084	90	0	108.8056	0.0218	90	0	792.866	1.306	136	173
295	7.6408	0.0049	11.6047	0.0072	9.312	0.0082	90	0	108.6669	0.019	90	0	782.247	1.422	134	164
296	7.6463	0.0037	11.622	0.0066	9.3326	0.0055	90	0	108.7945	0.0121	90	0	785.119	1.084	139	171
297	7.6573	0.0096	11.6408	0.0241	9.3532	0.0143	90	0	108.7394	0.0375	90	0	789.512	2.973	132	159
298	7.655	0.0044	11.6039	0.0152	9.3439	0.006	90	0	108.8208	0.0191	90	0	785.621	1.503	120	136
299	7.66	0.0042	11.6437	0.0118	9.3659	0.0052	90	0	108.7875	0.0144	90	0	790.852	1.432	129	154
300	7.6304	0.0047	11.5853	0.0123	9.3215	0.0056	90	0	108.7294	0.0143	90	0	780.384	1.521	130	146
301	7.6579	0.003	11.6107	0.0091	9.3448	0.0041	90	0	108.8052	0.0107	90	0	786.521	1.116	125	145
302	7.654	0.004	11.6179	0.0092	9.352	0.0046	90	0	108.8143	0.0147	90	0	787.178	1.238	126	142
303	7.646	0.004	11.6034	0.0079	9.3451	0.0042	90	0	108.8206	0.0204	90	0	784.762	1.106	119	136
304	7.6432	0.0059	11.6186	0.01	9.3337	0.0064	90	0	108.7517	0.0388	90	0	784.864	1.507	120	133
305	7.6588	0.0051	11.6239	0.0047	9.364	0.0049	90	0	108.9053	0.0327	90	0	788.664	0.988	133	158
306	7.6616	0.0085	11.6461	0.007	9.3759	0.0094	90	0	108.7968	0.0843	90	0	791.975	1.436	125	145
307	7.6663	0.0073	11.6416	0.0085	9.362	0.0132	90	0	108.505	0.0778	90	0	792.344	2.553	120	135
308	7.653	0.0063	11.6331	0.0084	9.3528	0.0102	90	0	108.5783	0.0605	90	0	789.274	2.094	130	152
309	7.6563	0.0065	11.6454	0.0079	9.3504	0.0091	90	0	108.7513	0.0487	90	0	789.434	1.944	133	154
310	7.6402	0.0047	11.608	0.0056	9.3296	0.006	90	0	108.699	0.0324	90	0	783.742	1.295	139	187