Supporting Information

Polymorphism in two biologically active dihydroprimidinium hydrochloride derivatives: quantitative inputs towards the energetics associated with crystal packing.

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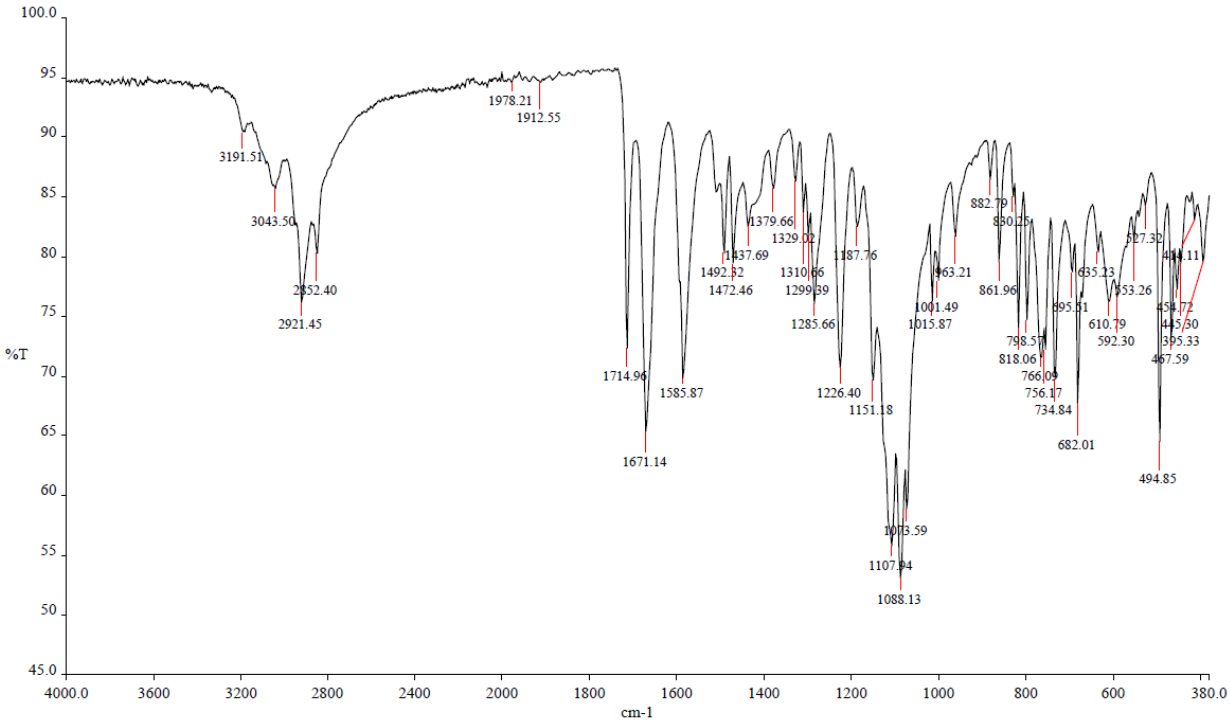
Section I: Experimental Characterization:

Figure S1: IR spectra of A: Recorded on a Nicolet 6700 FT-IR spectrometry

(a) A Form I:



(b) A Form II:

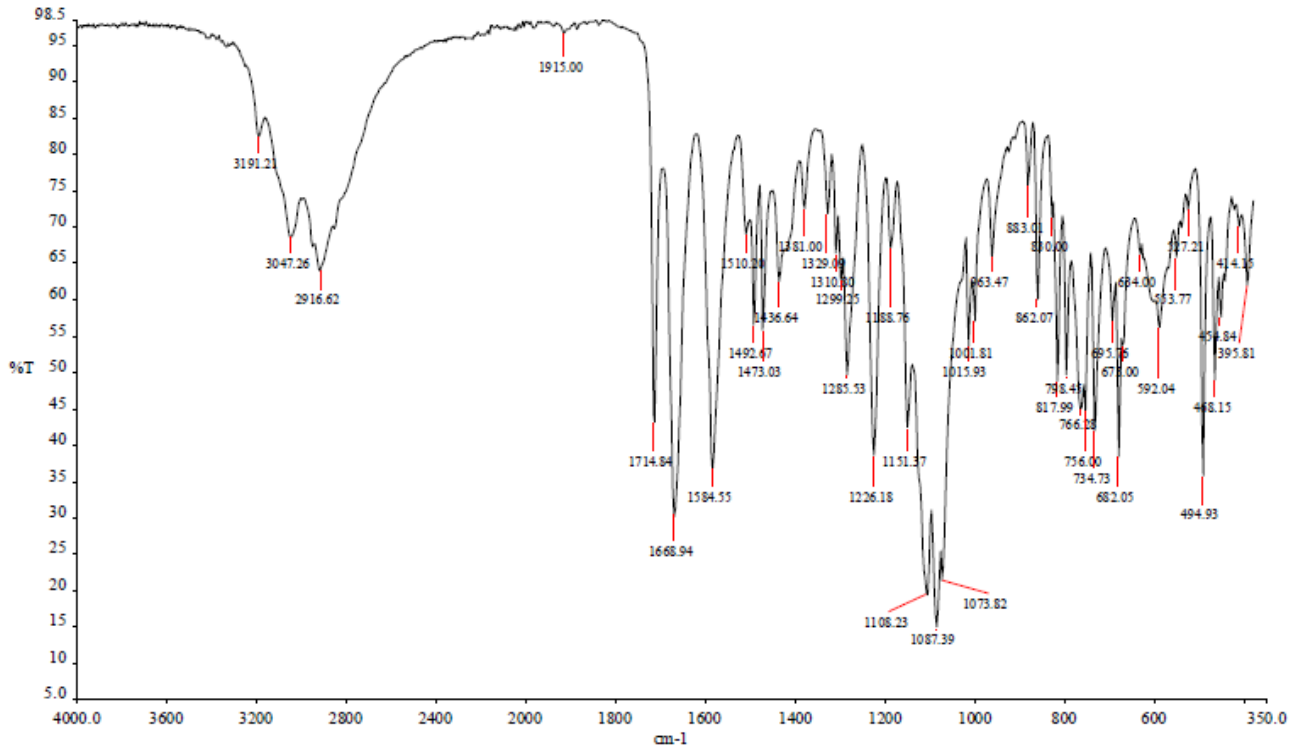
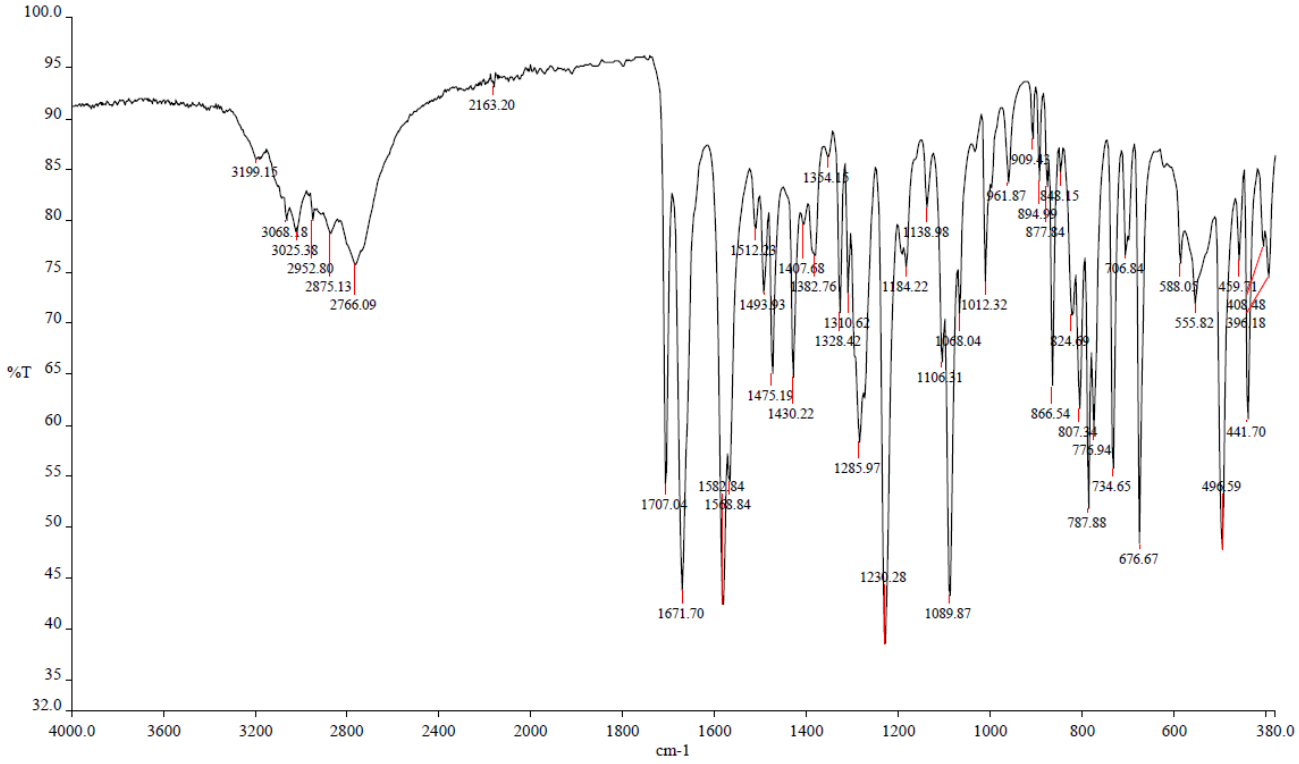


Figure S2: IR spectra of B.

(a) B:



(b) B·H_2O:

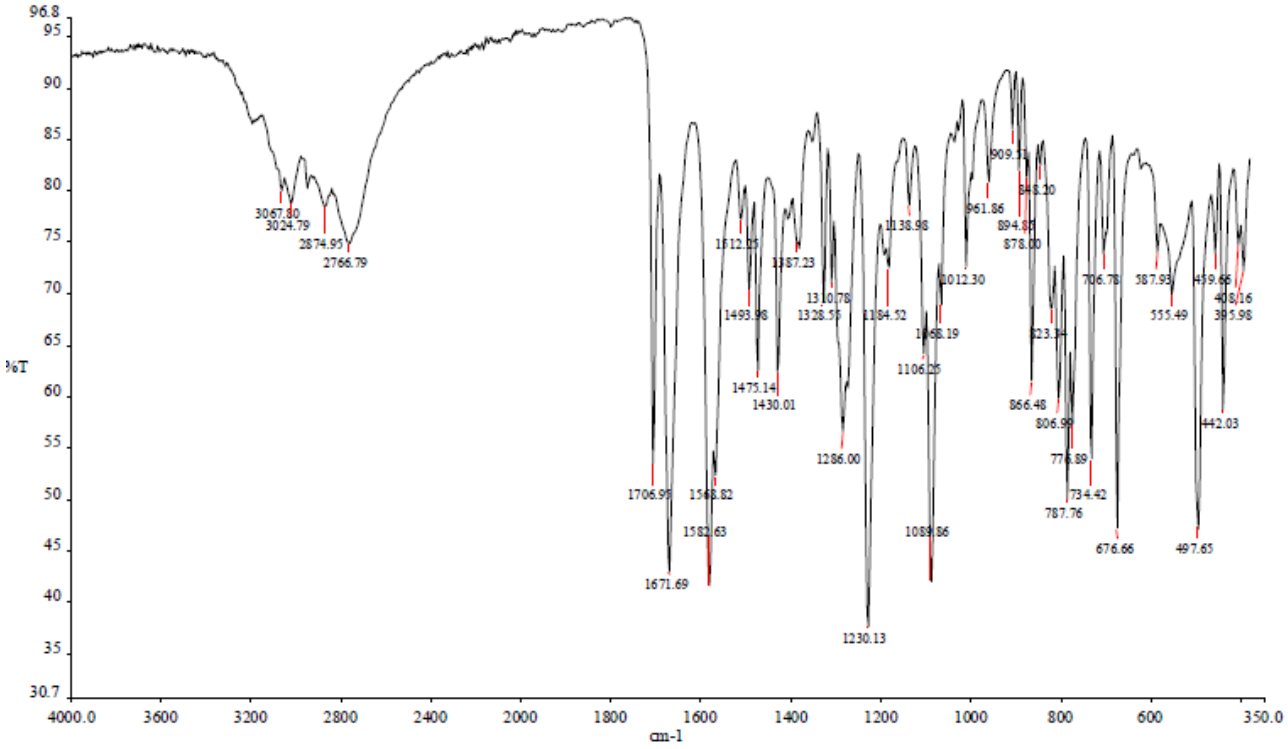
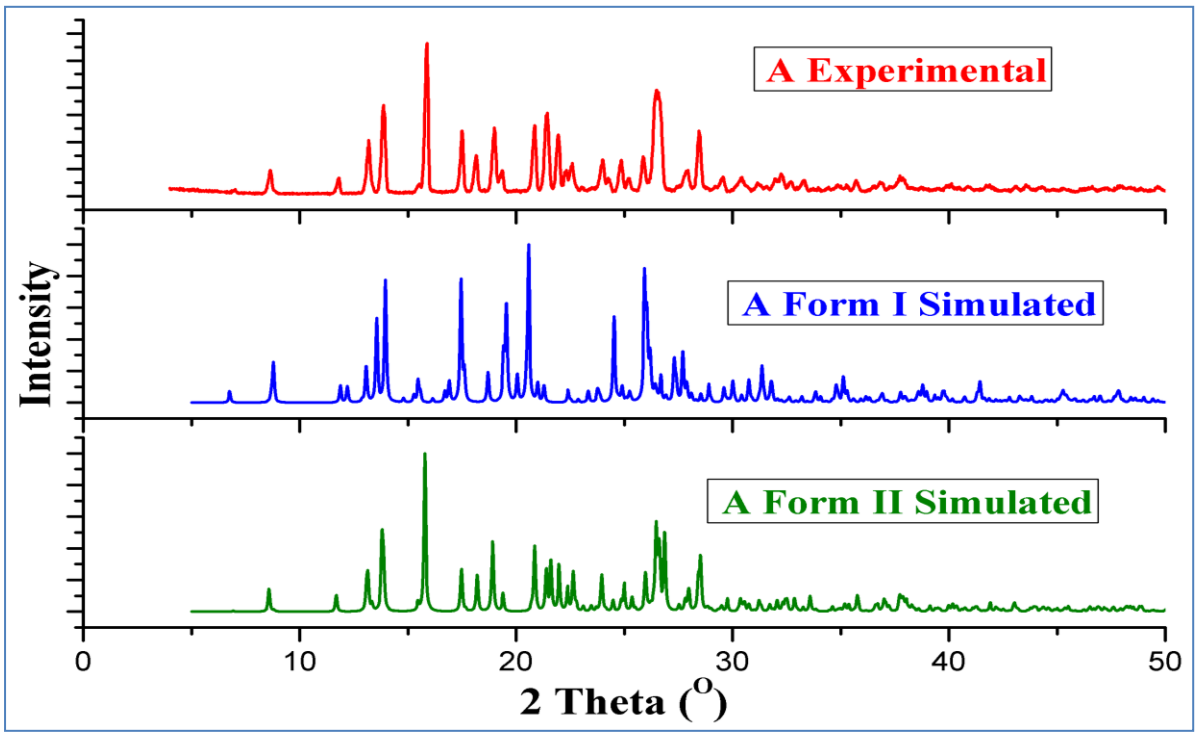
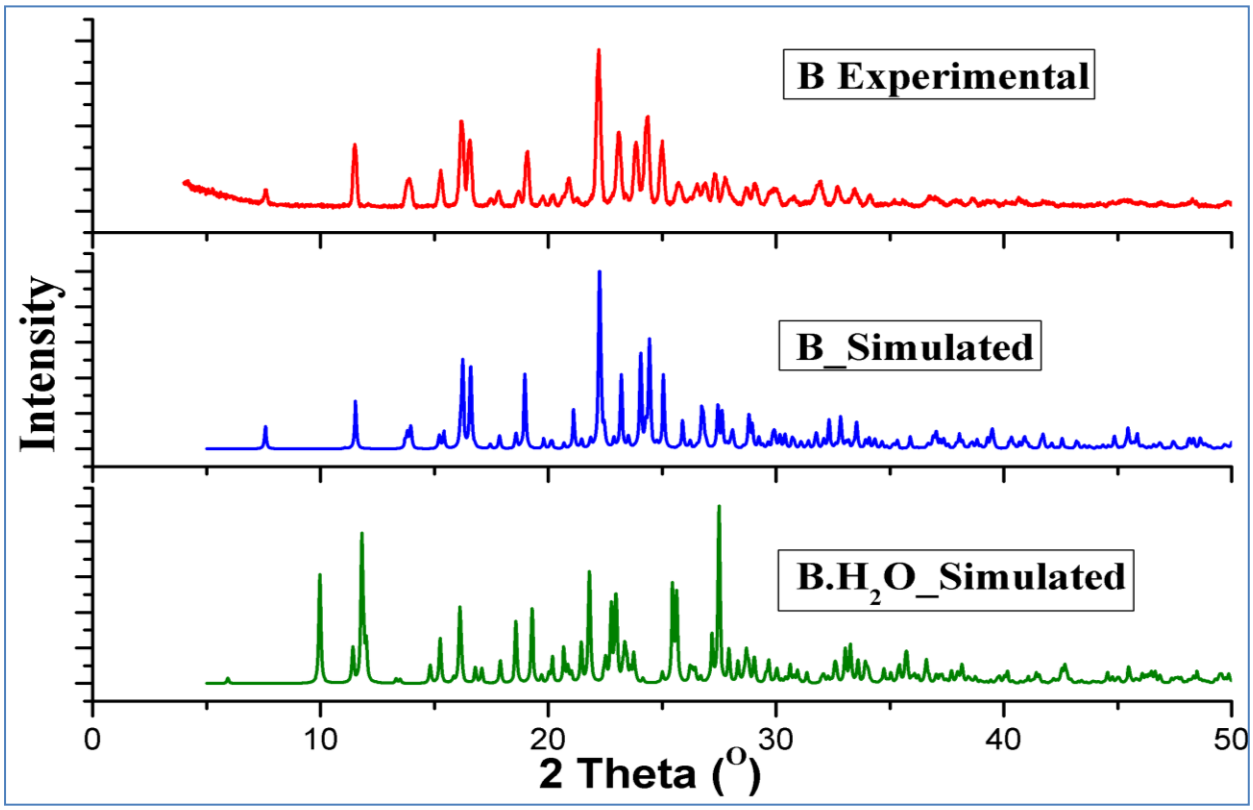


Figure S3: Comparison of the simulated diffraction pattern with the experimental PXRD (PXRD measurements were performed on a Bruker AXS D8 Advance X-ray diffractometer using Cu radiation with 1.5418Å):

(a) A



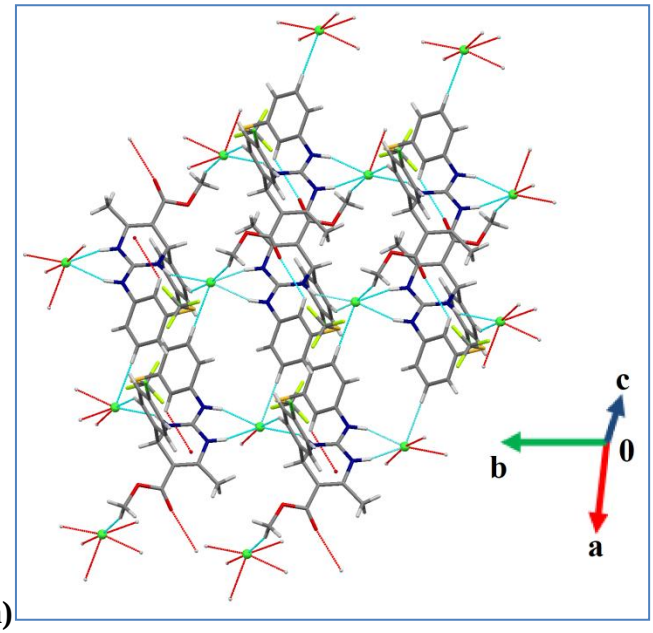
(b) B



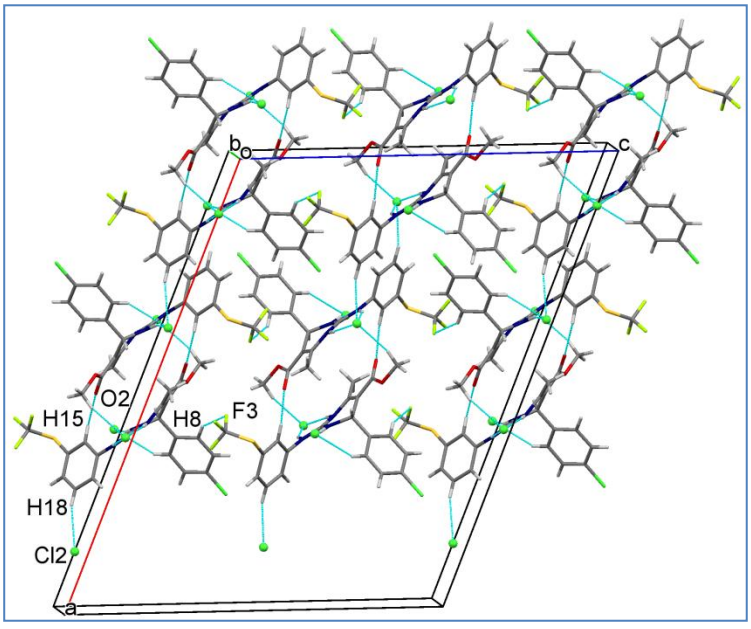
Section IIA: Packing diagrams of all the crystal structures:

A Form I:

(a)



(b)



A Form II:

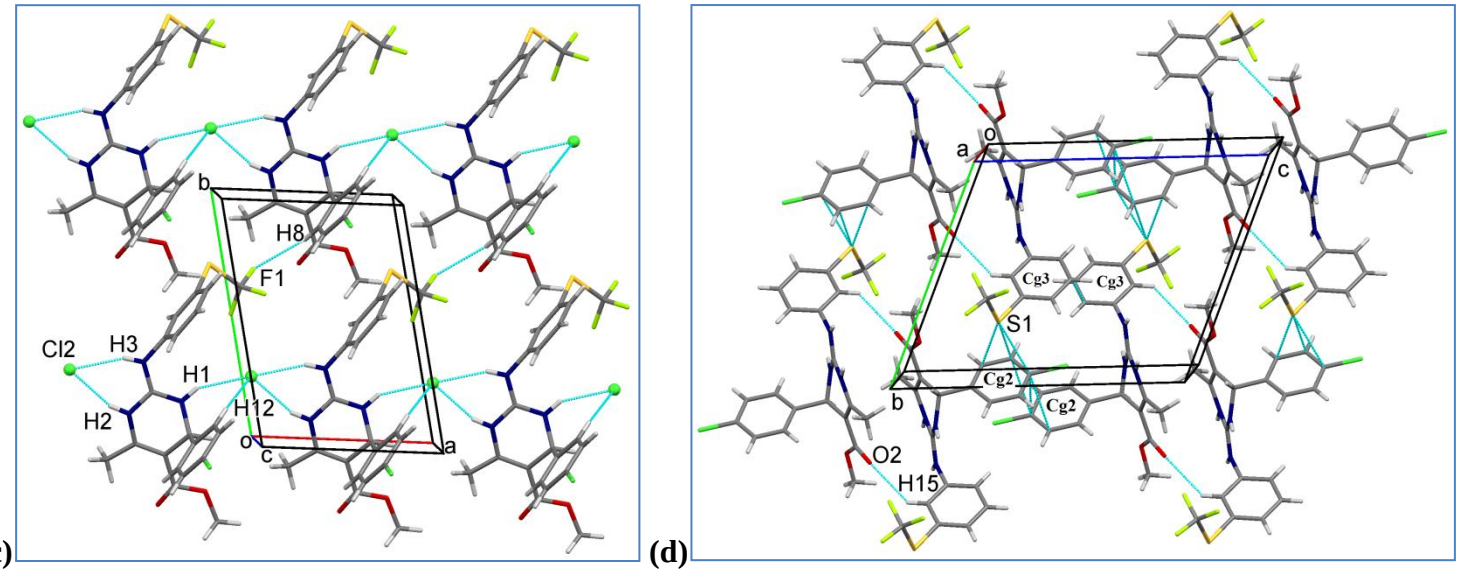
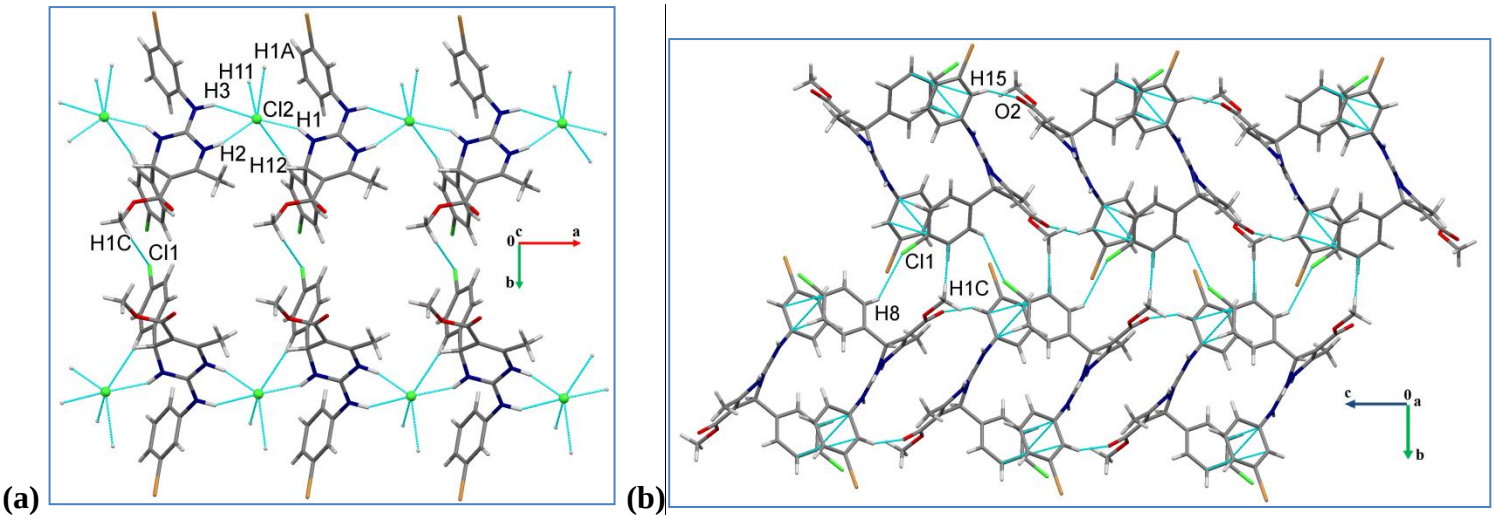


Figure S4: Molecular packing in **A Form I** [(a) – (b)] and in **A Form II** [(c) – (d)].

B:



B·H_2O:

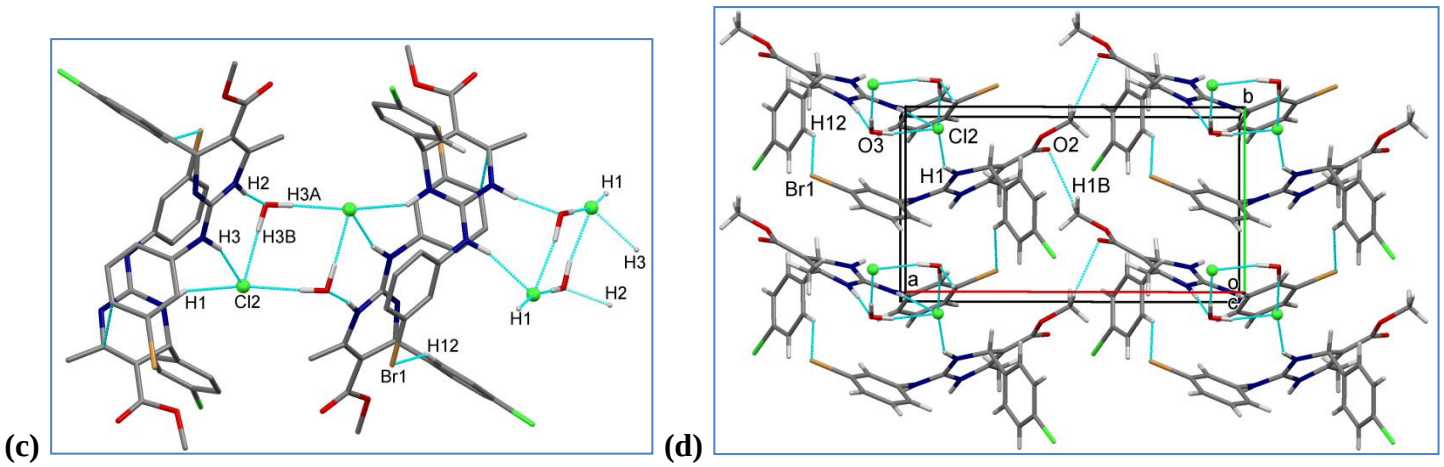


Figure S5: Displaying packing of molecules in **B** [(a) – (b)] and in **B·H$_2$O** [(c) – (d)].

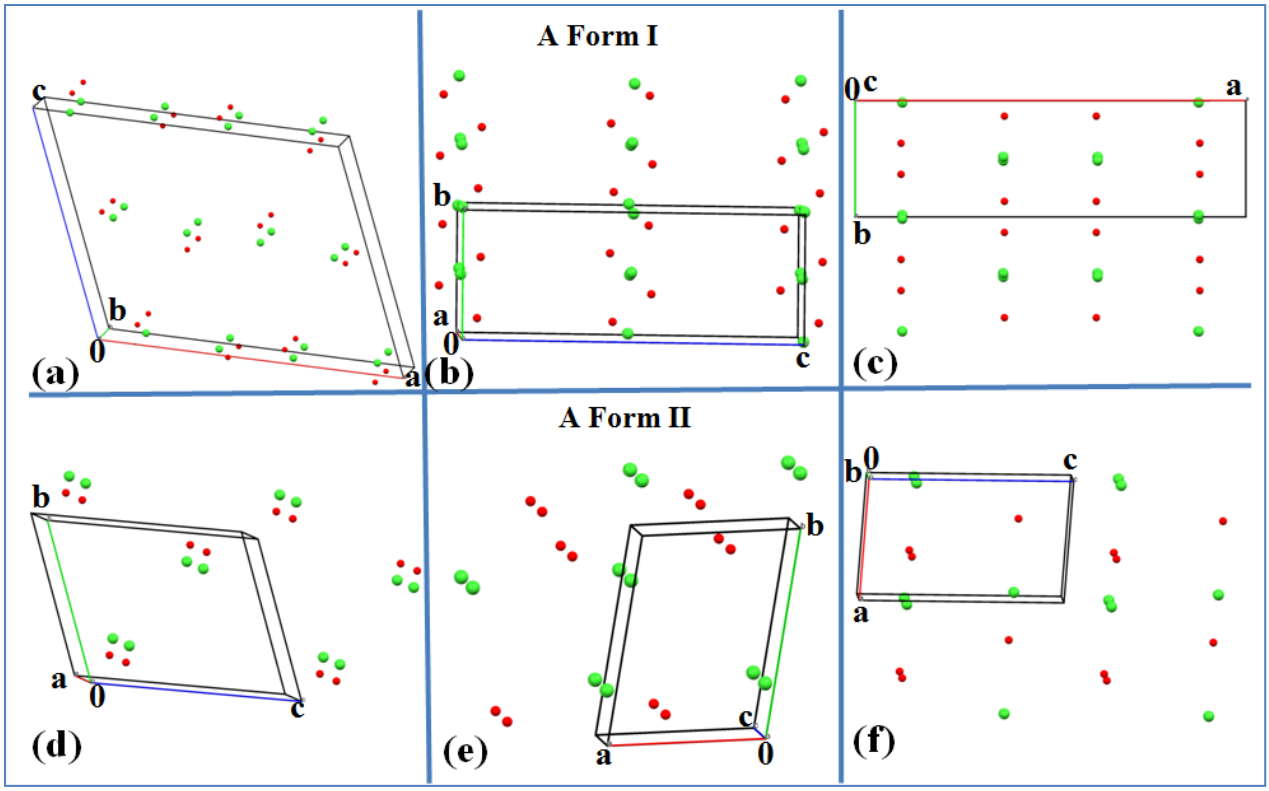


Figure S6 (a) – (f): Arrrangement of the ion pairs (the green ball and the red ball represent chloride ion and centroid of dihydropyrimidinium cation part respectively) in **A Form I** [(a) – (c)] and **Form II** [(d) – (f)].

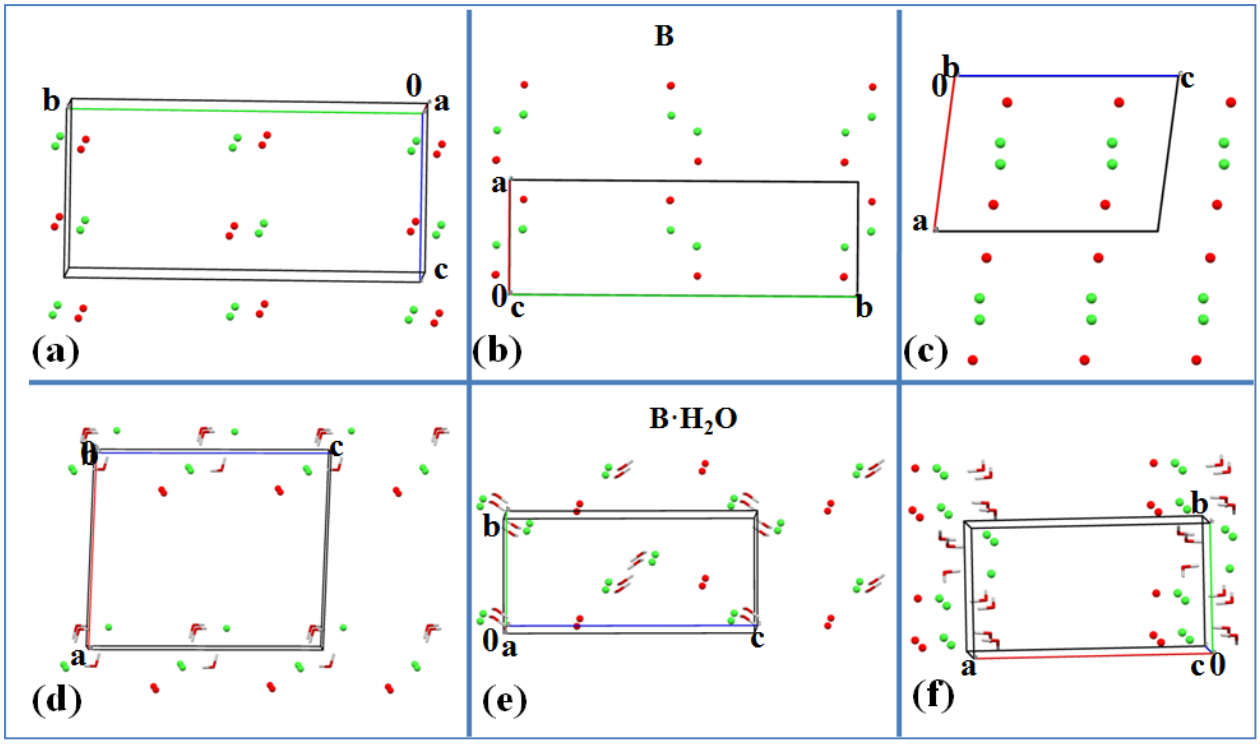


Figure S7 (a) – (f): Arrrangement of the ion pairs (the green ball and the red ball represent chloride ion and centroid of dihydropyrimidinium cation part respectively) in **B** [(a) – (c)] and **B·H$_2$O** [(d) – (f)].

Section IIB: XPAC Analysis

The XPAC method allows for the identification of similar packing arrangements present between two crystal structures. In this program, common structural motifs present in crystal structures to be compared are termed as 'supramolecular constracts' (SC). It may be 0D similarity, 1D similarity (row of molecules match), 2D similarity (layer of molecules match) and 3D similarity (isostructural). XPAC also defines the dissimilarity index 'X' which is a measure of how far the two crystal structures deviate from perfect geometrical similarity.

For XPAC analysis the circled atoms, labeled with C2, C3, C4, C6, C7, C8, C12-C15, C19, N1-N3, O1, O2, ,were consider for '**corresponding ordered sets of points**' (COSPs) [**Fig S5**]. The filter setting a/p/d: 10/14/1.50 was applied for all comparisons.

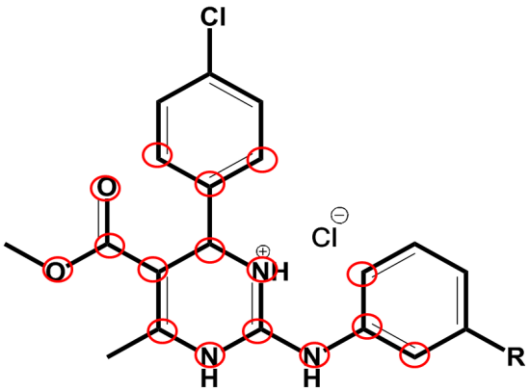


Figure S8: Selection of atoms for COSP denoted with red circles in all structures.

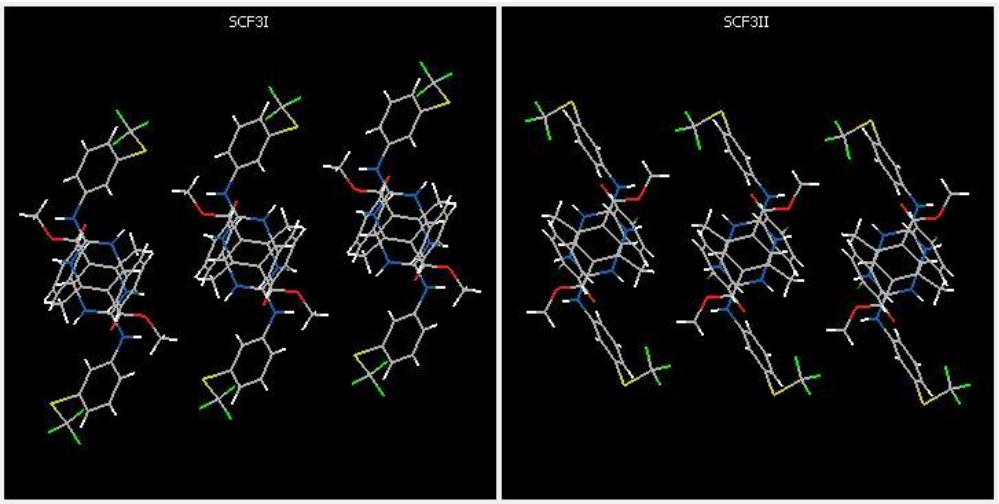


Figure S9(a): Comparison of the crystal packing between **A Form I** and **A Form II** by XPAC, depicting 1D SC.

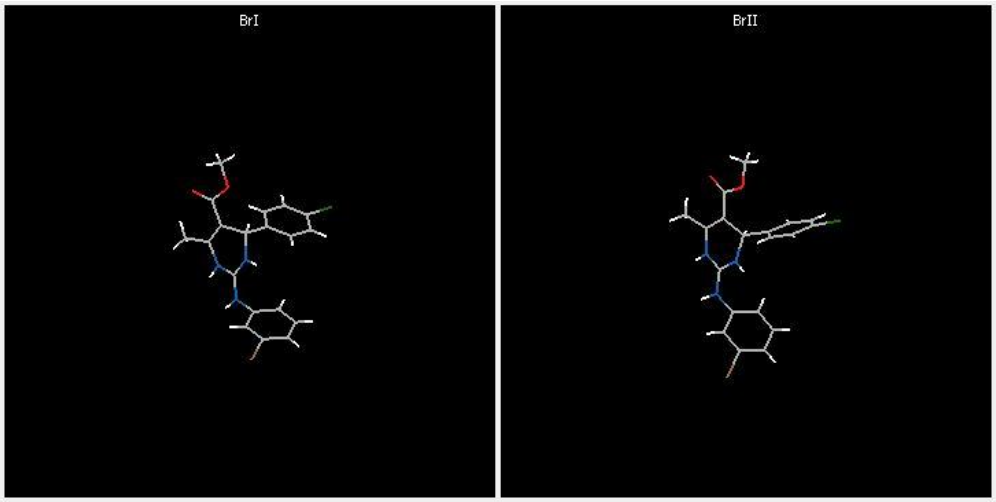


Figure S9(b): Comparison of the crystal packing between **B Form I** and **B Form II** by XPAC, depicting 0D SC.

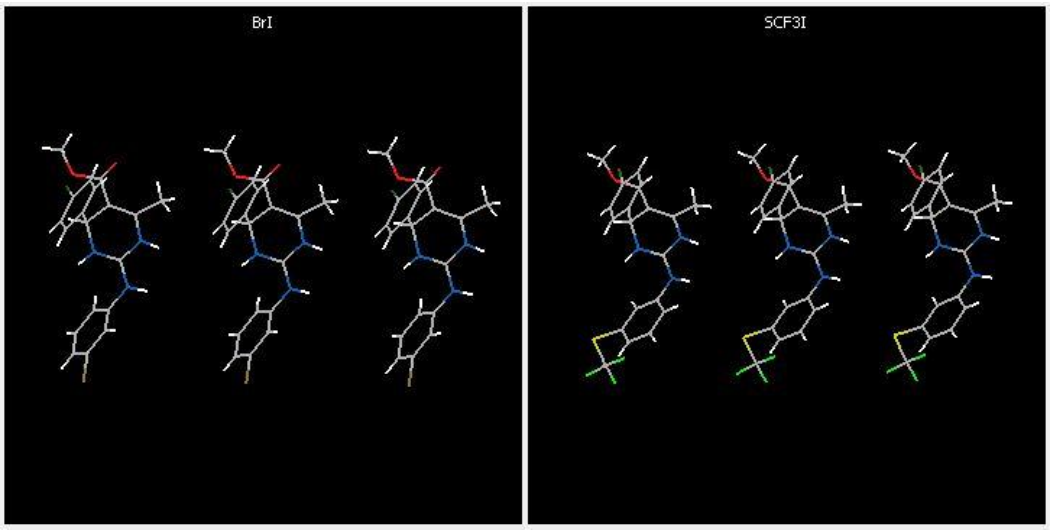


Figure S9(c): Comparison of the crystal packing between **B** and **A Form I** by XPAC, depicting 1D SC.

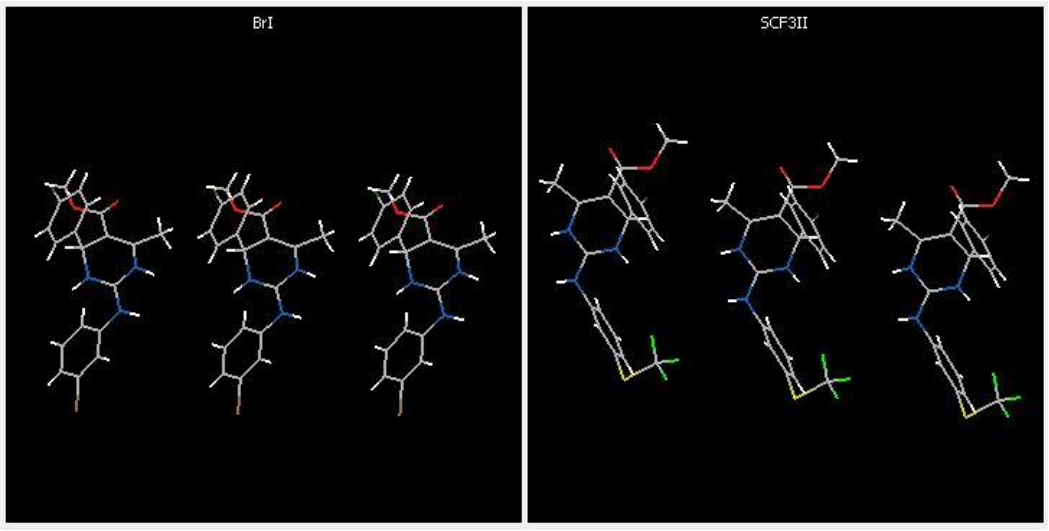


Figure S9(d): Comparison of the crystal packing between **B** and **A Form II** by XPAC, depicting 1D SC.

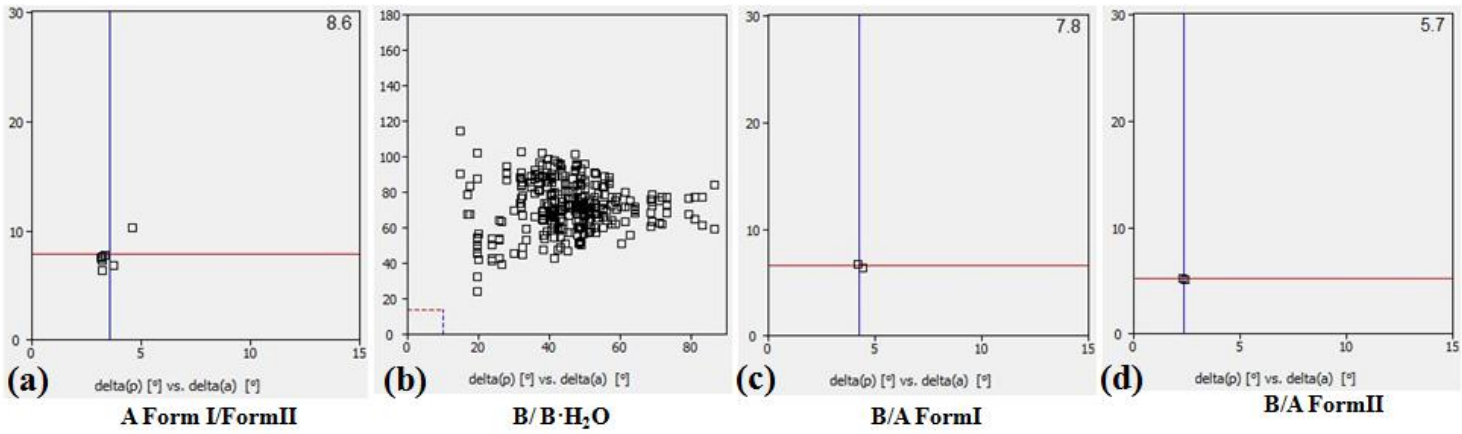


Figure S10: XPAC plots δp [y-axis] against δa [x-axis] (both in °), displaying the degree of similarity. Upper right corner is the dissimilarity index X, vertical and horizontal lines are the mean values of δa and δp, respectively.

Section IIIA: Results from Conformational analysis and Theoretical Calculations**:**

Table S1: Ring puckering and least squares plane analysis: Values in *italic* are obtained from B3LYP/6-311+G* calculation

	Ring puckering analysis of monocyclic ring C3-C4-N2-C13-N1-C6				**Deviation (Å) of C6 & N2 from plane C3/C4/C13/N1**	
	Puckering amplitude (Q, Å)	Phi, φ (°)	Theta, θ (°)	Conformation [**36**]	**C6**	**N2**
A Form I	0.382(3)	235.3(4)	103.7(5)	Boat	0.440(3) *0.335*	0.210(2) *0.088*
A Form II	0.352(2)	230.4(4)	107.3(3)	Boat	0.426(2) *0.335*	0.159(2) *0.113*
B	0.395(3)	235.6(5)	104.5(4)	Boat	0.460(3) *0.330*	0.211(3) *0.110*
B•H2O	0.285 (2)	352.5(3)	108.4(3)	Boat	0.286(2) *0.346*	0.113(2) *0.112*

Table S2: Selected Torsion Angles (º) represented as blue arrow in the scheme 1. Values in *italics* are obtained from theoretical B3LYP/6-311+G* calculation.

	Torsion 1(º) **O2-C2- C3- C6**	**Torsion 2(º)** **C3-C6-C7-C12**	**Torsion 3(º)** **C14-N3-C13-N2**	**Torsion 4(º)** **C13-N3-C14-C19**	**Torsion 5(º)** **C20-S1-C16-C15**
A Form I	171.3(3) *176.09*	177.8(2) *135.35*	179.1(2) *178.46*	129.8(3) *-134.93*	98.0(2) *85.66*
A Form II	178.0(2) *174.62*	176.3(2) *136.54*	172.8(2) *176.30*	78.3(3) *-59.84*	82.9(2) *-95.44*
B	177.3(3) *-173.35*	170.6(3) *-137.37*	173.8(3) *-176.82*	67.2(4) *55.98*	------
B•H2O	174.6(2) *172.06*	61.8(3) *-46.45*	165.6(2) *173.27*	52.3(3) *-54.25*	------

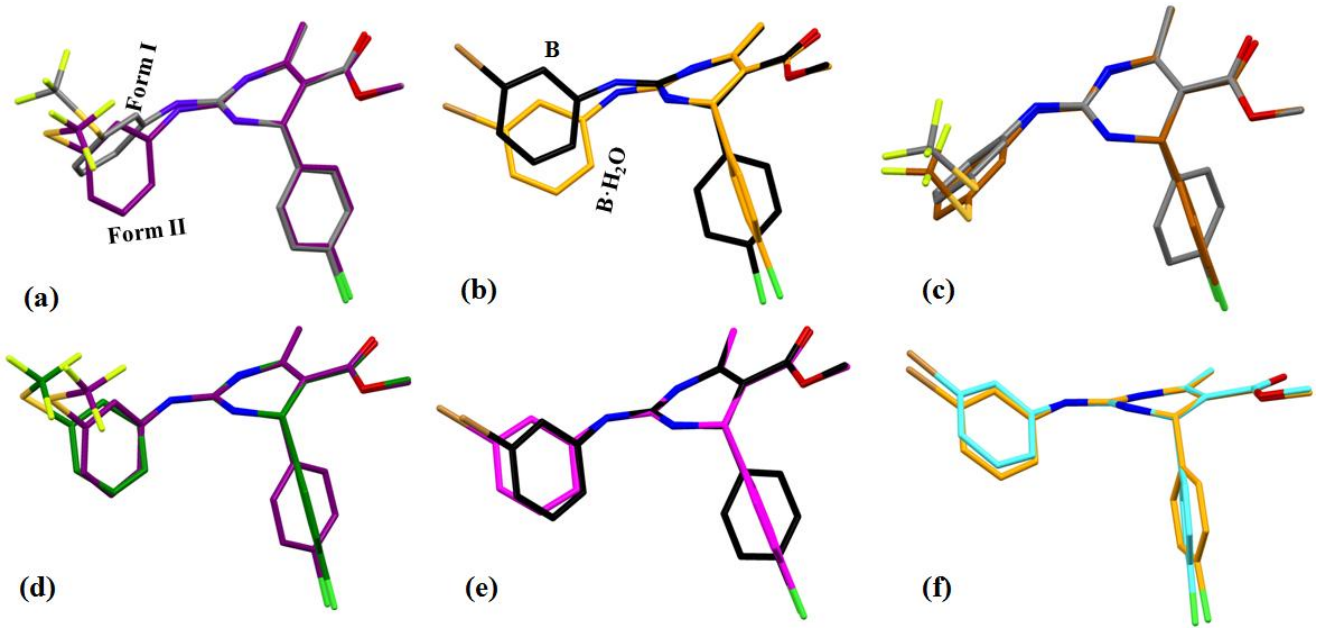


Figure S11: **(a)** Molecular overlay of the two forms of **A**. **(b)** Molecular overlay of the **B/B·H_2O**. **(c)** Molecular overlay of the **A Form I** with its optimized geometry (C- atoms are Brown). **(d)** Molecular overlay of the **A Form II** with its optimized geometry (C- atoms are Green). **(e)** Molecular overlay of the **B** with its optimized geometry (C- atoms are Magenta). **(f)** Molecular overlay of the **B·H_2O** with its optimized geometry (C- atoms are Cyan).

Table S3: lists of interaction energy of molecular at DFT+Disp (B97-D)/aug-cc-pVTZ (**in bold**). For comparison, counter poise corrected interaction energy of the molecular pairs for A Form I was also calculated at MP2/6-311G** (*in italic*)

Molecular motifs	**Interaction Energy (kcal/mol)**	**Counter Poise corrected Interaction Energy (kcal/mol)**	**BSSE (kcal/mol)**
A Form I			
I	-109.52 *-110.49*	-109.38 *-106.27*	0.14 *4.22*
II	-96.36 *-98.25*	-96.21 *-92.66*	0.15 *5.59*
III	-61.98 *-58.60*	-61.92 *-57.16*	0.06 *1.44*
IV	-55.85 *-51.11*	-55.79 *-49.60*	0.06 *1.51*
V	21.76 20.10	22.39 *24.94*	0.63 *4.84*

VI	28.31 *29.42*	28.66 *31.40*	0.35 *1.98*
VII	29.02 *27.01*	29.77 *32.17*	0.75 *5.16*
VIII	19.22 *17.72*	19.74 *21.59*	0.52 *3.87*
IX	22.57 *21.48*	22.88 *24.55*	0.31 *3.07*
X	23.02 22.20	24.06 28.98	1.04 6.78
A Form II			
I	-108.28	-108.13	0.15
II	-92.18	-92.01	0.17
III	-59.93	-59.88	0.05
IV	-53.14	-53.10	0.04
V	21.82	22.23	0.41
VI	26.67	27.08	0.41
VII	26.77	27.46	0.69
VIII	32.48	32.99	0.51
IX	22.16	22.78	0.62
X	24.96	26.09	1.13
B			
I	-107.05	-106.91	0.14
II	-94.16	-94.01	0.15
III	-62.98	-62.92	0.06
IV	-61.30	-61.20	0.10
V	20.04	20.29	0.25
VI	28.39	29.24	0.85
VII	28.80	29.80	1.00
VIII	28.65	29.12	0.47
B·H_2O			
I	-93.82	-93.71	0.11
II	-89.67	-89.54	0.13
III	-7.41	-7.23	0.18
IV	-13.81	-13.78	0.03
V	-13.59	-13.56	0.03
VI	-0.92	-0.83	0.09
VII	22.61	22.98	0.37
VIII	31.66	32.52	0.86
IX	29.61	29.72	0.11
X	18.81	18.85	0.04

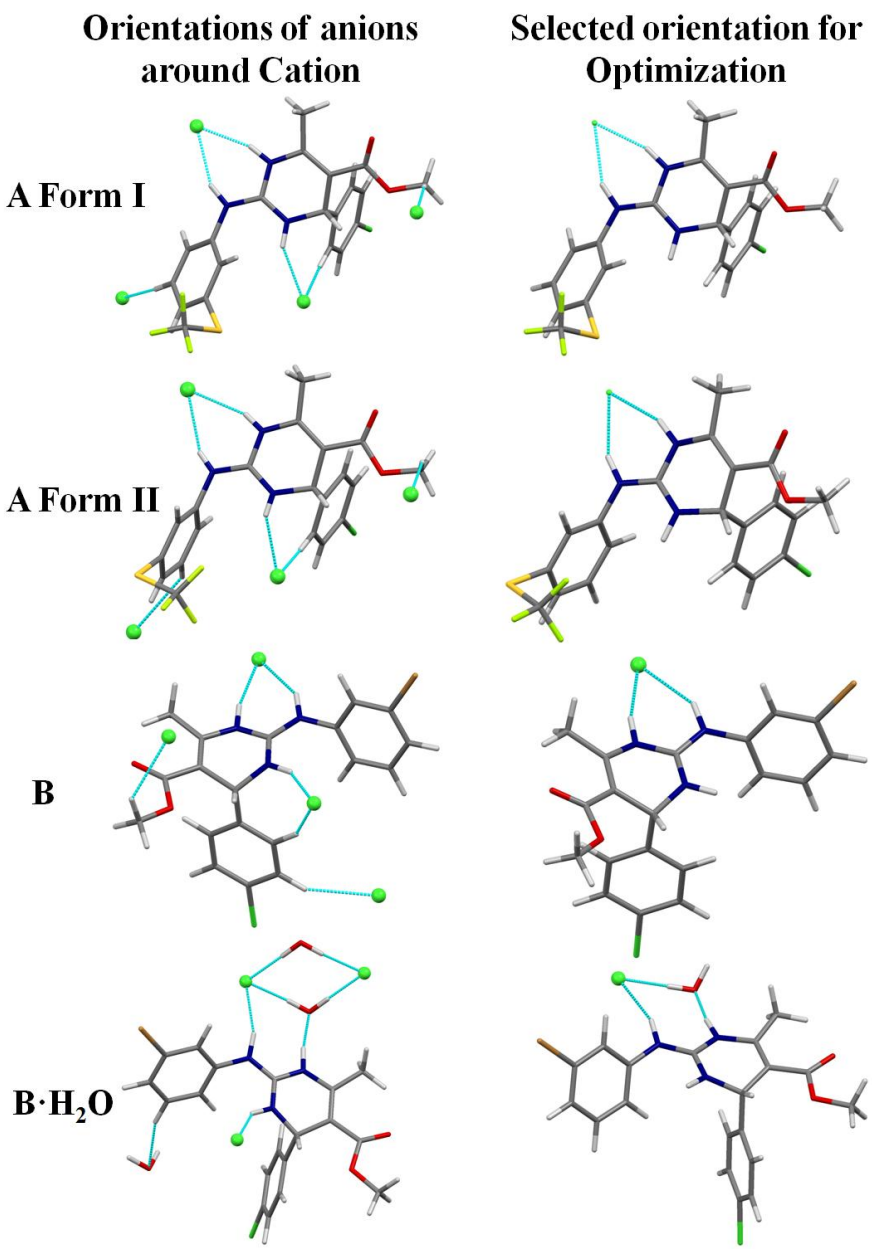
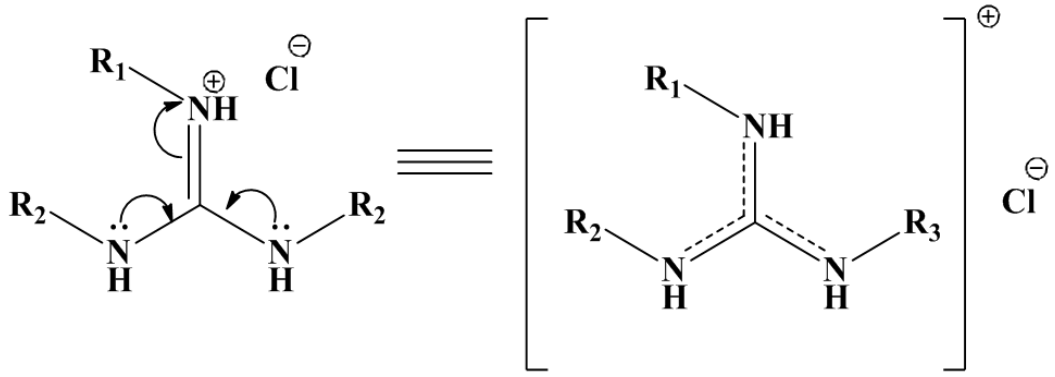


Figure S12: Most stable orientations (selected from single point energy calculations for all possible orientations) of Cation and anion, considered for geometry optimization.

Section IIIB: EUGEN method results



The positive charge was considered to be delocalized over the three Nitrogen atoms in all molecules. Each nitrogen atom was considered having an individual charge of +0.333333333 and the stoichiometry of the cation was taken as 3 for the calculations. The details of the output files are given below:

OUTPUT file: **A Form I**

program madelung
Begin counting lines...
Reached end of file
Number of lines counted = 37
Reading data from Madelung-input...
natoms before 32
Name of structure is SCF3I
28.1740000000000 7.76820000000000 21.9407000000000
90.0000000000000 112.101000000000 90.0000000000000
32 16 0.0000100
8 0.1108000000 0.3637000000 0.5434000000N 0.3333333330 1
9 0.0951000000 0.6483000000 0.5572000000N 0.3333333330 1
10 0.1428000000 0.5821000000 0.4956000000N 0.3333333330 1
56 0.8892000000 0.3637000000 0.9566000000N 0.3333333330 2
57 0.9049000000 0.6483000000 0.9428000000N 0.3333333330 2
58 0.8572000000 0.5821000000 1.0044000000N 0.3333333330 2
104 0.6108000000 0.8637000000 0.5434000000N 0.3333333330 3
105 0.5951000000 1.1483000000 0.5572000000N 0.3333333330 3
106 0.6428000000 1.0821000000 0.4956000000N 0.3333333330 3
152 0.3892000000 0.8637000000 0.9566000000N 0.3333333330 4
153 0.4049000000 1.1483000000 0.9428000000N 0.3333333330 4
154 0.3572000000 1.0821000000 1.0044000000N 0.3333333330 4
200 0.8892000000 0.6363000000 0.4566000000N 0.3333333330 5
201 0.9049000000 0.3517000000 0.4428000000N 0.3333333330 5
202 0.8572000000 0.4179000000 0.5045000000N 0.3333333330 5
248 0.1108000000 0.6363000000 0.0434000000N 0.3333333330 6
249 0.0951000000 0.3517000000 0.0572000000N 0.3333333330 6
250 0.1428000000 0.4179000000 -0.0044000000N 0.3333333330 6
296 0.3892000000 0.1363000000 0.4566000000N

OUTPUT file: **A Form II**

program madelung
Begin counting lines...
Reached end of file
Number of lines counted = 13
Reading data from Madelung-input...
natoms before 8
Name of structure is SCF3FormII
7.70050000000000 11.2405000000000 13.7322000000000
111.249000000000 90.9070000000000 99.7690000000000
8 4 0.0000100
8 0.6339000000 0.1398000000 0.2110000000N 0.3333333330 1
9 0.3328000000 0.0813000000 0.1749000000N 0.3333333330 1
10 0.4562000000 0.2962000000 0.2660000000N 0.3333333330 1
56 0.3661000000 0.8602000000 0.7890000000N 0.3333333330 2
57 0.6672000000 0.9187000000 0.8251000000N 0.3333333330 2
58 0.5438000000 0.7038000000 0.7340000000N 0.3333333330 2
97 0.9586000000 0.7469000000 0.7626000000Cl -1.0000000000 3
98 0.0414000000 0.2531000000 0.2374000000Cl -1.0000000000 4

The dipole moment of the unit cell is 0.00 compared to 0.01
Absolute Convergence
Minimum distance for each reference atom
1 N 3.14217515032691 0.333333333000000
2 N 3.13546754040507 0.333333333000000
3 N 3.14466059950297 0.333333333000000
4 N 3.14217515032691 0.333333333000000
5 N 3.13546754040506 0.333333333000000
6 N 3.14466059950297 0.333333333000000
7 Cl 3.13546754040506 -1.00000000000000
8 Cl 3.13546754040507 -1.00000000000000
For Ees calculations the following distance was seleceted as minimum
3.13546754040506
Electrostatic interactions for each reference atom within the unit cell
8 -7.131449699691819E-002
9 -0.106158307289560
10 -0.105810427872574
56 -7.131449699691819E-002

0.3333333330 7
297 0.4049000000 -0.1483000000 0.4428000000N
0.3333333330 7
298 0.3572000000 -0.0821000000 0.5045000000N
0.3333333330 7
344 0.6108000000 0.1363000000 0.0434000000N
0.3333333330 8
345 0.5951000000 -0.1483000000 0.0572000000N
0.3333333330 8
346 0.6428000000 -0.0821000000 -0.0045000000N
0.3333333330 8
385 0.3793000000 0.5157000000 0.5001000000Cl -
1.0000000000 9
386 0.6207000000 0.5157000000 0.9999000000Cl -
1.000000000010
387 0.8793000000 0.0157000000 0.5001000000Cl -
1.000000000011
388 0.1207000000 0.0157000000 0.9999000000Cl -
1.000000000012
389 0.6207000000 0.4843000000 0.4999000000Cl -
1.000000000013
390 0.3793000000 0.4843000000 0.0001000000Cl -
1.000000000014
391 0.1207000000 0.9843000000 0.4999000000Cl -
1.000000000015
392 0.8793000000 0.9843000000 0.0001000000Cl -
1.000000000016

The dipole moment of the unit cell is 0.00 compared to 0.01
Absolute Convergence
Minimum distance for each reference atom

1 N	3.14250633684583	0.333333333000000
2 N	3.09770690986220	0.333333333000000
3 N	3.19413210776253	0.333333333000000
4 N	3.14250639223057	0.333333333000000
5 N	3.09770687038318	0.333333333000000
6 N	3.19413206258576	0.333333333000000
7 N	3.14250633684583	0.333333333000000
8 N	3.09770690986220	0.333333333000000
9 N	3.19413210776253	0.333333333000000
10 N	3.14250639223057	0.333333333000000
11 N	3.09770687038318	0.333333333000000
12 N	3.19413206258576	0.333333333000000
13 N	3.14250633684583	0.333333333000000
14 N	3.09770690986220	0.333333333000000
15 N	3.19435857713412	0.333333333000000
16 N	3.14250639223057	0.333333333000000
17 N	3.09770687038318	0.333333333000000
18 N	3.19413206258576	0.333333333000000
19 N	3.14250633684583	0.333333333000000
20 N	3.09770690986220	0.333333333000000
21 N	3.19435857713412	0.333333333000000
22 N	3.14250639223057	0.333333333000000
23 N	3.09770687038318	0.333333333000000
24 N	3.19435853214817	0.333333333000000
25 Cl	3.09770690986220	-1.00000000000000
26 Cl	3.09770687038318	-1.00000000000000
27 Cl	3.09770690986220	-1.00000000000000
28 Cl	3.09770687038318	-1.00000000000000
29 Cl	3.09770690986220	-1.00000000000000
30 Cl	3.09770687038318	-1.00000000000000
31 Cl	3.09770690986220	-1.00000000000000
32 Cl	3.09770687038318	-1.00000000000000

For Ees calculations the following distance was seleceted as minimum
3.09770687038318
Electrostatic interactions for each reference atom within the unit cell

8	-6.853902312984182E-002
9	-0.107545334725556
10	-0.103518091959346
56	-3.903198682789315E-002
57	-3.292497426651955E-002
58	-4.311933799238908E-002
104	-0.105647044145228
57	-0.106158307289560
58	-0.105810427872574
97	-0.295602975711311
98	-0.295602975711311

DATA FOR ATOM 1 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.319380	-0.101643	0.030329
2	-0.320513	-0.102003	0.000360
3	-0.320605	-0.102033	0.000029
4	-0.320636	-0.102043	0.000010

DATA FOR ATOM 2 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.316951	-0.101086	0.005073
2	-0.314246	-0.100223	0.000863
3	-0.313594	-0.100015	0.000208
4	-0.313323	-0.099929	0.000086
5	-0.313186	-0.099885	0.000044
6	-0.313106	-0.099860	0.000025
7	-0.313057	-0.099844	0.000016
8	-0.313023	-0.099833	0.000011
9	-0.313000	-0.099826	0.000007

DATA FOR ATOM 3 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.347524	-0.110512	0.004702
2	-0.346983	-0.110340	0.000172
3	-0.346905	-0.110316	0.000025
4	-0.346875	-0.110306	0.000010

DATA FOR ATOM 4 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.319380	-0.101643	0.030329
2	-0.320513	-0.102003	0.000360
3	-0.320605	-0.102033	0.000029
4	-0.320636	-0.102043	0.000010

DATA FOR ATOM 5 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.316951	-0.101086	0.005073
2	-0.314246	-0.100223	0.000863
3	-0.313594	-0.100015	0.000208
4	-0.313323	-0.099929	0.000086
5	-0.313186	-0.099885	0.000044
6	-0.313106	-0.099860	0.000025
7	-0.313057	-0.099844	0.000016
8	-0.313023	-0.099833	0.000011
9	-0.313000	-0.099826	0.000007

DATA FOR ATOM 6 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.347524	-0.110512	0.004702
2	-0.346983	-0.110340	0.000172
3	-0.346905	-0.110316	0.000025
4	-0.346875	-0.110306	0.000010

DATA FOR ATOM 7 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.251553	-0.399160	0.103557
2	-1.262739	-0.402728	0.003568
3	-1.263568	-0.402992	0.000264
4	-1.263872	-0.403089	0.000097
5	-1.264029	-0.403139	0.000050
6	-1.264121	-0.403168	0.000029
7	-1.264179	-0.403187	0.000019
8	-1.264218	-0.403199	0.000012
9	-1.264246	-0.403208	0.000009

105 -6.298999356513908E-002
106 -6.634111523837702E-002
152 -5.789276831789804E-002
153 -4.993382730534779E-002
154 -4.908355633520314E-002
200 -6.854209545472564E-002
201 -0.107548197047767
202 -0.103509781030382
248 -3.903603525599027E-002
249 -3.292935487714773E-002
250 -4.312330333362359E-002
296 -0.105647783176847
297 -6.299082407678440E-002
298 -6.633883559353476E-002
344 -5.789701573258814E-002
345 -4.993744786957562E-002
346 -4.908470274278812E-002
385 -0.261683999464646
386 -0.191213786241317
387 -0.293803929761613
388 -9.510528881950943E-002
389 -0.261685367521903
390 -0.191198793490988
391 -0.293818963060238
392 -9.509809986077465E-002

DATA FOR ATOM 1 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.336531	-0.107090	0.038551
2	-0.347399	-0.110548	0.003458
3	-0.348739	-0.110975	0.000426
4	-0.348845	-0.111009	0.000034
5	-0.348810	-0.110997	0.000011
6	-0.348773	-0.110986	0.000012
7	-0.348748	-0.110978	0.000008

DATA FOR ATOM 2 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.327931	-0.105862	0.001683
2	-0.336861	-0.108745	0.002883
3	-0.338218	-0.109183	0.000438
4	-0.338361	-0.109230	0.000046
5	-0.338345	-0.109224	0.000005

DATA FOR ATOM 3 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.363648	-0.113849	0.010331
2	-0.369999	-0.115837	0.001988
3	-0.371016	-0.116156	0.000318
4	-0.371146	-0.116196	0.000041
5	-0.371147	-0.116196	0.000000

DATA FOR ATOM 4 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.329138	-0.104737	0.065706
2	-0.344779	-0.109715	0.004977
3	-0.347404	-0.110550	0.000835
4	-0.348035	-0.110751	0.000201
5	-0.348263	-0.110823	0.000073
6	-0.348379	-0.110860	0.000037
7	-0.348448	-0.110882	0.000022
8	-0.348494	-0.110897	0.000015
9	-0.348526	-0.110907	0.000010
10	-0.348550	-0.110915	0.000007

DATA FOR ATOM 5 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.317390	-0.102460	0.069535
2	-0.333196	-0.107562	0.005103
3	-0.336364	-0.108585	0.001023

DATA FOR ATOM 8 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.251553	-0.399160	0.103557
2	-1.262739	-0.402728	0.003568
3	-1.263568	-0.402992	0.000264
4	-1.263872	-0.403089	0.000097
5	-1.264029	-0.403139	0.000050
6	-1.264121	-0.403168	0.000029
7	-1.264179	-0.403187	0.000019
8	-1.264218	-0.403199	0.000012
9	-1.264246	-0.403208	0.000009

Average Madelung constant of cation is -0.9805

Average Madelung constant of anion is -1.2642

Average Madelung constant of salt is -1.1224

Minimum distance in the crystal is 3.1355

Electrostatic lattice energy is -497.0 kJ/mol

4	-0.337240	-0.108868	0.000283
5	-0.337591	-0.108981	0.000113
6	-0.337776	-0.109041	0.000060
7	-0.337889	-0.109077	0.000036
8	-0.337963	-0.109101	0.000024
9	-0.338016	-0.109118	0.000017
10	-0.338054	-0.109130	0.000012
11	-0.338082	-0.109140	0.000009

DATA FOR ATOM 6 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.354219	-0.110897	0.067777
2	-0.366672	-0.114795	0.003899
3	-0.369333	-0.115629	0.000833
4	-0.370129	-0.115878	0.000249
5	-0.370464	-0.115983	0.000105
6	-0.370644	-0.116039	0.000056
7	-0.370755	-0.116074	0.000035
8	-0.370828	-0.116097	0.000023
9	-0.370880	-0.116113	0.000016
10	-0.370917	-0.116125	0.000012
11	-0.370945	-0.116133	0.000009

DATA FOR ATOM 7 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.357720	-0.113833	0.008186
2	-0.350635	-0.111578	0.002254
3	-0.349051	-0.111074	0.000504
4	-0.348759	-0.110981	0.000093
5	-0.348701	-0.110963	0.000018
6	-0.348686	-0.110958	0.000005

DATA FOR ATOM 8 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.350044	-0.113001	0.050011
2	-0.341182	-0.110140	0.002861
3	-0.338789	-0.109368	0.000772
4	-0.338351	-0.109226	0.000141
5	-0.338271	-0.109201	0.000026
6	-0.338253	-0.109195	0.000006

DATA FOR ATOM 9 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.370393	-0.115960	0.049619
2	-0.372791	-0.116711	0.000751
3	-0.371676	-0.116362	0.000349
4	-0.371335	-0.116255	0.000107
5	-0.371231	-0.116223	0.000032
6	-0.371188	-0.116209	0.000013
7	-0.371164	-0.116202	0.000007

DATA FOR ATOM 10 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.354416	-0.112781	0.054888
2	-0.349647	-0.111264	0.001517
3	-0.348569	-0.110921	0.000343
4	-0.348474	-0.110891	0.000030
5	-0.348514	-0.110903	0.000013
6	-0.348554	-0.110916	0.000013
7	-0.348582	-0.110925	0.000009

DATA FOR ATOM 11 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.343530	-0.110898	0.060964
2	-0.339046	-0.109451	0.001448
3	-0.337720	-0.109023	0.000428
4	-0.337711	-0.109020	0.000003

DATA FOR ATOM 12 N

Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.362629	-0.113530	0.064446
2	-0.370327	-0.115940	0.002410
3	-0.370455	-0.115980	0.000040
4	-0.370606	-0.116027	0.000047
5	-0.370748	-0.116071	0.000044
6	-0.370844	-0.116102	0.000030
7	-0.370908	-0.116122	0.000020
8	-0.370950	-0.116135	0.000013
9	-0.370980	-0.116144	0.000009

DATA FOR ATOM 13 N
Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.336544	-0.107094	0.038552
2	-0.347413	-0.110553	0.003459
3	-0.348753	-0.110979	0.000426
4	-0.348860	-0.111013	0.000034
5	-0.348824	-0.111002	0.000011
6	-0.348787	-0.110990	0.000012
7	-0.348762	-0.110982	0.000008

DATA FOR ATOM 14 N
Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.327943	-0.105866	0.001682
2	-0.336875	-0.108750	0.002883
3	-0.338231	-0.109188	0.000438
4	-0.338375	-0.109234	0.000046
5	-0.338358	-0.109229	0.000005

DATA FOR ATOM 15 N
Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.363652	-0.113842	0.010332
2	-0.370004	-0.115831	0.001989
3	-0.371022	-0.116149	0.000319
4	-0.371152	-0.116190	0.000041
5	-0.371152	-0.116190	0.000000

DATA FOR ATOM 16 N
Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.329158	-0.104744	0.065708
2	-0.344800	-0.109721	0.004978
3	-0.347426	-0.110557	0.000835
4	-0.348056	-0.110758	0.000201
5	-0.348285	-0.110830	0.000073
6	-0.348400	-0.110867	0.000037
7	-0.348470	-0.110889	0.000022
8	-0.348516	-0.110904	0.000015
9	-0.348548	-0.110914	0.000010
10	-0.348571	-0.110921	0.000007

DATA FOR ATOM 17 N
Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.317410	-0.102466	0.069537
2	-0.333218	-0.107569	0.005103
3	-0.336386	-0.108592	0.001023
4	-0.337263	-0.108875	0.000283
5	-0.337614	-0.108988	0.000113
6	-0.337798	-0.109048	0.000060
7	-0.337911	-0.109084	0.000036
8	-0.337986	-0.109108	0.000024
9	-0.338038	-0.109125	0.000017
10	-0.338076	-0.109138	0.000012
11	-0.338105	-0.109147	0.000009

DATA FOR ATOM 18 N
Iteration Madelung constant Ees a.u. Difference in Ees

1	-0.354233	-0.110901	0.067778
2	-0.366687	-0.114800	0.003899

3	-0.369349	-0.115633	0.000833
4	-0.370144	-0.115883	0.000249
5	-0.370480	-0.115988	0.000105
6	-0.370660	-0.116044	0.000056
7	-0.370771	-0.116079	0.000035
8	-0.370844	-0.116102	0.000023
9	-0.370896	-0.116118	0.000016
10	-0.370933	-0.116130	0.000012
11	-0.370961	-0.116138	0.000009

DATA FOR ATOM 19 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.357729	-0.113836	0.008188
2	-0.350645	-0.111581	0.002254
3	-0.349060	-0.111077	0.000504
4	-0.348768	-0.110984	0.000093
5	-0.348711	-0.110966	0.000018
6	-0.348695	-0.110961	0.000005

DATA FOR ATOM 20 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.350054	-0.113004	0.050013
2	-0.341194	-0.110144	0.002860
3	-0.338801	-0.109371	0.000772
4	-0.338363	-0.109230	0.000141
5	-0.338283	-0.109204	0.000026
6	-0.338264	-0.109198	0.000006

DATA FOR ATOM 21 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.370388	-0.115951	0.049612
2	-0.372787	-0.116702	0.000751
3	-0.371672	-0.116353	0.000349
4	-0.371330	-0.116246	0.000107
5	-0.371226	-0.116213	0.000032
6	-0.371183	-0.116200	0.000013
7	-0.371160	-0.116192	0.000007

DATA FOR ATOM 22 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.354429	-0.112785	0.054888
2	-0.349662	-0.111268	0.001517
3	-0.348584	-0.110925	0.000343
4	-0.348489	-0.110895	0.000030
5	-0.348529	-0.110908	0.000013
6	-0.348569	-0.110921	0.000013
7	-0.348597	-0.110929	0.000009

DATA FOR ATOM 23 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.343544	-0.110903	0.060965
2	-0.339062	-0.109456	0.001447
3	-0.337736	-0.109028	0.000428
4	-0.337727	-0.109025	0.000003

DATA FOR ATOM 24 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.362623	-0.113520	0.064435
2	-0.370326	-0.115931	0.002411
3	-0.370455	-0.115972	0.000040
4	-0.370606	-0.116019	0.000047
5	-0.370747	-0.116063	0.000044
6	-0.370844	-0.116093	0.000030
7	-0.370908	-0.116113	0.000020
8	-0.370950	-0.116127	0.000013
9	-0.370980	-0.116136	0.000009

DATA FOR ATOM 25 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees

1	-1.146895	-0.370240	0.108556
2	-1.178023	-0.380289	0.010049
3	-1.182785	-0.381826	0.001537
4	-1.183606	-0.382091	0.000265
5	-1.183785	-0.382149	0.000058
6	-1.183844	-0.382168	0.000019
7	-1.183874	-0.382177	0.000010

DATA FOR ATOM 26 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.156060	-0.373199	0.181985
2	-1.181359	-0.381366	0.008167
3	-1.184478	-0.382373	0.001007
4	-1.184627	-0.382421	0.000048
5	-1.184466	-0.382369	0.000052
6	-1.184330	-0.382325	0.000044
7	-1.184238	-0.382295	0.000030
8	-1.184174	-0.382275	0.000020
9	-1.184130	-0.382260	0.000014
10	-1.184097	-0.382250	0.000011
11	-1.184073	-0.382242	0.000008

DATA FOR ATOM 27 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.195895	-0.386058	0.092254
2	-1.187735	-0.383424	0.002634
3	-1.184385	-0.382343	0.001081
4	-1.183813	-0.382158	0.000185
5	-1.183774	-0.382145	0.000013
6	-1.183804	-0.382155	0.000010

DATA FOR ATOM 28 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.150949	-0.371549	0.276443
2	-1.171277	-0.378111	0.006562
3	-1.176005	-0.379637	0.001526
4	-1.178761	-0.380527	0.000890
5	-1.180410	-0.381059	0.000532
6	-1.181412	-0.381383	0.000323
7	-1.182050	-0.381589	0.000206
8	-1.182478	-0.381727	0.000138
9	-1.182779	-0.381824	0.000097
10	-1.182997	-0.381895	0.000071
11	-1.183162	-0.381948	0.000053
12	-1.183288	-0.381988	0.000041
13	-1.183387	-0.382020	0.000032
14	-1.183466	-0.382046	0.000026
15	-1.183530	-0.382067	0.000021
16	-1.183583	-0.382084	0.000017
17	-1.183627	-0.382098	0.000014
18	-1.183664	-0.382110	0.000012
19	-1.183696	-0.382120	0.000010
20	-1.183722	-0.382129	0.000009

DATA FOR ATOM 29 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.146919	-0.370248	0.108562
2	-1.178046	-0.380296	0.010048
3	-1.182808	-0.381833	0.001537
4	-1.183629	-0.382098	0.000265
5	-1.183807	-0.382156	0.000058
6	-1.183867	-0.382175	0.000019
7	-1.183896	-0.382185	0.000010

DATA FOR ATOM 30 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.156056	-0.373197	0.181998
2	-1.181351	-0.381363	0.008166
3	-1.184470	-0.382370	0.001007

4	-1.184619	-0.382418	0.000048
5	-1.184457	-0.382366	0.000052
6	-1.184322	-0.382322	0.000044
7	-1.184229	-0.382292	0.000030
8	-1.184166	-0.382272	0.000020
9	-1.184121	-0.382257	0.000014
10	-1.184089	-0.382247	0.000011
11	-1.184064	-0.382239	0.000008

DATA FOR ATOM 31 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.195942	-0.386073	0.092254
2	-1.187785	-0.383440	0.002633
3	-1.184435	-0.382359	0.001081
4	-1.183862	-0.382174	0.000185
5	-1.183823	-0.382161	0.000013
6	-1.183853	-0.382171	0.000010

DATA FOR ATOM 32 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.150948	-0.371548	0.276450
2	-1.171277	-0.378111	0.006563
3	-1.176004	-0.379637	0.001526
4	-1.178761	-0.380527	0.000890
5	-1.180409	-0.381059	0.000532
6	-1.181411	-0.381382	0.000323
7	-1.182049	-0.381588	0.000206
8	-1.182477	-0.381727	0.000138
9	-1.182778	-0.381824	0.000097
10	-1.182996	-0.381894	0.000071
11	-1.183161	-0.381947	0.000053
12	-1.183287	-0.381988	0.000041
13	-1.183386	-0.382020	0.000032
14	-1.183465	-0.382046	0.000026
15	-1.183529	-0.382066	0.000021
16	-1.183582	-0.382083	0.000017
17	-1.183626	-0.382098	0.000014
18	-1.183663	-0.382110	0.000012
19	-1.183695	-0.382120	0.000010
20	-1.183721	-0.382128	0.000009

Average Madelung constant of cation is -1.0578

Average Madelung constant of anion is -1.1839

Average Madelung constant of salt is -1.1208

Minimum distance in the crystal is 3.0977

Electrostatic lattice energy is -502.4 kJ/mol

OUTPUT file: **B**

```
program madelung
 Begin counting lines...
 Reached end of file
 Number of lines counted =          21
 Reading data from Madelung-input...
 natoms before          16
 Name of structure is Br1
   7.72940000000000       23.2900000000000
11.0671000000000
   90.0000000000000       97.6080000000000
90.0000000000000
 16  8 0.0000100
  5      0.8029000000      0.0070000000      0.7220000000N
0.3333333330 1
  6      1.0854000000      0.0282000000      0.6954000000N
0.3333333330 1
```

OUTPUT file: **B·H_2O**

```
program madelung
 Begin counting lines...
 Reached end of file
 Number of lines counted =          21
 Reading data from Madelung-input...
 natoms before          16
 Name of structure is Br2
   7.72940000000000       23.2900000000000
11.0671000000000
   90.0000000000000       97.6080000000000
90.0000000000000
 16  8 0.0000100
  5      0.8454000000      0.6487000000      0.2167000000N
0.3333333330 1
  7      0.8327000000      0.5430000000      0.3360000000N
0.3333333330 1
```

7 1.0279000000 -0.0556000000 0.7931000000N 0.3333333330 1
49 0.1971000000 0.5070000000 0.7780000000N 0.3333333330 2
50 -0.0854000000 0.5282000000 0.8046000000N 0.3333333330 2
51 -0.0279000000 0.4444000000 0.7069000000N 0.3333333330 2
93 0.1971000000 0.9930000000 0.2780000000N 0.3333333330 3
94 -0.0854000000 0.9718000000 0.3046000000N 0.3333333330 3
95 -0.0279000000 1.0556000000 0.2069000000N 0.3333333330 3
137 0.8029000000 0.4930000000 0.2220000000N 0.3333333330 4
138 1.0854000000 0.4718000000 0.1954000000N 0.3333333330 4
139 1.0279000000 0.5556000000 0.2931000000N 0.3333333330 4
177 0.5689000000 0.0377000000 0.2567000000Cl - 1.0000000000 5
178 0.4311000000 0.5377000000 0.2434000000Cl - 1.0000000000 6
179 0.4311000000 0.9623000000 0.7434000000Cl - 1.0000000000 7
180 0.5689000000 0.4623000000 0.7567000000Cl - 1.0000000000 8

The dipole moment of the unit cell is 0.00 compared to 0.01
Absolute Convergence
Minimum distance for each reference atom
1 N 3.09496329368641 0.333333333000000
2 N 3.06624449325737 0.333333333000000
3 N 3.26232570270591 0.333333333000000
4 N 3.09474282059357 0.333333333000000
5 N 3.06618050283718 0.333333333000000
6 N 3.26265246919452 0.333333333000000
7 N 3.09474274301138 0.333333333000000
8 N 3.06618064296548 0.333333333000000
9 N 3.26265244053800 0.333333333000000
10 N 3.09496337123052 0.333333333000000
11 N 3.06624435308356 0.333333333000000
12 N 3.26232573137765 0.333333333000000
13 Cl 3.06618064296548 -1.00000000000000
14 Cl 3.06624435308356 -1.00000000000000
15 Cl 3.06624449325737 -1.00000000000000
16 Cl 3.06618050283718 -1.00000000000000
For Ees calculations the following distance was seleceted as minimum
3.06618050283718
Electrostatic interactions for each reference atom within the unit cell
5 -6.818599903243396E-002
6 -6.150704634055237E-002
7 -5.238460151069108E-002
49 -0.128621245293808
50 -7.969855912118778E-002
51 -9.209445940752217E-002
93 -6.817314975682542E-002
94 -6.149888970678721E-002
95 -5.237781472237221E-002
137 -0.128603863208839
138 -7.968929791511936E-002
139 -9.208687103693680E-002
177 -0.158900927529270
178 -0.199851490908815
179 -0.158871747406372
180 -0.199840025887786

DATA FOR ATOM 1 N
Iteration Madelung constant Ees a.u. Difference in Ees

1 -0.480665 -0.155306 0.087120
2 -0.484136 -0.156427 0.001121

9 0.9663000000 0.5113000000 0.2747000000N 0.3333333330 1
49 0.1546000000 0.1487000000 0.2833000000N 0.3333333330 2
51 0.1673000000 0.0430000000 0.1640000000N 0.3333333330 2
53 0.0337000000 0.0113000000 0.2253000000N 0.3333333330 2
93 0.1546000000 0.3513000000 0.7833000000N 0.3333333330 3
95 0.1673000000 0.4570000000 0.6640000000N 0.3333333330 3
97 0.0337000000 0.4887000000 0.7253000000N 0.3333333330 3
137 0.8454000000 0.8513000000 0.7167000000N 0.3333333330 4
139 0.8327000000 0.9570000000 0.8360000000N 0.3333333330 4
141 0.9663000000 0.9887000000 0.7747000000N 0.3333333330 4
177 0.9026000000 0.8864000000 0.0916000000Cl - 1.0000000000 5
178 0.0974000000 0.3864000000 0.4084000000Cl - 1.0000000000 6
179 0.0974000000 0.1136000000 0.9084000000Cl - 1.0000000000 7
180 0.9026000000 0.6136000000 0.5916000000Cl - 1.0000000000 8

The dipole moment of the unit cell is 0.00 compared to 0.01
Absolute Convergence
Minimum distance for each reference atom
1 N 4.19436299146301 0.333333333000000
2 N 3.25464112347699 0.333333333000000
3 N 3.35872790433248 0.333333333000000
4 N 4.19436291323554 0.333333333000000
5 N 3.25464127227643 0.333333333000000
6 N 3.35872771557540 0.333333333000000
7 N 4.19436299146301 0.333333333000000
8 N 3.25464112347699 0.333333333000000
9 N 3.35872790433248 0.333333333000000
10 N 4.19436291323554 0.333333333000000
11 N 3.25464127227643 0.333333333000000
12 N 3.35872771557540 0.333333333000000
13 Cl 3.25464127227643 -1.00000000000000
14 Cl 3.25464112347699 -1.00000000000000
15 Cl 3.25464127227643 -1.00000000000000
16 Cl 3.25464112347699 -1.00000000000000
For Ees calculations the following distance was seleceted as minimum
3.25464112347699
Electrostatic interactions for each reference atom within the unit cell
5 -0.101509612321270
7 -0.112281034263648
9 -8.741991170603053E-002
49 -6.303208154485176E-002
51 -4.681031342132440E-002
53 -4.861380525270805E-002
93 -0.101509612321270
95 -0.112281034263648
97 -8.741991170603057E-002
137 -6.303208154485178E-002
139 -4.681031342132439E-002
141 -4.861380525270807E-002
177 -0.145393804404929
178 -0.280622127947168
179 -0.145393804404929
180 -0.280622127947168

DATA FOR ATOM 1 N
Iteration Madelung constant Ees a.u. Difference in Ees

1 -0.389678 -0.092905 0.008605
2 -0.377709 -0.090052 0.002853

3	-0.484797	-0.156641	0.000214
4	-0.485049	-0.156722	0.000081
5	-0.485172	-0.156762	0.000040
6	-0.485242	-0.156784	0.000023
7	-0.485285	-0.156798	0.000014
8	-0.485314	-0.156808	0.000009

DATA FOR ATOM 2 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.459855	-0.149973	0.088466
2	-0.463385	-0.151125	0.001151
3	-0.463778	-0.151253	0.000128
4	-0.463937	-0.151305	0.000052
5	-0.464017	-0.151331	0.000026
6	-0.464062	-0.151345	0.000015
7	-0.464090	-0.151354	0.000009

DATA FOR ATOM 3 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.489894	-0.150167	0.097783
2	-0.497171	-0.152398	0.002231
3	-0.498351	-0.152759	0.000362
4	-0.498760	-0.152885	0.000126
5	-0.498953	-0.152944	0.000059
6	-0.499061	-0.152977	0.000033
7	-0.499127	-0.152997	0.000020
8	-0.499171	-0.153011	0.000013
9	-0.499201	-0.153020	0.000009

DATA FOR ATOM 4 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.484387	-0.156519	0.027898
2	-0.484950	-0.156701	0.000182
3	-0.485152	-0.156766	0.000065
4	-0.485245	-0.156797	0.000030
5	-0.485293	-0.156812	0.000016
6	-0.485321	-0.156821	0.000009

DATA FOR ATOM 5 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.463170	-0.151058	0.071359
2	-0.464135	-0.151372	0.000315
3	-0.464109	-0.151364	0.000008

DATA FOR ATOM 6 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.498516	-0.152795	0.060700
2	-0.499430	-0.153075	0.000280
3	-0.499426	-0.153073	0.000002

DATA FOR ATOM 7 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.480616	-0.155301	0.087128
2	-0.484086	-0.156422	0.001121
3	-0.484747	-0.156636	0.000214
4	-0.484999	-0.156717	0.000081
5	-0.485122	-0.156757	0.000040
6	-0.485192	-0.156779	0.000023
7	-0.485235	-0.156793	0.000014
8	-0.485264	-0.156803	0.000009

DATA FOR ATOM 8 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.459829	-0.149968	0.088469
2	-0.463360	-0.151119	0.001151
3	-0.463752	-0.151247	0.000128
4	-0.463912	-0.151299	0.000052
5	-0.463991	-0.151325	0.000026

3	-0.375783	-0.089592	0.000459
4	-0.375277	-0.089472	0.000121
5	-0.375063	-0.089421	0.000051
6	-0.374945	-0.089393	0.000028
7	-0.374872	-0.089375	0.000017
8	-0.374824	-0.089364	0.000012
9	-0.374790	-0.089356	0.000008

DATA FOR ATOM 2 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.364830	-0.112095	0.000186
2	-0.360504	-0.110766	0.001329
3	-0.359863	-0.110569	0.000197
4	-0.359690	-0.110516	0.000053
5	-0.359614	-0.110493	0.000023
6	-0.359571	-0.110480	0.000013
7	-0.359545	-0.110471	0.000008

DATA FOR ATOM 3 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.351698	-0.104712	0.017292
2	-0.348479	-0.103753	0.000958
3	-0.347759	-0.103539	0.000214
4	-0.347520	-0.103468	0.000071
5	-0.347404	-0.103433	0.000034
6	-0.347338	-0.103414	0.000020
7	-0.347297	-0.103401	0.000012
8	-0.347269	-0.103393	0.000008

DATA FOR ATOM 4 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.375719	-0.089577	0.026545
2	-0.374699	-0.089334	0.000243
3	-0.374414	-0.089266	0.000068
4	-0.374459	-0.089277	0.000011
5	-0.374516	-0.089290	0.000013
6	-0.374553	-0.089299	0.000009

DATA FOR ATOM 5 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.353732	-0.108685	0.061875
2	-0.358172	-0.110050	0.001364
3	-0.358804	-0.110244	0.000194
4	-0.359059	-0.110322	0.000078
5	-0.359193	-0.110363	0.000041
6	-0.359270	-0.110387	0.000024
7	-0.359319	-0.110402	0.000015
8	-0.359351	-0.110412	0.000010

DATA FOR ATOM 6 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.341601	-0.101705	0.053092
2	-0.346216	-0.103080	0.001374
3	-0.346716	-0.103228	0.000149
4	-0.346897	-0.103282	0.000054
5	-0.346988	-0.103309	0.000027
6	-0.347041	-0.103325	0.000016
7	-0.347073	-0.103335	0.000010

DATA FOR ATOM 7 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.389678	-0.092905	0.008605
2	-0.377709	-0.090052	0.002853
3	-0.375783	-0.089592	0.000459
4	-0.375277	-0.089472	0.000121
5	-0.375063	-0.089421	0.000051
6	-0.374945	-0.089393	0.000028
7	-0.374872	-0.089375	0.000017
8	-0.374824	-0.089364	0.000012

6	-0.464036	-0.151340	0.000015
7	-0.464064	-0.151349	0.000009

DATA FOR ATOM 9 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.489890	-0.150151	0.097773
2	-0.497167	-0.152381	0.002230
3	-0.498347	-0.152743	0.000362
4	-0.498756	-0.152868	0.000125
5	-0.498949	-0.152927	0.000059
6	-0.499056	-0.152960	0.000033
7	-0.499123	-0.152981	0.000020
8	-0.499166	-0.152994	0.000013
9	-0.499197	-0.153003	0.000009

DATA FOR ATOM 10 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.484381	-0.156506	0.027903
2	-0.484945	-0.156688	0.000182
3	-0.485146	-0.156753	0.000065
4	-0.485240	-0.156784	0.000030
5	-0.485288	-0.156799	0.000016
6	-0.485316	-0.156808	0.000009

DATA FOR ATOM 11 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.463142	-0.151045	0.071356
2	-0.464106	-0.151360	0.000314
3	-0.464080	-0.151351	0.000009

DATA FOR ATOM 12 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.498462	-0.152794	0.060707
2	-0.499377	-0.153074	0.000280
3	-0.499372	-0.153072	0.000002

DATA FOR ATOM 13 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.770403	-0.251258	0.092357
2	-0.776189	-0.253145	0.001887
3	-0.777442	-0.253554	0.000409
4	-0.777944	-0.253718	0.000164
5	-0.778194	-0.253799	0.000081
6	-0.778336	-0.253846	0.000046
7	-0.778425	-0.253875	0.000029
8	-0.778484	-0.253894	0.000019
9	-0.778526	-0.253907	0.000013
10	-0.778556	-0.253917	0.000010

DATA FOR ATOM 14 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.779222	-0.254129	0.054278
2	-0.780003	-0.254384	0.000255
3	-0.779408	-0.254190	0.000194
4	-0.779126	-0.254098	0.000092
5	-0.778981	-0.254050	0.000047
6	-0.778897	-0.254023	0.000027
7	-0.778845	-0.254006	0.000017
8	-0.778810	-0.253995	0.000011
9	-0.778785	-0.253987	0.000008

DATA FOR ATOM 15 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.770317	-0.251225	0.092353
2	-0.776103	-0.253112	0.001887
3	-0.777356	-0.253520	0.000409
4	-0.777857	-0.253684	0.000164
5	-0.778107	-0.253765	0.000081
6	-0.778255	-0.253813	0.000048
7	-0.778342	-0.253841	0.000028
8	-0.778394	-0.253858	0.000017
9	-0.778426	-0.253868	0.000010
10	-0.778446	-0.253875	0.000006

DATA FOR ATOM 16 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.779222	-0.254129	0.054278
2	-0.780003	-0.254384	0.000255
3	-0.779408	-0.254190	0.000194
4	-0.779126	-0.254098	0.000092
5	-0.778981	-0.254050	0.000047
6	-0.778897	-0.254023	0.000027
7	-0.778845	-0.254006	0.000017
8	-0.778810	-0.253995	0.000011
9	-0.778785	-0.253987	0.000008

DATA FOR ATOM 8 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.364830	-0.112095	0.000186
2	-0.360504	-0.110766	0.001329
3	-0.359863	-0.110569	0.000197
4	-0.359690	-0.110516	0.000053
5	-0.359614	-0.110493	0.000023
6	-0.359571	-0.110480	0.000013
7	-0.359545	-0.110471	0.000008

DATA FOR ATOM 9 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.351698	-0.104712	0.017292
2	-0.348479	-0.103753	0.000958
3	-0.347759	-0.103539	0.000214
4	-0.347520	-0.103468	0.000071
5	-0.347404	-0.103433	0.000034
6	-0.347338	-0.103414	0.000020
7	-0.347297	-0.103401	0.000012
8	-0.347269	-0.103393	0.000008

DATA FOR ATOM 10 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.375719	-0.089577	0.026545
2	-0.374699	-0.089334	0.000243
3	-0.374414	-0.089266	0.000068
4	-0.374459	-0.089277	0.000011
5	-0.374516	-0.089290	0.000013
6	-0.374553	-0.089299	0.000009

DATA FOR ATOM 11 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.353732	-0.108685	0.061875
2	-0.358172	-0.110050	0.001364
3	-0.358804	-0.110244	0.000194
4	-0.359059	-0.110322	0.000078
5	-0.359193	-0.110363	0.000041
6	-0.359270	-0.110387	0.000024
7	-0.359319	-0.110402	0.000015
8	-0.359351	-0.110412	0.000010

DATA FOR ATOM 12 N

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.341601	-0.101705	0.053092
2	-0.346216	-0.103080	0.001374
3	-0.346716	-0.103228	0.000149
4	-0.346897	-0.103282	0.000054
5	-0.346988	-0.103309	0.000027
6	-0.347041	-0.103325	0.000016
7	-0.347073	-0.103335	0.000010

DATA FOR ATOM 13 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.081389	-0.332261	0.186867
2	-1.121821	-0.344683	0.012423
3	-1.129680	-0.347098	0.002415
4	-1.132362	-0.347922	0.000824
5	-1.133631	-0.348312	0.000390
6	-1.134348	-0.348532	0.000220
7	-1.134796	-0.348670	0.000138
8	-1.135095	-0.348762	0.000092
9	-1.135304	-0.348826	0.000064
10	-1.135457	-0.348873	0.000047
11	-1.135571	-0.348908	0.000035
12	-1.135659	-0.348935	0.000027
13	-1.135728	-0.348956	0.000021
14	-1.135783	-0.348973	0.000017

6	-0.778249	-0.253812	0.000046
7	-0.778338	-0.253841	0.000029
8	-0.778397	-0.253860	0.000019
9	-0.778439	-0.253874	0.000013
10	-0.778468	-0.253883	0.000010

DATA FOR ATOM 16 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-0.779147	-0.254110	0.054270
2	-0.779927	-0.254364	0.000254
3	-0.779331	-0.254170	0.000194
4	-0.779049	-0.254078	0.000092
5	-0.778904	-0.254031	0.000047
6	-0.778820	-0.254003	0.000027
7	-0.778768	-0.253986	0.000017
8	-0.778732	-0.253975	0.000011
9	-0.778708	-0.253967	0.000008

Average Madelung constant of cation is -1.4487

Average Madelung constant of anion is -0.7786

Average Madelung constant of salt is -1.1137

Minimum distance in the crystal is 3.0662

Electrostatic lattice energy is -504.3 kJ/mol

15	-1.135828	-0.348987	0.000014
16	-1.135865	-0.348999	0.000011
17	-1.135896	-0.349008	0.000009

DATA FOR ATOM 14 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.115380	-0.342704	0.062082
2	-1.134039	-0.348438	0.005733
3	-1.135929	-0.349018	0.000581
4	-1.136141	-0.349083	0.000065
5	-1.136161	-0.349089	0.000006

DATA FOR ATOM 15 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.081389	-0.332261	0.186867
2	-1.121821	-0.344683	0.012423
3	-1.129680	-0.347098	0.002415
4	-1.132362	-0.347922	0.000824
5	-1.133631	-0.348312	0.000390
6	-1.134348	-0.348532	0.000220
7	-1.134796	-0.348670	0.000138
8	-1.135095	-0.348762	0.000092
9	-1.135304	-0.348826	0.000064
10	-1.135457	-0.348873	0.000047
11	-1.135571	-0.348908	0.000035
12	-1.135659	-0.348935	0.000027
13	-1.135728	-0.348956	0.000021
14	-1.135783	-0.348973	0.000017
15	-1.135828	-0.348987	0.000014
16	-1.135865	-0.348999	0.000011
17	-1.135896	-0.349008	0.000009

DATA FOR ATOM 16 Cl

Iteration	Madelung constant	Ees a.u.	Difference in Ees
1	-1.115380	-0.342704	0.062082
2	-1.134039	-0.348438	0.005733
3	-1.135929	-0.349018	0.000581
4	-1.136141	-0.349083	0.000065
5	-1.136161	-0.349089	0.000006

Average Madelung constant of cation is -1.0813

Average Madelung constant of anion is -1.1360

Average Madelung constant of salt is -1.1087

Minimum distance in the crystal is 3.2546

Electrostatic lattice energy is -473.0 kJ/mol

Section IV: Hirshfeld surfaces and Fingerprint plots analysis

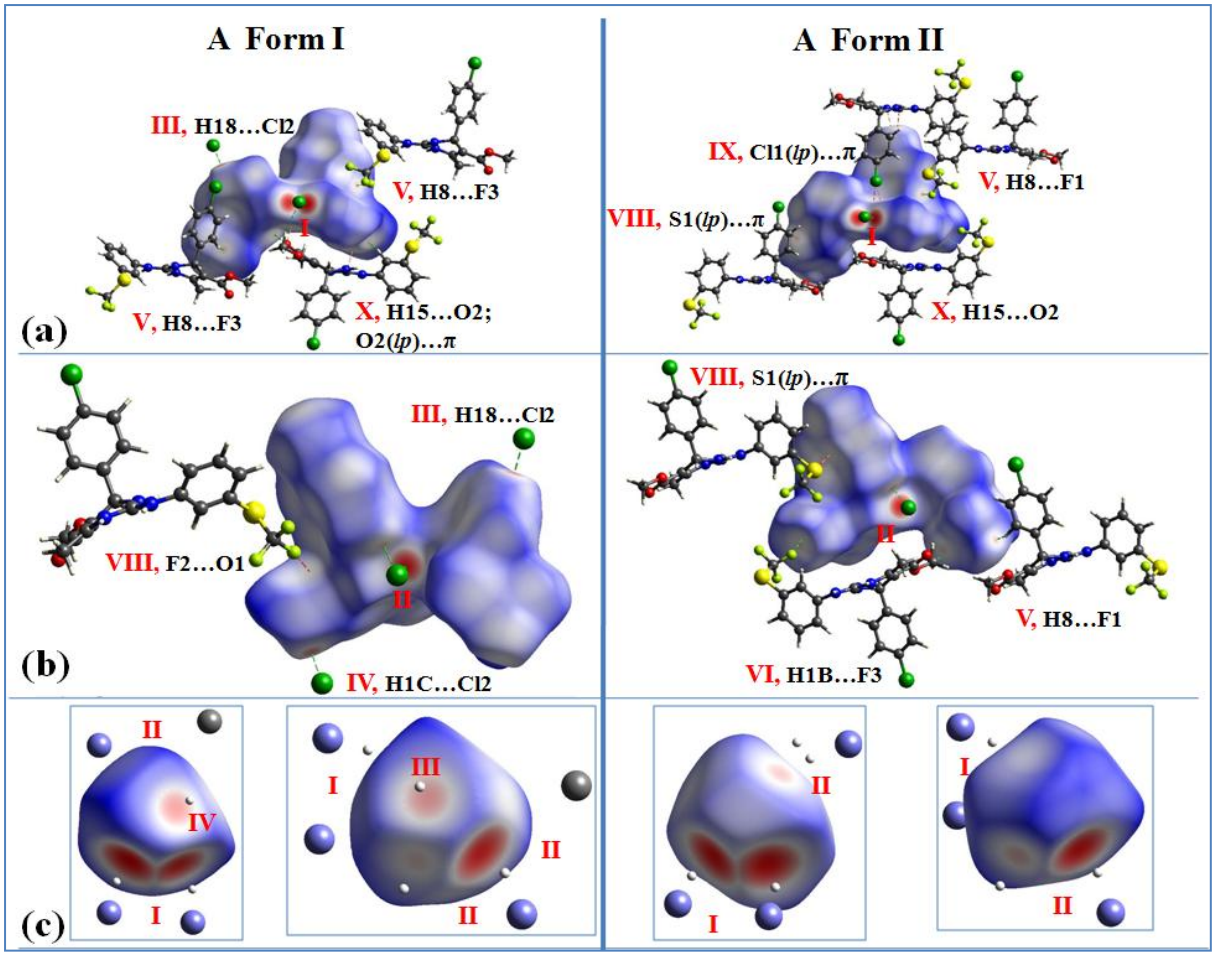


Figure S13: Comparison of the Hirshfeld surface mapped with d_{norm} and 2D-finger print plot between **A Form I** (left column) and **A Form II** (right column) **(a)** front view **(b)** back view **(c)** d_{norm} for chloride ion

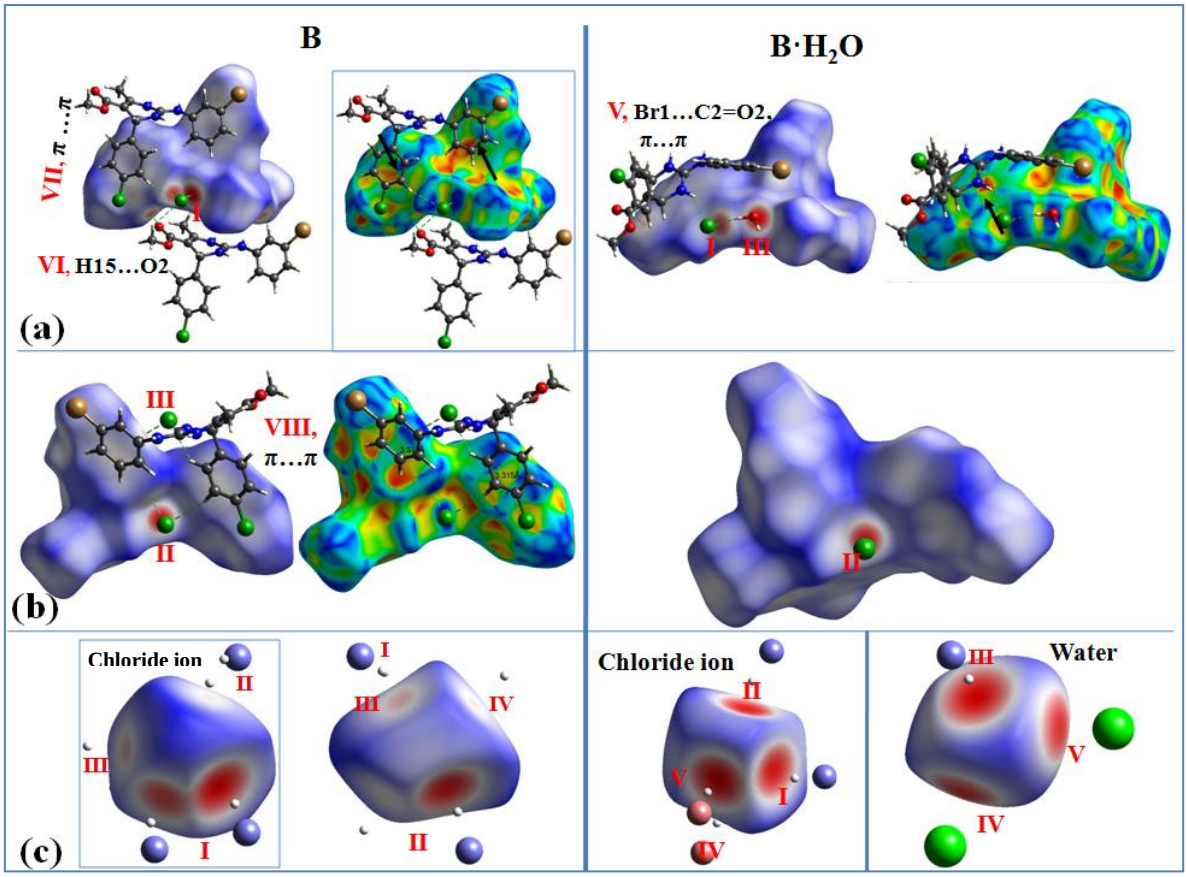
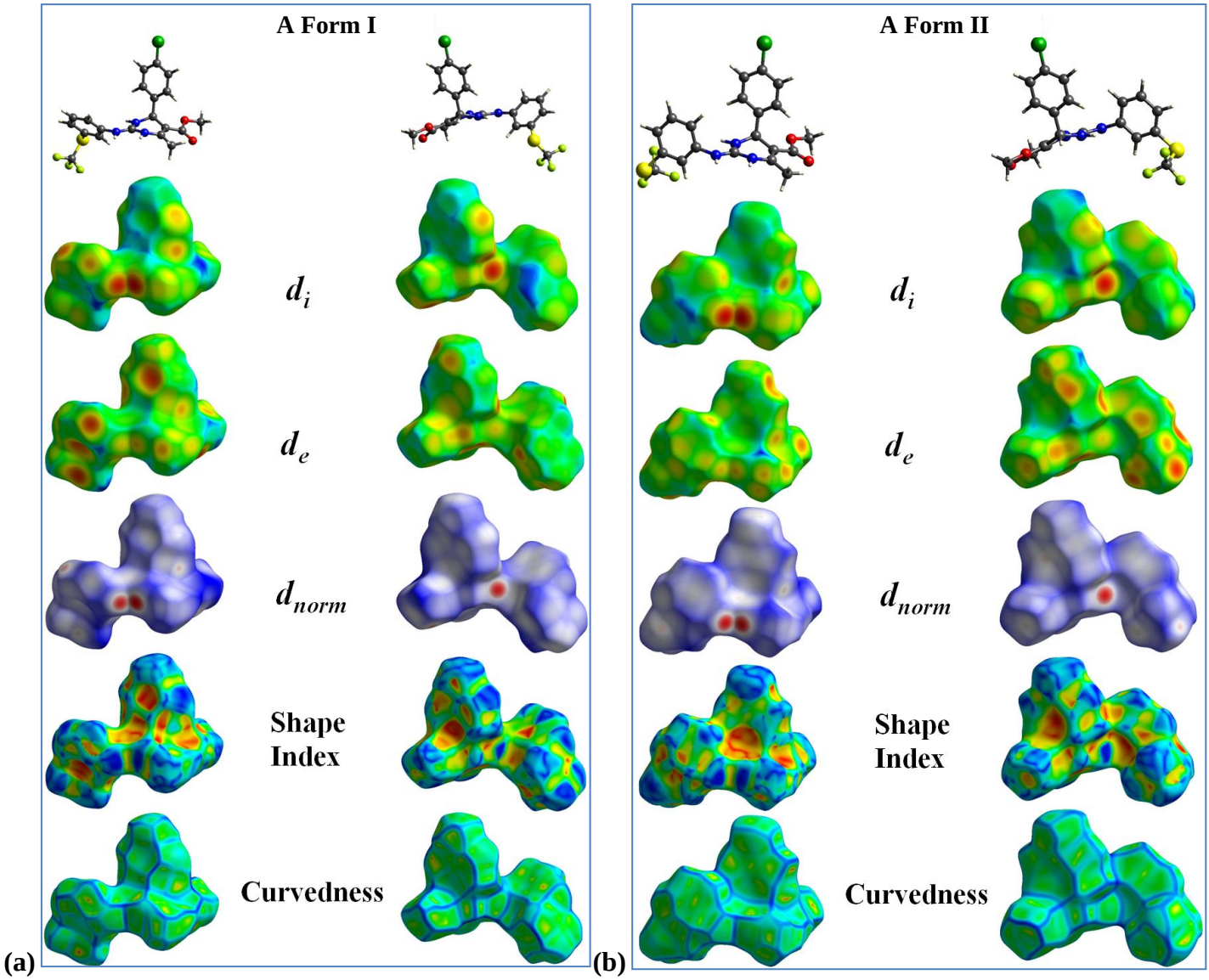


Figure S14: Comparison of the Hirshfeld surface and 2D-finger print plot between **B** (left column) and **B·H$_2$O** (right column) **(a)** mapped with d_{norm} and shape index, front view **(b)** mapped with d_{norm} and shape index for **B** and d_{norm} for **B·H$_2$O**, back view **(c)** d_{norm} for chloride ion and water molecule for **B·H$_2$O.**


A Form I
d_i
d_e
d_{norm}
Shape Index
Curvedness
A Form II
d_i
d_e
d_{norm}
Shape Index
Curvedness

(a) (b)

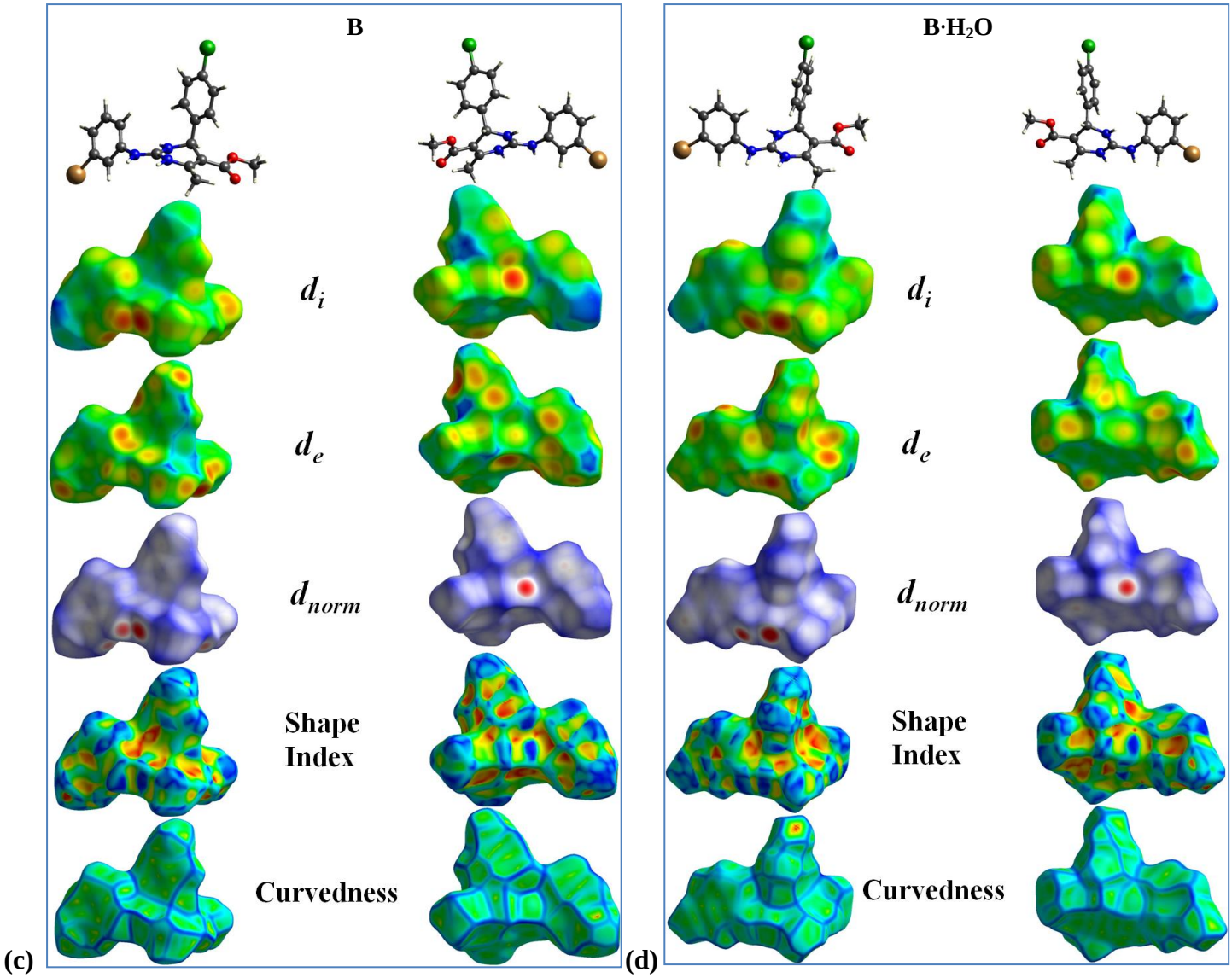
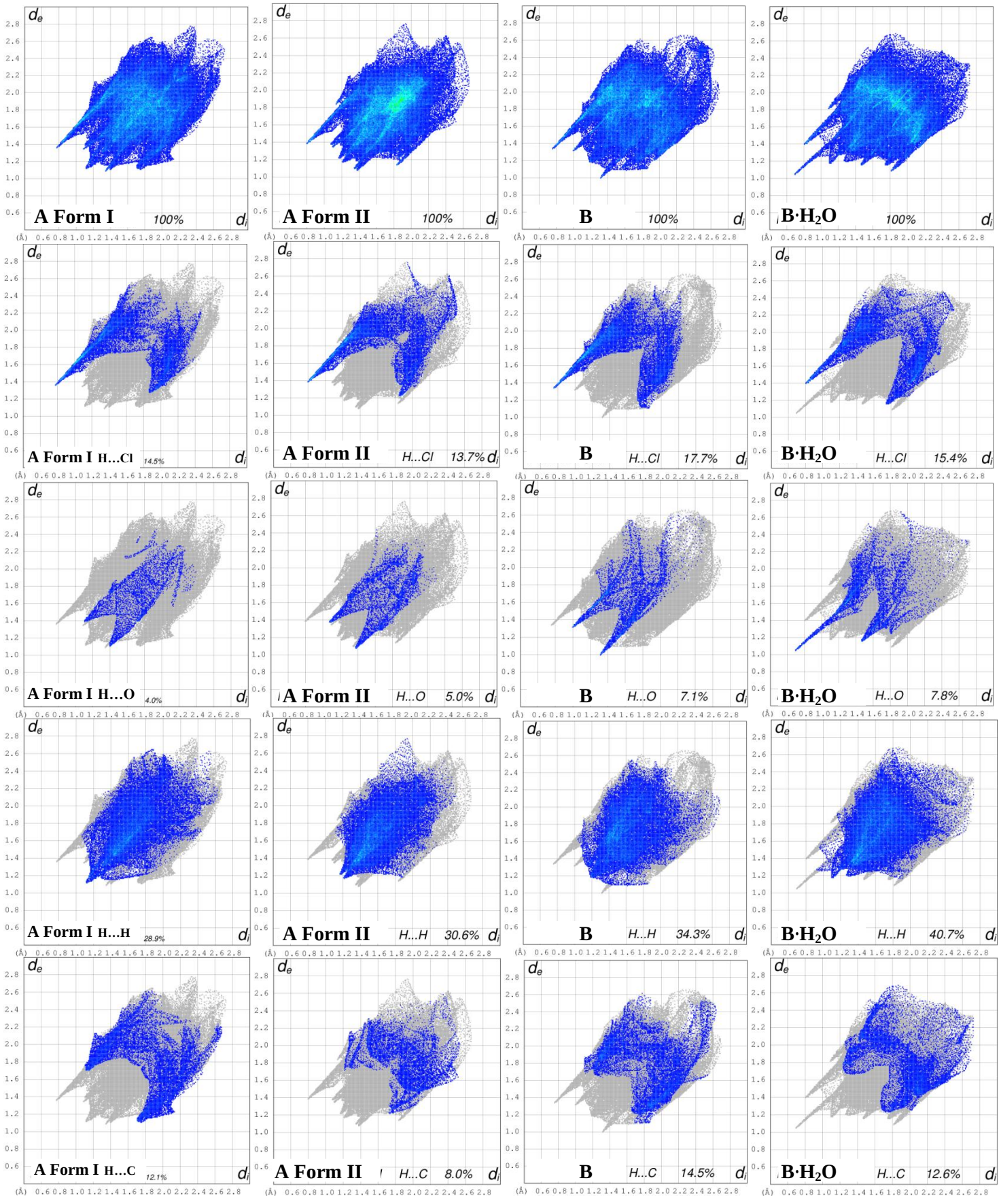


Figure S15: Hirshfeld surfaces of the four crystal structures mapped with different properties. Left column (front view) while right column (back view) (a) for **A Form I** (b) for **A Form II** (c) for **B** (d) for **B·H$_2$O**.


A Form I 100%
A Form II 100%
B 100%
B·H2O 100%
A Form I H...Cl 14.5%
A Form II H...Cl 13.7%
B H...Cl 17.7%
B·H2O H...Cl 15.4%
A Form I H...O 4.0%
A Form II H...O 5.0%
B H...O 7.1%
B·H2O H...O 7.8%
A Form I H...H 28.9%
A Form II H...H 30.6%
B H...H 34.3%
B·H2O H...H 40.7%
A Form I H...C 12.1%
A Form II H...C 8.0%
B H...C 14.5%
B·H2O H...C 12.6%

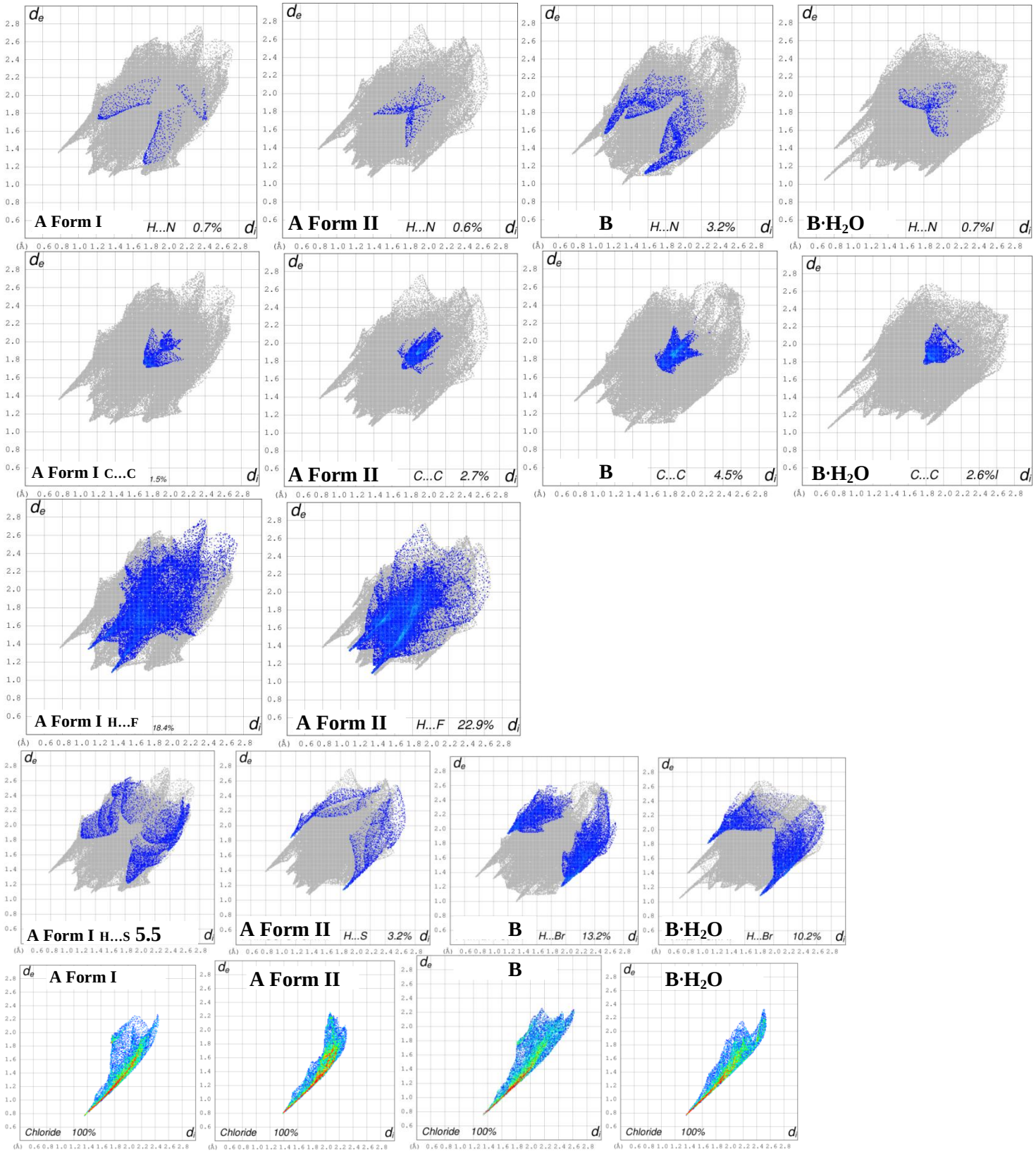


Figure S16: Comparison of the full fingerprint plots and decomposed fingerprint plots into various intermolecular interactions for **A Form I**, **A Form II**, **B** and **B·H$_2$O**.