

Supporting Information

for

**Does Hydrogen Bonding Matter in Crystal Engineering? Crystal Structures
of Salts of Isomeric Ions.**

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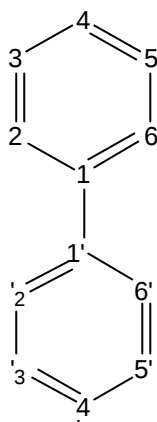
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Supplementary Data Tables.

The numbering of Hbond donor contact points on bipyridinium and pyridyl-pyridinium fragments **B**, **C**, **D** and **E** have been assigned according to the following diagram.



Fragments in the structures of **4**, **5a**, **6**, **7** and **8** contain no symmetry equivalent hydrogen atoms, however, in the structures of **1**, **2**, **3** and **5b**, the following symmetry conditions apply.

1. $2 = 2? = 6 = 6?$, $3 = 3? = 5 = 5?$, $4 = 4?$.

2. $2 = 6?$, $3 = 5?$, $4 = 4?$, $5 = 3?$, $6 = 2?$.

3. $2 = 6?$, $3 = 5?$, $4 = 4?$, $5 = 3?$, $6 = 2?$.

5b. $2 = 6$, $2? = 6?$, $3 = 5$, $3? = 5$.

Structure	Position	Contact Type	Bond Length /	Bond Angle / °
			Å	DH ^{xxx} Cl
			H ^{xxx} Cl	
1	2	CH...Cl	2.83	130.5
	3	CH...Cl	2.98	150.0
	3	CH...Cl	2.96	114.1
	4	NH...Cl	2.40	136.4
2	2	CH...Cl	2.82	120.3
	3	NH...Cl	2.43	131.7
	3	NH...Cl	2.22	137.1
	4	CH...Cl	3.08	109.0

	4	CH...Cl	2.70	163.3
	5	CH...Cl	2.85	137.5
	6	CH...Cl	2.73	165.7
3	2	NH...Cl	2.30	161.4
	4	CH...Cl	3.00	138.8
	4	CH...Cl	2.75	158.6
	5	CH...Cl	2.65	163.2
	5	CH...Cl	3.10	127.9
	6	CH...Cl	3.11	127.3
4	2	CH...Cl	2.65	160.1
	3	CH...Cl	2.88	120.0
	4	NH...Cl	2.72	130.4
	4	NH...Cl	2.44	151.5
	5	CH...Cl	2.70	175.5
	6	CH...Cl	2.86	136.6
	6	CH...Cl	2.93	121.2
	6?	CH...Cl	2.69	151.9
	4?	CH...Cl	2.80	138.7
	4?	CH...Cl	2.74	145.7
	3?	CH...Cl	2.69	168.4
	3?	CH...Cl	2.99	120.6
	2?	CH...Cl	2.74	133.3
	2?	CH...Cl	3.03	112.3

Table S1: Intermolecular NH and CH...Cl Contacts For Salts **1** – **4**.

Structure	Position	Contact Type	Bond Length /	Bond Angle / °
			Å H...Cl	DH...Cl
5a	2	CH...Cl	2.80	134.0
	3	CH...Cl	2.81	119.1
	4	NH _{xxx} Cl	2.64	131.1
	4	NH _{xxx} Cl	2.62	138.0

	6?	CH...Cl	2.90	133.2
	5?	CH...Cl	2.94	116.3
	4?	NH _{xxx} Cl	2.59	137.5
	4?	NH _{xxx} Cl	2.62	133.6
	3?	CH...Cl	2.82	119.8
	2?	CH...Cl	2.89	126.8
5b	2	CH...Cl	2.88	171.6
	3	CH...Cl	3.00	169.6
	3	CH...Cl	2.97	114.1
	4	NH...Cl	2.51	139.9
	2?	CH...Cl	3.02	147.0
	2?	CH...Cl	3.00	133.2
	3?	CH...Cl	2.89	134.9
	3?	CH...Cl	3.01	151.8
	3?	CH...Cl	2.95	112.9
	4?	NH...Cl	2.47	139.0
6	2	CH...Cl	2.64	163.5
	2	CH...Cl	3.12	110.7
	3	NH...Cl	2.29	172.9
	4	CH...Cl	2.63	175.7
	5	CH...Cl	2.85	161.2
	5	CH...Cl	2.96	122.6
	6	CH...Cl	2.86	127.7
	6?	CH...Cl	3.13	108.1
	6?	CH...Cl	2.77	137.2
	5?	CH...Cl	2.99	112.0

4?	CH...Cl	2.77	130.0
4?	CH...Cl	2.75	155.5
3?	NH...Cl	2.19	169.2
2?	CH...Cl	2.64	171.9
2	CH...Cl	2.51	158.4
3	NH...Cl	2.27	166.5
3	NH...Cl	3.04	112.1
4	CH...Cl	2.60	170.2
5	CH...Cl	2.89	140.2
5	CH...Cl	3.87	130.8
6	CH...Cl	3.12	165.9
6?	CH...Cl	2.74	141.6
5?	NH...Cl	2.55	148.1
5?	NH...Cl	3.13	126.3
5?	NH...Cl	2.84	124.2
4?	CH...Cl	2.66	128.4
4?	CH...Cl	2.86	157.6
3?	CH...Cl	3.15	158.0
3?	CH...Cl	2.91	118.9
2?	CH...Cl	2.92	118.1

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2	NH...Cl	2.21	155.5
3	CH...Cl	2.73	148.4
4	CH...Cl	2.67	171.4
5	CH...Cl	3.03	108.4
6	CH...Cl	2.79	118.0
6	CH...Cl	2.90	118.5
6?	NH...Cl	2.30	170.4

5?	CH...Cl	2.82	171.1
4?	CH...Cl	2.83	147.2
4?	CH...Cl	2.80	135.7
3?	CH...Cl	2.88	123.2
2?	CH...Cl	2.84	118.6
2	NH...Cl	2.26	164.8
3	CH...Cl	2.90	155.5
3	CH...Cl	2.90	117.7
4	CH...Cl	2.72	171.2
5	CH...Cl	2.90	148.4
5	CH...Cl	2.94	128.0
6?	NH...Cl	2.19	153.0
4?	CH...Cl	2.78	144.4
4?	CH...Cl	2.74	137.4
3?	CH...Cl	2.94	160.9
2?	CH...Cl	2.78	133.9

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2	CH...Cl	2.50	177.7
3	CH...Cl	3.12	114.2
3	CH...Cl	2.89	166.7
4	NH...Cl	2.87	136.3
4	NH...Cl	2.59	146.5
5	CH...Cl	3.06	107.6
5	CH...Cl	3.14	173.4
5	CH...Cl	3.01	115.6
6	CH...Cl	2.77	125.4
6?	CH...Cl	2.61	151.8
5?	CH...Cl	2.57	153.8

5?	CH...Cl	3.06	105.0
4?	CH...Cl	2.67	167.3
3?	CH...Cl	2.98	112.7
3?	CH...Cl	3.04	156.9
3?	CH...Cl	2.85	116.3
2?	CH...Cl	2.89	114.6
2?	CH...Cl	2.79	154.5
2	CH...Cl	2.59	173.9
3	CH...Cl	2.77	167.0
3	CH...Cl	3.01	105.7
4	NH...Cl	2.36	170.7
5	CH...Cl	2.79	150.3
5	CH...Cl	2.69	132.0
6	CH...Cl	2.95	119.6
6?	CH...Cl	3.07	132.6
6?	CH...Cl	2.74	111.0
5?	CH...Cl	2.88	153.3
5?	CH...Cl	3.10	121.1
4?	CH...Cl	2.86	131.7
4?	CH...Cl	2.79	152.3
3?	CH...Cl	3.02	109.8
2?	CH...Cl	2.88	118.8
2?	CH...Cl	2.97	153.1

Table S2: Intermolecular NH and CH...Cl Contacts For Salts **5** – **8**.