

**Table S1**

Intermolecular interactions with distances shorter-than the sum of van der Waals radii for dications of I and II [Å and °].

Structure	$D\text{--H}\dots A$	$d(D\text{--H})$	$d(\text{H}\dots A)$	$d(D\dots A)$	$\angle(D\text{H}A)$	Label	Figure
Dication of I							
	C3—H1c3...O2	0.960 (2)	2.383 (1)	3.263 (2)	152.2 (1)	1	3
	C7—H1c7...O2 <sup>i</sup>	0.960 (2)	2.481 (1)	3.332 (2)	147.6 (1)	2	3
	C1—H2c1...O2 <sup>i</sup>	0.960 (1)	2.604 (1)	3.326(2)	132.28 (8)	3	3
	C3—H1c3...O3	0.960 (2)	2.576 (1)	3.220 (2)	124.6 (1)	4	3
	C4—H1c4...O3 <sup>ii</sup>	0.960 (2)	2.467 (1)	3.379 (2)	158.6 (1)	5	3
	C1—H1c1...O2 <sup>iii</sup>	0.960 (1)	2.495 (1)	3.389 (2)	154.81 (8)	6	3
	C3...O4 <sup>iv</sup>	—	—	3.000(2) <sup>a</sup>	—	7	3
	N2...O4 <sup>iv</sup>	—	—	2.997 (2) <sup>b</sup>	—	8	3
	C1—H1c1...O4 <sup>iv</sup>	0.960 (1)	2.630 (1)	3.129 (2)	112.69 (8)	9	3
	C5...C5 <sup>v</sup>	—	—	3.297 (2) <sup>c</sup>	—	10	3
	C5—H1c5...O3 <sup>vi</sup>	0.960 (2)	2.528 (1)	3.245 (2)	131.5 (1)	11	3
	C5...C4 <sup>vi</sup>	—	—	3.354 (2) <sup>c</sup>	—	12	3
Dication of II							
	C1—H2c1...O1 <sup>i</sup>	0.960 (1)	2.365 (1)	3.320 (2)	172.93 (8)	1	3
	C7—H1c7...O2 <sup>i</sup>	0.960 (1)	2.448 (1)	3.355 (2)	157.56 (8)	2	3
	C3—H1c3...O2	0.960 (1)	2.517 (1)	3.279 (2)	136.39 (8)	3	3
	C3—H1c3...O1 <sup>ii</sup>	0.960 (1)	2.410 (1)	3.072 (2)	125.75 (8)	4	3
	C7—H1c7...O4 <sup>iii</sup>	0.960 (1)	2.594 (1)	3.185 (2)	120.06 (8)	5	3
	C1—H1c1...O2	0.960 (1)	2.711 (1)	3.358 (2)	125.27 (8)	6	3
	N2...O2 <sup>iv</sup>	—	—	2.996 (1) <sup>b</sup>	—	7	3
	C5—H1c5...O1 <sup>v</sup>	0.960 (1)	2.343 (1)	3.063 (2)	131.36 (9)	8	3
	C5—H1c5...O3 <sup>vi</sup>	0.960 (1)	2.543 (1)	3.177 (2)	123.64 (9)	9	3
	C4—H1c4...O3 <sup>vi</sup>	0.960 (1)	2.600 (1)	3.204 (2)	121.18 (9)	10	3

Symmetry transformations used to generate equivalent atoms for dication of I: (i):  $-x, -y + 1, -z$ ; (ii):  $-x + 1, -y + 1, -z + 1$ ; (iii):  $-x + 1, -y + 1, -z$ ; (iv)  $x, y + 1, z$ ; (v):  $-x, -y + 2, -z + 1$ ;

(vi):  $-x, -y + 1, -z + 1$ . for dication of II: (i):  $-x + 1, -y + 1, -z$ ; (ii):  $x, -y - 1/2, z - 1/2$ ; (iii):  $x, y + 1, z$ ; (iv)  $-x + 1, y + 1/2, -z + 1/2$ ; (v):  $-x, -y + 1, -z$ ; (vi):  $-x, y + 1/2, -z + 1/2$ . <sup>a</sup>The distance between O and C( $sp^2$ ) atoms. <sup>b</sup>The distance between O and N( $sp^2$ ) atoms. <sup>c</sup>The distance between two C( $sp^2$ ) atoms.