Article

Synthesis, Crystal Structure, and Hirshfeld Surface Analysis of Hexachloroplatinate and Tetraclorouranylate of 3-Carboxypyridinium. Halogen Bonds and π-Interactions vs Hydrogen Bonds

Anton Petrovich Novikov *, Mikhail Alexandrovich Volkov, Alexey Vladimirovich Safonov and Mikhail Semenovich Grigoriev

Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninskii prospect 31-4, 119071 Moscow, Russia; mendeleev93@yandex.ru (M.A.V.); alexeysafonof@gmail.com (A.V.S.); mickgrig@mail.ru (M.S.G.)
* Correspondence: tony.novickoff@yandex.ru

Table S1. Bond Lengths for **I** at 100 K.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pt[1]	Cl1	2.3180(8)	N1	C2	1.340(4)
Pt[1]	Cl1[1]	2.3180(8)	N1	C6	1.337(4)
Pt[1]	Cl2[1]	2.3090(8)	C2	C3	1.391(4)
Pt[1]	Cl2	2.3090(8)	C3	C4	1.388(5)
Pt[1]	Cl3	2.3107(8)	C3	C7	1.495(5)
Pt[1]	Cl3[1]	2.3107(8)	C4	C5	1.384(5)
O[1]	C7	1.236(4)	C5	C6	1.371(5)
O[2]	C7	1.323(5)			

[1]1-X, 1-Y, 1-Z

Table S2. Bond Angles for **I** at 100 K.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	Pt1	Cl1[1]	180.0	Cl3[1]	Pt1	Cl1	89.57(3)
Cl2	Pt1	Cl1	89.06(3)	Cl3[1]	Pt1	Cl3	180.00(3)
Cl2	Pt1	Cl1[1]	90.94(3)	C6	N1	C2	122.6(3)
Cl2[1]	Pt1	Cl1[1]	89.06(3)	N1	C2	C3	119.4(3)
Cl2[1]	Pt1	Cl1	90.94(3)	C2	C3	C7	117.2(3)
Cl2	Pt1	Cl2[1]	180.0	C4	C3	C2	118.7(3)
Cl2	Pt1	Cl3	90.89(3)	C4	C3	C7	124.1(3)
Cl2	Pt1	Cl3[1]	89.11(3)	C5	C4	C3	120.1(3)
Cl2[1]	Pt1	Cl3	89.11(3)	C6	C5	C4	119.0(3)
Cl2[1]	Pt1	Cl3[1]	90.89(3)	N1	C6	C5	120.2(3)
Cl3[1]	Pt1	Cl1[1]	90.43(3)	O1	C7	O2	124.0(3)
Cl3	Pt1	Cl1[1]	89.57(3)	O1	C7	C3	119.8(3)
Cl3	Pt1	Cl1	90.43(3)	O2	C7	C3	116.2(3)

[1]1-X, 1-Y, 1-Z

Table S3. Torsion Angles for **I** at 100 K.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C2	C3	C4	0.0(5)	C3	C4	C5	C6	−0.9(5)
N1	C2	C3	C7	−179.3(3)	C4	C3	C7	O1	151.1(3)
C2	N1	C6	C5	0.1(5)	C4	C3	C7	O2	−28.8(5)
C2	C3	C4	C5	0.6(5)	C4	C5	C6	N1	0.5(5)
C2	C3	C7	O1	−29.8(5)	C6	N1	C2	C3	−0.4(5)
C2	C3	C7	O2	150.4(3)	C7	C3	C4	C5	179.8(3)

Table S4. Bond Lengths for **I** at 296 K.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pt1	Cl1[1]	2.3220(6)	N1	C2	1.340(3)
Pt1	Cl1	2.3220(6)	N1	C6	1.335(3)
Pt1	Cl2	2.3144(5)	C2	C3	1.375(3)
Pt1	Cl2[1]	2.3145(5)	C3	C4	1.392(3)
Pt1	Cl3	2.3139(5)	C3	C7	1.496(3)
Pt1	Cl3[1]	2.3139(5)	C4	C5	1.375(4)
O1	C7	1.231(3)	C5	C6	1.365(4)
O2	C7	1.317(4)			

[1]1-X, 1-Y, 1-Z

Table S5. Bond Angles for **I** at 296 K.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1[1]	Pt1	Cl1	180.0	Cl3	Pt1	Cl2[1]	89.18(2)
Cl2[1]	Pt1	Cl1	90.87(2)	Cl3	Pt1	Cl3[1]	180.0
Cl2	Pt1	Cl1[1]	90.86(2)	C6	N1	C2	122.5(2)
Cl2	Pt1	Cl1	89.14(2)	N1	C2	C3	120.3(2)
Cl2[1]	Pt1	Cl1[1]	89.14(2)	C2	C3	C4	117.7(2)
Cl2	Pt1	Cl2[1]	180.0	C2	C3	C7	118.2(2)
Cl3[1]	Pt1	Cl1[1]	90.49(2)	C4	C3	C7	124.1(2)
Cl3	Pt1	Cl1	90.49(2)	C5	C4	C3	120.5(2)
Cl3	Pt1	Cl1[1]	89.51(2)	C6	C5	C4	119.4(3)
Cl3[1]	Pt1	Cl1	89.51(2)	N1	C6	C5	119.6(3)
Cl3[1]	Pt1	Cl2[1]	90.82(2)	O1	C7	O2	124.0(2)
Cl3[1]	Pt1	Cl2	89.18(2)	O1	C7	C3	119.5(2)
Cl3	Pt1	Cl2	90.81(2)	O2	C7	C3	116.5(2)

[1]1-X,1-Y,1-Z

Table S6. Hydrogen Bonds for **I** at 296 K**.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O2	H2B	Cl1[1]	0.86(2)	2.71(3)	3.531(3)	161(8)
O2	H2B	Cl3[1]	0.86(2)	2.86(7)	3.434(3)	126(7)
O2	H2C	Cl3[2]	0.87(2)	2.66(4)	3.451(3)	152(6)
N1	H1A	O1[3]	0.86	1.93	2.762(3)	162.3

[1]1-X,1-Y,2-Z; [2]-1/2+X,1/2-Y,1/2+Z; [3]-1/2+X,3/2-Y,-1/2+Z

Table S7. Torsion Angles for **I** at 296 K.

Table 7 Torsion Angles for NicPt_RT.								
A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
N1	C2	C3	C4	0.3(4)	C3	C4	C5	C6	-1.1(4)
N1	C2	C3	C7	-178.9(2)	C4	C3	C7	O1	151.5(2)
C2	N1	C6	C5	0.2(4)	C4	C3	C7	O2	-28.2(4)
C2	C3	C4	C5	0.6(4)	C4	C5	C6	N1	0.7(4)
C2	C3	C7	O1	-29.4(4)	C6	N1	C2	C3	-0.7(4)
C2	C3	C7	O2	151.0(3)	C7	C3	C4	C5	179.7(3)

Table S8. Bond Lengths for **II** at 100 K.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
U1	Cl1[1]	2.6461(8)	N1	C2	1.341(4)
U1	Cl1	2.6461(8)	N1	C6	1.342(4)
U1	Cl2	2.6694(7)	C2	C3	1.383(4)
U1	Cl2[1]	2.6694(7)	C3	C4	1.394(4)
U1	O1[1]	1.780(2)	C3	C7	1.512(4)
U1	O1	1.780(2)	C4	C5	1.389(4)
O2	C7	1.235(4)	C5	C6	1.378(4)
O3	C7	1.334(4)			

[1]1-X,1-Y,-Z

Table S9. Bond Angles for **II** at 100 K.

Table 5 Bond Angles for U9.							
Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Cl1[1]	U1	Cl1	180.0	O1[1]	U1	Cl2	90.14(8)
Cl1	U1	Cl2	89.47(2)	O1	U1	O1[1]	180.0
Cl1	U1	Cl2[1]	90.53(2)	C2	N1	C6	123.3(3)
Cl1[1]	U1	Cl2	90.53(2)	N1	C2	C3	119.2(3)
Cl1[1]	U1	Cl2[1]	89.47(2)	C2	C3	C4	118.9(3)
Cl2[1]	U1	Cl2	180.000(17)	C2	C3	C7	122.9(3)
O1	U1	Cl1	89.81(8)	C4	C3	C7	118.2(3)
O1	U1	Cl1[1]	90.19(8)	C5	C4	C3	120.1(3)
O1[1]	U1	Cl1[1]	89.81(8)	C6	C5	C4	118.8(3)
O1[1]	U1	Cl1	90.19(8)	N1	C6	C5	119.6(3)
O1[1]	U1	Cl2[1]	89.86(8)	O2	C7	O3	124.4(3)
O1	U1	Cl2	89.86(8)	O2	C7	C3	118.4(3)

O1	U1	Cl2[1]	90.14(8)	O3	C7	C3	117.2(3)

[1]1-X,1-Y,-Z

Table S10. Torsion Angles for **II** at 100 K.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C2	C3	C4	1.8(4)	C3	C4	C5	C6	0.4(5)
N1	C2	C3	C7	−178.1(3)	C4	C3	C7	O2	15.5(4)
C2	N1	C6	C5	−1.6(5)	C4	C3	C7	O3	−162.5(3)
C2	C3	C4	C5	−2.0(5)	C4	C5	C6	N1	1.4(5)
C2	C3	C7	O2	−164.6(3)	C6	N1	C2	C3	0.0(5)
C2	C3	C7	O3	17.4(4)	C7	C3	C4	C5	177.9(3)

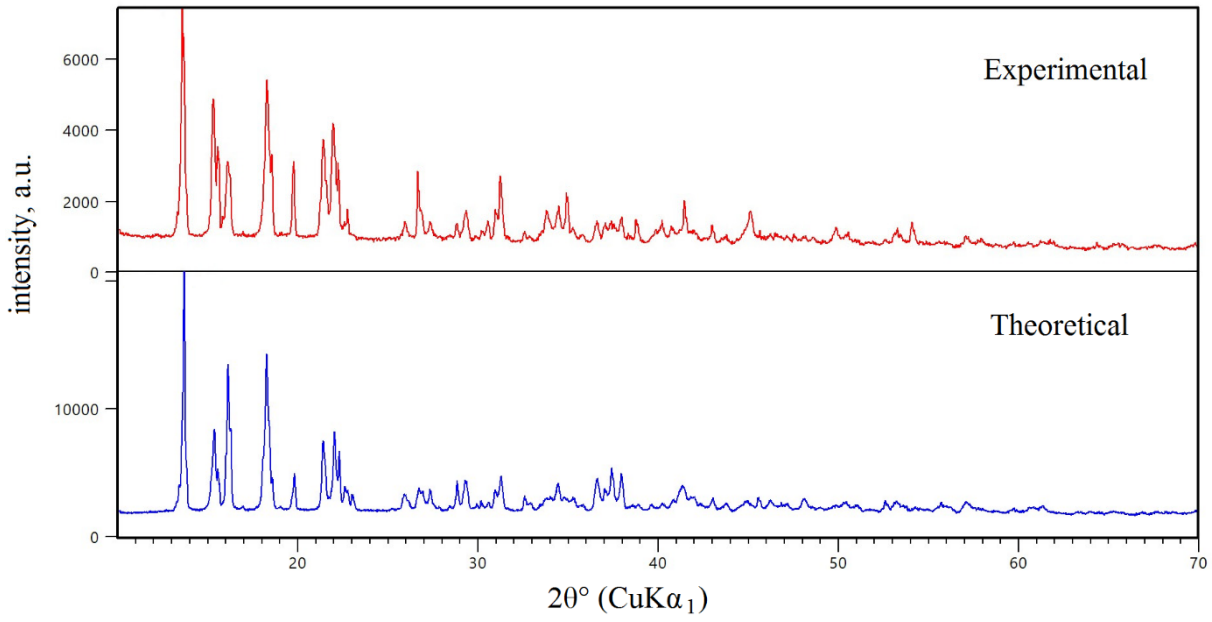

Figure S1. Experimental and theoretical powder XRD spectra of **I** at 296 K.

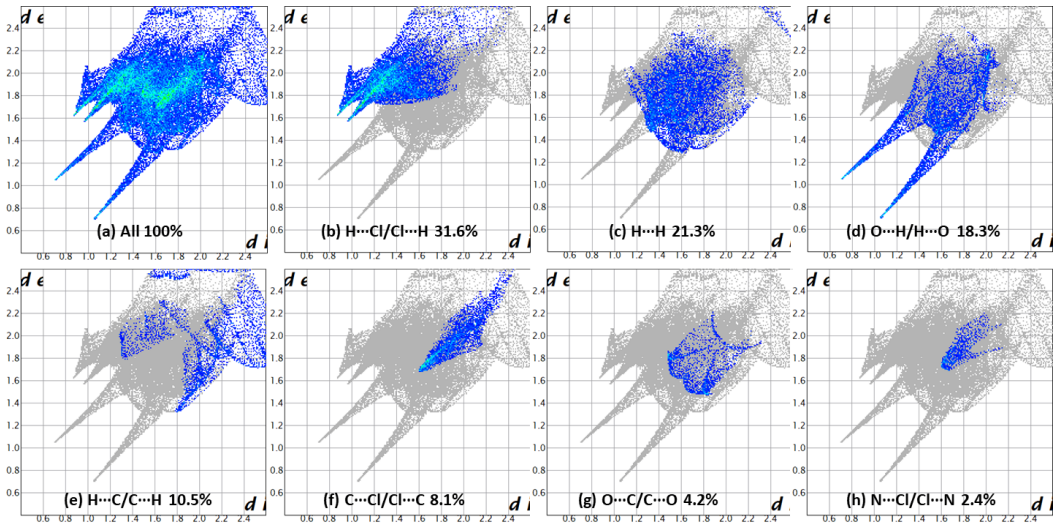

Figure S2. The 2D fingerprint plots of interatomic interactions for cation in **I** at 100 K show the percentages of contacts contributed to the total Hirshfeld surface area of the molecules.

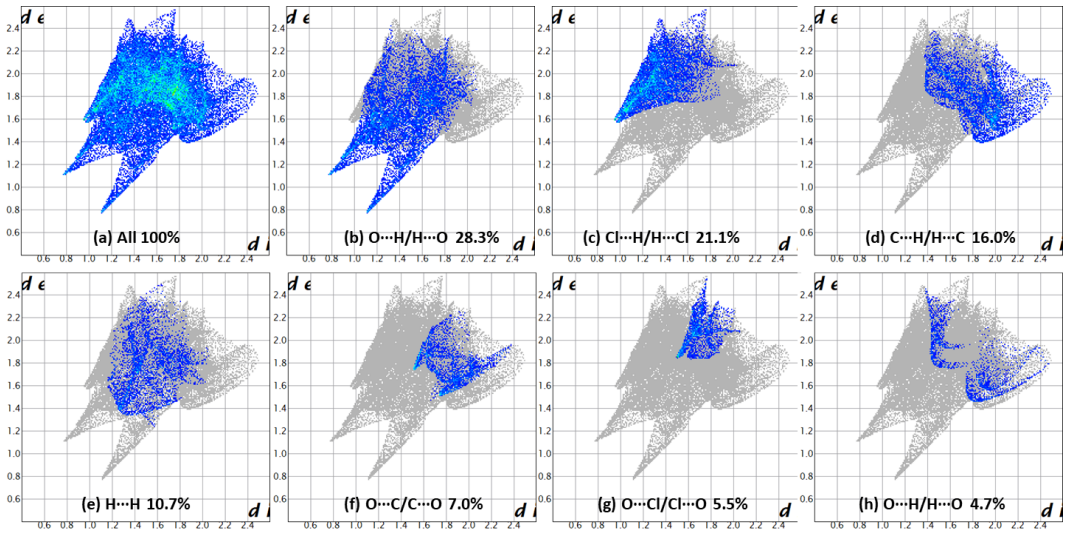

Figure S3. The 2D fingerprint plots of interatomic interactions for cation in **II** at 100 K show the percentages of contacts contributed to the total Hirshfeld surface area of the molecules.

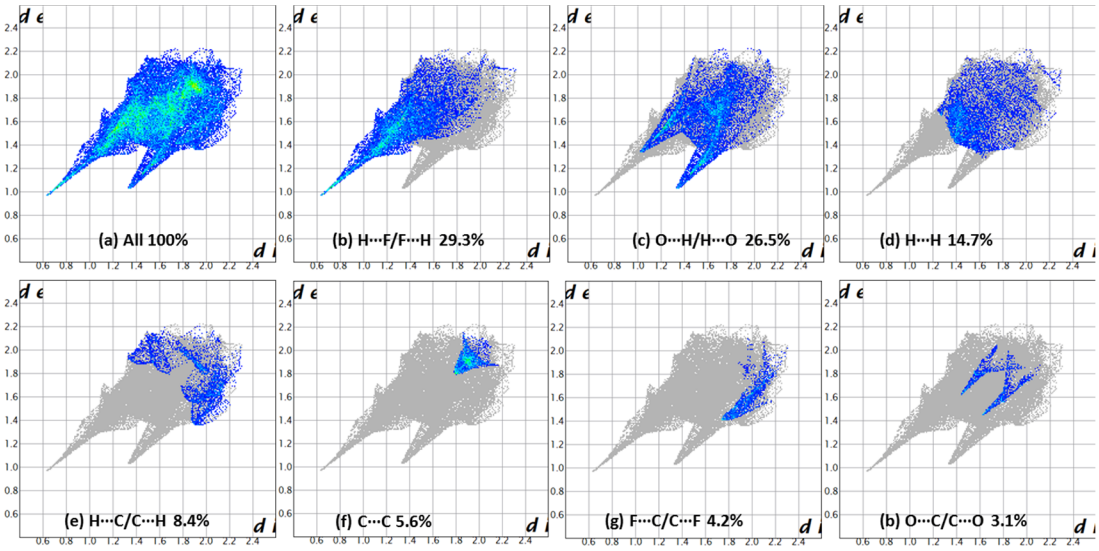

Figure S4. The 2D fingerprint plots of interatomic interactions for cation in **III** at 100 K showing the percentages of contacts contributed to the total Hirshfeld surface area of the molecules.

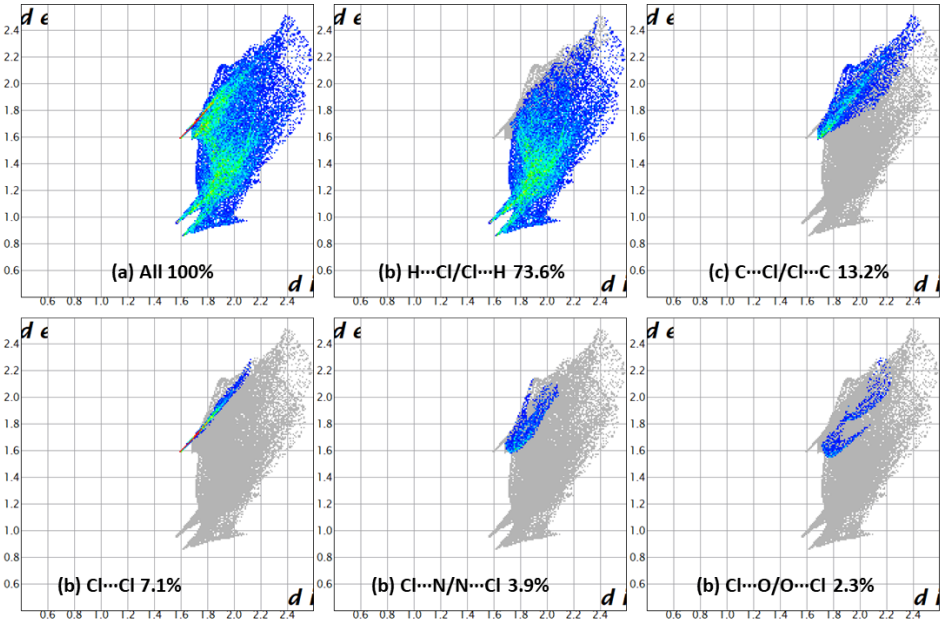

Figure S5. The 2D fingerprint plots of interatomic interactions for anion in **I** at 100 K show the percentages of contacts contributed to the total Hirshfeld surface area of the molecules.

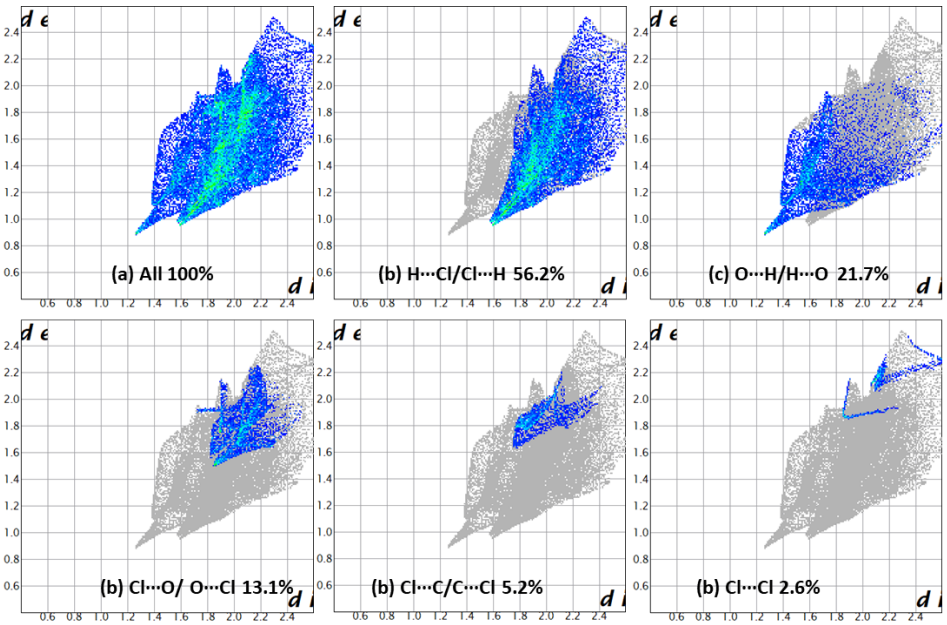

Figure S6. The 2D fingerprint plots of interatomic interactions for anion in **II** at 100 K show the percentages of contacts contributed to the total Hirshfeld surface area of the molecules.

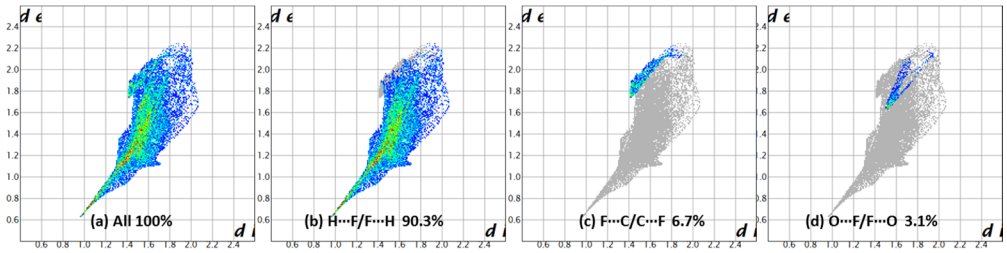

Figure S7. The 2D fingerprint plots of interatomic interactions for anion in **III** at 100 K showing the percentages of contacts contributed to the total Hirshfeld surface area of the molecules.