

Table S 1. The main interatomic distances in the structure of $C_6H_{15}N_2O_4 \cdot I_3$.

Atoms	Distance, Å	Atoms	Distance, Å
I1-I2	2.9243(7)	N4-H4B	0.84(5)
O5-C1	1.233(4)	N4-H4C	0.94(7)
O6-C1	1.277(4)	N4-H4A	0.90(4)
N4-C2	1.489(5)	C2-H2	0.98(5)
O6-H6	0.79(3)	C3-H3B	0.90(7)
C1-C2	1.516(4)	C3-H3C	0.95(6)
C2-C3	1.517(5)	C3-H3A	0.98(6)

Table S 2. The main valence angles (in degrees) in the structure of $[C_6H_{15}N_2O_4]^{+1}I_3^{-1}$

Atoms	Angle degree	Atoms	Angle degree
I1-I2-I1_a	180.00	H4B-N4-H4C	104(5)
C1-O6-H6	116(8)	C2-N4-H4A	109(3)
O5-C1-C2	118.9(3)	N4-C2-H2	106(3)
O6-C1-C2	114.1(3)	C1-C2-H2	109(2)
O5-C1-O6	127.0(3)	C3-C2-H2	112(3)
C1-C2-C3	111.2(3)	C2-C3-H3B	107(4)
N4-C2-C1	108.3(3)	C2-C3-H3C	110(3)
N4-C2-C3	110.3(3)	C2-C3-H3A	111(3)
C2-N4-H4B	105(4)	H3A-C3-H3C	107(5)
C2-N4-H4C	112(4)	H3B-C3-H3C	112(5)
H4A-N4-H4B	113(5)	H3A-C3-H3B	111(5)
H4A-N4-H4C	114(5)		

Table S 3. Hydrogen bonds in the structure $C_6H_{15}N_2O_4 \cdot I_3$.

D—H $\cdots$ A	D-H (Å)	H $\cdots$ A (Å)	D-A (Å)	Angle D-H $\cdots$ A (°)	Sym. code
N4--H4A $\cdots$ O5	0.90(4)	1.88(4)	2.772(4)	173(5)	x, y, z
N4--H4B $\cdots$ O6	0.84(5)	2.21(5)	2.842(4)	132(5)	x, y, z
N4--H4C $\cdots$ I1	0.94(7)	2.90(7)	3.643(3)	137(5)	x, 1+y, z
N4--H4C $\cdots$ I1	0.94(7)	3.04(7)	3.633(3)	123(5)	2-x, 0.5+y, 0.5-z
O6--H6 $\cdots$ O6	0.79(3)	1.68(3)	2.459(3)	174.00	x, y, z

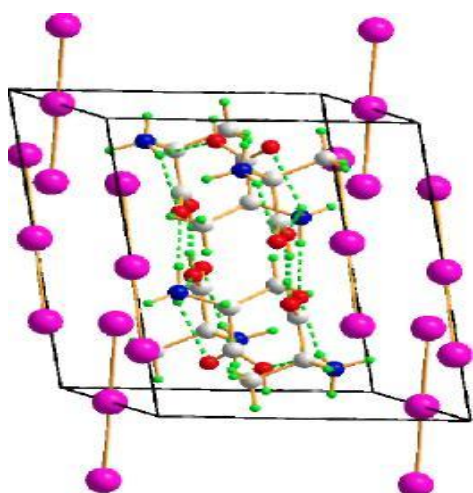


Fig.S1 Perspective view of the structure of $\text{C}_6\text{H}_{15}\text{N}_2\text{O}_4 \cdot \text{I}_3$. The planes parallel to (100) formed by the molecules of $\text{C}_6\text{H}_{15}\text{N}_2\text{O}_4$ and the polyanion of I_3 are visible

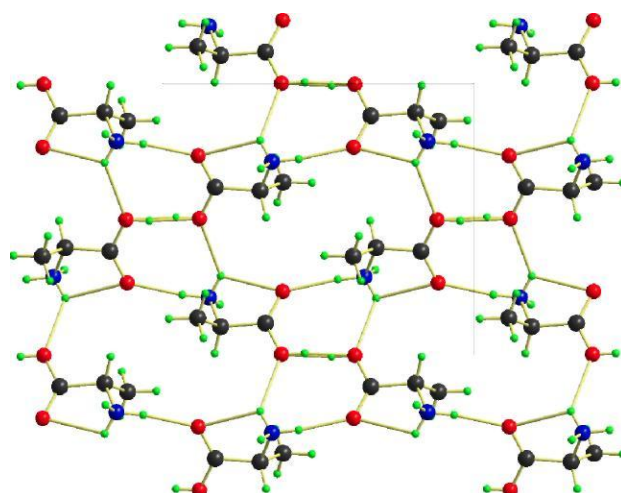


Fig.S2 A two-dimensional network of $\text{C}_6\text{H}_{15}\text{N}_2\text{O}_4$ dimers. Both the hydrogen bonds forming the dimers and the hydrogen bonds linking the dimers into a two-dimensional network parallel to (100) are shown.

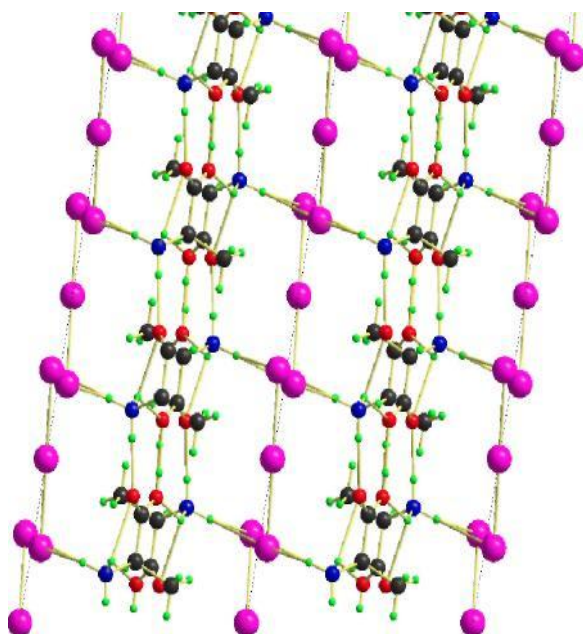


Fig.S3 Projection of the structure onto the (010) plane. Hydrogen bonds between the dimer and polyanion layers are shown.

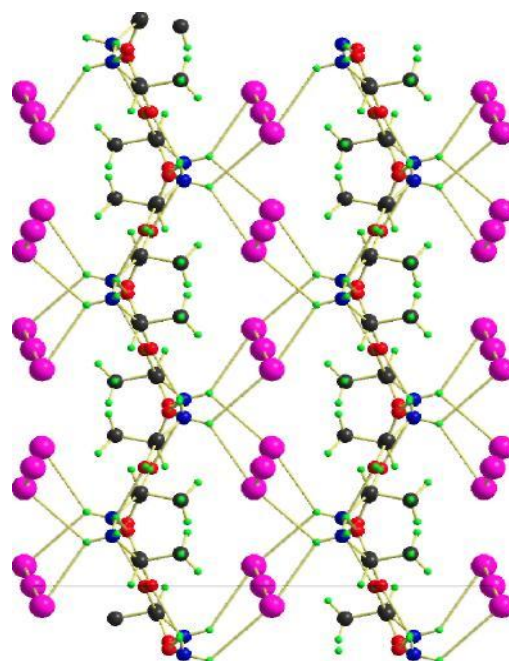


Fig.S4 Projection of the structure onto the (001) plane. Hydrogen bonds between the dimer and polyanion layers are shown.