Supplemental Material

Substituent swap affect the crystal structure and properties of N-benzyl-4-amino-1, 2, 4-triazole related organic salts

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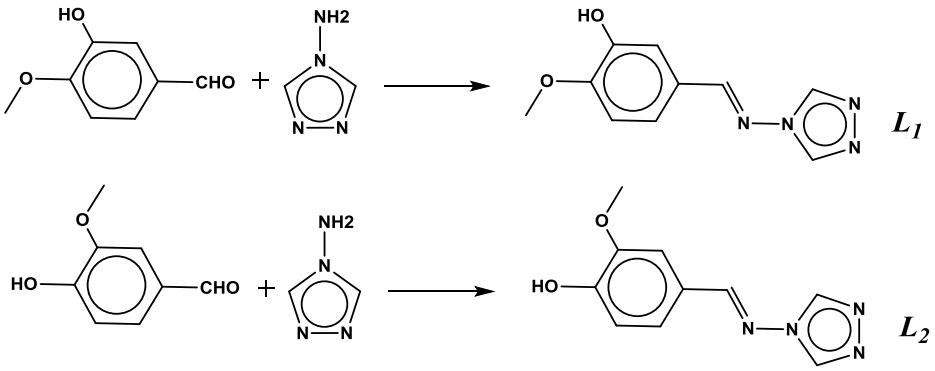

Scheme S1 The synthetic route of L_1 and L_2.

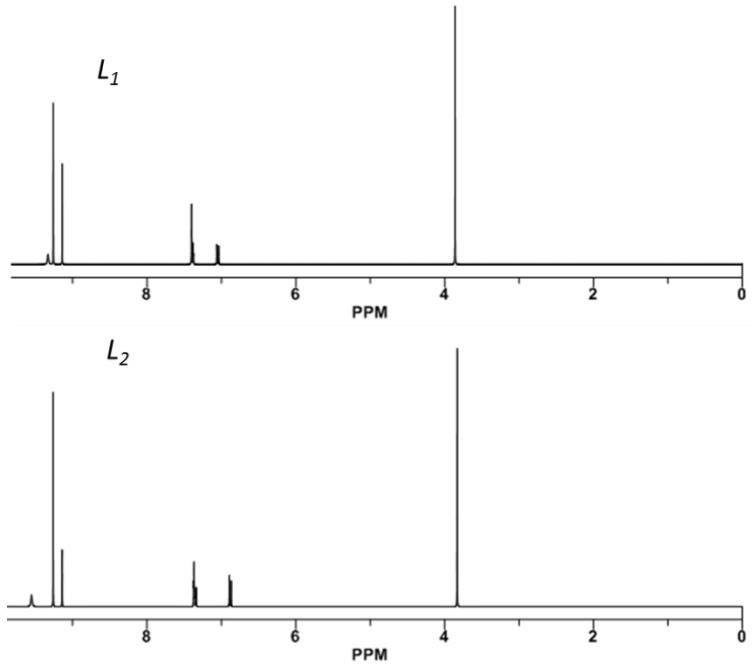

Fig S1 ^{1}HNMR of compounds L_1 and L_2.

Table: S1 Crystal data and structure refinement for ligand L_1 and salts **1-6**.

Complex	L_1	**1**	**2**	**3**
Formula	$C_{10}H_{10}N_4O_2$	$C_{10}H_{11}N_5O_5$	$C_{20}H_{21}ClN_8O_8$	$C_{20}H_{25}N_8O_9P$
Formula weight	218.22	281.24	536.90	552.45
Crystal system	Monoclinic	Monoclinic	Triclinic	Orthorhombic
Space group	*P21/c*	*P 21/c*	*P -1*	*Pca21*
a/ Å	5.4220(11)	8.8062(18)	8.0110(16)	21.2012(14)
b/ Å	10.436(2)	17.518(4)	11.071(2)	7.069(3)
c/ Å	17.944(4)	8.1176(16)	13.968(3)	17.137
α/ °	90.00	90.00	100.75(3)	90.00
β/°	91.20(3)	103.15(3)	91.99(3)	90.00
λ/°	90.00	90.00	108.46(3)	90.00
V, Å ^{3}	1015.1(4)	1219.4(4)	1148.6(5)	2568.2(12)
Z	4	4	2	4
D calc (Mg m^{-3})	1.428	1.532	1.552	1.429
T/K	293(2)	293(2)	293(2)	293(2)
μ (mm^{-1})	0.104	0.125	0.233	0.172
Cryst dimensions	0.2×0.1×0.1	0.2×0.2×0.2	0.2×0.1×0.1	0.3×0.1×0.1
No. of reflns collected	1869	2776	4234	5235
No. of unique reflns	1186	1614	2983	3532
No. of params	146	187	335	352
Goodness-of-fit on F^2	1.002	1.169	1.059	1.069
R1,wR2 (I>2σ(I)	0.0561, 0.1331	0.0875, 0.1798	0.0581, 0.1522	0.0923, 0.2198
R1,wR2 (all data)	0.1000, 0.1581	0.1555, 0.2043	0.0863, 0.1712	0.1354 , 0.2440
CCDC NO.	1526868	1526869	1526870	1526871

Complex	**4**	**5**	**6**
Formula	$C_{10}H_{11}N_5O_5$	$C_{10}H_{11}ClN_4O_6$	$C_{10}H_{13}N_4O_6P$
Formula weight	281.24	318.68	316.21
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*Pn*	*Pn*	*Pn*
a/ Å	4.2000(8)	4.4190(9)	4.4091(9)
b/ Å	8.5070(17)	8.5810(17)	8.6022(17)
c/ Å	17.069(3)	17.499(4)	17.525(4)
α/°	90.00	90.00	90.00
β/°	94.05(3)	91.35(3)	91.34(3)
λ/°	90.00	90.00	90.00
V, Å ^{3}	608.3(2)	663.4(2)	664.5(2)
Z	2	2	2
D calc (Mg m^{-3})	1.535	1.595	1.580
T/K	293(2)	293(2)	293(2)
μ (mm^{-1})	0.126	0.324	0.243
Cryst dimensions	0.3×0.2×0.1	0.2×0.1×0.1	0.3×0.1×0.1
No. of reflns collected	1278	1390	2636
No. of unique reflns	1162	1201	2092
No. of params	181	190	196
Goodness-of-fit on F^2	1.001	1.080	0.995
R1,wR2 (I>2σ(I)	0.0404, 0.1162	0.0553,0.1418	0.0558,0.1205
R1,wR2 (all data)	0.0458, 0.1226	0.0681,0.1530	0.0750,0.1404
CCDC NO.	1526872	1526873	1526874

Table: S2 Selected H-bond lengths and angles of ligand L_1 and salts **1-6**.

D-H···A(Å)(symmetry mode)	H···A(Å)	D···A(Å)	D-H··A(deg)
L_1			
O2-H2A···N2(1+x, 1+y, z)	1.98	2.72	146.00
O2-H2A···N1(1+x, 1+y, z)	2.55	3.17	130.54
C9-H9A···N1(-x, 1/2+y, 1/2-y)	2.61	3.49	160.49
Salt **1**			
N5-H5…O3(1-x, 1-y, 1-z)	1.76	2.71	160.76
N5-H5…O5(-x, 1/2+y, -1/2+z)	2.56	2.95	104.13
O5-H5A…O2(x, 1/2-y, 1/2+y)	1.85	2.66	171.35
Salt **2**			
O3-H3B…N5(-1+x, -1+y, z)	2.01	2.83	162.46
N6-H6…N2(x, 2+y, z)	1.82	2.67	170.92
O1-H1A…N1(1+x, -1+y, z)	2.08	2.81	149.62
Salt **3**			
N8-H8A…O2(x, -1+y, z)	1.75	2.61	171.00
O8-H8…O3(1/2-x, -1+y, 1/2+z)	1.92	2.66	150.42
O1-H1A…O2W	1.99	2.59	129.82
Salt **4**			
O1-H1A…O4(-3/2+x, 1-y, 1/2+z)	1.80	2.62	178.56
N1-H1B…O1(3/2+x, 1-y, -1/2+z)	2.25	2.85	127.06
N1-H1B…O2(3/2+x, 1-y, -1/2+z)	1.98	2.79	157.94
Salt **5**			
N1-H1…O2(-3/2+x, 1-y, 1/2+z)	1.98	2.77	154.18
O1-H1A…N1(3/2+x, 1-y, -1/2+z)	2.09	2.92	164.96
Salt **6**			
N3-H3A…O1(3/2+x, 1-y, -1/2+z)	1.98	2.77	154.25
O6-H6…O4(-1/2+x, 1-y, 1/2+z)	1.84	2.66	175.18
O5-H5…O2(1+x, y, z)	1.79	2.59	167.27

Table: S3 The solubility of salts **1-6**.

Salts	Solubility[m]
1	0.312
2	0.025
3	0.505
4	0.252
5	0.233
6	0.284

Table: S4 the crystallization of ligands L_1, L_2 in aqueous solution with various anion mixtures

Entry	Ligand	Anion mixture/mol (1:1)	Crystalline product
1	L_1	ClO_4^-/NO_3^-	$L_1 \cdot HL_1^+ \cdot ClO4^-$
2	L_1	$ClO_4^-/H_2PO_4^-$	$L_1 \cdot HL_1^+ \cdot ClO4^-$
3	L_2	ClO_4^-/NO_3^-	$HL_2^+ \cdot NO_3^-/HL_2^+ \cdot ClO_4^-$
4	L_2	$ClO_4^-/H_2PO_4^-$	$HL_2^+ \cdot ClO_4^-/HL_2^+ \cdot H_2PO_4^-$

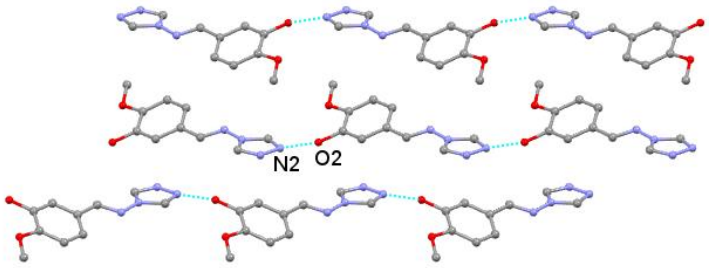

Fig. S2: The views of hydrogen bonds connection of L_1.

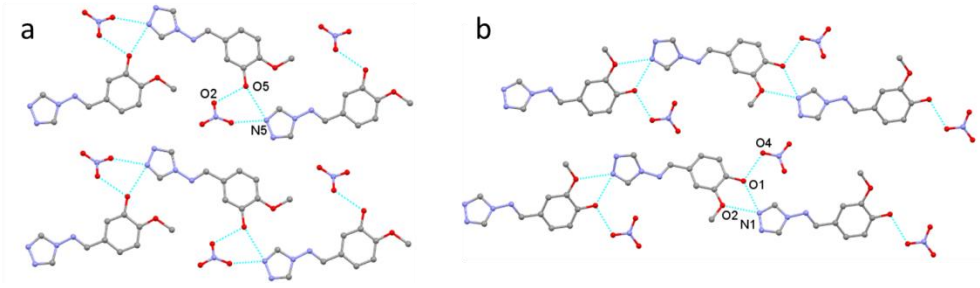

Fig. S3: (a) The view of hydrogen bonds interaction of salt **1**. (b) The view of hydrogen bonds interaction of salt **4**. The hydrogen atoms are omitted for clarity.

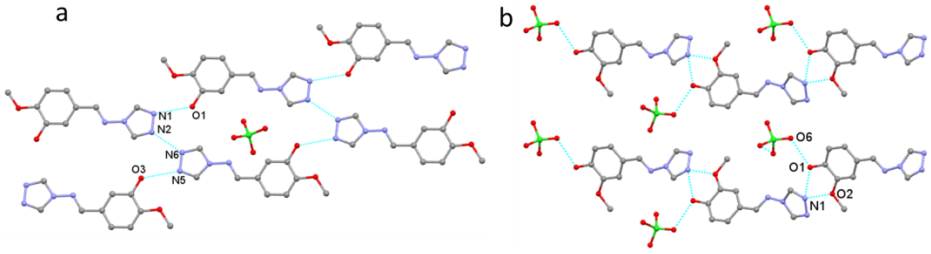

Fig. S4: X-ray crystal structure of the salt **2** and **5**. The mainly hydrogen bonding interaction (a and b).

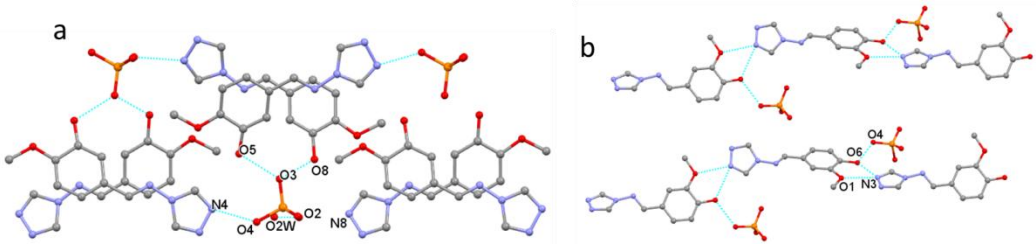

Fig. S5: (a) The hydrogen bonding interaction of salts **3** and **6** (a and b).

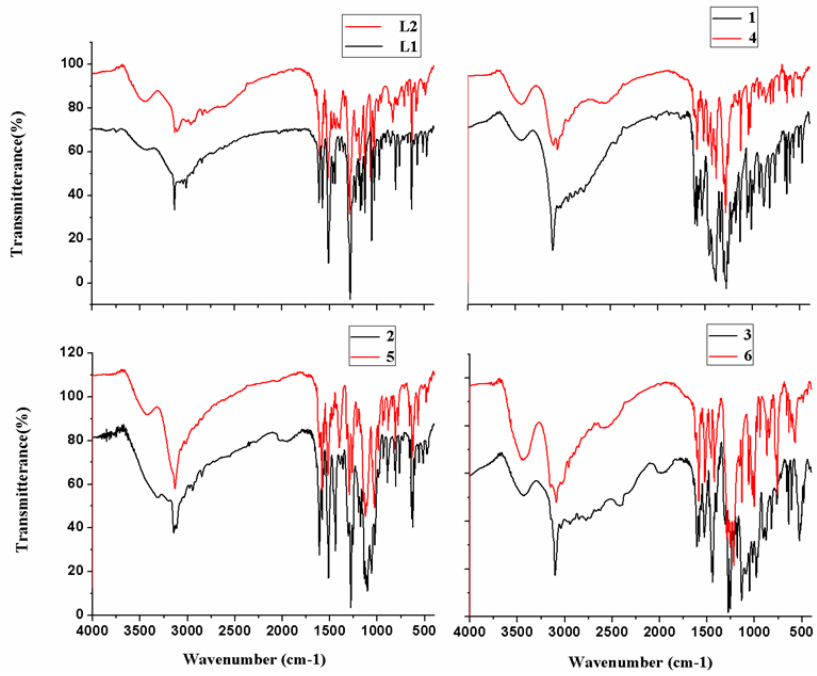

Fig. S6: IR spectrum of the ligands L_1, L_2 and salts **1**-**6**.

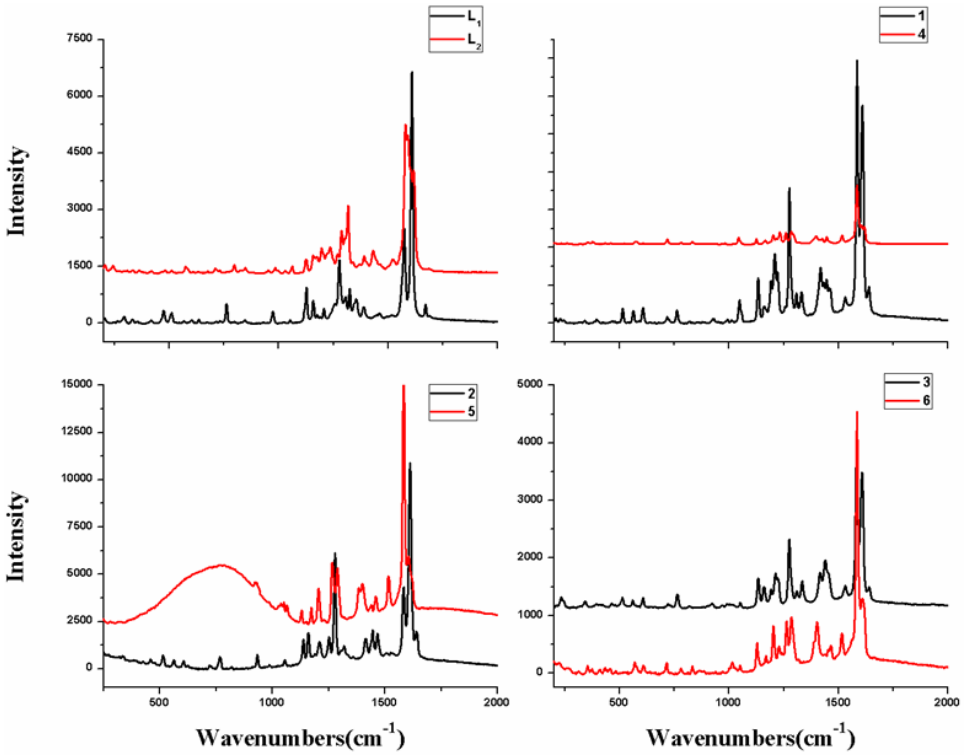

Fig.S7 Raman spectra of the ligands L_1, L_2 and salts **1-6.**

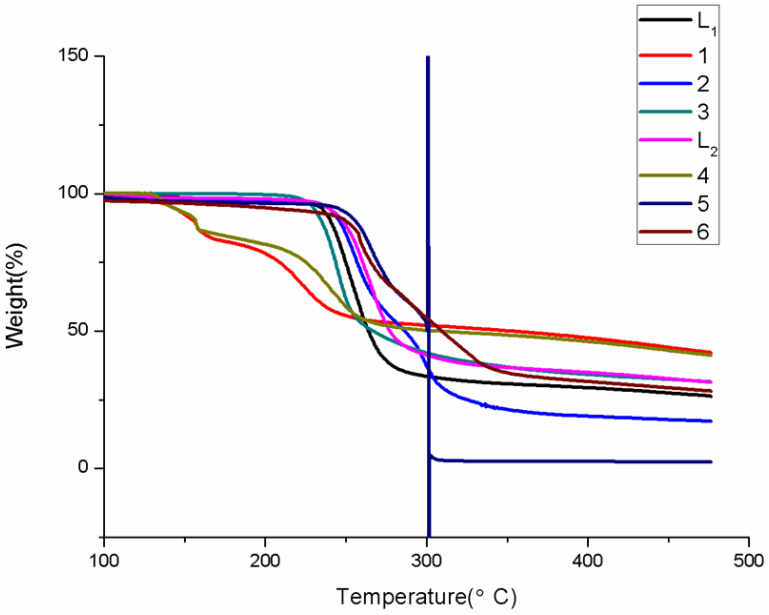

Fig. S8: Thermogravimetric analysis (TGA) curves of ligands L_1, L_2 and salts **1-6**.