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Inorganic anion-assisted supramolecular assemblies of bent dipyridines: effects of anionic geometries on the hydrogen-bonding networks

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Table S1. Hydrogen-bonding Distances and Parameters for the complex of **1**−**7** (Å, °)

Compound	D–H···A	D–H	H···A	D···A	D–H···A	Symmetry Code
1	N1–H3···O8	0.86	1.82	2.670(3)	170	1+x, 3/2−y, 1/2+z
	N4–H8···O2	0.86	1.88	2.710(3)	161	x, y, 1+z
	N4–H8···O3	0.86	2.41	3.120(3)	140	x, y, 1+z
	O8–H11···O4	0.85	2.21	2.977(3)	149	−x, 2−y, 1−z
	O8–H11···N2	0.85	2.56	3.073(3)	120	1−x, 2−y, 1−z
	O8–H12···N2	0.85	2.52	3.333(3)	161	−1+x, y, −1+z
	O9–H13···O5	0.76	2.10	2.849(3)	168	x, 3/2−y, 1/2+z
	O9–H14···O7	0.85	2.24	2.919(3)	137	
	C1–H1···O9	0.93	2.55	3.451(3)	163	x, 3/2−y, 1/2+z
	C2–H2···O2	0.93	2.34	3.243(4)	163	1−x, −1/2+y, 3/2−z
	C3–H4···O7	0.93	2.34	3.217(4)	157	1+x, y, z
	C4–H5···O4	0.93	2.49	3.412(4)	175	1+x, y, z
	C10–H7···O5	0.93	2.56	3.194(4)	126	x, y, 1+z
	C11–H9···O9	0.93	2.39	3.258(4)	155	1−x, 2−y, 2−z
	C12–H10···O6	0.93	2.40	3.330(3)	174	1−x, 1/2+y, 3/2−z
2	N1–H3···O3	0.86	1.73	2.582(3)	170	
	N4–H8···O4	0.86	1.76	2.607(3)	168	x, 1+y, z
	O2–H11···O5	0.82	1.72	2.514(3)	162	−x, y, 3/2−z
	C2–H2···O3	0.93	2.53	3.452(4)	174	1/2−x, 1/2-y, 2−z
	C4–H5···N2	0.93	2.49	3.384(4)	162	−x, 1−y, 1−z
	C12–H10···O2	0.93	2.44	3.248(4)	145	x, 1−y, −1/2+z
3	O4–H1(O4)···O5	0.88	1.91	2.761(11)	161	
	O4–H2(O4)···I10	0.87	2.86	3.393(8)	121	1−x, 1−y, 1−z
	N1–H3···O5	0.86	1.83	2.684(9)	176	1−x, −y, 1−z
	O5–H1(O5)···I2	0.85	2.90	3.709(6)	160	−1+x, y, z
	O5–H2(O5)···I11	0.85	2.69	3.484(7)	157	−1+x, y, z
	N8–H17···I10	0.86	2.76	3.441(7)	137	x, 1+y, z
	N9–H22···N5	0.86	1.85	2.674(9)	161	2−x, 1−y, −z
	N12–H27···O4	0.86	1.84	2.683(11)	167	−x, 2−y, 1−z
	C10–H7···I10	0.93	2.99	3.677(9)	132	1−x, 1−y, 1−z
	C11–H9···I4	0.93	3.03	3.842(11)	146	1−x, 1−y, 1−z

	C21–H15···N3	0.93	2.62	3.360(11)	137	1−x, 1−y, 1−z
	C22–H16···I11	0.93	3.05	3.739(9)	132	1−x, 2−y, 1−z
	C33–H25···N11	0.93	2.54	2.855(11)	100	
	C35–H28···I7	0.93	3.02	3.792(10)	142	1−x, 2−y, −z
4	N4–H7···N8	0.86	1.90	2.737(6)	165	2−x, 1−y, 1−z
	N5–H12···N1	0.86	1.90	2.707(6)	157	1−x, −y, −z
	O3–H19···F10	0.85	2.30	3.135(15)	168	1−x, 1−y, 1−z
	O3–H20···N3	0.85	2.58	3.393(14)	161	
	C1–H1···F8	0.93	2.51	3.331(15)	147	1−x, −y, 1−z
	C2–H2···O3	0.93	2.25	3.159(14)	167	x, −1+y, z
	C4–H4···N6	0.93	2.54	3.267(6)	135	1−x, 1−y, −z
	C9–H5···F9	0.93	2.42	3.355(7)	177	1−x, −y, 1−z
	C10–H6···F3	0.93	2.51	3.235(8)	135	1−x, −y, 1−z
	C11–H8···F12	0.93	2.39	3.315(7)	171	1−x, 1−y, 1−z
	C13–H10···F6	0.93	2.43	3.35(2)	170	1+x, y, z
	C21–H15···F6	0.93	2.41	3.329(15)	171	1+x, y, z
5	N1–H3···F1	0.86	2.31	2.901(5)	126	2−x, −y, 2−z
	N1–H3···F2	0.86	2.12	2.811(6)	137	1−x, −y, 2−z
	N4–H8···O2	0.86	1.78	2.628(6)	169	−1/2+x, 3/2−y, 1/2+z
	O2–H11···F4	0.96	2.12	2.855(15)	132	1−x, 1− y, 1−z
	O2–H12···F5'	0.96	2.22	2.834(12)	120	
	C2–H2···F3	0.93	2.40	3.242(6)	150	−1+x, y, z
	C4–H5···F6	0.93	2.50	3.384(6)	158	3/2−x, −1/2+y, 3/2−z
	C9–H6···F7'	0.93	2.38	3.303(10)	175	−x, 1−y, 1−z
	C10–H7···F4	0.93	2.49	3.180(16)	131	1/2−x, 1/2+y, 3/2−z
	C10–H7···F4'	0.93	2.18	2.990(17)	145	1/2−x, 1/2+y, 3/2−z
	C12–H10···N3	0.93	2.40	3.317(6)	169	2−x, 1−y, 2−z
6	C2–H2···F4	0.93	2.41	3.282(3)	156	x, y, 1+z
	C3–H3···F4	0.93	2.45	3.343(4)	162	1−x, −y, 1−z
	C9–H5···N3	0.93	2.47	3.239(4)	141	1−x, 1−y, −z
	C10–H6···F2	0.93	2.52	3.347(3)	149	−x, 1−y, −z
	C11–H8···F2	0.93	2.46	3.271(3)	146	x, 1+y, z
7	N1–H3···O3	0.86	2.53	3.143(2)	129	x, y, 1+z
	N1–H3···O6	0.86	1.81	2.654(2)	166	x, y, 1+z
	N2–H6···O3	0.86	1.93	2.752(2)	161	x, 1/2−y, 1/2+z
	N3–H7···O5	0.86	1.91	2.732(2)	159	1+x, 1/2−y, 1/2+z
	N4–H10···O4	0.86	1.73	2.578(2)	170	1+x, y, z
	C3–H1···O6	0.93	2.44	3.309(2)	156	1+x, y, 1+z
	C5–H4···O1	0.93	2.38	3.215(3)	150	−1+x, y, z
	C6–H5···O5	0.93	2.47	3.095(2)	125	x, 1/2−y, 1/2+z
	C9–H8···O5	0.93	2.43	3.264(2)	150	1+x, 1/2−y, 1/2+z
	C10–H9···O2	0.93	2.25	3.123(3)	157	1+x, y, z
	C11–H11···O3	0.93	2.53	3.131(2)	122	

Table S2. Weak Intermolecular Interactions for the Complex of 1−7 (Å)

Compound	Weak Interactions	Shortest Atom-Atom Distance	Anion/Centroid -Centroid Distance
1	N6–O6···Cg1	3.111	3.228
	N6–O5···Cg2	3.216	3.766
2	P1–O3···Cg1	3.165	3.440
	Cg2···Cg3(C2···C11)	3.285	3.741
	Cg1···Cg1(C6···C6)	3.398	3.287
	Cg1···Cg1(C7···C7)	3.295	3.287
3	I3···I9	3.837	
	I1···I6	3.922	
	Cg2···Cg1(C2···C7)	3.235	3.589
	Cg7···Cg4^{i}(C19···N11)	3.162	3.400
4	P1–F5···Cg1	2.999	3.312
	P1–F6'···Cg4	3.019	3.175
	P1–F1···Cg2	3.041	3.722
	P2–F12···Cg3	3.122	3.490
	P2–F8···Cg1	3.044	3.051
	Cg4···Cg5(N6···C15)	3.181	3.418
5	B1–F1···Cg3	3.166	3.633
	B1–F3···Cg2	3.136	2.978
	B1–F4···Cg3	2.827	3.287
	B1–F4'···Cg3	2.916	3.112
	B2–F5'···Cg1	3.080	3.133
	Cg3···Cg1(C12···C7)	3.395	3.820
6	B1–F1···Cg1	2.974	2.940
	B1–F3···Cg3	3.156	3.706
	B1–F4···Cg3	3.165	3.963
	N2–H10···Cg2	2.859	3.452
7	S1–O4···Cg1^{i}	3.088	3.774
	S1–O5···Cg1^{i}	3.095	4.229

Cg1 = centroid of the O1C6N2N3C7 ring, Cg1^{i} = centroid of the N1C4C3C2C6C5 ring, Cg2 = centroid of the N1C2C1C5C4C3 ring, Cg3 = centroid of the N4C10C9C8C12C11 ring, Cg4 = Cg7 = centroid of the O2C18N6N7C19 ring, Cg4^{i} = centroid of the O3C30N10N11C31 ring, Cg5 = centroid of the N5C14C13C17C16C15 ring.

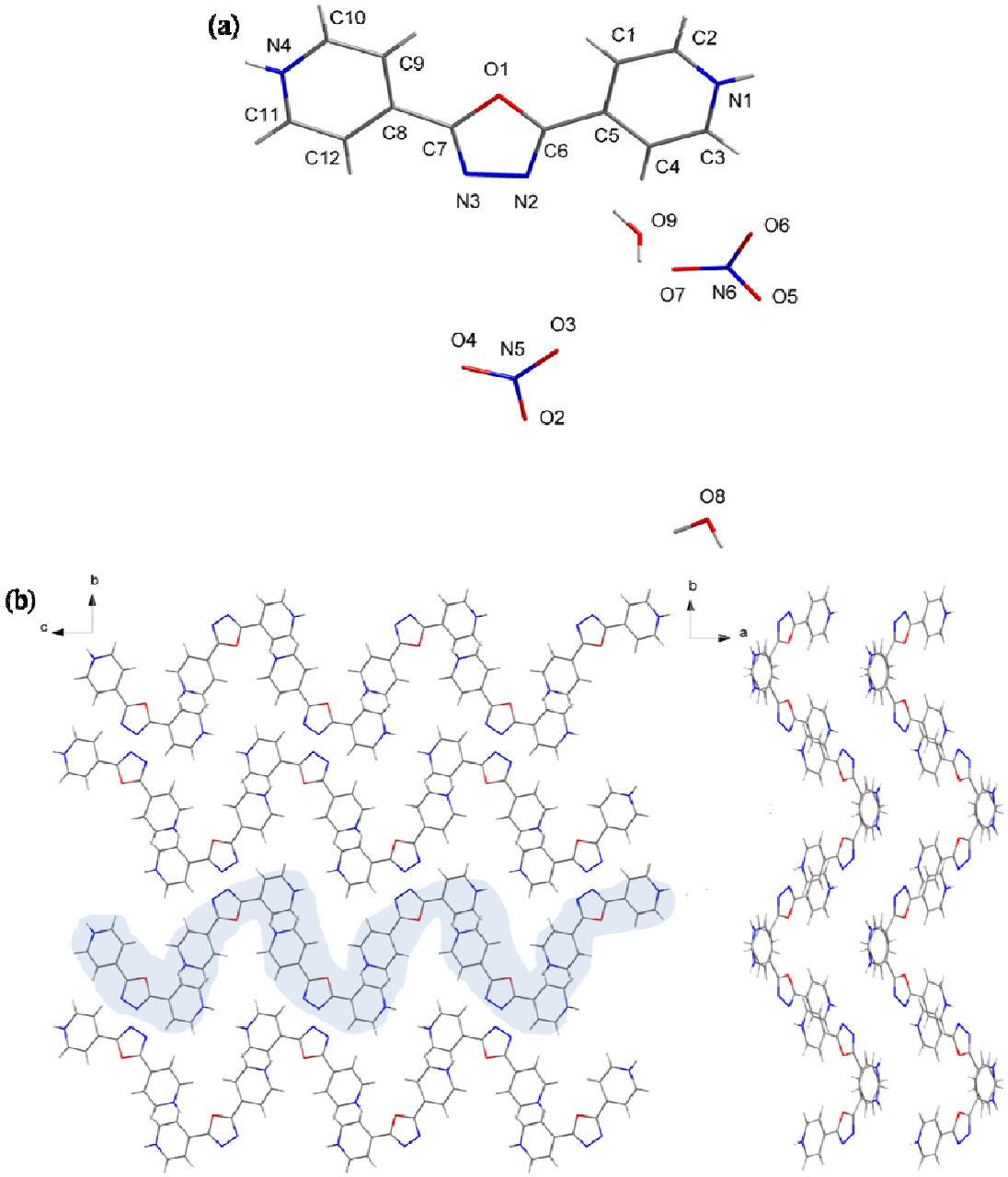


Fig. S1 (a) The asymmetric unit of **1** together with the numbering scheme; (b) Separate molecular structure of 4-H_2bpo^{2+}cations.

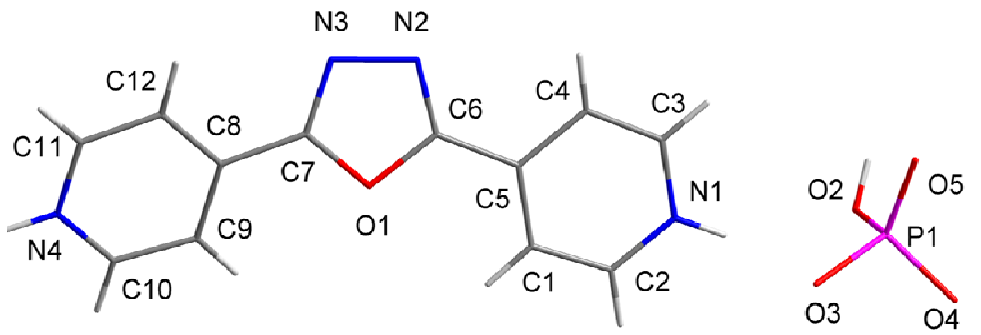
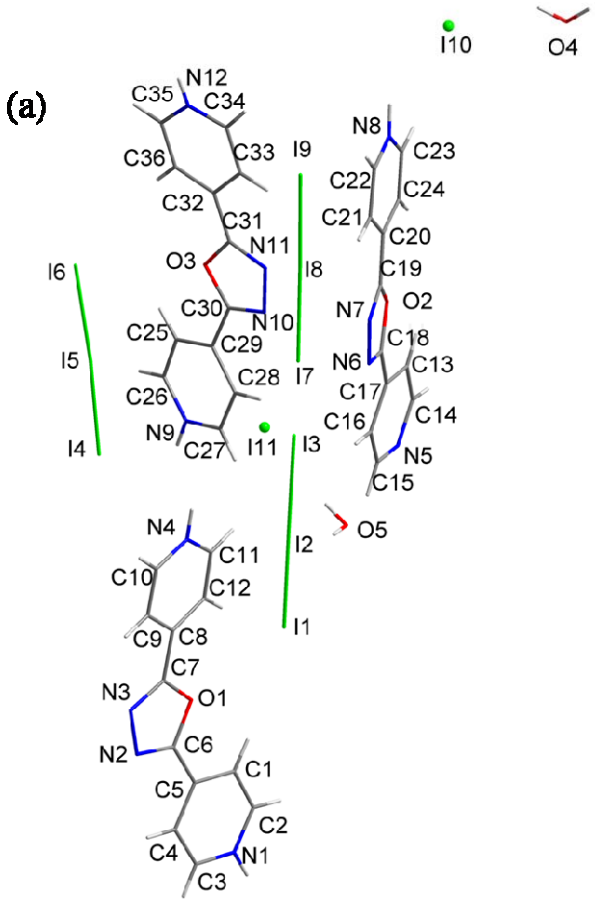


Fig. S2 The asymmetric unit of **2** together with the numbering scheme.



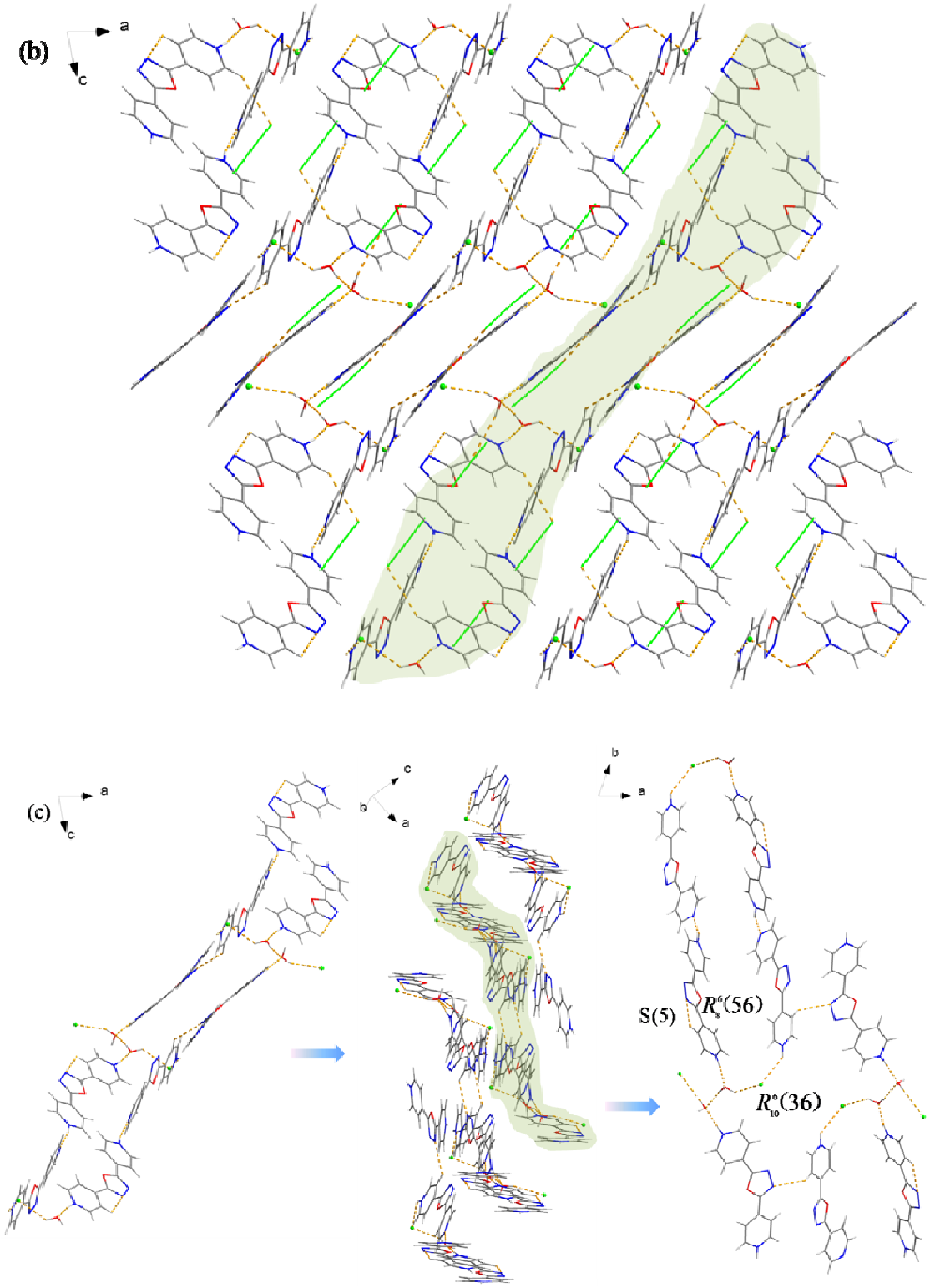


Fig. S3 (a) The asymmetric unit of **3** together with the numbering scheme where ball-and-stick model was used for I^- ions for clarity; (b) The 3D hydrogen-bonding network parallel to the *ac*-plane; (c) Independent molecular structure with I_3^- anions deleted and the side view as well as a moiety of structure in pale green viewed along

the *c*-axis.

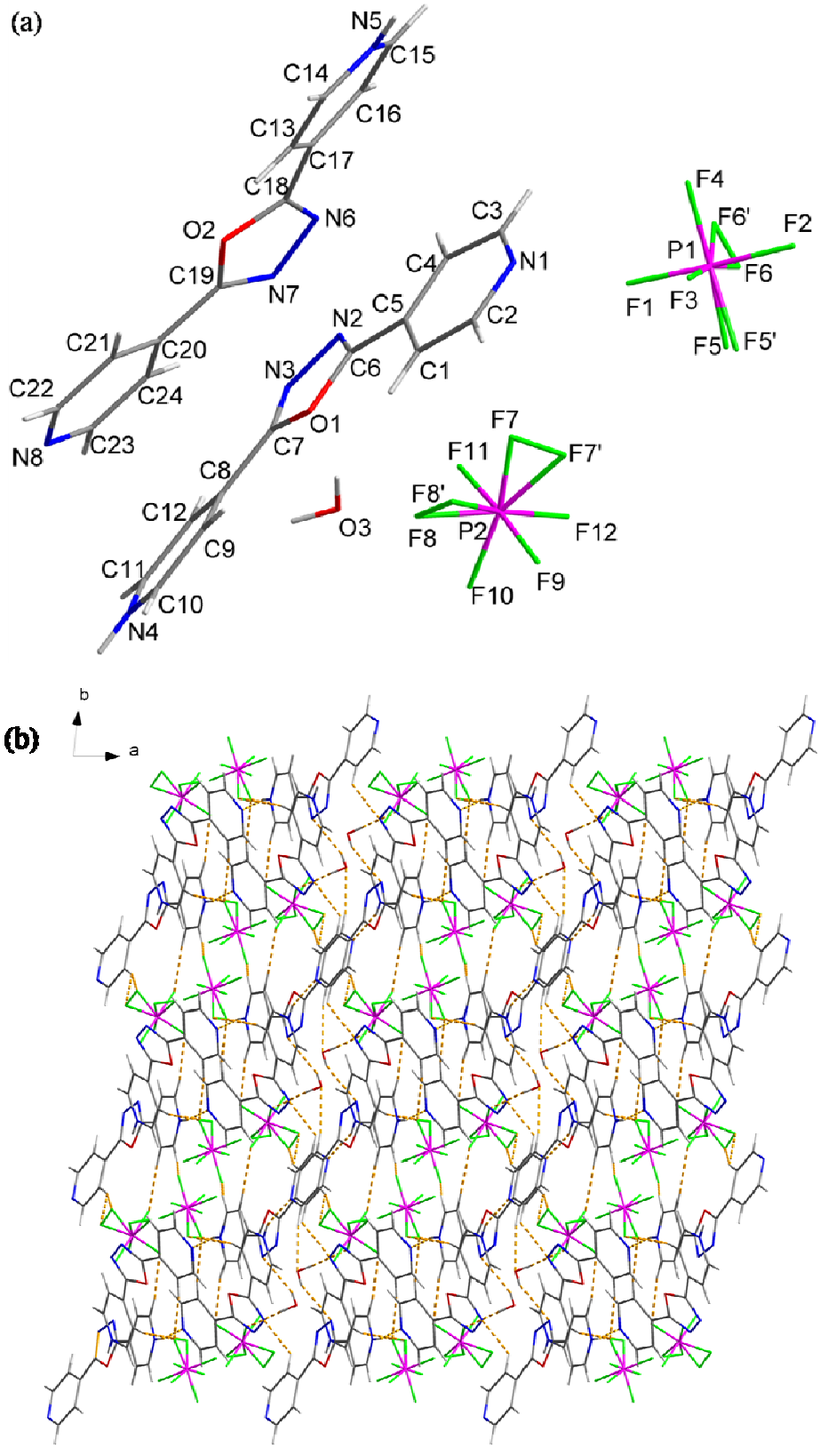


Fig. S4 (a) The asymmetric unit of **4** together with the numbering scheme; (b) The 3D

hydrogen-bonding network parallel to the *ab*-plane.

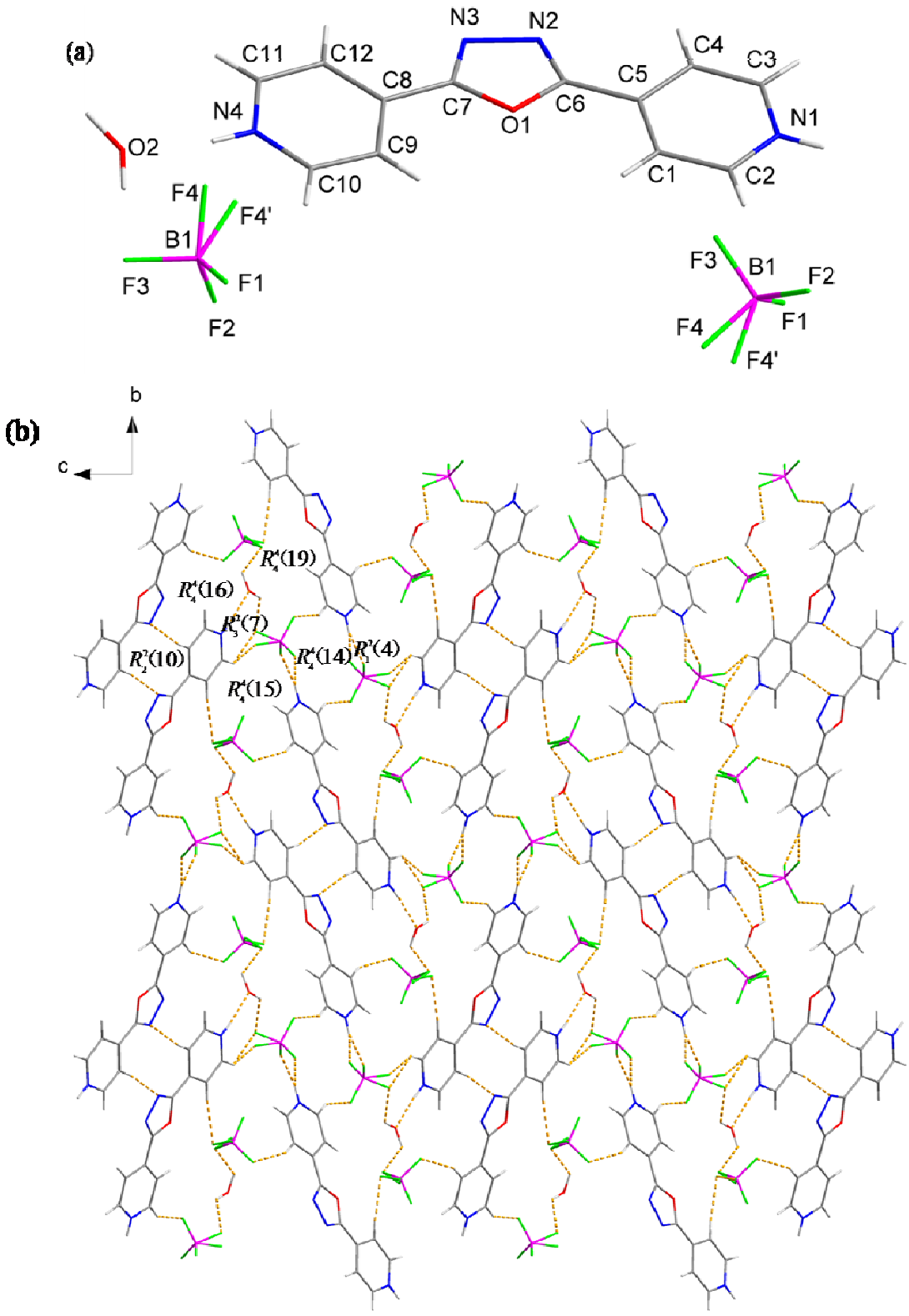


Fig. S5 (a) The asymmetric unit of **5** together with the numbering scheme; (b) The 3D hydrogen-bonding network parallel to the *bc*-plane.

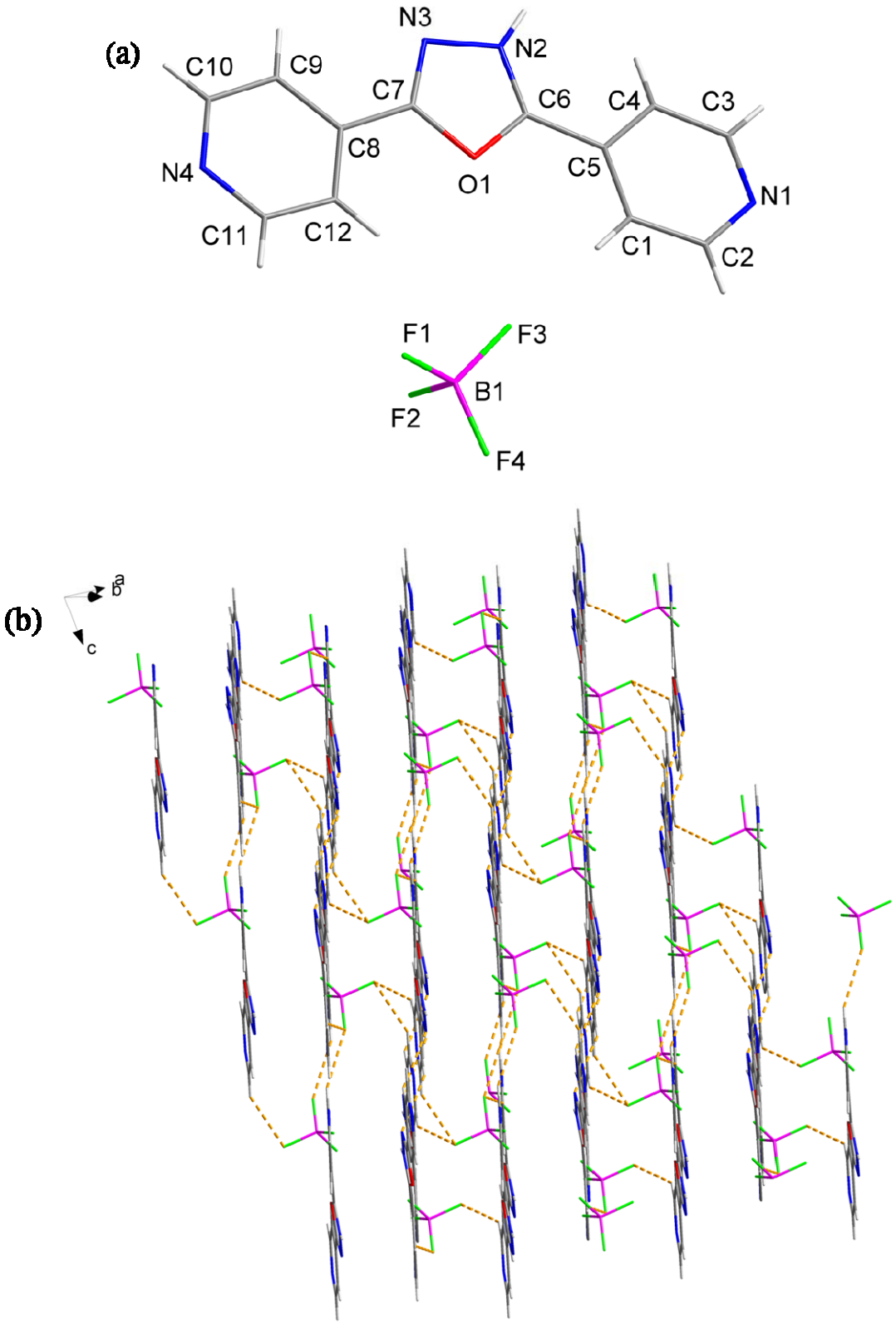


Fig. S6 (a) The asymmetric unit of **6** together with the numbering scheme; (b) A side view of the 3D crystal packing.

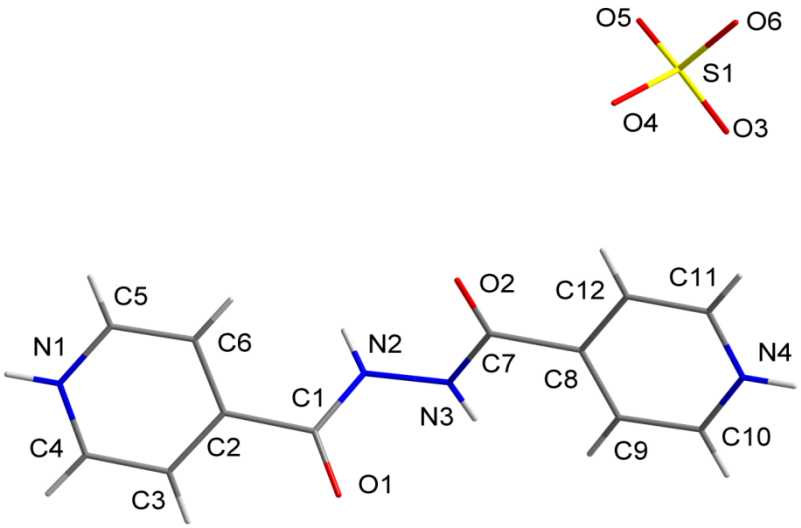


Fig. S7 The asymmetric unit of **7** together with the numbering scheme.

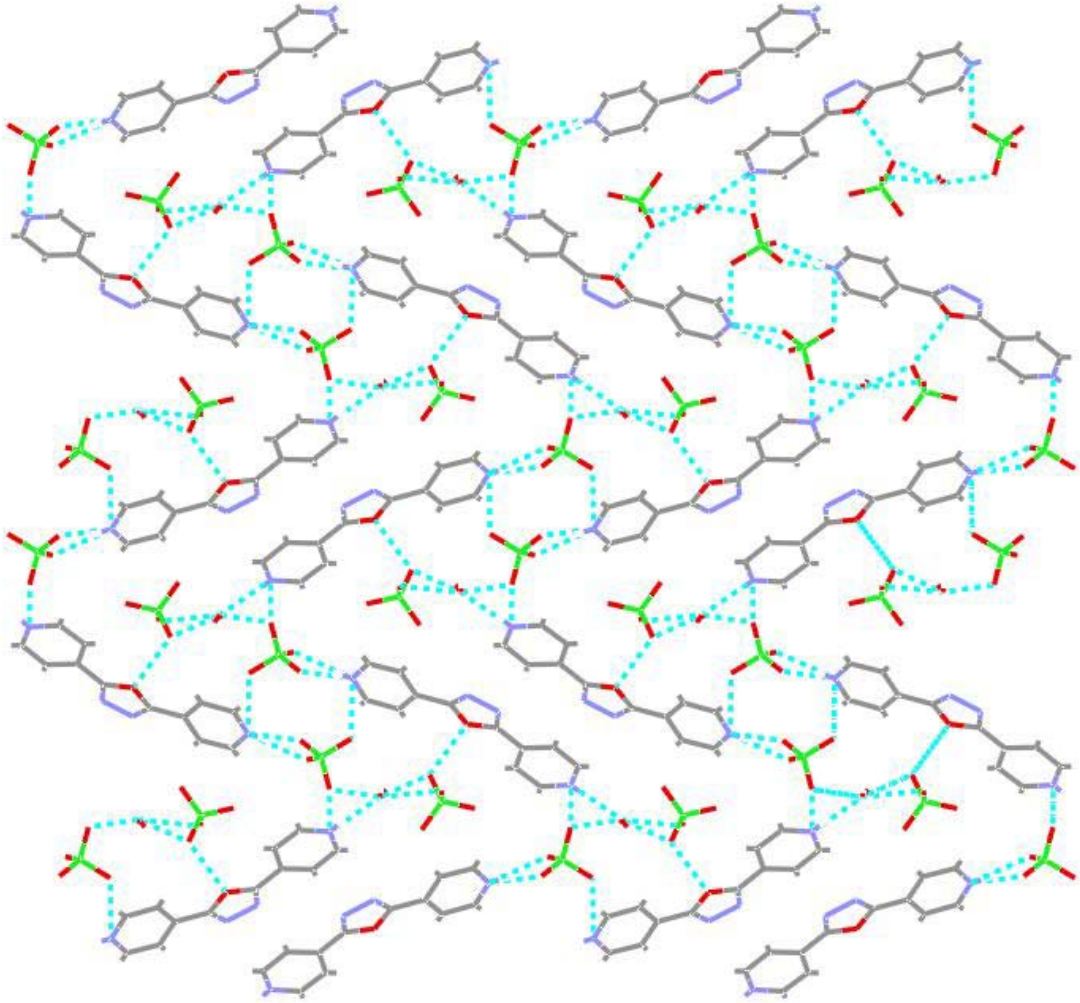


Fig. S8 The crystal packing of perchlorate in ref. 44.

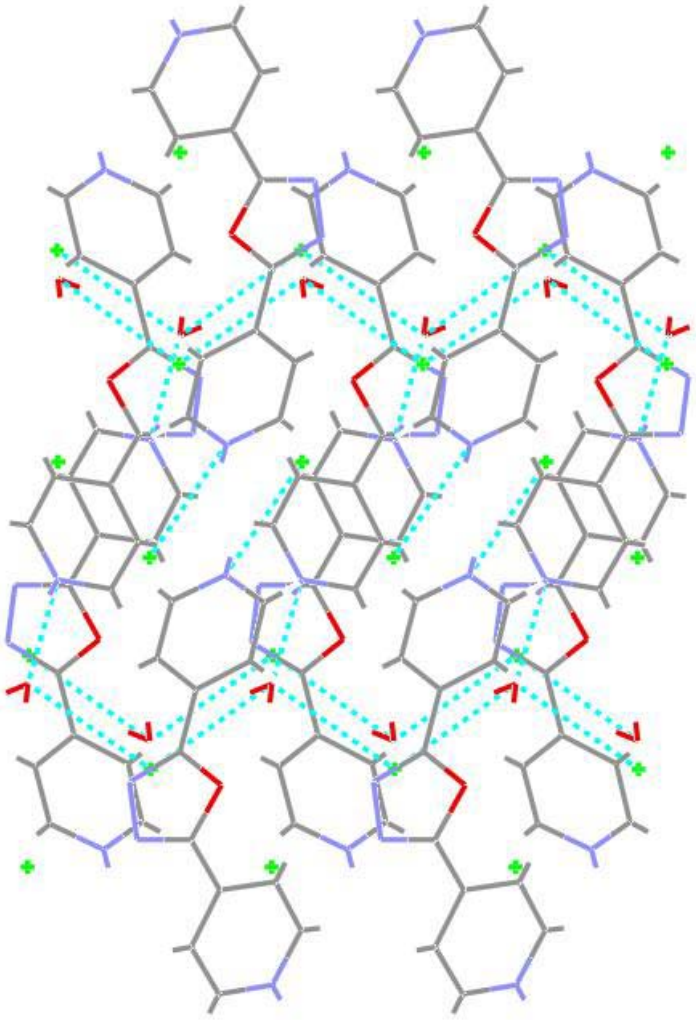


Fig. S9 The crystal packing of bromide in ref. 45.