Two UV Optical Crystals with Strong Optical Anisotropy, Large Band Gaps and α-BBO Type Structure

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Table S1. Crystal data and structure refinement for compounds **1** and **2**.

	Compound **1**	Compound **2**
Formula	$C_{12}H_{25}N_{24}PF_6$	$C_9H_{21}N_{18}OPF_6$
Dcalc./ g cm^{-3}	1.709	1.733
m/mm^{-1}	1.229	2.137
Formula Weight	650.53	542.41
Colour	colourless	colourless
T/K	293(2)	293(2)
Crystal System	trigonal	monoclinic
Space Group	$R\bar{3}c$	$P2_1/n$
a/Å	10.8117(8)	12.9123(3)
b/Å	10.8117(8)	10.9021(2)
c/Å	37.472(4)	15.2051(4)
a/°	90	90
b/°	90	103.770(2)
g/°	120	90
V/Å^3	3793.4(7)	2078.92(8)
Z	6	4
Z'	0.166667	1
Wavelength/Å	1.3405	1.54184
Radiation type	Ga K*a*	Cu K*a*
Qmin/°	4.590	2.992
Qmax/°	60.579	77.167
Measured Refl's.	4249	14828
Indep't Refl's	955	4266
Refl's I≥2 *s*(I)	755	3389
*R*int	0.0377	0.0918
Parameters	98	394
Restraints	0	741
Largest Peak	0.354	1.049
Deepest Hole	-0.344	-1.087
GooF	1.046	1.120
wR_2 (all data)[a]	0.1465	0.1935
wR_2	0.1368	0.1833
R_1 (all data)[b]	0.0590	0.1265
R_1	0.0491	0.0790

[a] $wR_2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$; [b] $R_1 = \sum||Fo|-|Fc||/\sum|Fo|$

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å2\times 10^3$) for compound **1**. *Ueq* is defined as 1/3 of the trace of the orthogonalized *Uij*.

Atom	x	y	z	*Ueq*
N1	8644.3(14)	-1175.2(13)	5440.2(4)	34.4(4)
N2	7741.5(17)	336.6(18)	5439.1(5)	45.2(5)
C1	8876.0(16)	168.7(16)	5440.5(4)	31.7(4)
N3	9645.2(18)	2249.0(18)	6334.2(6)	55.1(6)
N4	11172.6(14)	1362.5(14)	6332.1(4)	37.5(4)
C2	9823.0(17)	1106.2(17)	6332.3(5)	35.4(4)
P1	6666.67	3333.33	5833.33	33.7(4)
F1	5669(13)	2299(10)	6113(3)	126(3)
F2	7616(9)	4507(7)	6121(2)	77.2(16)
F3	7500(20)	2620(20)	5901(4)	201(7)

Table S3. Anisotropic Displacement Parameters ($\times 10^4$) for compound **1**. The anisotropic displacement factor exponent takes the form: *-2p2[h2a*2 × U11+ ... +2hka* × b* × U12]*.

Atom	*U11*	*U22*	*U33*	*U23*	*U13*	*U12*
N1	28.3(7)	27.9(7)	45.5(8)	0.1(6)	1.0(6)	13.1(5)
N2	30.6(8)	35.8(8)	72.1(11)	-2.5(7)	-1.3(7)	18.8(6)
C1	30.5(8)	31.0(8)	33.6(8)	-0.8(6)	-0.4(6)	15.4(6)
N3	34.7(8)	29.9(8)	102.9(15)	1.1(8)	1.1(9)	17.8(6)
N4	28.7(7)	28.0(7)	54.3(9)	0.5(6)	-0.5(6)	13.1(5)
C2	31.0(8)	30.1(8)	45.1(9)	-0.9(7)	-0.3(7)	15.2(6)
P1	26.1(4)	26.1(4)	48.9(6)	0	0	13.04(19)
F1	144(9)	72(5)	99(6)	37(4)	73(7)	8(5)
F2	66(3)	58(3)	88(4)	-30(3)	-29(3)	16(3)
F3	325(16)	289(14)	174(12)	-35(17)	-53(18)	291(15)

Table S4. Bond Lengths in Å for compound **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.3454(19)	P1	F33	1.467(7)
N1	C11	1.3513(19)	P1	F35	1.467(7)
N2	C1	1.327(2)	P1	F36	1.467(7)
N3	C2	1.342(2)	P1	F34	1.467(7)
N4	C2	1.342(2)	P1	F37	1.467(7)
N4	C22	1.3455(19)	F1	F25	1.278(11)
P1	F1	1.520(5)	F1	F23	0.985(10)
P1	F13	1.520(5)	F1	F34	1.460(16)
P1	F14	1.520(5)	F1	F35	1.074(16)
P1	F15	1.520(5)	F2	F36	1.663(15)
P1	F16	1.520(5)	F2	F33	1.004(16)
P1	F17	1.520(5)	F3	F36	1.42(4)
P1	F3	1.467(7)	F3	F34	1.64(4)

11-y,-1+x-y,+z; 22+y-x,1-x,+z; 31-y,+x-y,+z; 44/3-x,2/3-x+y,7/6-z; 51+y-x,1-x,+z; 61/3-y+x,2/3-y,7/6-z; 71/3+y,-1/3+x,7/6-z

Table S5.ond Angles in ° for compound **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C11	115.39(15)	F34	P1	F16	58.5(7)
N1	C1	N12	124.61(14)	F33	P1	F1	135.0(10)
N2	C1	N12	117.87(14)	F37	P1	F36	117.1(3)
N2	C1	N1	117.53(15)	F36	P1	F35	58(2)
C2	N4	C22	114.11(15)	F33	P1	F37	117.0(3)
N3	C2	N41	117.28(15)	F3	P1	F34	117.0(3)
N3	C2	N4	116.83(16)	F3	P1	F33	58(2)
N4	C2	N41	125.89(15)	F33	P1	F34	175(2)
F13	P1	F14	87.5(9)	F37	P1	F35	175(2)
F13	P1	F15	135.2(10)	F37	P1	F34	58(2)
F16	P1	F1	87.5(9)	F34	P1	F35	117.0(3)
F15	P1	F14	77.5(7)	F36	P1	F34	68(2)
F17	P1	F1	135.2(10)	F33	P1	F36	117.1(3)
F17	P1	F13	77.5(7)	F3	P1	F35	117.0(3)
F17	P1	F15	87.4(9)	F3	P1	F36	175(2)
F16	P1	F14	135.2(10)	F33	P1	F35	68.0(19)
F17	P1	F14	140.0(12)	F3	P1	F37	68(2)
F1	P1	F14	77.5(7)	F24	F1	P1	68.6(4)
F13	P1	F1	140.0(12)	F25	F1	P1	75.4(5)
F17	P1	F16	77.5(7)	F25	F1	F24	126.0(12)
F15	P1	F1	77.5(7)	F24	F1	F37	74.4(10)
F13	P1	F16	77.5(7)	F25	F1	F34	58.2(13)
F16	P1	F15	140.0(12)	F25	F1	F37	118.4(15)
F37	P1	F16	42.1(7)	F37	F1	P1	58.9(4)
F37	P1	F1	58.5(7)	F34	F1	P1	66.3(6)
F3	P1	F14	119.4(9)	F34	F1	F24	130.8(9)
F36	P1	F17	119.4(9)	F34	F1	F37	66(2)
F34	P1	F13	100.1(11)	P1	F2	F33	53.6(3)
F34	P1	F17	135.0(10)	F15	F2	P1	62.9(4)
F34	P1	F14	83.7(10)	F14	F2	P1	67.7(4)
F35	P1	F16	135.0(10)	F14	F2	F15	113.9(11)
F34	P1	F1	42.1(7)	F14	F2	F33	117.4(8)
F35	P1	F17	100.1(11)	F14	F2	F35	65.3(12)
F3	P1	F17	58.5(7)	F15	F2	F33	57.8(7)
F3	P1	F13	135.0(10)	F35	F2	P1	64.3(5)
F37	P1	F14	135.0(10)	F35	F2	F15	121.2(13)
F3	P1	F15	42.1(7)	F35	F2	F33	71(2)
F33	P1	F16	119.4(9)	P1	F3	F23	60.7(5)
F33	P1	F15	58.5(7)	P1	F3	F37	56.0(10)
F36	P1	F1	100.1(11)	F15	F3	P1	71.6(5)
F37	P1	F15	100.1(11)	F17	F3	P1	62.6(5)
F35	P1	F1	119.4(9)	F15	F3	F17	111.1(15)
F36	P1	F15	135.0(10)	F15	F3	F23	132.2(8)
F35	P1	F13	58.5(7)	F17	F3	F23	47.8(7)
F34	P1	F15	119.4(9)	F17	F3	F37	79.8(13)
F3	P1	F16	100.1(11)	F15	F3	F33	70.0(19)
F35	P1	F15	83.7(10)	F15	F3	F37	113.4(18)
F33	P1	F14	100.1(11)	F24	F3	P1	77.6(7)
F33	P1	F13	83.7(10)	F24	F3	F17	139.8(10)
F36	P1	F14	58.5(7)	F24	F3	F15	56.5(8)
F37	P1	F13	119.4(9)	F24	F3	F23	108.6(19)
F35	P1	F14	42.1(7)	F24	F3	F37	74(2)
F36	P1	F13	42.1(7)	F24	F3	F33	120.2(19)
F3	P1	F1	83.7(10)	F33	F3	P1	61.0(10)
F33	P1	F17	42.1(7)	F33	F3	F17	43.7(10)
F36	P1	F16	83.7(10)	F33	F3	F23	87.5(11)
F37	P1	F17	83.7(10)	F37	F3	F23	35.4(7)

11-y,-1+x-y,+z; 22+y-x,1-x,+z; 31/3-y+x,2/3-y,7/6-z; 41+y-x,1-x,+z; 51-y,+x-y,+z; 61/3+y,-1/3+x,7/6-z; 74/3-x,2/3-x+y,7/6-z

Table S6. Torsion Angles in ° for compound **1**.

Atom	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Atom	Angle/°
C11	N1	C1	N12	0.2(3)	F15	P1	F3	F27	13.8(10)
C11	N1	C1	N2	179.79(11)	F15	P1	F3	F23	-106.2(12)
C22	N4	C2	N3	179.63(12)	F17	P1	F3	F27	-68.6(13)
C22	N4	C2	N41	-0.1(3)	F14	P1	F3	F23	58.5(8)
F13	P1	F1	F24	33.2(10)	F1	P1	F3	F23	-19.9(18)
F13	P1	F1	F23	-105.8(6)	F1	P1	F3	F27	100.0(6)
F14	P1	F1	F24	112.9(7)	F16	P1	F3	F37	50.0(10)
F15	P1	F1	F23	116.7(10)	F14	P1	F3	F36	137(2)
F16	P1	F1	F23	47.3(6)	F16	P1	F3	F36	-96.3(13)
F16	P1	F1	F24	-173.8(12)	F17	P1	F3	F37	36.1(17)
F14	P1	F1	F23	-26.0(10)	F13	P1	F3	F36	130.4(8)
F17	P1	F1	F24	-37.3(10)	F15	P1	F3	F37	118.5(13)
F15	P1	F1	F24	-104.4(14)	F17	P1	F3	F36	-110.2(12)
F17	P1	F1	F23	-176.2(8)	F14	P1	F3	F37	-76.9(19)
F16	P1	F1	F33	-112.5(17)	F1	P1	F3	F36	58.5(9)
F14	P1	F1	F33	174.2(17)	F1	P1	F3	F37	-155.2(10)
F15	P1	F1	F36	32.5(12)	F13	P1	F3	F37	-83.4(14)
F14	P1	F1	F36	-110.2(17)	F15	P1	F3	F36	-27.8(12)
F16	P1	F1	F36	-36.9(11)	F34	P1	F1	F24	37.6(12)
F17	P1	F1	F33	24.0(15)	F37	P1	F1	F24	125.0(19)
F13	P1	F1	F33	94.4(19)	F33	P1	F1	F23	160(2)
F13	P1	F1	F36	170.0(14)	F3	P1	F1	F23	16.3(13)
F15	P1	F1	F33	-43.1(16)	F35	P1	F1	F23	-160.1(7)
F17	P1	F1	F36	99.6(14)	F37	P1	F1	F23	-13.9(11)
F16	P1	F2	F13	155.9(10)	F3	P1	F1	F24	155.2(9)
F17	P1	F2	F14	-148.6(9)	F36	P1	F1	F24	-137(2)
F13	P1	F2	F14	134.5(17)	F35	P1	F1	F24	-21.2(17)
F17	P1	F2	F13	76.9(16)	F33	P1	F1	F24	-61.3(14)
F1	P1	F2	F14	70.2(8)	F34	P1	F1	F23	-101.3(16)
F14	P1	F2	F13	-134.5(17)	F36	P1	F1	F23	84.2(10)
F1	P1	F2	F13	-64.2(8)	F3	P1	F1	F36	-68(2)
F16	P1	F2	F14	-69.6(12)	F3	P1	F1	F33	-143.5(13)
F13	P1	F2	F37	-157.0(19)	F35	P1	F1	F33	40(2)
F13	P1	F2	F34	-72.4(14)	F37	P1	F1	F36	-98.1(5)
F14	P1	F2	F37	68.5(9)	F36	P1	F1	F33	-76(3)
F16	P1	F2	F34	83.5(16)	F35	P1	F1	F36	115.6(9)
F17	P1	F2	F37	-80.1(10)	F34	P1	F1	F33	98.9(7)
F17	P1	F2	F34	5(2)	F33	P1	F1	F36	76(3)
F1	P1	F2	F37	138.7(13)	F37	P1	F1	F33	-174(2)
F1	P1	F2	F34	-136.6(18)	F34	P1	F1	F36	174(2)
F16	P1	F2	F37	-1.1(13)	F34	P1	F2	F14	-153(2)
F14	P1	F2	F34	153(2)	F35	P1	F2	F14	170.2(7)
F16	P1	F3	F14	127(2)	F37	P1	F2	F14	-68.5(9)
F13	P1	F3	F16	-133.3(15)	F33	P1	F2	F13	-27.9(10)
F14	P1	F3	F16	-127(2)	F35	P1	F2	F13	35.7(17)
F17	P1	F3	F14	113.0(15)	F34	P1	F2	F13	72.4(14)
F15	P1	F3	F16	68.5(15)	F36	P1	F2	F14	34.7(13)
F1	P1	F3	F14	-78.3(17)	F3	P1	F2	F13	-147.9(10)
F1	P1	F3	F16	154.8(9)	F36	P1	F2	F13	-100(2)
F13	P1	F3	F14	-6.5(19)	F37	P1	F2	F13	157.0(19)
F17	P1	F3	F16	-13.9(18)	F3	P1	F2	F14	-13.4(14)
F15	P1	F3	F14	-164.6(10)	F33	P1	F2	F14	106.6(16)
F14	P1	F3	F27	178.4(18)	F3	P1	F2	F37	55.1(18)
F16	P1	F3	F27	-54.8(7)	F35	P1	F2	F34	-37(2)
F13	P1	F3	F23	52.0(19)	F37	P1	F2	F34	85(3)
F16	P1	F3	F23	-175(2)	F36	P1	F2	F37	103.2(5)
F13	P1	F3	F27	171.9(9)	F3	P1	F2	F34	139.8(13)
F17	P1	F3	F23	171.4(13)	F35	P1	F2	F37	-121.3(8)
F36	P1	F2	F34	-172(3)	F37	P1	F3	F23	135(2)

F33	P1	F2	F37	175.1(19)	F33	P1	F3	F27	73.4(13)
F33	P1	F2	F34	-100.2(8)	F34	P1	F3	F23	100.0(15)
F34	P1	F2	F37	-85(3)	F36	P1	F3	F23	-78(2)
F37	P1	F3	F14	76.9(19)	F34	P1	F3	F27	-140.1(10)
F37	P1	F3	F16	-50.0(10)	F37	P1	F3	F27	-104.8(12)
F33	P1	F3	F16	128.2(14)	F36	P1	F3	F27	41.5(7)
F33	P1	F3	F14	-104.9(13)	F33	P1	F3	F23	-46.5(17)
F36	P1	F3	F16	96.3(13)	F33	P1	F3	F36	31.9(17)
F34	P1	F3	F14	41.6(17)	F37	P1	F3	F36	-146.3(17)
F34	P1	F3	F16	-85.3(16)	F34	P1	F3	F37	-35.3(19)
F36	P1	F3	F14	-137(2)	F36	P1	F3	F37	146.3(17)
F34	P1	F3	F36	178.4(6)	F33	P1	F3	F37	178.2(8)

11-y,-1+x-y,+z; 22+y-x,1-x,+z; 31+y-x,1-x,+z; 41-y,+x-y,+z; 51/3+y,-1/3+x,7/6-z; 64/3-x,2/3-x+y,7/6-z; 71/3-y+x,2/3-y,7/6-z

Table S7. Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å2\times 10^3$) for compound **1**. *Ueq* is defined as 1/3 of the trace of the orthogonalized *Uij*.

Atom	x	y	z	*Ueq*
H2A	7900(30)	1180(30)	5440(6)	54
H2B	6950(30)	-340(30)	5432(6)	54
H3A	8760(30)	2150(30)	6310(7)	66
H3B	10300(30)	3040(30)	6285(7)	66
H	11500(500)	3333.33	5833.33	700(600)

Table S8. Aomic Occupancies for all atoms that are not fully occupied in compound **1**.

Atom	Occupancy
F1	0.3333
F2	0.3333
F3	0.3333
H	0.3333

Table S9. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å2 \times 10^3$) for compound **2**. *Ueq* is defined as 1/3 of the trace of the orthogonalized *Uij*.

Atom	x	y	z	*Ueq*
N1	-2238.8(19)	3227(2)	6549.4(17)	23.5(5)
N2	2041(2)	1075(3)	9199(2)	35.7(7)
N3	5388(2)	1005(2)	4265(2)	36.3(7)
N4	4620.1(19)	3281(2)	9777.7(17)	23.0(5)
N5	5668(2)	1560(3)	9991(2)	36.6(7)
N6	3575.1(19)	1255(2)	3902.7(17)	24.0(5)
C1	-1273(2)	3700(3)	6760.8(19)	23.0(6)
C2	3616(2)	3706(3)	9556.5(19)	22.1(6)
C3	-496(2)	1740(3)	6912(2)	25.2(6)
N7	4057(2)	4899(2)	4032(2)	36.3(7)
N8	2723.6(19)	3021(2)	9349.4(18)	24.6(5)
N9	-3245(2)	1484(2)	6351(2)	32.1(6)
N10	-1444(2)	1206(2)	6709.8(17)	26.3(6)
N11	-1126(2)	4898(2)	6796.1(19)	32.0(6)
N12	3867.4(19)	1254(2)	9598.9(18)	25.4(5)
C4	4688(2)	2050(3)	9781.5(19)	22.5(6)
C5	3897(2)	3689(3)	3980(2)	24.1(6)
C6	4548(2)	1765(3)	4103(2)	23.2(6)
N13	3492(2)	4927(2)	9536(2)	32.6(6)
N14	2879.0(19)	3300(2)	3766.8(17)	24.3(5)
N15	1779(2)	1618(3)	3548(2)	36.0(7)
N16	-383.0(19)	2979(2)	6949.8(17)	25.9(5)
N17	384(2)	1080(3)	7090(2)	37.6(7)
N18	4765.0(19)	2970(2)	4147.7(18)	24.9(5)
C7	2904(2)	1801(3)	9393(2)	23.6(6)
C8	-2284(2)	1989(3)	6541(2)	23.3(6)
C9	2777(2)	2074(3)	3743(2)	23.0(6)
P1	3767.5(6)	2503.1(7)	6768.4(5)	26.9(2)
F1	3656(7)	3693(6)	7349(6)	56.5(19)
F3	2752(6)	1912(9)	7006(8)	61(2)
F2	3897(10)	1341(7)	6207(7)	76(2)
F4	4780(6)	3137(8)	6557(9)	71(2)
F5	4528(6)	1900(7)	7643(5)	58.5(19)
F6	3033(9)	3168(9)	5918(6)	74(2)
F1B	3943(15)	3538(13)	7512(9)	70(4)
F2B	3579(11)	1424(11)	6032(9)	54(3)
F3B	2824(9)	3251(13)	6137(10)	57(3)
F4B	4702(9)	1718(13)	7357(13)	69(3)
F5B	2947(10)	1902(13)	7275(8)	44(3)
F6B	4587(10)	3037(12)	6225(9)	54(3)
O1	1509(4)	4048(6)	7557(5)	54.2(18)
O1B	1371(10)	4447(11)	7073(11)	48(3)

Table S10. Anisotropic Displacement Parameters ($\times 10^4$) for compound **2**. The anisotropic displacement factor exponent takes the form: *-2p2[h2a*2 × U11+ ... +2hka* × b* × U12]*

Atom	*U11*	*U22*	*U33*	*U23*	*U13*	*U12*
N1	24.3(11)	12.1(11)	32.5(12)	-1.1(9)	3.9(9)	0.5(9)
N2	24.8(13)	14.3(13)	65.1(18)	-6.0(12)	5.0(12)	-4.9(10)
N3	27.3(13)	12.6(13)	64.7(18)	-0.7(12)	2.2(12)	3.8(10)
N4	21.7(11)	11.3(11)	34.5(12)	-1.3(9)	4.1(9)	-1.2(8)
N5	23.1(13)	15.4(13)	68.2(19)	-1.1(12)	5.1(12)	1.2(10)
N6	25.0(11)	11.5(11)	34.2(12)	-1.2(9)	4.6(9)	-0.5(9)
C1	27.4(13)	14.5(13)	26.2(12)	-0.5(10)	4.4(10)	0.2(10)
C2	24.8(12)	12.3(12)	28.4(12)	0.5(10)	4.7(10)	-1.0(10)
C3	29.6(13)	18.3(13)	26.5(12)	0.9(10)	4.7(10)	3.1(11)
N7	28.2(13)	7.2(12)	68.9(19)	-2.4(12)	2.4(13)	-1.2(10)
N8	22.7(11)	13.1(11)	36.0(12)	-1.1(9)	2.8(9)	0.0(9)

N9	26.3(13)	14.0(12)	53.3(16)	-2.5(11)	4.4(11)	-3.8(10)
N10	29.7(12)	13.5(11)	34.7(12)	-0.2(9)	6.0(10)	1.5(9)
N11	30.9(13)	11.1(13)	50.6(16)	-1.7(10)	3.1(12)	-3.4(10)
N12	24.5(11)	13.0(11)	37.9(12)	-1.6(9)	5.9(9)	-1.0(9)
C4	23.8(12)	14.2(12)	29.0(12)	-1.3(10)	5.3(10)	1.0(10)
C5	26.0(12)	13.6(13)	31.9(13)	0.1(10)	5.4(10)	-0.4(10)
C6	25.6(13)	13.6(13)	29.1(12)	0.3(10)	4.1(10)	0.1(10)
N13	28.2(13)	9.8(12)	55.7(16)	1.4(11)	1.9(12)	-0.3(10)
N14	23.5(11)	11.5(11)	36.4(12)	0.1(9)	4.2(9)	0.6(9)
N15	23.1(13)	14.3(13)	68.4(19)	-1.2(12)	6.3(12)	-1.6(10)
N16	23.2(11)	17.1(12)	34.8(12)	0.7(9)	1.6(9)	-1.1(9)
N17	32.1(14)	22.6(14)	54.3(17)	0.4(12)	2.8(12)	10.0(11)
N18	23.4(11)	12.9(11)	36.9(12)	-1.0(9)	4.4(9)	-1.7(9)
C7	24.5(12)	15.3(13)	30.1(13)	-1.8(10)	4.8(10)	-0.3(10)
C8	27.8(13)	13.4(12)	27.9(12)	-0.7(10)	5.5(10)	0.5(10)
C9	26.2(12)	12.6(12)	30.2(13)	-0.7(10)	6.7(10)	-1.2(10)
P1	26.5(4)	11.1(4)	41.3(5)	0.2(3)	4.4(3)	1.4(3)
F1	59(3)	27(3)	78(4)	-25(2)	5(3)	-2(2)
F3	45(3)	53(3)	83(4)	-7(3)	13(3)	-19(2)
F2	90(5)	52(3)	86(4)	-28(3)	17(3)	27(3)
F4	58(3)	71(3)	92(5)	12(3)	33(3)	-14(2)
F5	64(3)	56(3)	48(3)	10(2)	-1(2)	18(2)
F6	82(4)	69(3)	61(3)	11(3)	0(3)	29(3)
F1B	80(6)	59(5)	63(5)	-20(4)	-2(4)	-10(4)
F2B	55(5)	42(4)	63(4)	-21(3)	11(3)	-8(3)
F3B	48(4)	55(4)	63(5)	21(4)	3(3)	17(3)
F4B	60(4)	62(5)	76(5)	21(4)	2(4)	22(3)
F5B	49(4)	44(4)	41(4)	3(3)	16(3)	-9(3)
F6B	52(4)	53(4)	58(5)	4(3)	19(3)	-16(3)
O1	39(2)	60(3)	61(3)	-12(3)	8(2)	-4(2)
O1B	47(4)	39(5)	58(5)	-7(4)	15(4)	-8(3)

Table S11. Bond Lengths in Å for compound **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.317(4)	N12	C4	1.346(4)
N1	C8	1.351(4)	N12	C7	1.347(4)
N2	C7	1.341(4)	C5	N14	1.345(4)
N3	C6	1.340(4)	C5	N18	1.341(4)
N4	C2	1.342(4)	C6	N18	1.342(4)
N4	C4	1.345(4)	N14	C9	1.343(4)
N5	C4	1.341(4)	N15	C9	1.347(4)
N6	C6	1.341(4)	P1	F1	1.594(5)
N6	C9	1.341(4)	P1	F3	1.578(6)
C1	N11	1.319(4)	P1	F2	1.559(6)
C1	N16	1.365(4)	P1	F4	1.578(6)
C2	N8	1.347(4)	P1	F5	1.595(5)
C2	N13	1.341(4)	P1	F6	1.585(6)
C3	N10	1.323(4)	P1	F1B	1.575(9)
C3	N16	1.359(4)	P1	F2B	1.602(8)
C3	N17	1.318(4)	P1	F3B	1.586(8)
N7	C5	1.335(4)	P1	F4B	1.573(8)
N8	C7	1.349(4)	P1	F5B	1.592(8)
N9	C8	1.325(4)	P1	F6B	1.599(8)
N10	C8	1.357(4)			

Table S12.Bond Angles in ° for compound **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C8	115.5(3)	N6	C9	N14	126.3(3)
C2	N4	C4	113.8(2)	N6	C9	N15	116.6(3)
C6	N6	C9	113.7(2)	N14	C9	N15	117.1(3)
N1	C1	N11	121.1(3)	F1	P1	F5	89.6(4)
N1	C1	N16	121.8(3)	F3	P1	F1	90.9(5)
N11	C1	N16	117.1(3)	F3	P1	F5	91.2(4)
N4	C2	N8	126.1(3)	F3	P1	F6	90.2(5)
N13	C2	N4	116.9(3)	F2	P1	F1	179.1(4)
N13	C2	N8	117.0(3)	F2	P1	F3	89.8(5)
N10	C3	N16	122.1(3)	F2	P1	F4	92.4(5)
N17	C3	N10	120.8(3)	F2	P1	F5	89.8(4)
N17	C3	N16	117.0(3)	F2	P1	F6	92.7(5)
C2	N8	C7	114.0(2)	F4	P1	F1	86.8(5)
C3	N10	C8	114.9(3)	F4	P1	F3	177.7(5)
C4	N12	C7	113.6(3)	F4	P1	F5	88.5(4)
N4	C4	N12	126.5(3)	F4	P1	F6	89.9(5)
N5	C4	N4	117.1(3)	F6	P1	F1	87.9(5)
N5	C4	N12	116.4(3)	F6	P1	F5	177.1(5)
N7	C5	N14	117.0(3)	F1B	P1	F2B	178.4(8)
N7	C5	N18	117.1(3)	F1B	P1	F3B	91.4(7)
N18	C5	N14	125.9(3)	F1B	P1	F5B	86.9(8)
N3	C6	N6	117.3(3)	F1B	P1	F6B	96.3(8)
N3	C6	N18	116.5(3)	F3B	P1	F2B	89.3(7)
N6	C6	N18	126.2(3)	F3B	P1	F5B	90.0(6)
C9	N14	C5	113.8(2)	F3B	P1	F6B	90.4(6)
C3	N16	C1	119.1(3)	F4B	P1	F1B	91.2(7)
C5	N18	C6	114.0(2)	F4B	P1	F2B	88.1(6)
N2	C7	N8	116.5(3)	F4B	P1	F3B	177.3(7)
N2	C7	N12	117.6(3)	F4B	P1	F5B	90.5(7)
N12	C7	N8	125.9(3)	F4B	P1	F6B	88.9(7)
N1	C8	N10	126.6(3)	F5B	P1	F2B	91.6(7)
N9	C8	N1	117.0(3)	F5B	P1	F6B	176.7(7)
N9	C8	N10	116.4(3)	F6B	P1	F2B	85.1(7)

Table S13. Torsion Angles in ° for compound **2**.

Atom	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Atom	Angle/°
N1	C1	N16	C3	0.5(4)	C4	N4	C2	N8	0.0(4)
N3	C6	N18	C5	180.0(3)	C4	N4	C2	N13	-179.7(3)
N4	C2	N8	C7	1.0(4)	C4	N12	C7	N2	179.8(3)
N6	C6	N18	C5	0.7(4)	C4	N12	C7	N8	0.9(4)
C1	N1	C8	N9	178.5(3)	C5	N14	C9	N6	-0.4(4)
C1	N1	C8	N10	-1.3(4)	C5	N14	C9	N15	179.0(3)
C2	N4	C4	N5	179.6(3)	C6	N6	C9	N14	0.1(4)
C2	N4	C4	N12	-0.7(4)	C6	N6	C9	N15	-179.3(3)
C2	N8	C7	N2	179.6(3)	N13	C2	N8	C7	-179.3(3)
C2	N8	C7	N12	-1.5(4)	N14	C5	N18	C6	-1.1(4)
C3	N10	C8	N1	0.9(4)	N16	C3	N10	C8	0.2(4)
C3	N10	C8	N9	-178.8(3)	N17	C3	N10	C8	-179.9(3)
N7	C5	N14	C9	-178.8(3)	N17	C3	N16	C1	179.3(3)
N7	C5	N18	C6	178.7(3)	N18	C5	N14	C9	0.9(4)
N10	C3	N16	C1	-0.9(4)	C7	N12	C4	N4	0.3(4)
N11	C1	N16	C3	-179.3(3)	C7	N12	C4	N5	-179.9(3)
C9	N6	C6	N3	-179.5(3)	C8	N1	C1	N11	-179.7(3)
C9	N6	C6	N18	-0.2(4)	C8	N1	C1	N16	0.5(4)

Table S14. Hydrogen Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for compound **2**. *Ueq* is defined as 1/3 of the trace of the orthogonalized *Uij*.

Atom	x	y	z	*Ueq*
H2A	2114.58	291.13	9208.79	43
H2B	1413.99	1394.43	9064.25	43
H3A	5290.78	224.68	4238.48	44
H3B	6024.67	1298.9	4395.12	44
H5A	6219.05	2029.19	10115.25	44
H5B	5746.22	776.09	10001.02	44
H7A	4695.51	5186.61	4168.56	44
H7B	3521.24	5391.83	3929.48	44
H9A	-3804.12	1940.8	6240.95	38
H9B	-3310.03	698.32	6338.52	38
H11A	-1665.94	5383.97	6680.17	38
H11B	-490.02	5193.21	6935.13	38
H13A	4041.5	5398.65	9660.82	39
H13B	2862.23	5239.63	9397.09	39
H15A	1679.84	837.13	3530.7	43
H15B	1241.22	2106.86	3440.19	43
H16	241.26	3304.7	7090.65	31
H17A	347.41	292.67	7075.07	45
H17B	995.27	1437.64	7220.96	45
H1A	1920(50)	4070(80)	7210(40)	81
H1B	1740(60)	3670(70)	8030(30)	81
H1BA	1180(130)	4760(110)	6570(40)	72
H1BB	1530(140)	4930(100)	7500(60)	72

Table S15. Atomic Occupancies for all atoms that are not fully occupied in compound **2**.

Atom	Ocupancy
F1	0.62(2)
F3	0.62(2)
F2	0.62(2)
F4	0.62(2)
F5	0.62(2)
F6	0.62(2)
F1B	0.38(2)
F2B	0.38(2)
F3B	0.38(2)
F4B	0.38(2)
F5B	0.38(2)
F6B	0.38(2)
O1	0.694(15)
H1A	0.694(15)
H1B	0.694(15)
O1B	0.306(15)
H1BA	0.306(15)
H1BB	0.306(15)

Table S16. Hydrogen bonds for compound **1**.

Donor-H	Acceptor	[ARU]	D···A/Å	D-H···A/°
N2-H2A	F3	[1555.01]	3.131(19)	132(2)
N2-H2A	F1	[17656.01]	3.272(15)	162(3)'
N2-H2A	F2	[18556.01]	2.965(11)	133(3)"
N2-H2B	N4	[16536.03]	3.065(2)	172(2)
N3-H3A	F3	[1555.01]	3.02(2)	139(2)
N3-H3A	F1	[2655.01]	3.020(14)	141(2)'
N3-H3A	F2	[3665.01]	3.156(13)	163(2)"
N3-H3B	N1	[16646.02]	3.084(2)	172(3)

Translation of ARU-Code to CIF and Equivalent Position Code

[2655.] = [2_655] = 1-y,x-y,z; [3665.] = [3_665] = 1-x+y,1-x,z;

[17656.] = [18_655] = 4/3-x,2/3-x+y,7/6-z; [18556.] = [17_555] = 1/3+x-y,2/3-y,7/6-z;

[16536.] = [16_535] = 1/3+y,-4/3+x,7/6-z; [16646.] = [16_645] = 4/3+y,-1/3+x,7/6-z.

Table S17. Hydrogen bonds for compound **2.**

Donor-H	Acceptor	[ARU]	D···A/Å	D-H···A/°
O1-H1A	F1	[1555.01]	2.890(11)	135(6)
O1-H1B	N8	[1555.03]	3.018(8)	164(6)
N2-H2A	F6	[2546.01]	3.174(10)	169
N2-H2B	N18	[4455.04]	3.101(4)	162
N3-H3A	F2	[3656.01]	2.868(9)	135
N3-H3B	N8	[4554.03]	3.171(4)	165
N5-H5A	F6	[4555.01]	3.058(12)	136
N5-H5B	N12	[3657.03]	3.160(4)	166
N7-H7A	F4	[3666.01]	2.878(9)	123
N7-H7B	N1	[3566.02]	3.079(3)	170
N9-H9A	F4	[1455.01]	3.198(9)	158
N9-H9B	N6	[3556.04]	3.028(3)	172
N11-H11A	N14	[3566.04]	2.965(3)	171
N11-H11B	F5	[2556.01]	2.985(8)	144
N13-H13A	N4	[3667.03]	3.104(3)	169
N13-H13B	F2	[2556.01]	3.393(12)	171
N15-H15A	N10	[3556.02]	3.121(4)	172
N15-H15B	F5	[4454.01]	3.324(8)	160
N16-H16A	O1	[1555.05]	2.666(6)	171
N17-H17A	F1	[2546.01]	2.921(8)	139
N17-H17B	F3	[1555.01]	3.221(9)	154

Translation of ARU-Code to CIF and Equivalent Position Code

[3566.] = [3_566] = -x,1-y,1-z; [4455.] = [4_566] = -1/2+x,1/2-y,1/2+z;

[1455.] = [1_455] = -1+x,y,z; [3556.] = [3_556] = -x,-y,1-z;

[2556.] = [2_556] = 1/2-x,1/2+y,3/2-z; [2546.] = [2_546] = 1/2-x,-1/2+y,3/2-z;

[3667.] = [3_667] = 1-x,1-y,2-z.

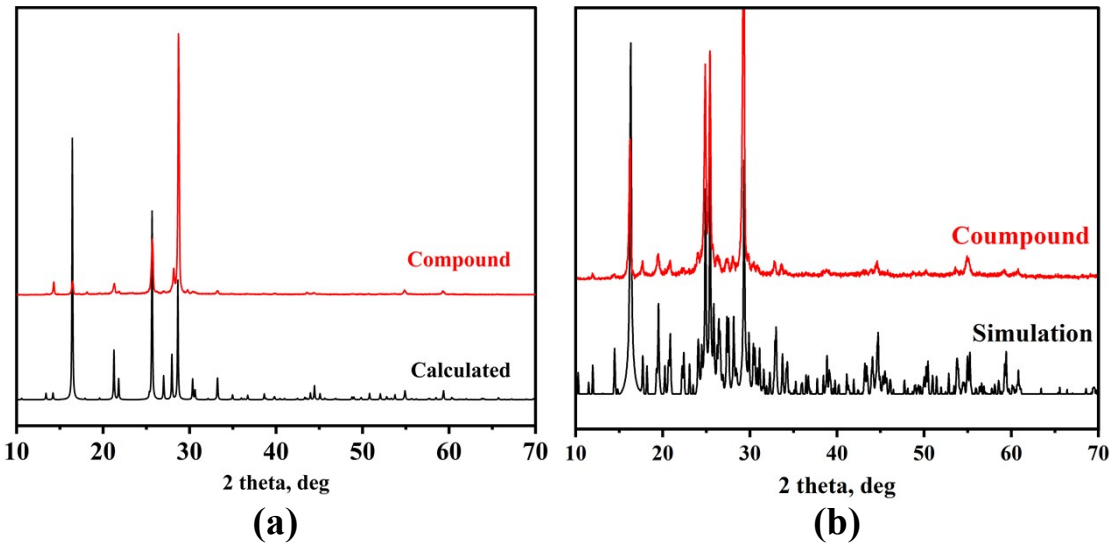

Fig. S1. Experimental and calculated XRD patterns of (a) compound **1**, (b) compound **2**.

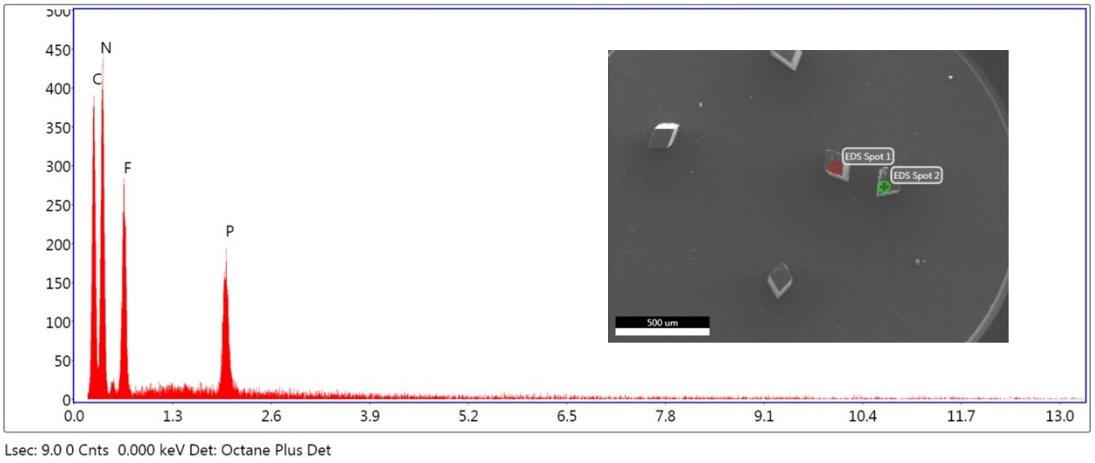

Fig. S2. EDS spectrum of compound **1**.

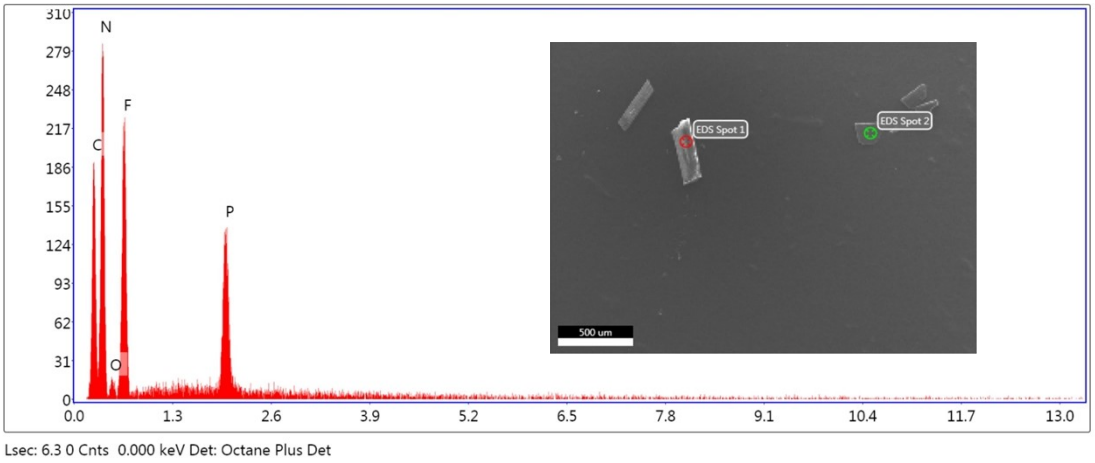

Fig. S3. EDS spectrum of compound **2**.

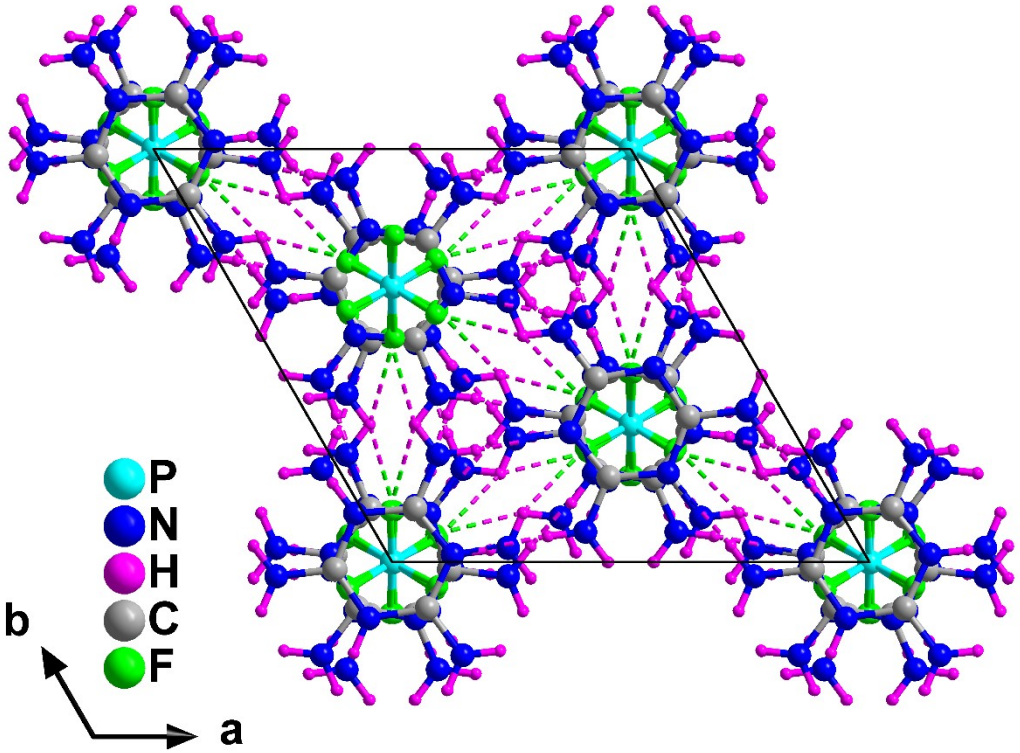

Fig. S4. The H-bond of compound **1** view along as *c* axis.

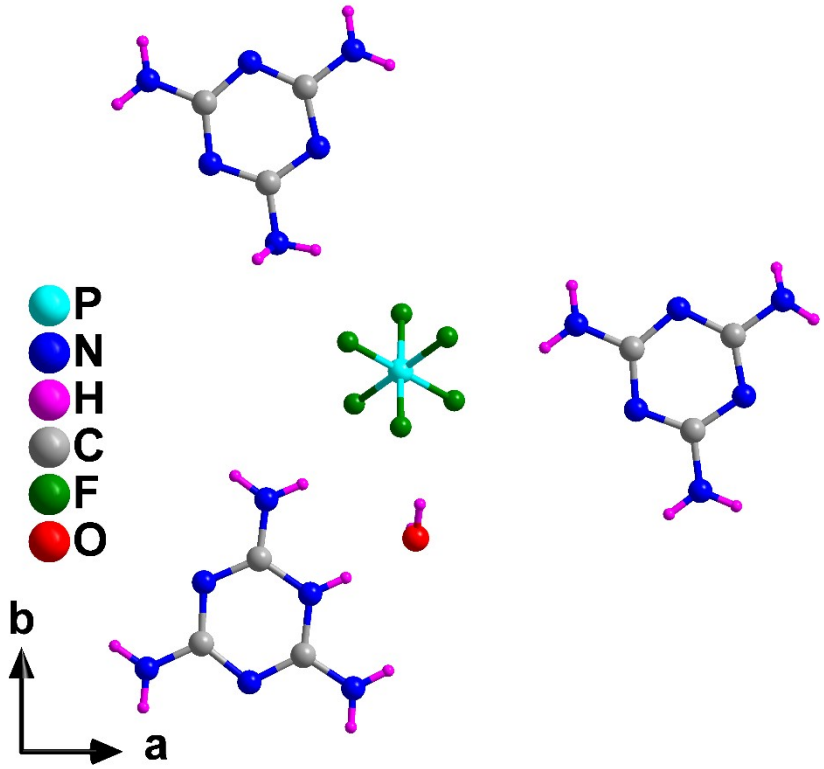

Fig. S5. The asymmetric unit of compound **2**.

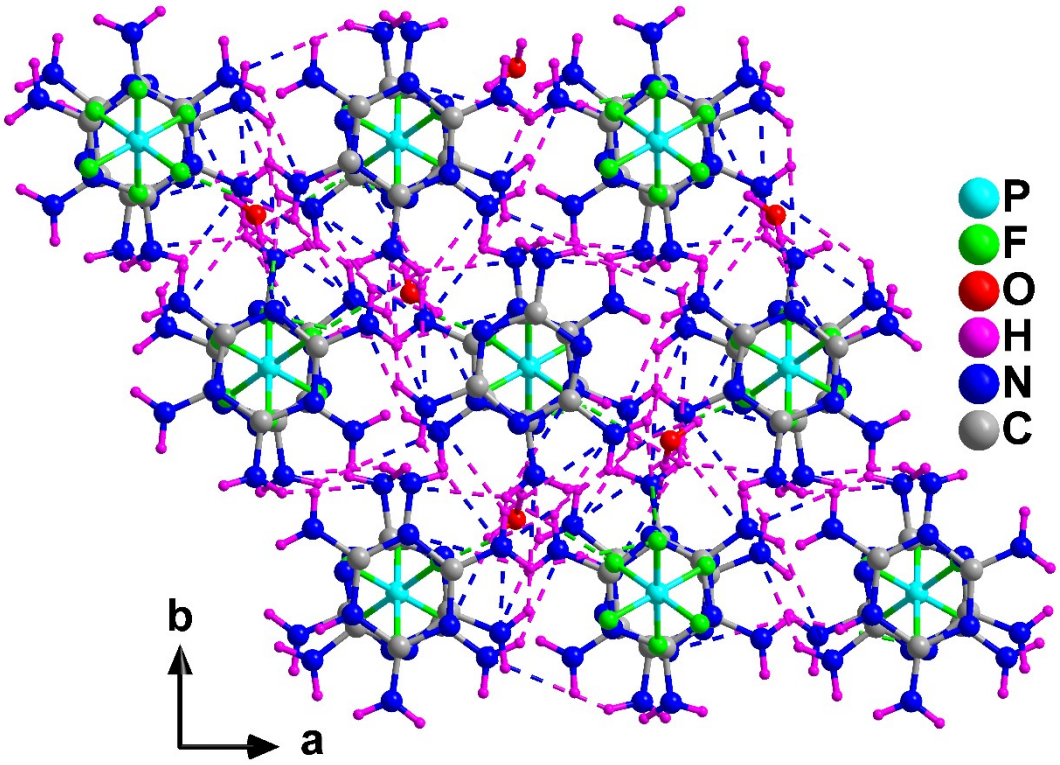

Fig. S6. The H-bond of compound **2** views along as *c* axis.

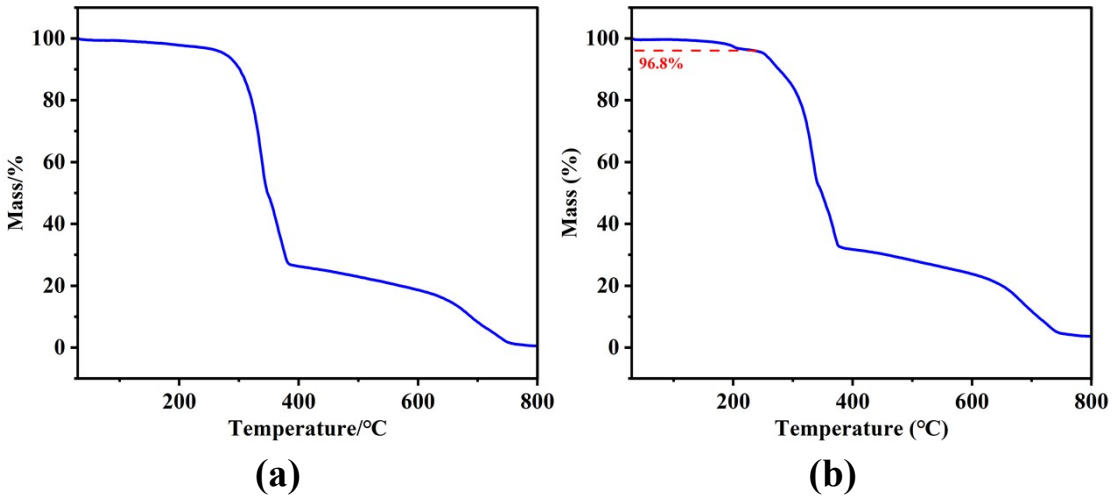

Fig. S7. Thermal analyses for compounds **1** (a) and **2** (b).

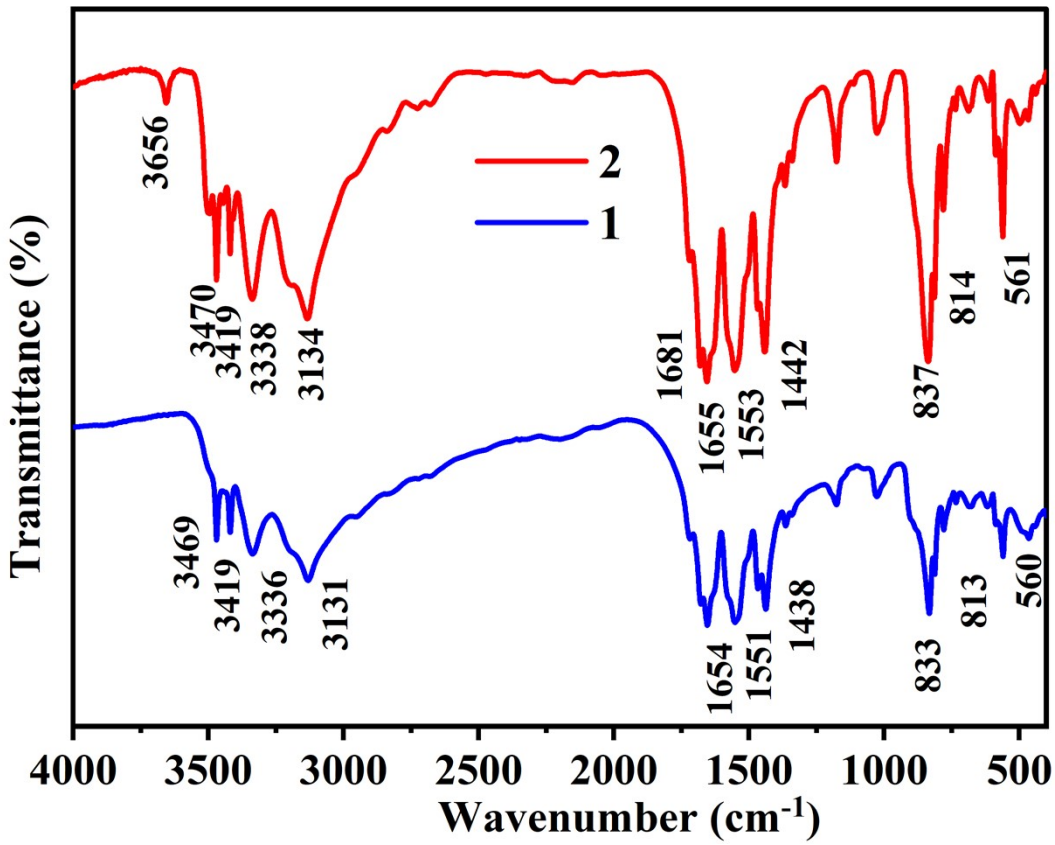

Fig. S8. The IR spectrum of compounds **1** and **2**.