Supporting Information

Photochromic and Room Temperature Phosphorescent D-A Hybrid Crystals Regulated by Core-Substituted Naphthalenediimides

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1. Materials and instrumentations

$H_3PW_{12}O_{40}$, methanol (MeOH) and N-methylpyrrolidone (NMP) were obtained from commercial sources and were used without further purification. The organic ligand H_2BDMPy-Br_2NDI and H_2BDMPy-I_2NDI were synthesized following the literatures.[1-3] The infrared spectra were obtained in the range of 400-4000 cm^{-1} from a PerkinElmer FT-IR spectrophotometer and power X-ray diffraction (PXRD) was recorded on a Rigaku MiniFlex-II X-Ray diffractometer. UV-vis diffuse reflectance spectra (DRS) were recorded on a Varian Cary 500 UV-vis spectrophotometer equipped with an integrating sphere at room temperature. The photochromism experiment was performed in air. The irradiation source was a 300 W xenon lamp equipped with a filter to provide a wavelength range of 420-780 nm. The distance between the light source and the sample was fixed at 15.0 cm. Photoluminescence spectra and lifetimes at room temperature were recorded on an Edinburgh FLS 980 luminescence spectrometer. The photoluminescence quantum yields were measured on a Hamammatus C11347-11 absolute luminescence quantum yield measurement system equipped with an integrating sphere apparatus and a 150 W xenon light source. Electron paramagnetic resonance (EPR) measurements were obtained using a Bruker A300 instrument operating in the X-band at the room temperature.

2. X-ray crystallographic study

Crystal data for the complexes **1** and **2** were collected on a Rigaku Saturn 724 CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å) at 295 K and reduction were performed by using the program CrysAlisPro.[4] The structures were solved by the direct method and different Fourier syntheses. All calculations were performed by full-matrix least-squares

methods on F^2 by using the SHELXTL program, all non-hydrogen atoms were refined with anisotropic thermal parameters and the hydrogen atoms were fixed at calculated positions and refined by a riding mode.[5, 6]

3. Molecular orbital calculation

Molecular structure has been used for the evaluation of its molecular orbital energy through density functional theory (DFT) computations using the Gaussian 09 suite of programs.[7] A hybrid functional, B3LYP, was adopted. Geometry was optimized using the LANL2DZ basis set.[8]

4. Related figures of hybrid 1

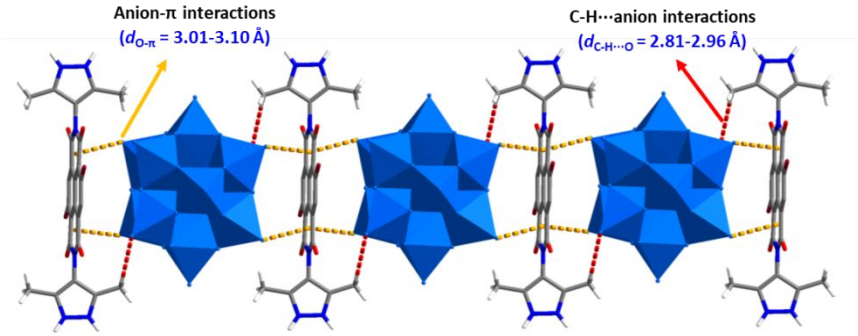

Figure S1. The 1-D long chain of hybrid **1**.

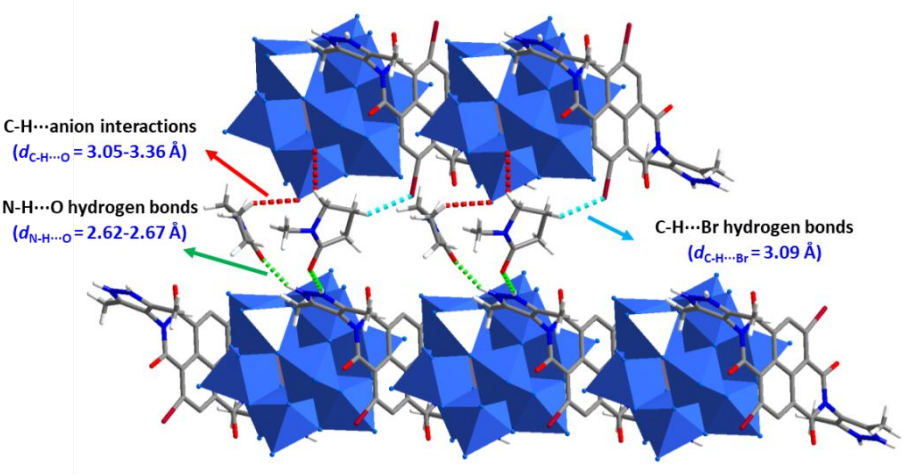

Figure S2. The hydrogen bonds between adjacent1-D long chains for hybrid **1**.

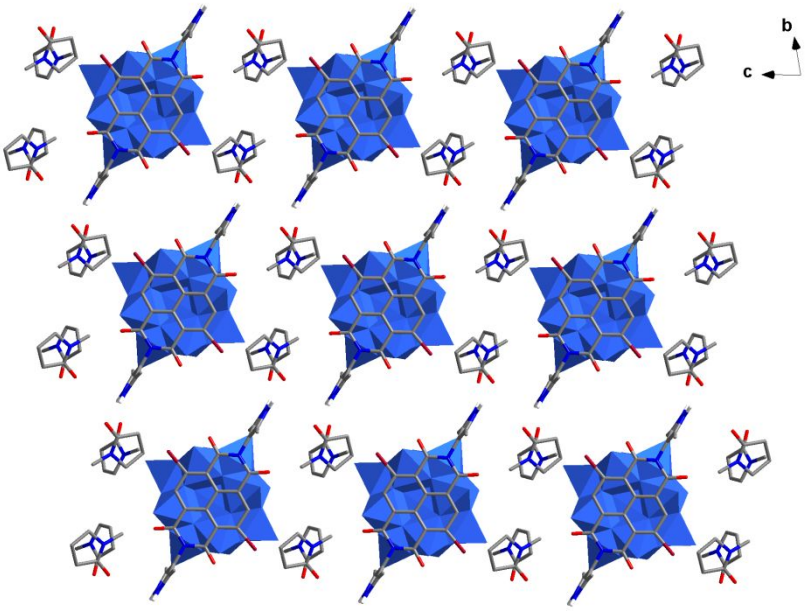

Figure S3. The supramolecular structure of hybrid **1** along a axis.

5. PXRD patterns analysis

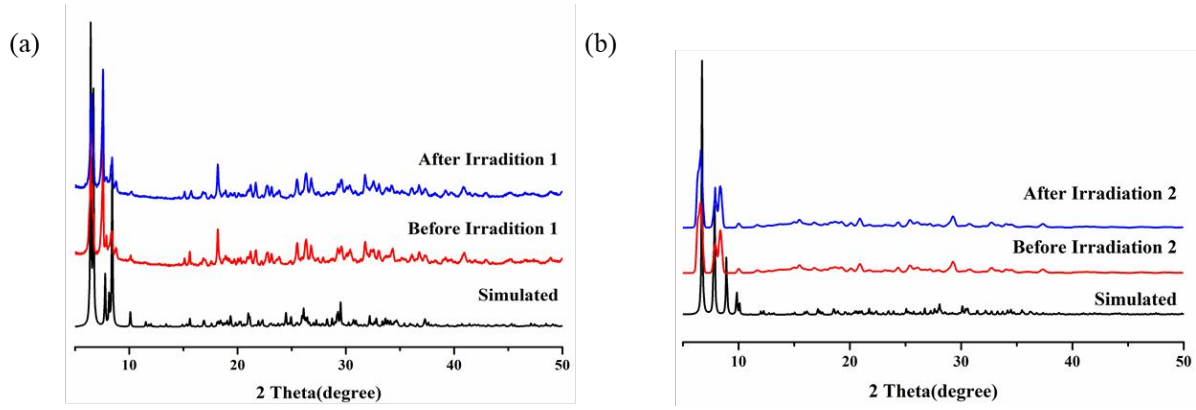

Figure S4. PXRD patterns of hybrids **1** (a) and **2** (b).

6. Infrared spectral analysis

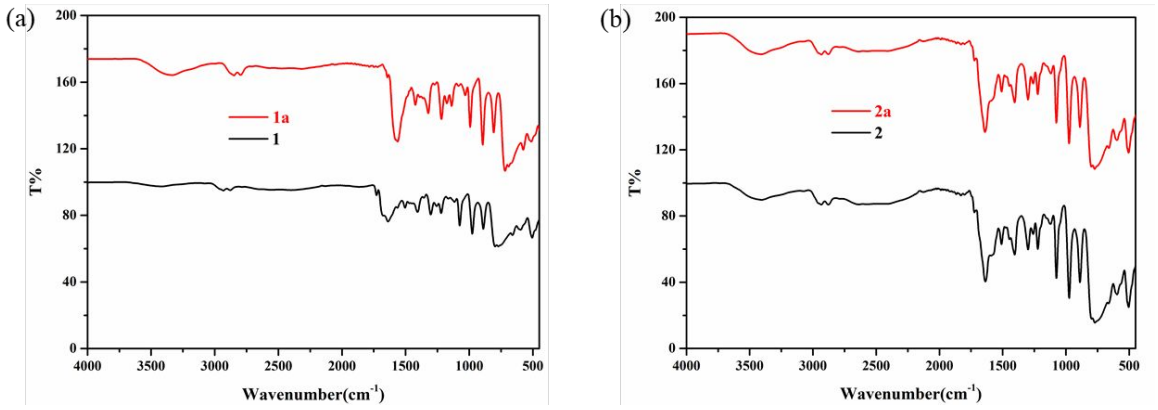

Figure S5. Infrared spectra of hybrids **1** (a) and **2** (b).

7. Absorption spectra of organic ligands

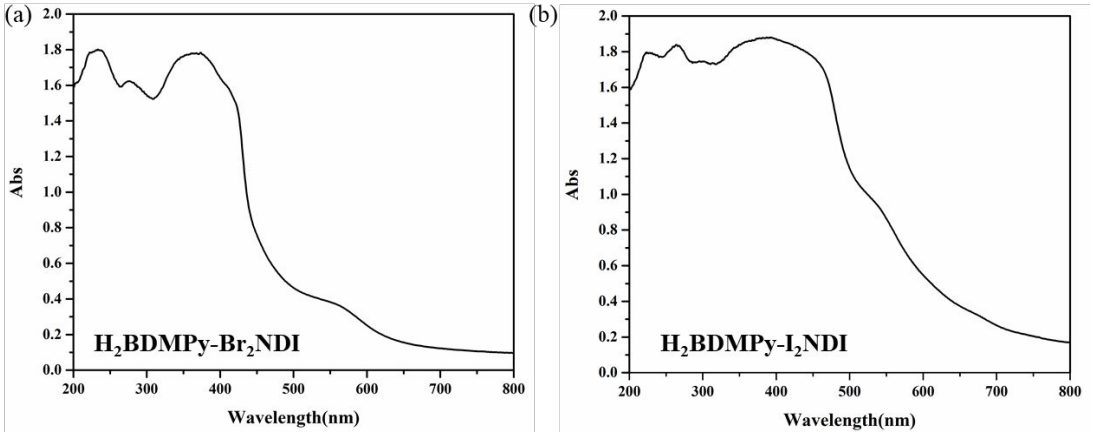

Figure S6. The absorption spectra of organic ligands H_2BDMPy-Br_2NDI (a) and H_2BDMPy-I_2NDI (b).

8. Crystal datum and structure refinement data

Table S1. Crystal datum and structure refinement parameters for the crystals **1** and **2**

Complexes	**1**	**2**
Empirical formula	$C_{44}H_{52}Br_2N_{10}O_{48}PW_{12}$	$C_{42}H_{64}I_2N_9O_{48}PW_{12}$
Formula weight	3885.94	3585.41
Temperature/K	296.15	296.15
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a/Å	13.0871(18)	13.2935(8)
b/Å	14.727(2)	13.4723(8)
c/Å	15.153(2)	15.1868(10)
α/°	71.810(4)	75.092(2)
β/°	66.548(4)	83.712(2)
γ/°	65.680(4)	70.447(2)
Volume/Å^3	2402.8(6)	2475.9(3)
Z	1	1
ρ_{calc}g/cm^3	2.686	2.405
μ/mm^{-1}	15.228	14.577

F(000)	1743.0	1565.0
Reflections collected	69179	43407
Independent reflections	8414	8714
Data/restraints/parameters	8414/482/561	8714/18/423
Goodness-of-fit on F^2	1.076	1.049
$R_1{}^a$, $wR_2{}^b$ ($I>2\sigma(I)$)	$R_1 = 0.0956$, $wR_2 = 0.2380$	$R_1 = 0.0527$, $wR_2 = 0.1288$
$R_1{}^a$, $wR_2{}^b$ (all data)	$R_1 = 0.1208$, $wR_2 = 0.2544$	$R_1 = 0.0682$ $wR_2 = 0.1399$

$R_1 = \sum \big| \, |F_0| - |F_c| \, \big| / \sum |F_0|$. $wR_2 = \{\sum[w(F_0^2-F_c)^2]/ \sum[w(F_0^2)^2]\}^{1/2}$

Table S2. Bond lengths for the crystal **1**

Atom	Length/Å	Atom	Length/Å	Atom	Length/Å	Atom	Length/Å
W001-O2[1]	2.45(4)	P008-O1[1]	1.54(4)	W004-O3[1]	2.45(4)	C00M-C011	1.40(4)
W001-O00A	1.92(2)	P008-O1	1.54(4)	W004-O00K	1.84(2)	C00Q-C00X	1.40(4)
W001-O4	2.46(4)	P008-O3[1]	1.49(4)	W004-O00O	1.90(2)	C00V-C00Z	1.43(5)
W001-O00B	1.88(2)	P008-O3	1.49(4)	W004-O00S	1.92(2)	C00V-C01C	1.44(5)
W001-O00C	1.87(2)	O2-O4[1]	1.59(5)	W004-O14	1.68(2)	C00X-C013	1.46(4)
W001-O00D	1.87(2)	O1-O3[1]	1.82(5)	W005-O1	2.49(4)	C00Z-C018	1.30(5)
W001-O00L	1.66(2)	Br07-Br00[2]	2.73(2)	W005-O00H	1.67(2)	C018-C01B	1.51(5)
W002-O2[1]	2.50(4)	Br07-C00Q	1.89(3)	W005-O00N[1]	1.89(2)	O016-C30	1.30(7)
W002-O00A	1.86(2)	Br00-C00I	1.88(4)	W005-O00S	1.86(2)	N20-C30	1.22(7)
W002-O3[1]	2.48(4)	O009-C00E	1.22(4)	W005-O00Y[1]	1.92(3)	N20-C34	1.42(8)
W002-O00O	1.91(2)	O00G-C013	1.24(4)	W005-O010	1.89(3)	N20-C38	1.46(6)
W002-O00P	1.67(2)	N00F-C00E	1.37(4)	W006-O1[1]	2.41(4)	C01D-C01H	1.58(8)
W002-O00U	1.89(2)	N00F-C00Z	1.44(4)	W006-O00C	1.90(2)	C01D-C34	1.54(7)
W002-O010	1.89(3)	N00F-C013	1.40(4)	W006-O00J	1.66(3)	C01H-C30	1.46(8)
W003-O1[1]	2.50(4)	N00W-N012	1.36(4)	W006-O00R	1.88(2)	O01K-C019	1.17(7)
W003-O00D[1]	1.90(2)	N00W-C018	1.35(4)	W006-O00U	1.94(2)	N017-C019	1.33(8)
W003-O00K	1.95(2)	N012-C00V	1.32(4)	W006-O00Y	1.85(3)	N017-C01A	1.40(7)
W003-O00N	1.89(3)	C00E-C011	1.51(4)	P008-O2[1]	1.47(4)	N017-C35	1.41(7)
W003-O00R	1.85(2)	C00I-C00Q[2]	1.39(5)	P008-O2	1.47(4)	C014-C35	1.46(2)
W003-O13	1.67(2)	C00I-C011	1.35(5)	P008-O4[1]	1.47(4)	C014-C39	1.39(2)
W004-O4[1]	2.52(4)	C00M-C00M[2]	1.42(6)	P008-O4	1.47(4)	C019-C39	1.41(8)

[1]2-X, 1-Y, 1-Z; [2]1-X, 1-Y, 1-Z

Table S3. Bond lengths for the crystal **2**

Atom	Length/Å	Atom	Length/Å	Atom	Length/Å	Atom	Length/Å
W001-O00D	1.892(11)	W006-O2[1]	2.399(19)	W006-O2[1]	1.918(13)	C00J-C00R[2]	1.37(2)
W001-O00E	1.875(15)	W006-O014	1.890(15)	W006-O014	2.500(16)	C00K-C00Q	1.388(18)
W001-O00F	1.874(13)	W006-O016	1.869(15)	W006-O016	2.427(18)	C00K-C00T	1.45(2)
W001-O00L	1.880(11)	I07-C00R	2.126(12)	I07-C00R	1.890(15)	C00P-C00Q	1.423(17)
W001-O00X	1.673(10)	P008-O2[1]	1.60(2)	P008-O2[1]	1.674(11)	C00P-C00R	1.378(19)
W001-O4[1]	2.465(15)	P008-O2	1.60(2)	P008-O2	1.902(13)	C00P-C00V	1.47(2)
W001-O1[1]	2.397(18)	P008-O4[1]	1.484(16)	P008-O4[1]	2.429(17)	C00Q-C00Q[2]	1.45(3)
W002-O00D	1.875(11)	P008-O4	1.484(16)	P008-O4	1.874(13)	O2-O4[1]	1.80(2)
W002-O00I[1]	1.857(15)	P008-O1[1]	1.498(17)	P008-O1[1]	1.902(14)	N010-N011	1.34(2)
W002-O00M	1.913(14)	P008-O1	1.498(17)	P008-O1	1.662(11)	N010-C017	1.43(3)
W002-O00S	1.906(12)	P008-O3	1.533(18)	P008-O3	1.854(14)	N011-C018	1.38(2)
W002-O4[1]	2.471(15)	P008-O3[1]	1.533(18)	P008-O3[1]	1.856(13)	C015-C017	1.39(2)
W002-O15	1.686(10)	O00A-C00V	1.226(16)	O00A-C00V	2.482(17)	C015-C018	1.41(3)
W002-O3[1]	2.416(17)	O00B-C00T	1.222(16)	O00B-C00T	1.905(13)	C017-C20	1.45(3)
W003-O00L	1.910(13)	N00G-C00T	1.391(17)	N00G-C00T	1.888(14)	C018-C0AA	1.49(3)
W003-O00N	1.681(10)	N00G-C00V	1.439(19)	N00G-C00V	1.874(14)	O4-O1	1.60(2)
W003-O00O	1.878(14)	N00G-C015	1.42(2)	N00G-C015	1.910(14)	O4-O3	1.66(2)
W003-O00S[1]	1.879(13)	C00J-C00K	1.371(18)	C00J-C00K	1.647(14)	O1-O3[1]	1.72(2)

[1]1-X, 1-Y, 1-Z; [2]2-X, 1-Y, 1-Z

Table S4. Bond angles for the crystal **1**

Atom	Angle/°	Atom	Angle/°	Atom	Angle/°	Atom	Angle/°
O2[1]-W001-O4	37.8(13)	O2[1]-P008-O3[1]	70(2)	O00B[1]-W004-O3[1]	93.7(12)	W002-O00U-W006	137.3(14)
O00A-W001-O2[1]	63.4(11)	O2-P008-O3[1]	110(2)	O00B[1]-W004-O00S	88.1(11)	W006-O00Y-W005[1]	141.0(14)
O00A-W001-O4	90.7(11)	O4-P008-O2	115(2)	O3[1]-W004-O4[1]	39.3(13)	W005-O010-W002	139.7(13)
O00B-W001-O2[1]	93.4(12)	O4[1]-P008-O2[1]	115(2)	O00K-W004-O4[1]	65.1(11)	C00Q-Br07-Br002	67.8(11)
O00B-W001-O00A	155.9(9)	O4[1]-P008-O2	65(2)	O00K-W004-O00B[1]	87.6(11)	C00E-N00F-C00Z	116(3)
O00B-W001-O4	65.6(11)	O4-P008-O2[1]	65(2)	O00K-W004-O3[1]	90.1(11)	C00E-N00F-C013	125(3)
O00C-W001-O2[1]	64.9(11)	O4-P008-O4[1]	180(3)	O00K-W004-O00O	85.8(10)	C013-N00F-C00Z	118(3)
O00C-W001-O00A	86.9(10)	O4[1]-P008-O1[1]	74(2)	O00K-W004-O00S	154.0(10)	C018-N00W-N012	109(3)
O00C-W001-O4	90.5(12)	O4[1]-P008-O1	106(2)	O00O-W004-O4[1]	93.3(11)	C00V-N012-N00W	109(3)
O00C-W001-O00B	88.9(11)	O4-P008-O1	74(2)	O00O-W004-O00B[1]	156.9(10)	O009-C00E-N00F	122(3)
O00D-W001-O2[1]	90.3(11)	O4-P008-O1[1]	106(2)	O00O-W004-O3[1]	64.3(12)	O009-C00E-C011	120(3)
O00D-W001-O00A	86.4(10)	O4[1]-P008-O3[1]	69(2)	O00O-W004-O00S	88.3(10)	N00F-C00E-C011	118(3)
O00D-W001-O4	65.2(11)	O41-P008-O3	111(2)	O00S-W004-O4[1]	90.2(12)	C00Q2-C00I-Br00	108(2)

O00D-W001-O00B	87.3(10)	O4-P008-O3[1]	111(2)	O00S-W004-O3[1]	64.7(11)	C011-C00I-Br00	129(3)
O00D-W001-O00C	154.7(10)	O4-P008-O3	69(2)	O14-W004-O4[1]	160.2(14)	C011-C00I-C00Q[2]	122(3)
O00L-W001-O2[1]	161.2(13)	O1-P008-O11	180	O14-W004-O00B[1]	101.5(11)	C00X-C00M-C00M[2]	121(3)
O00L-W001-O00A	104.0(11)	O3[1]-P008-O1	74(2)	O14-W004-O3[1]	160.5(14)	C00X-C00M-C011	122(3)
O00L-W001-O4	161.0(13)	O3-P008-O1	106(2)	O14-W004-O00K	102.7(12)	C011-C00M-C00M[2]	117(4)
O00L-W001-O00B	100.1(11)	O3-P008-O1[1]	74(2)	O14-W004-O00O	101.5(12)	C00I2-C00Q-Br07	113(2)
O00L-W001-O00C	102.1(11)	O3[1]-P008-O1[1]	106(2)	O14-W004-O00S	103.3(12)	C00I2-C00Q-C00X	119(3)
O00L-W001-O00D	103.2(11)	O3[1]-P008-O3	180(3)	O00H-W005-O1	158.8(13)	C00X-C00Q-Br07	128(2)
O00A-W002-O2[1]	63.0(11)	W001[1]-O2-W002[1]	92.0(14)	O00H-W005-O00N1	102.9(12)	N012-C00V-C00Z	106(3)
O00A-W002-O3[1]	93.1(11)	P008-O2-W001[1]	129(2)	O00H-W005-O00S	102.2(11)	N012-C00V-C01C	124(3)
O00A-W002-O00O	156.0(10)	P008-O2-W002[1]	125(2)	O00H-W005-O00Y1	102.3(12)	C00Z-C00V-C01C	130(3)
O00A-W002-O00U	89.6(10)	P008-O2-O4[1]	57(2)	O00H-W005-O010	101.8(11)	C00M-C00X-C00Q	120(3)
O00A-W002-O010	87.3(10)	O4[1]-O2-W001[1]	72(2)	O00N1-W005-O1	64.0(12)	C00M-C00X-C013	121(3)
O3[1]-W002-O2[1]	40.2(12)	O4[1]-O2-W002[1]	136(3)	O00N1-W005-O00Y1	85.3(11)	C00Q-C00X-C013	119(3)
O00O-W002-O2[1]	93.9(12)	W002-O00A-W001	140.1(12)	O00S-W005-O1	91.5(12)	C00V-C00Z-N00F	123(3)
O00O-W002-O3[1]	63.3(11)	W001-O4-W004[1]	91.0(13)	O00S-W005-O00N1	154.9(11)	C018-C00Z-N00F	129(3)
O00P-W002-O21	159.6(12)	P008-O4-W001	128(2)	O00S-W005-O00Y1	88.0(11)	C018-C00Z-C00V	109(3)
O00P-W002-O00A	101.9(11)	P008-O4-W004[1]	125(2)	O00S-W005-O010	88.0(11)	C00I-C011-C00E	121(3)
O00P-W002-O3[1]	160.2(12)	P008-O4-O2[1]	57(2)	O00Y1-W005-O1	61.7(12)	C00I-C011-C00M	121(3)
O00P-W002-O00O	102.0(11)	O2[1]-O4-W001	71(2)	O010-W005-O1	94.7(12)	C00M-C011-C00E	118(3)
O00P-W002-O00U	100.4(12)	O2[1]-O4-W0041	135(3)	O010-W005-O00N1	88.3(11)	O00G-C013-N00F	119(3)
O00P-W002-O010	101.7(12)	W001-O00B-W004[1]	138.9(12)	O010-W005-O00Y1	155.9(11)	O00G-C013-C00X	125(3)
O00U-W002-O2[1]	67.5(11)	W005-O1-W003[1]	91.1(14)	O00C-W006-O11	91.9(12)	N00F-C013-C00X	116(3)
O00U-W002-O3[1]	92.4(12)	W006[1]-O1-W003[1]	92.8(13)	O00C-W006-O00U	86.6(10)	N00W-C018-C01B	120(3)
O00U-W002-O00O	87.1(10)	W006[1]-O1-W005	93.0(13)	O00J-W006-O11	160.3(14)	C00Z-C018-N00W	108(3)
O00U-W002-O010	157.9(10)	P008-O1-W003[1]	122(2)	O00J-W006-O00C	102.9(11)	C00Z-C018-C01B	132(3)
O010-W002-O2[1]	91.7(12)	P008-O1-W005	123(2)	O00J-W006-O00R	105.7(12)	C30-N20-C34	114(5)
O010-W002-O3[1]	65.9(12)	P008-O1-W006[1]	126(2)	O00J-W006-O00U	100.2(12)	C30-N20-C38	131(6)
O010-W002-O00O	86.8(10)	P008-O1-O31	52.0(18)	O00J-W006-O00Y	102.4(12)	C34-N20-C38	113(5)
O00D[1]-W003-O1[1]	93.7(11)	O3[1]-O1-W003[1]	130(2)	O00R-W006-O11	61.0(12)	C34-C01D-C01H	101(5)
O00D[1]-W003-O00K	87.5(10)	O3[1]-O1-W005	70.7(18)	O00R-W006-O00C	151.2(11)	C30-C01H-C01D	102(4)
O00K-W003-O1[1]	91.0(11)	O3[1]-O1-W006[1]	133(2)	O00R-W006-O00U	85.7(10)	O016-C30-C01H	123(5)
O00N-W003-O1[1]	63.8(12)	W001-O00C-W006	142.2(13)	O00U-W006-O11	93.5(12)	N20-C30-O016	122(6)
O00N-W003-O00D[1]	87.5(11)	W004[1]-O3-W002[1]	92.5(13)	O00Y-W006-O11	64.1(13)	N20-C30-C01H	115(7)
O00N-W003-O00K	154.0(11)	P008-O3-W002[1]	125(2)	O00Y-W006-O00C	90.5(11)	N20-C34-C01D	104(5)
O00R-W003-O11	59.6(12)	P008-O3-W004[1]	128(2)	O00Y-W006-O00R	86.1(11)	C019-N017-C01A	121(6)
O00R-W003-O00D[1]	151.9(11)	P008-O3-O1[1]	54.4(18)	O00Y-W006-O00U	157.3(11)	C019-N017-C35	111(6)
O00R-W003-O00K	84.8(11)	O1[1]-O3-W002[1]	130(2)	O21-P008-O2	180(3)	C01A-N017-C35	127(5)
O00R-W003-O00N	87.7(11)	O1[1]-O3-W004[1]	129(2)	O2-P008-O1	72(2)	C39-C014-C35	106(5)
O13-W003-O1[1]	158.2(13)	W001-O00D-W0031	140.8(13)	O2-P008-O11	108(2)	O01K-C019-N017	126(7)

O13-W003-O00D[1]	103.4(11)	W004-O00K-W003	141.0(14)	O21-P008-O11	72(2)	O01K-C019-C39	125(7)
O13-W003-O00K	103.0(11)	W005[1]-O00N-W003	140.5(15)	O21-P008-O1	108(2)	N017-C019-C39	108(6)
O13-W003-O00N	103.0(12)	W004-O00O-W002	138.9(14)	O2-P008-O3	70(2)	N017-C35-C014	102(5)
O13-W003-O00R	104.6(12)	W003-O00R-W006	145.0(15)	O21-P008-O3	110(2)	C014-C39-C019	105(6)
O00B[1]-W004-O4[1]	64.0(11)	W005-O00S-W004	140.5(13)				

[1]2-X, 1-Y, 1-Z; [2]1-X, 1-Y, 1-Z

Table S5. Bond angles for the crystal **2**

Atom	Angle/°	Atom	Angle/°	Atom	Angle/°	Atom	Angle/°
O00D-W001-O4[1]	63.3(5)	O4-P008-O4[1]	180.0(11)	O00S[1]-W003-O00W	87.3(6)	P008-O2-W004[1]	122.9(9)
O00D-W001-O1[1]	92.3(6)	O4-P008-O1[1]	115.0(9)	O00S[1]-W003-O1[1]	94.7(7)	P008-O2-W005[1]	119.6(9)
O00E-W001-O00D	87.7(5)	O4-P008-O1	65.0(9)	O00S[1]-W003-O3	62.1(7)	P008-O2-W006[1]	124.7(8)
O00E-W001-O00L	87.4(6)	O4[1]-P008-O1	115.0(9)	O00W-W003-O1[1]	89.8(7)	P008-O2-O4[1]	51.4(8)
O00E-W001-O4[1]	90.4(6)	O4[1]-P008-O1[1]	65.0(9)	O00W-W003-O3	66.0(6)	O4[1]-O2-W004[1]	135.2(10)
O00E-W001-O1[1]	65.6(6)	O4-P008-O3[1]	113.2(8)	O3-W003-O1[1]	40.9(6)	O4[1]-O2-W005[1]	130.2(10)
O00F-W001-O00D	85.8(5)	O4[1]-P008-O3	113.2(8)	O00E-W004-O00O	87.2(5)	O4[1]-O2-W006[1]	73.3(8)
O00F-W001-O00E	154.0(6)	O4[1]-P008-O3[1]	66.8(8)	O00E-W004-O2[1]	94.5(6)	N01[1]-N010-C017	116.8(16)
O00F-W001-O00L	88.3(6)	O4-P008-O3	66.8(8)	O00E-W004-O016	153.9(7)	N010-N011-C018	101.8(18)
O00F-W001-O4[1]	64.2(6)	O1-P008-O2[1]	105.6(9)	O00H-W004-O00E	104.1(6)	W004-O012-W005	140.8(8)
O00F-W001-O1[1]	89.5(6)	O1[1]-P008-O2[1]	74.4(9)	O00H-W004-O00O	102.8(6)	W005-O014-W006	141.3(9)
O00L-W001-O00D	156.1(6)	O1[1]-P008-O2	105.6(9)	O00H-W004-O2[1]	157.1(7)	C017-C015-N00G	124.9(18)
O00L-W001-O4[1]	93.3(6)	O1-P008-O2	74.4(9)	O00H-W004-O012	102.5(7)	C017-C015-C018	108.4(17)
O00L-W001-O1[1]	64.4(6)	O1-P008-O1[1]	180	O00H-W004-O016	102.0(7)	C018-C015-N00G	126.7(15)
O00X-W001-O00D	102.4(6)	O1-P008-O3	110.8(9)	O00O-W004-O2[1]	91.3(6)	W006-O016-W004	141.6(10)
O00X-W001-O00E	102.9(7)	O1-P008-O3[1]	69.2(9)	O012-W004-O00E	89.5(6)	N010-C017-C20	125.4(17)
O00X-W001-O00F	103.0(7)	O1[1]-P008-O3	69.2(9)	O012-W004-O00O	154.5(6)	C015-C017-N010	101.3(18)
O00X-W001-O00L	101.5(7)	O1[1]-P008-O3[1]	110.8(9)	O012-W004-O2[1]	63.8(6)	C015-C017-C20	133(2)
O00X-W001-O4[1]	160.3(7)	O3-P008-O2	77.3(10)	O012-W004-O016	86.8(6)	N011-C018-C015	111.6(18)
O00X-W001-O1[1]	161.2(7)	O3[1]-P008-O2	102.7(10)	O016-W004-O00O	85.1(7)	N011-C018-C0AA	117(2)
O1[1]-W001-O4[1]	38.5(6)	O3-P008-O2[1]	102.7(10)	O016-W004-O21	60.8(7)	C015-C018-C0AA	131.4(16)
O00D-W002-O00M	89.9(6)	O3[1]-P008-O2[1]	77.3(10)	O00C-W005-O00M	101.3(6)	W001[1]-O4-W002[1]	91.9(5)
O00D-W002-O00S	155.5(7)	O3-P008-O3[1]	180.0(12)	O00C-W005-O00W[1]	100.8(6)	P008-O4-W001[1]	126.4(9)
O00D-W002-O4[1]	63.4(5)	W002-O00D-W001	140.9(7)	O00C-W005-O2[1]	158.0(7)	P008-O4-W002[1]	126.3(9)
O00D-W002-O3[1]	94.6(6)	W001-O00E-W004	141.4(7)	O00C-W005-O012	103.3(6)	P008-O4-O21	57.1(8)
O00I[1]-W002-O00D	85.7(6)	W006[1]-O00F-W001	142.8(7)	O00C-W005-O014	103.1(7)	P008-O4-O1	57.9(9)
O00I[1]-W002-O00M	154.7(7)	C00T-N00G-C00V	124.1(11)	O00M-W005-O00W[1]	88.7(6)	P008-O4-O3	58.0(8)
O00I[1]-W002-O00S	86.8(6)	C00T-N00G-C015	120.4(12)	O00M-W005-O2[1]	94.5(7)	O2[1]-O4-W001[1]	129.3(9)
O00I[1]-W002-O4[1]	64.8(6)	C015-N00G-C00V	115.4(12)	O00M-W005-O012	86.5(6)	O2[1]-O4-W002[1]	128.3(10)
O00I[1]-W002-O3[1]	89.6(7)	W002[1]-O00I-W006	142.0(8)	O00M-W005-O014	155.5(7)	O1-O4-W001[1]	68.5(8)
O00M-W002-O4[1]	91.0(7)	C00R2-C00J-C00K	120.2(13)	O00W[1]-W005-O2[1]	94.6(6)	O1-O4-W002[1]	135.6(11)

O00M-W002-O3[1]	65.8(6)	C00J-C00K-C00Q	121.8(13)	O00W[1]-W005-O012	155.8(7)	O1-O4-O2[1]	92.6(11)
O00S-W002-O00M	87.0(6)	C00J-C00K-C00T	118.5(12)	O00W[1]-W005-O014	88.8(7)	O1-O4-O3	99.7(14)
O00S-W002-O4[1]	92.4(6)	C00Q-C00K-C00T	119.7(12)	O012-W005-O2[1]	62.3(6)	O3-O4-W001[1]	138.3(11)
O00S-W002-O3[1]	62.0(7)	W001-O00L-W003	139.5(9)	O014-W005-O2[1]	61.4(7)	O3-O4-W002[1]	68.3(8)
O15-W002-O00D	101.4(6)	W005-O00M-W002	140.2(8)	O014-W005-O012	85.9(6)	O3-O4-O2[1]	89.7(11)
O15-W002-O00I[1]	101.0(7)	W003-O00O-W004	140.8(7)	O00F[1]-W006-O00I	85.8(5)	W0011-O1-W003[1]	93.1(6)
O15-W002-O00M	104.3(7)	C00Q-C00P-C00V	118.2(12)	O00F[1]-W006-O2[1]	92.4(6)	P008-O1-W001[1]	130.1(10)
O15-W002-O00S	103.0(6)	C00R-C00P-C00Q	119.3(13)	O00F[1]-W006-O014	86.9(6)	P008-O1-W003[1]	123.6(9)
O15-W002-O4[1]	158.7(6)	C00R-C00P-C00V	122.5(12)	O00I-W006-O2[1]	92.2(6)	P008-O1-O4	57.1(8)
O15-W002-O3[1]	161.4(6)	C00K-C00Q-C00P	123.2(13)	O00U-W006-O00F1	103.5(7)	P008-O1-O3[1]	56.4(8)
O31-W002-O4[1]	39.7(5)	C00K-C00Q-C00Q[2]	118.3(14)	O00U-W006-O00I	103.1(7)	O4-O1-W001[1]	73.1(9)
O00L-W003-O00W	85.9(6)	C00P-C00Q-C00Q[2]	118.5(15)	O00U-W006-O2[1]	158.5(7)	O4-O1-W003[1]	139.3(12)
O00L-W003-O1[1]	61.8(6)	C00J[2]-C00R-I07	112.7(10)	O00U-W006-O014	102.8(8)	O4-O1-O3[1]	98.4(13)
O00L-W003-O3	93.8(6)	C00J[2]-C00R-C00P	121.8(12)	O00U-W006-O016	103.1(8)	O3[1]-O1-W001[1]	139.5(12)
O00N-W003-O00L	101.5(6)	C00P-C00R-I07	125.5(11)	O014-W006-O00I	154.0(7)	O3[1]-O1-W003[1]	67.3(8)
O00N-W003-O00O	102.7(7)	W0031-O00S-W002	140.3(10)	O014-W006-O2[1]	63.2(6)	W002[1]-O3-W003	94.6(7)
O00N-W003-O00S[1]	102.9(7)	O00B-C00T-N00G	117.9(13)	O016-W006-O00F[1]	153.4(7)	P008-O3-W002[1]	127.0(9)
O00N-W003-O00W	102.7(7)	O00B-C00T-C00K	124.1(12)	O016-W006-O00I	88.9(6)	P008-O3-W003	126.3(9)
O00N-W003-O1[1]	158.7(6)	N00G-C00T-C00K	118.0(12)	O016-W006-O2[1]	61.8(7)	P008-O3-O4	55.2(8)
O00N-W003-O3	160.4(6)	O00A-C00V-N00G	118.0(13)	O016-W006-O014	86.6(6)	P008-O3-O1[1]	54.5(8)
O00O-W003-O00L	88.2(6)	O00A-C00V-C00P	125.3(14)	O2-P008-O2[1]	180.0(8)	O4-O3-W002[1]	71.9(8)
O00O-W003-O00S[1]	87.9(6)	N00G-C00V-C00P	116.7(11)	O4-P008-O2	108.5(9)	O4-O3-W003	139.7(13)
O00O-W003-O00W	154.6(6)	W005[1]-O00W-W003	139.7(7)	O4[1]-P008-O2	71.5(9)	O4-O3-O1[1]	96.0(12)
O00O-W003-O1[1]	65.8(6)	W004[1]-O2-W005[1]	92.9(6)	O4[1]-P008-O2[1]	108.5(9)	O1[1]-O3-W002[1]	143.1(13)
O00O-W003-O3	89.8(6)	W006[1]-O2-W004[1]	95.1(7)	O4-P008-O2[1]	71.5(9)	O1[1]-O3-W003	71.9(8)
O00S[1]-W003-O00L	155.5(7)	W006[1]-O2-W005[1]	93.8(7)				

[1]1-X, 1-Y, 1-Z; [2]2-X, 1-Y, 1-Z

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