Supporting Information

An Optoelectronic Duple Bistable Phosphate with Ultrahigh Thermal Stability

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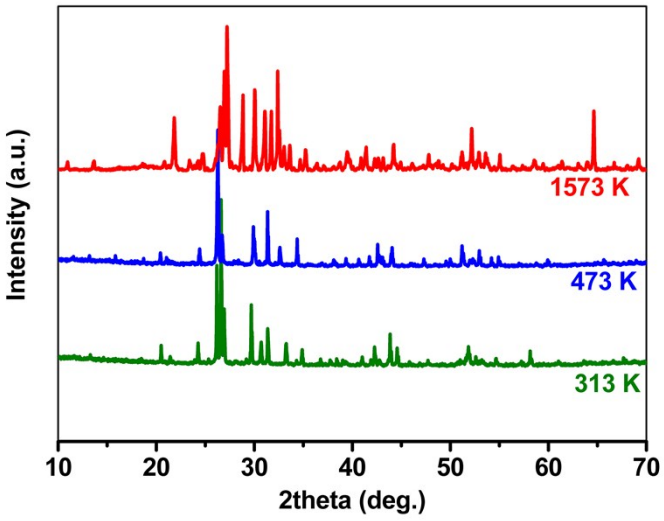

Fig. S1. Experimental XRD patterns for **1**. The two curves at the bottom were measured at 313 K and 473 K, respectively. The top curve was measured at room temperature on the sintered **1** sample during 1573 K.

Table S1. Crystal data and structure refinement for 1 in LTP and HTP.

formula	$CsCdPO_4$ (LTP)	$CsCdPO_4$ (HTP)
formula weight (g/mol)	340.28	
crystal system	monoclinic	orthorhombic
space group	$P2_1$ (4)	*Pnma* (62)
a (Å)	9.0589(4)	9.3971(8)
b (Å)	5.6406(2)	5.6764(6)
c (Å)	9.4634(4)	9.3171(11)
B	90.244(4)	90
V (Å^3)	483.55(4)	496.99(9)
Z	4	4
crystal size (mm^3)	0.25 × 0.13 × 0.08	0.12 × 0.1 × 0.07
ρ_{calcd} (g/cm^3)	4.67386	4.548
temperature (K)	100(2)	460(2)
μ (mm^{-1})	12.160	11.831
F (000)	600	600
data/restraints/parameters	1968/1/128	556/30/65
R (int)	0.0411	0.0180
GOF (F^2)	1.022	1.113
Flack parameter	0.35(4)	
final *R* indices $[F_0^2 > 2\sigma(F_c^2)]^{a)}$	R_1 = 0.0306, wR_2 = 0.0738	R_1 = 0.0388, wR_2 = 0.1106
final *R* indices (all data)[a]	R_1 = 0.0325, wR_2 = 0.0724	R_1 = 0.0444, wR_2 = 0.1048

[a)] $R_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$ and $wR_2 = [\Sigma[w(F_0^2-F_c^2)^2]/\Sigma[w(F_0^2)^2]]^{1/2}$ for $F_o^2 > 2\sigma(F_c^2)$

Table S2. Atom coordinates and equivalent isotropic displacement parameters for 1 in LTP.

Atom	Wyck.	Site	*x/a*	*y/b*	*z/c*	U_{eq} (Å^2)[a)]	BVS
Cs1	2a	1	0.17753(6)	0.88599(9)	0.01413(6)	0.0234(2)	1.31
Cs2	2a	1	0.32266(6)	0.92720(11)	0.51357(6)	0.0259(2)	0.91
Cd1	2a	1	0.59641(7)	0.87802(13)	0.16327(7)	0.0235(2)	2.03
Cd2	2a	1	0.07374(7)	0.43844(12)	0.34128(7)	0.0231(2)	1.91
P1	2a	1	0.6014(3)	0.8789(5)	–0.1889(3)	0.0222(5)	4.84
P2	2a	1	–0.0824(2)	0.9023(5)	0.3071(2)	0.0227(5)	4.93
O1	2a	1	0.6844(6)	0.9028(14)	–0.0460(7)	0.0273(14)	
O2	2a	1	0.6948(7)	0.9909(13)	–0.3068(7)	0.0318(17)	
O3	2a	1	0.4491(7)	1.0058(11)	–0.1841(8)	0.0302(16)	
O4	2a	1	0.4213(7)	1.1147(12)	0.2248(7)	0.0258(15)	
O5	2a	1	–0.0060(7)	0.8322(13)	0.4475(7)	0.0296(16)	
O6	2a	1	–0.0089(8)	1.1196(11)	0.2402(8)	0.0294(16)	
O7	2a	1	–0.0606(8)	0.6853(11)	0.2102(7)	0.0250(15)	
O8	2a	1	–0.2476(7)	0.9476(14)	0.3328(7)	0.0305(16)	

[a)] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Atom coordinates and equivalent isotropic displacement parameters for 1 in HTP.

Atom	Wyck.	Site	*x/a*	*y/b*	*z/c*	U_{eq} (Å^2)[a)]
Cs1	4c	.m.	0.01272(10)	1/4	0.18222(10)	0.0657(4)
Cd1	4c	.m.	0.16093(9)	1/4	0.58469(11)	0.0567(4)
P1	4c	.m.	0.3044(3)	1/4	-0.0920(3)	0.0458(7)
O1	8d	1	0.2313(16)	0.482(2)	-0.0469(16)	0.068(4)
O2	8d	1	0.194(3)	0.153(6)	-0.195(3)	0.105(6)
O3	8d	1	0.283(3)	0.414(4)	0.028(3)	0.077(5)
O4	4c	.m.	0.449(2)	1/4	-0.183(2)	0.107(5)
O5	4c	.m.	0.314(2)	1/4	-0.244(3)	0.105(5)
O6	4c	.m.	0.447(2)	1/4	-0.010(3)	0.114(5)

[a)] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S4. Selected bond distances and angles for 1 in LTP.

Bonds	Bond distances (Å)	Bonds	Bond distances /angels (Å)/(°)	Bonds	Bond angels (°)
Cs1—O1^{ii}	3.013(7)	Cd2—O2^{ii}	2.144(7)	O2^{ii}—Cd2—O7	111.2(3)
Cs1—O1^{iii}	3.186(7)	Cd2—O5^{vi}	2.177(7)	O6^{ix}—Cd2—O7	95.0(3)
Cs1—O3	3.173(7)	Cd2—O6^{ix}	2.169(7)	O5^{vi}—Cd2—O7	121.9(3)
Cs1—O4	3.237(7)	Cd2—O7	2.224(7)	O2^{ii}—Cd2—O5	102.7(2)
Cs1—O6	3.032(7)	P1—O1	1.539(7)	O6^{ix}—Cd2—O5	143.2(3)
Cs1—O6^{iv}	3.218(8)	P1—O2	1.550(6)	O5^{vi}—Cd2—O5	78.22(14)
Cs1—O7	3.067(7)	P1—O3	1.555(7)	O7—Cd2—O5	61.2(2)
Cs1—O7^{i}	2.909(7)	P1—O4^{ii}	1.542(7)	O2—P1—O4^{ii}	108.0(4)
Cs2—O2^{ii}	3.147(7)	P2—O5	1.547(7)	O2—P1—O1	109.3(4)
Cs2—O2^{iii}	3.736(8)	P2—O6	1.533(8)	O4^{ii}—P1—O1	109.9(4)
Cs2—O3^{v}	3.109(7)	P2—O7	1.542(7)	O2—P1—O3	108.8(4)
Cs2—O4	3.067(7)	P2—O8	1.538(7)	O4^{ii}—P1—O3	109.5(4)
Cs2—O5	3.087(7)	O1—Cd1—O3^{ii}	102.7(3)	O1—P1—O3	111.2(4)
Cs2—O5^{vii}	3.687(7)	O1—Cd1—O4	119.1(3)	O6—P2—O8	110.9(4)
Cs2—O8^{vi}	3.147(7)	O3^{ii}—Cd1—O4	116.0(3)	O6—P2—O7	109.4(4)
Cs2—O8^{vii}	3.347(7)	O1—Cd1—O8^{xi}	115.4(2)	O8—P2—O7	110.7(4)
Cd1—O1	2.143(6)	O3^{ii}—Cd1—O8^{xi}	103.5(3)	O6—P2—O5	111.4(4)
Cd1—O3^{ii}	2.149(6)	O4—Cd1—O8^{xi}	99.6(3)	O8—P2—O5	109.8(4)
Cd1—O4	2.156(7)	O2^{ii}—Cd2—O5^{vi}	117.2(3)	O7—P2—O5	104.5(4)
Cd1—O8^{xi}	2.169(7)	O6^{ix}—Cd2—O5^{vi}	94.5(3)		

Symmetry codes: (i) −x, 0.5+y, −z; (ii) 1−x, −0.5+y, −z; (iii) 1−x, 0.5+y, −z; (iv) −x, −0.5+y, −z; (v) x, y, 1+z; (vi) −x, −0.5+y, 1−z; (vii) −x, 0.5+y, 1−z; (viii) x, y, −1+z; (ix) x, −1+y, z; (xi) 1+x, y, z.

Table S5. Selected bond distances and angles for 1 in HTP.

Bonds	Bond distances (Å)	Bonds	Bond distance /angels (Å)/(°)	Bonds	Bond angels (°)
Cs1—O1	3.243(16)	O2—Cd1^{xvi}	2.15(3)	O2^{xi}—Cd1—O4^{vi}	74.5(9)
Cs1—O1^{v}	3.243(16)	O3—Cd1^{xiv}	2.05(2)	O2^{x}—Cd1—O4^{vi}	74.5(9)
Cs1—O1^{iii}	3.026(14)	O4—Cd1^{xvii}	2.19(2)	O3^{vii}—Cd1—O1^{ix}	112.4(10)
Cs1—O1^{iv}	3.026(14)	O5—Cd1^{xvi}	2.15(2)	O3^{vii}—Cd1—O1^{vii}	25.1(7)
Cs1—O2^{i}	3.01(3)	O6—Cd1^{xvii}	2.12(2)	O3^{ix}—Cd1—O1^{vii}	112.4(10)
Cs1—O2^{ii}	3.01(3)	O1—P1—O6	104.6(7)	O3^{ix}—Cd1—O1^{ix}	25.1(7)
Cs1—O3	3.06(3)	O1^{v}—P1—O1	117.2(12)	O3^{vii}—Cd1—O2^{x}	116.4(12)
Cs1—O3^{v}	3.06(3)	O1^{v}—P1—O4	121.4(6)	O3^{vii}—Cd1—O2^{xi}	88.2(12)
Cs1—O4^{vii}	3.123(9)	O1^{v}—P1—O6	104.6(7)	O3^{ix}—Cd1—O2^{x}	88.2(12)
Cs1—O4^{viii}	3.123(9)	O2—P1—O1	100.3(14)	O3^{ix}—Cd1—O2^{xi}	116.4(12)
Cs1—O5^{vii}	3.345(11)	O2—P1—O1^{v}	63.8(13)	O3^{vii}—Cd1—O3^{ix}	137.2(17)
Cs1—O6^{vi}	3.11(2)	O2—P1—O4	104.0(12)	O3^{vii}—Cd1—O4^{vi}	110.0(9)
O1—Cs1^{iii}	3.026(14)	O2—P1—O6	155.1(13)	O3^{ix}—Cd1—O4^{vi}	110.0(9)
O1—Cs1^{xiv}	3.803(16)	O2^{v}—P1—O1	63.8(13)	O3^{vii}—Cd1—O5^{x}	91.0(8)
O2—Cs1^{ii}	3.01(3)	O2^{v}—P1—O4	104.0(12)	O3^{ix}—Cd1—O5^{x}	91.0(8)
O2—Cs1^{xv}	3.76(3)	O2^{v}—P1—O6	155.1(13)	O3^{vii}—Cd1—O6^{vi}	99.2(9)
O3—Cs1^{xvii}	3.58(3)	O3—P1—O1	36.0(11)	O3^{ix}—Cd1—O6^{vi}	99.2(9)
O4—Cs1^{xiv}	3.123(9)	O3—P1—O4	121.6(13)	O4^{vi}—Cd1—O1^{vii}	130.7(4)
O4—Cs1^{xv}	3.123(9)	O3—P1—O6	75.2(14)	O4^{vi}—Cd1—O1^{ix}	130.7(4)
O5—Cs1^{xiv}	3.345(11)	O3^{v}—P1—O1	105.6(13)	O5^{x}—Cd1—O1^{vii}	96.1(6)
O5—Cs1^{xv}	3.345(11)	O3^{v}—P1—O4	121.6(13)	O5^{x}—Cd1—O1^{ix}	96.1(6)
O6—Cs1^{xvii}	3.11(2)	O3^{v}—P1—O6	75.2(14)	O5^{x}—Cd1—O2^{x}	36.1(9)
P1—O1	1.545(12)	O5—P1—O1	107.4(7)	O5^{x}—Cd1—O2^{xi}	36.1(9)
P1—O1^{v}	1.545(12)	O5—P1—O4	54.4(11)	O5^{x}—Cd1—O4^{vi}	107.2(8)
P1—O2	1.51(3)	O5—P1—O6	116.1(13)	O6^{vi}—Cd1—O1^{vii}	104.6(6)
P1—O2^{v}	1.51(3)	O6—P1—O4	61.7(12)	O6^{vi}—Cd1—O1^{ix}	104.6(6)
P1—O3	1.47(2)	O1^{vii}—Cd1—O1^{ix}	87.4(7)	O6^{vi}—Cd1—O2^{x}	116.9(10)
P1—O3^{v}	1.47(2)	O2^{x}—Cd1—O1^{vii}	129.9(9)	O6^{vi}—Cd1—O2^{xi}	116.9(10)
P1—O4	1.60(2)	O2^{x}—Cd1—O1^{ix}	106.8(10)	O6^{vi}—Cd1—O4^{vi}	44.0(8)
P1—O5	1.42(2)	O2^{xi}—Cd1—O1^{vii}	106.8(10)	O6^{vi}—Cd1—O5^{x}	151.1(9)
P1—O6	1.55(2)	O2^{xi}—Cd1—O1^{ix}	129.9(9)		
O1—Cd1^{xiv}	2.199(13)	O2^{xi}—Cd1—O2^{x}	29.7(18)		

Symmetry codes: (i) −x, 0.5+y, −z; (ii) −x, −y, −z; (iii) −x, 1−y, −z; (iv) −x, −0.5+y, −z; (v) x, 0.5−y, z; (vi) −0.5+x, y, 0.5−z; (vii) 0.5−x, 1−y, 0.5+z; (viii) 0.5−x, −y, 0.5+z; (ix) 0.5−x, −0.5+y, 0.5+z; (x) x, y, 1+z; (xi) x, 0.5−y, 1+z; (xii) −x, 1−y, 1−z; (xiii) −x, −y, 1−z; (xiv) 0.5−x, 1−y, −0.5+z; (xv) 0.5−x, −y, −0.5+z; (xvi) x, y, −1+z; (xvii) 0.5+x, y, 0.5−z.

Table S6. Anisotropic displacement parameters for 1 in LTP.

Atom	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
Cs1	0.0245(3)	0.0232(3)	0.0224(3)	–0.0001(2)	0.0004(2)	0.0008(3)
Cs2	0.0268(3)	0.0272(4)	0.0239(3)	–0.0015(3)	–0.0008(2)	–0.0008(3)
Cd1	0.0243(3)	0.0241(4)	0.0220(3)	–0.0004(3)	0.0003(2)	0.0000(3)
Cd2	0.0235(3)	0.0239(4)	0.0220(3)	0.0002(3)	–0.0002(2)	0.0003(3)
P1	0.0226(11)	0.0227(13)	0.0213(11)	0.0000(11)	0.0006(9)	0.0023(11)
P2	0.0247(11)	0.0213(13)	0.0222(11)	0.0017(11)	–0.0006(8)	0.0011(11)
O1	0.024(3)	0.033(4)	0.025(3)	–0.003(3)	–0.005(2)	–0.002(3)
O2	0.023(3)	0.038(4)	0.034(4)	–0.001(3)	0.003(3)	0.010(3)
O3	0.025(4)	0.029(4)	0.037(4)	0.001(3)	0.001(3)	0.000(3)
O4	0.022(3)	0.028(4)	0.027(4)	0.002(3)	–0.003(3)	0.001(3)
O5	0.031(4)	0.034(4)	0.023(4)	0.004(3)	0.002(3)	0.001(3)
O6	0.034(4)	0.024(4)	0.030(4)	0.000(3)	–0.003(3)	–0.001(3)
O7	0.024(4)	0.027(4)	0.024(4)	–0.005(3)	–0.005(3)	–0.002(3)
O8	0.029(3)	0.036(4)	0.027(4)	–0.002(3)	0.006(3)	–0.001(3)

Table S7. Anisotropic displacement parameters for 1 in HTP.

Atom	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
Cs1	0.0595(6)	0.0692(6)	0.0683(6)	0.00000	0.0019(4)	0.00000
Cd1	0.0466(6)	0.0593(6)	0.0641(7)	0.00000	–0.0028(4)	0.00000
P1	0.0416(14)	0.0437(15)	0.0521(17)	0.00000	–0.0060(12)	0.00000
O1	0.09(1)	0.041(6)	0.073(10)	0.026(6)	–0.015(7)	–0.020(6)
O2	0.073(8)	0.156(16)	0.086(11)	–0.013(8)	–0.008(9)	–0.003(9)
O3	0.113(12)	0.052(10)	0.066(11)	–0.001(9)	–0.009(9)	–0.021(8)
O4	0.064(6)	0.164(13)	0.092(9)	0.00000	0.005(7)	0.00000
O5	0.073(7)	0.159(13)	0.083(9)	0.00000	–0.003(7)	0.00000
O6	0.064(8)	0.183(15)	0.094(10)	0.00000	–0.011(8)	0.00000