Supporting information

Direct X-ray detection made of zero-dimensional hybrid metal halide perovskite single crystal

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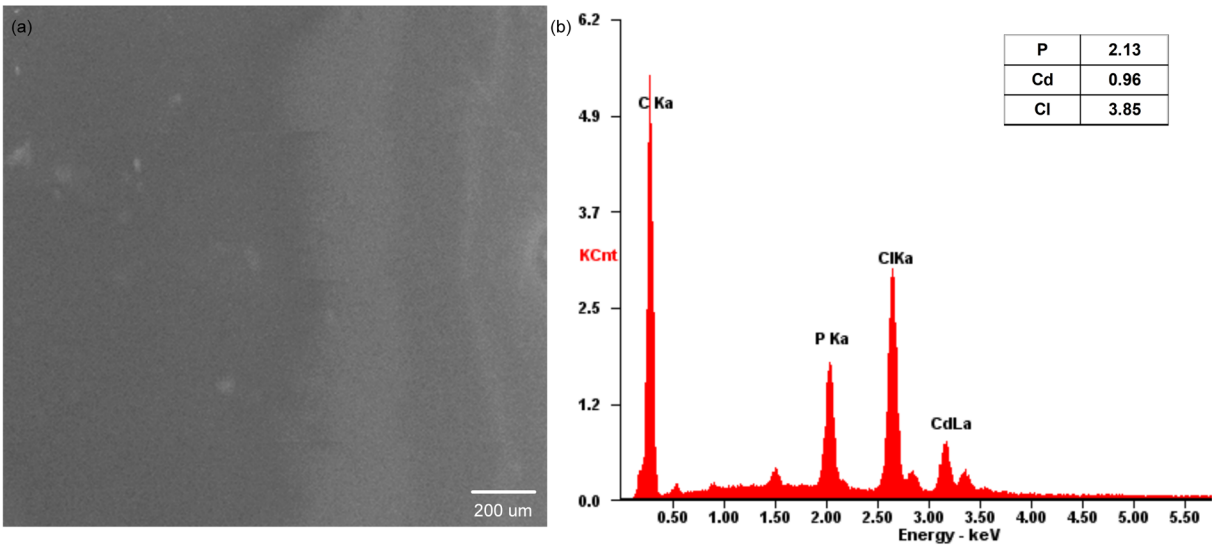

Figure S1. (a) SEM image of the $(C_{19}H_{18}P)_2CdCl_4$ SC surface; (b) EDS spectra of the three elements P, Cd and Cl.

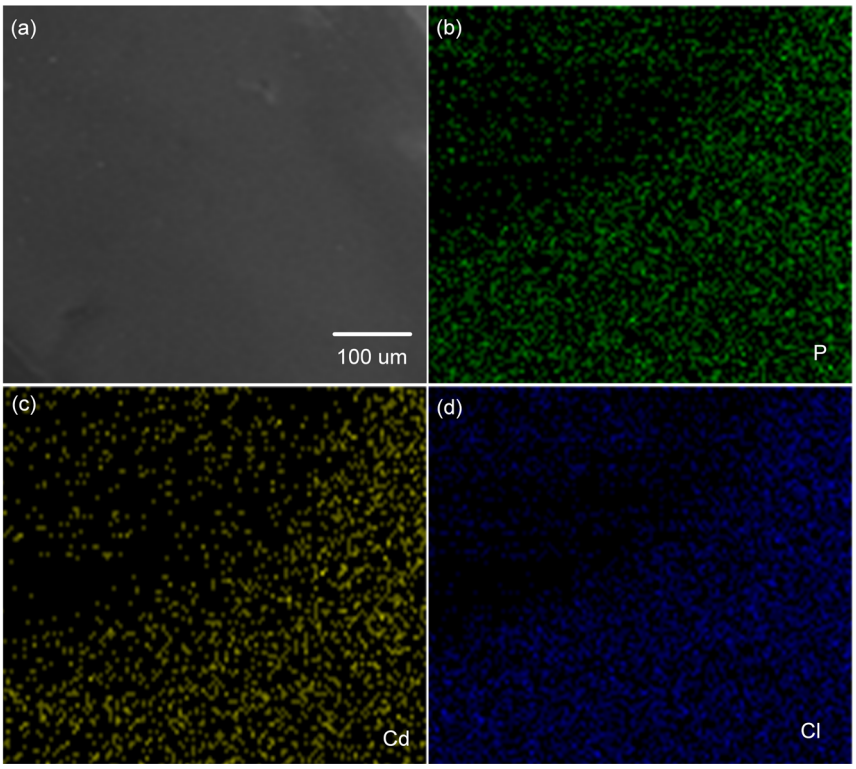

Figure S2. EDS mapping scanning measurement of the detected elements P, Cd and Cl.

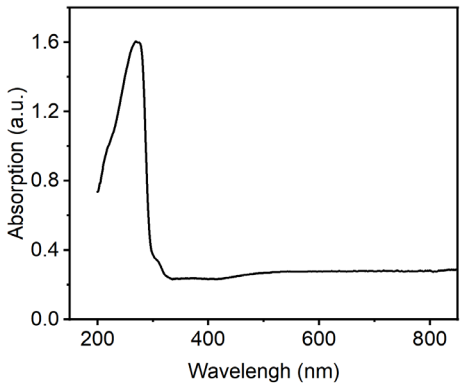

Figure S3. Absorption and photoluminescence spectra of the $(C_{19}H_{18}P)_2CdCl_4$ SC.

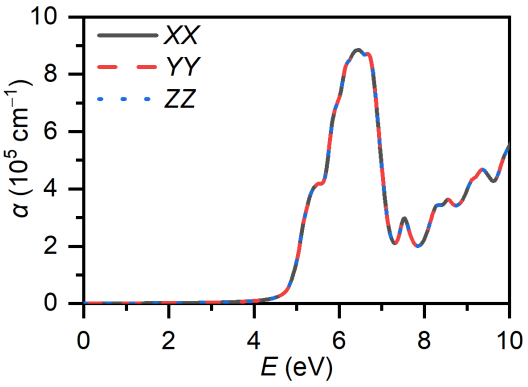

Figure S4. Optical absorption spectra of $(C_{19}H_{18}P)_2CdCl_4$ calculated based on the HSE functional.

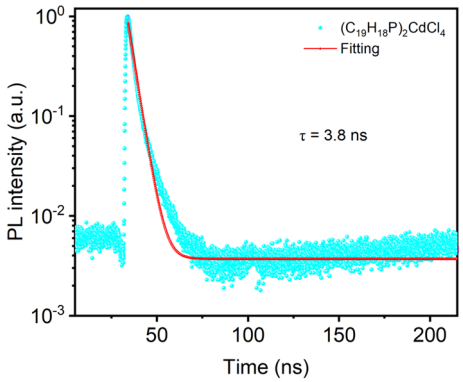

Figure S5. PL decay time of the $(C_{19}H_{18}P)_2CdCl_4$ crystals.

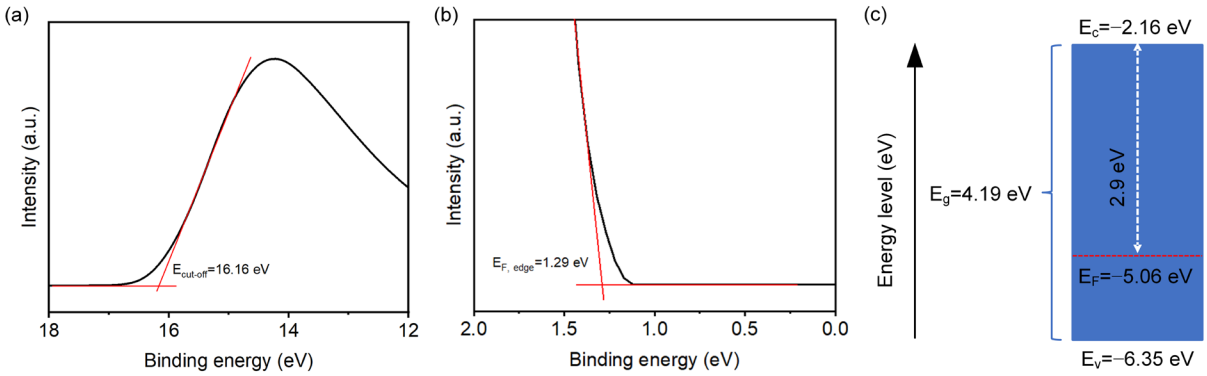

Figure S6. (a) UPS spectra of $(C_{19}H_{18}P)_2CdCl_4$. (b) Energy band diagram of the $(C_{19}H_{18}P)_2CdCl_4$ calculated from the bandgap and UPS results.

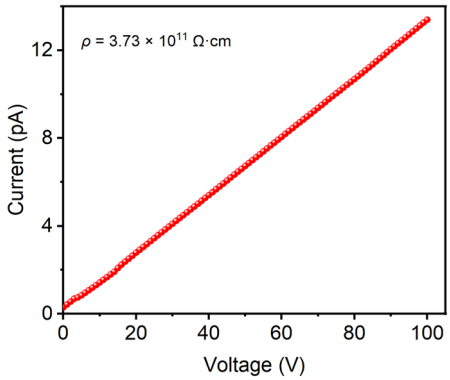

Figure S7. Resistivity measurement for $(C_{19}H_{18}P)_2CdCl_4$ SC.

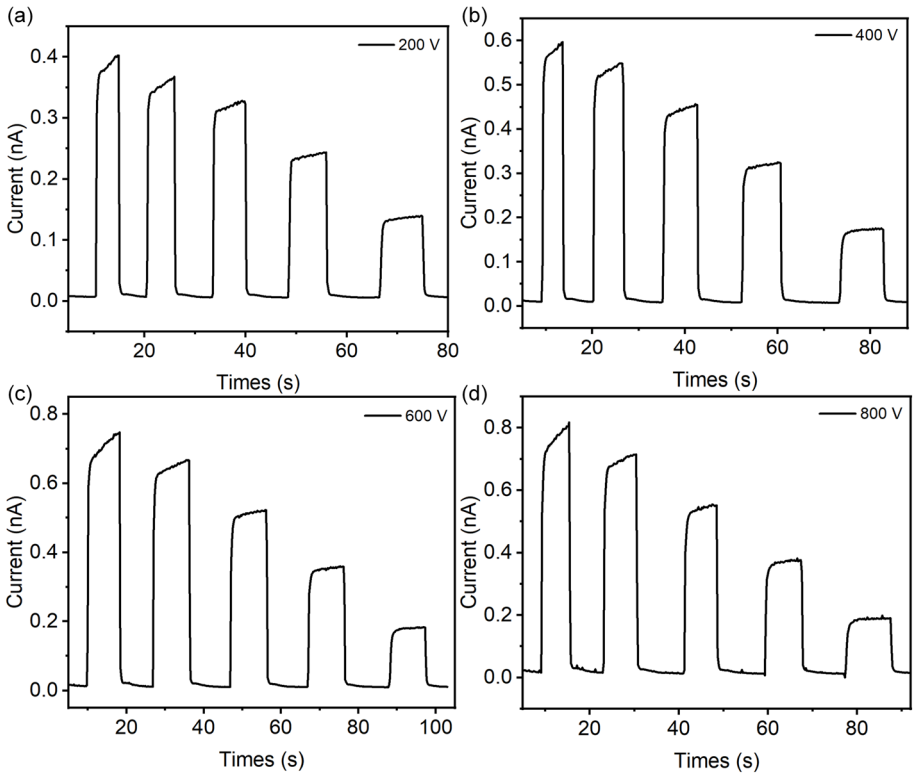

Figure S8. ON/OFF photocurrent response under various electric field and dose rates of the $(C_{19}H_{18}P)_2CdCl_4$ SC X-ray detector.

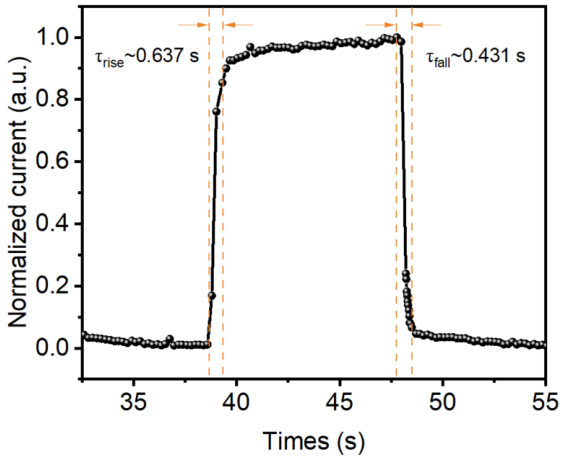

Figure S9. Single cycle on–off switching showing the rise and fall time. The rise and fall time of the device are defined as the time taken for the initial current to increase or decrease from initial to 90% of the on-state current, and vice versa. It is observed that the $(C_{19}H_{18}P)_2CdCl_4$ photodetector yields a rise/fall time of 0.637/0.431 s.

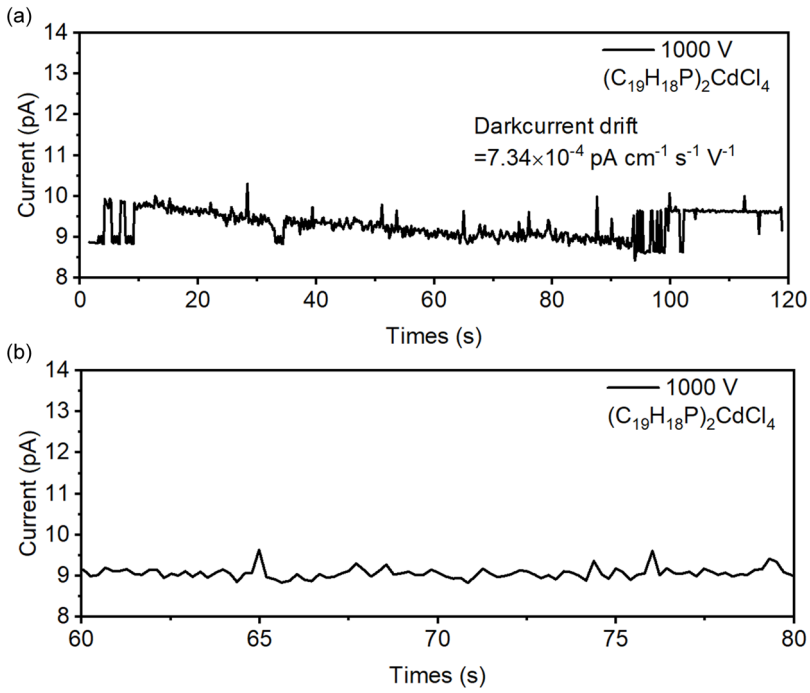

Figure S10. (a) Dark current drift of $(C_{19}H_{18}P)_2CdCl_4$ SC detector under 1000 V bias voltage. (b) Fluctuation of the dark current of $(C_{19}H_{18}P)_2CdCl_4$ device.

Table S1. Crystallographic information of $(C_{19}H_{18}P)_2CdCl_4$.

Compound	$(C_{19}H_{18}P)_2CdCl_4$
Empirical formula	$C_{38}H_{36}CdCl_4P_2$
Formula weight	808.81
Temperature/K	149.99(10)
Crystal system	cubic
Space group	$P2_13$
a/Å	15.49955(3)
b/Å	15.49955(3)
c/Å	15.49955(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3723.55(2)
Z	4
ρ_{calc} / g/cm^3	1.443
μ/mm^{-1}	8.343
F(000)	1640.0
Crystal size/mm^3	0.22 × 0.18 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.068 to 148.264
Index ranges	−18 ≤ h ≤ 18, −18 ≤ k ≤ 19, −19 ≤ l ≤ 19
Reflections collected	29156
Independent reflections	2539 [R_{int} = 0.0459, R_{sigma} = 0.0158]
Data/restraints/parameters	2539/0/139
Goodness-of-fit on F^2	1.056
Final R indexes [$I \geq 2\sigma$ (I)]	R_1 = 0.0201, wR_2 = 0.0567
Final R indexes [all data]	R_1 = 0.0201, wR_2 = 0.0567
Largest diff. peak/hole / e Å^{-3}	1.50/-0.27

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) of $(C_{19}H_{18}P)_2CdCl_4$. Ueq is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Cd1	5623.8(2)	5623.8(2)	5623.8(2)	21.58(12)
Cl1	5986.9(5)	4831.5(5)	6958.2(4)	26.82(17)
Cl2	4714.6(4)	4714.6(4)	4714.6(4)	28.8(3)
P1	7831.7(4)	2168.3(4)	7168.3(4)	22.8(3)
P2	4958.7(4)	−41.3(4)	5041.3(4)	21.1(2)
C14	4288.9(19)	−711.1(19)	5711.1(19)	28.9(10)
C12	4810(2)	1191(2)	6330(2)	31.7(7)
C4	6683(2)	854(2)	7570(2)	32.4(7)
C11	5198(2)	1726(2)	4916(2)	29.7(6)
C10	4876(3)	2020(2)	6652(2)	39.1(8)
C5	8075(2)	402(2)	7039(2)	29.7(6)
C1	6987(2)	−651(2)	7362(2)	35.6(7)
C13	4973.4(19)	1040.3(18)	5452.2(18)	23.3(6)
C3	7809(2)	−451(2)	7079(2)	34.5(7)
C2	6427(2)	−4(3)	7608(3)	39.1(8)
C6	7507.5(18)	1059.8(19)	7278.1(19)	23.3(6)
C8	5116(3)	2697(2)	6118(2)	37.4(8)
C9	5277(2)	2548(2)	5256(2)	35.2(7)
C7	7164.2(19)	2835.8(19)	7835.8(19)	33.9(12)

Table S3. Anisotropic Displacement Parameters ($Å^2×10^3$) for $(C_{19}H_{18}P)_2CdCl_4$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cd1	21.58(12)	21.58(12)	21.58(12)	−0.08(7)	−0.08(7)	−0.08(7)
Cl1	28.3(3)	31.2(4)	21.0(3)	1.7(3)	1.3(3)	6.4(3)
Cl2	28.8(3)	28.8(3)	28.8(3)	−4.2(3)	−4.2(3)	−4.2(3)
P1	22.8(3)	22.8(3)	22.8(3)	−3.7(3)	3.7(3)	3.7(3)
P2	21.1(2)	21.1(2)	21.1(2)	1.7(3)	1.7(3)	−1.7(3)
C14	28.9(10)	28.9(10)	28.9(10)	3.3(12)	3.3(12)	−3.3(12)
C12	42.2(18)	31.5(16)	21.3(14)	1.8(12)	−1.7(13)	2.6(14)
C4	24.2(15)	36.0(17)	37.1(16)	−1.5(13)	5.9(13)	1.0(12)
C11	36.5(16)	24.4(14)	28.3(15)	3.2(12)	1.3(13)	−1.1(12)
C10	52(2)	40.0(18)	25.1(15)	−5.2(14)	−6.9(14)	7.3(16)
C5	26.5(14)	27.2(15)	35.4(16)	1.5(12)	5.2(12)	3.1(12)
C1	38.6(17)	32.1(15)	36.1(17)	2.3(14)	−3.4(13)	−9.7(15)
C13	23.4(13)	24.3(13)	22.2(14)	1.5(11)	−0.3(11)	1.4(11)
C3	39.2(17)	25.8(16)	38.7(18)	2.3(13)	2.7(14)	4.3(13)
C2	30.8(17)	43.2(19)	43.2(19)	1.0(16)	5.4(14)	−9.7(14)
C6	23.1(13)	24.8(14)	22.0(13)	−1.0(11)	2.4(11)	2.3(11)
C8	46(2)	25.1(15)	40.6(18)	−7.6(14)	−14.7(16)	4.0(14)
C9	40.2(17)	23.4(14)	41.9(18)	4.0(13)	−5.4(15)	0.1(13)
C7	33.9(12)	33.9(12)	33.9(12)	−9.2(12)	9.2(12)	9.2(12)

Table S4. Bond Lengths for $(C_{19}H_{18}P)_2CdCl_4$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cd1	Cl1[1]	2.4702(7)	C12	C10	1.382(5)
Cd1	Cl1[1]	2.4703(7)	C12	C13	1.404(4)
Cd1	Cl1[2]	2.4702(7)	C4	C2	1.389(5)
Cd1	Cl2	2.4410(12)	C4	C6	1.393(4)
P1	C6	1.798(3)	C11	C13	1.393(4)
P1	C6[3]	1.798(3)	C11	C9	1.385(4)
P1	C6[4]	1.798(3)	C10	C8	1.387(5)
P1	C7	1.792(5)	C5	C3	1.387(4)
P2	C14	1.798(5)	C5	C6	1.396(4)
P2	C13[5]	1.793(3)	C1	C3	1.383(5)
P2	C13[6]	1.793(3)	C1	C2	1.380(5)
P2	C13	1.793(3)	C8	C9	1.378(5)

[1]+Y, +Z, +X; [2]+Z, +X, +Y; [3]1−Y, −1/2+Z, 3/2−X; [4]3/2−Z, 1−X, 1/2+Y; [5]1−Z, −1/2+X, 1/2−Y; [6]1/2+Y, 1/2−Z, 1−X

Table S5. Bond Angles for $(C_{19}H_{18}P)_2CdCl_4$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$Cl1^1$	Cd1	Cl1	109.801(18)	$C13^5$	P2	C13	108.95(10)
$Cl1^2$	Cd1	Cl1	109.798(18)	C10	C12	C13	119.4(3)
$Cl1^2$	Cd1	$Cl1^1$	109.799(18)	C2	C4	C6	119.6(3)
Cl2	Cd1	$Cl1^2$	109.142(18)	C9	C11	C13	119.8(3)
Cl2	Cd1	Cl1	109.141(18)	C12	C10	C8	120.6(3)
Cl2	Cd1	$Cl1^1$	109.142(18)	C3	C5	C6	119.8(3)
C6	P1	$C6^3$	109.33(10)	C2	C1	C3	120.3(3)
$C6^4$	P1	$C6^3$	109.33(10)	C12	C13	P2	119.8(2)
C6	P1	$C6^4$	109.33(10)	C11	C13	P2	120.3(2)
C7	P1	$C6^3$	109.61(10)	C11	C13	C12	119.8(3)
C7	P1	C6	109.62(10)	C1	C3	C5	120.1(3)
C7	P1	$C6^4$	109.61(10)	C1	C2	C4	120.3(3)
$C13^5$	P2	C14	109.99(10)	C4	C6	P1	120.4(2)
C13	P2	C14	109.99(10)	C4	C6	C5	119.8(3)
$C13^6$	P2	C14	109.99(10)	C5	C6	P1	119.8(2)
$C13^5$	P2	$C13^6$	108.95(10)	C9	C8	C10	120.0(3)
$C13^6$	P2	C13	108.94(10)	C8	C9	C11	120.5(3)

^{1}+Y, +Z, +X; ^{2}+Z, +X, +Y; ^{3}1−Y, −1/2+Z, 3/2−X; ^{4}3/2−Z, 1−X, 1/2+Y; ^{5}1−Z, −1/2+X, 1/2−Y; ^{6}1/2+Y, 1/2−Z, 1−X

Table S6. Torsion Angles for $(C_{19}H_{18}P)_2CdCl_4$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C14	P2	C13	C12	25.1(3)	C3	C1	C2	C4	0.3(5)
C14	P2	C13	C11	-158.8(2)	C2	C4	C6	P1	176.6(3)
C12	C10	C8	C9	1.2(6)	C2	C4	C6	C5	-1.0(5)
C10	C12	C13	P2	176.0(3)	C2	C1	C3	C5	-0.2(5)
C10	C12	C13	C11	-0.1(5)	C6[3]	P1	C6	C4	-98.5(3)
C10	C8	C9	C11	0.1(6)	C6[4]	P1	C6	C4	141.9(3)
C13[1]	P2	C13	C12	145.8(3)	C6[3]	P1	C6	C5	79.1(2)
C13[2]	P2	C13	C12	-95.5(3)	C6[4]	P1	C6	C5	-40.5(3)
C13[2]	P2	C13	C11	80.6(2)	C6	C4	C2	C1	0.3(5)
C13[1]	P2	C13	C11	-38.2(3)	C6	C5	C3	C1	-0.5(5)
C13	C12	C10	C8	-1.2(6)	C9	C11	C13	P2	-174.7(3)
C13	C11	C9	C8	-1.4(5)	C9	C11	C13	C12	1.4(5)
C3	C5	C6	P1	-176.5(3)	C7	P1	C6	C4	21.7(3)
C3	C5	C6	C4	1.1(5)	C7	P1	C6	C5	-160.7(2)

[1]1−Z, −1/2+X, 1/2−Y; [2]1/2+Y, 1/2−Z, 1−X; [3]3/2−Z, 1−X, 1/2+Y; [4]1−Y, −1/2+Z, 3/2−X

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $(C_{19}H_{18}P)_2CdCl_4$.

Atom	x	y	z	U(eq)
H14A	4524.97	-732.45	6283.3	43
H14B	4267.55	-1283.3	5475.03	43
H14C	3716.7	-475.04	5732.45	43
H12	4658.65	737.03	6692.46	38
H4	6305.27	1289.06	7738.87	39
H11	5294.37	1631.71	4331.37	36
H10	4758.17	2124.86	7230.97	47
H5	8629.39	536.04	6852.94	36
H1	6809.95	-1224.26	7385.84	43
H3	8184.13	-890	6915.65	41
H2	5875.6	-142.92	7799.38	47
H8	5169.17	3251.63	6341.98	45
H9	5438.79	3003.25	4900.6	42
H7A	6596.88	2872.12	7589.87	51
H7B	7410.12	3403.12	7872.12	51
H7C	7127.88	2589.88	8403.12	51

Table S8. Comparison of physical properties of $(C_{19}H_{18}P)_2CdCl_4$ and some related materials.

Materials	Dark current density (nA cm^{-2})	Electric field (V mm^{-1})	Dark current drift (pA cm^{-1} s^{-1} V^{-1})	$\mu\tau$ product (cm^2 V^{-1})	Sensitivity (μC Gy_{air-1} cm^{-2})	Ref.
$MA_3Bi_2I_9$ SC	~16	60	5.0×10^{-7}	2.87×10^{-3}	1947	1
$Cs_3Bi_2I_9$ SC	~18	50	-	7.97×10^{-4}	1652.3	2
$CsPbBr_3$ SC	~170	20	-	$\sim2.5\times10^{-3}$	1256	3, 4
a-Se	~0.5	10000	-	$\sim10^{-7}$	20	5, 6, 7
Rb_3Bi2I_9 SC	2.73	300	1.82×10^{-4}	2.51×10^{-3}	159.7	8
$MAPbBr_3$ SC	-	454.5	4.9×10^{-3}	1.4×10^{-2}	-	1
$Cs_2AgBiBr_6$ SC	0.15	25	-	-	105	9
TMCM-$CdCl_3$ SC	-	10	-	1.42×10^{-4}	128.9	10
CdZnTe	-	-	-	9.1×10^{-3}	-	11
$(C_{19}H_{18}P)_2CdCl_4$ SC	~20	333	7.34 × 10−4	8.53×10^{-4}	~143.6	This work

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