Supporting Information

Arsenic Containing Chalcophosphate Molecular Anions

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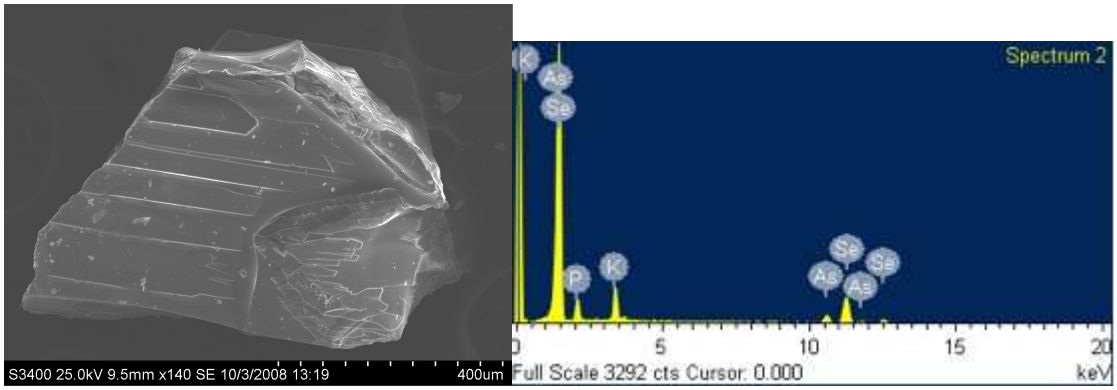

Figure S1. SEM micrograph and corresponding EDS spectrum of a $K_7As_3(P_2Se_6)_4$ crystal. The average composition of multiple scans was $K_{6.2}As_{3.0}P_{9.4}Se_{24.7}$.

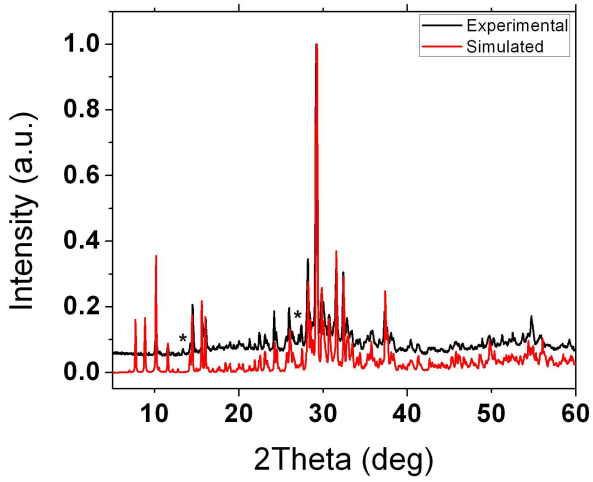

Figure S2. Experimental (black) and simulated (red) PXRD of $K_7As_3(P_2Se_6)_4$. Minor impurity peaks are denoted with an asterisk (*).

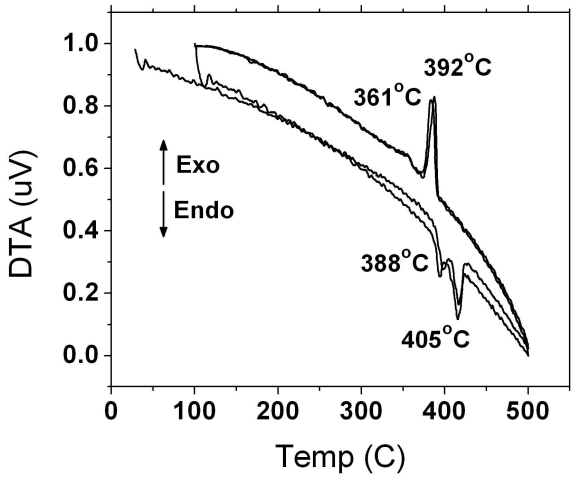

Figure S3. DTA of $K_7As_3(P_2Se_6)_4$. Melting and crystallization of the major product, **1**, are 388°C and 361°C, respectively, although the presence of the impurity is seen.

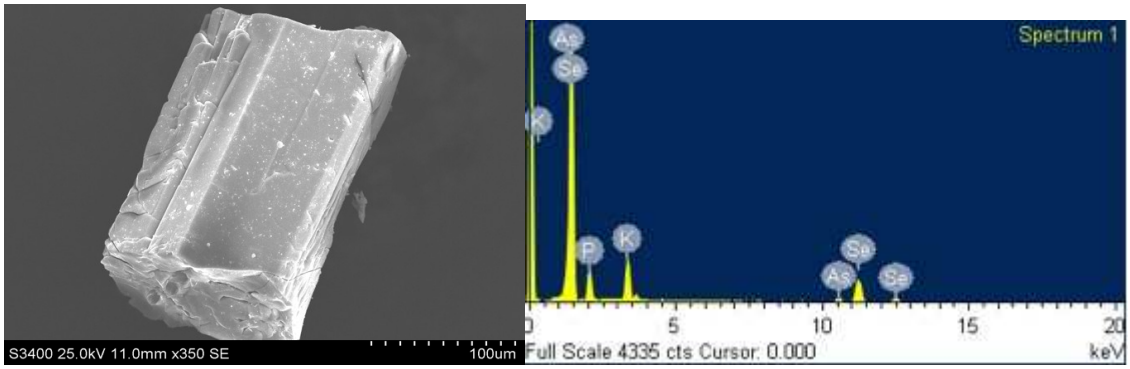

Figure S4. SEM micrograph and corresponding EDS spectrum of a $K_6As_2(P_2Se_6)_3$ crystal. The average composition of multiple scans was $K_{6.0}As_{2.0}P_{7.8}Se_{20.5}$.

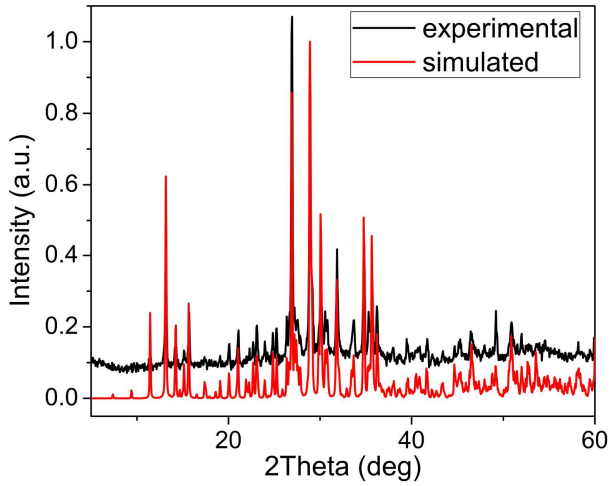

Figure S5. Experimental (black) and simulated (red) PXRD of $K_6As_2(P_2Se_6)_3$. All peaks match between the two patterns indicating a pure compound.

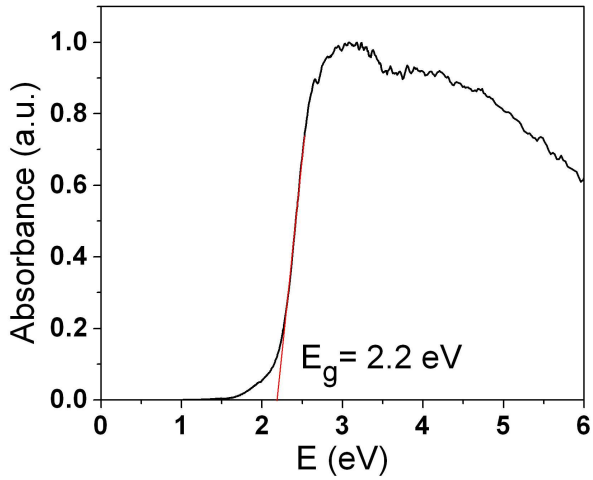

Figure S6. Diffuse reflectance spectrum of $K_6As_2(P_2Se_6)_3$. The sharp band gap transition at 2.2eV matches well with the orange color of the crystals.

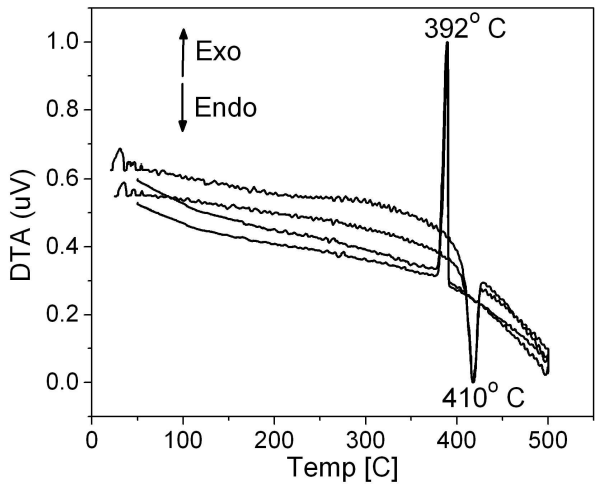

Figure S7. DTA of $K_6As_2(P_2Se_6)_3$. The pure compound melts congruently at 410°C and recrystallizes at 392°C with no significant shifts observed upon running multiple cycles.

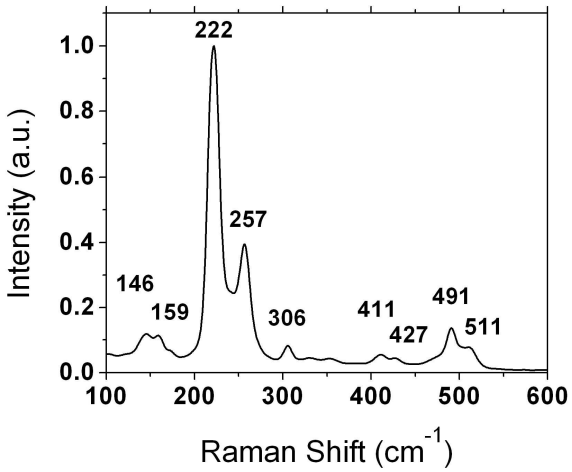

Figure S8. Raman spectrum of $K_6As_2(P_2Se_6)_3$. The strongest peak at 222 cm^{-1} can be assigned to the A_{1g} stretch of $[P_2Se_6]^{4-}$. All others are consistent with the anion as well.

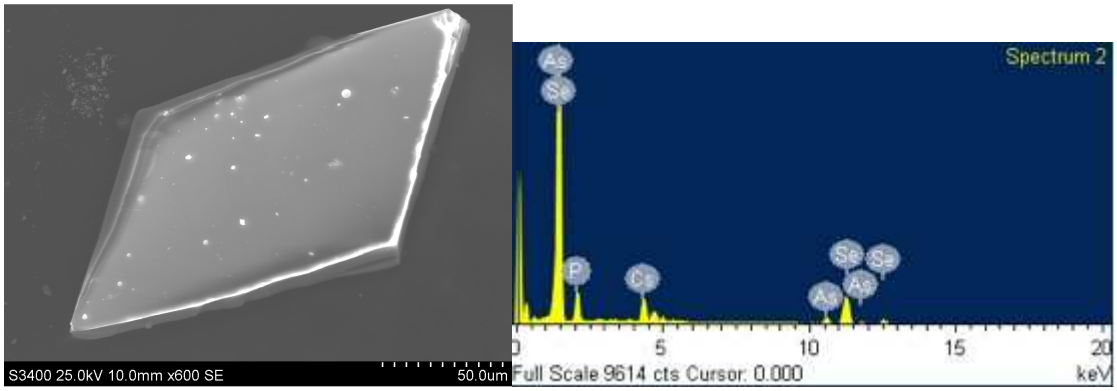

Figure S9. SEM micrograph and corresponding EDS spectrum of a $Cs_6As_2(P_2Se_6)_3$ crystal. The average composition of multiple scans was $Cs_{6.1}As_{2.0}P_{6.7}Se_{18.3}$.

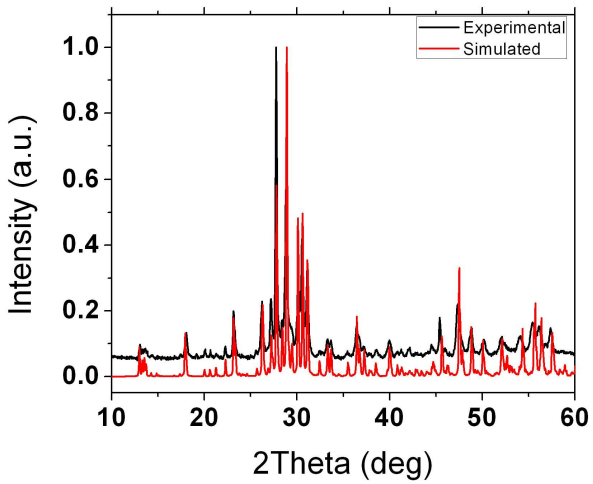

Figure S10. Experimental (black) and simulated (red) PXRD of $Cs_6As_2(P_2Se_6)_3$. All peaks match between the two patterns indicating a pure compound.

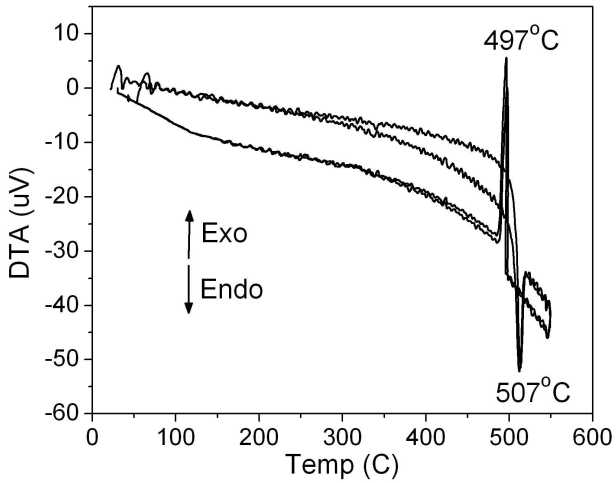

Figure S11. DTA of $Cs_6As_2(P_2Se_6)_3$. The pure compound melts congruently at 507°C and crystallizes at 497°C with no significant shifts observed upon running multiple cycles.

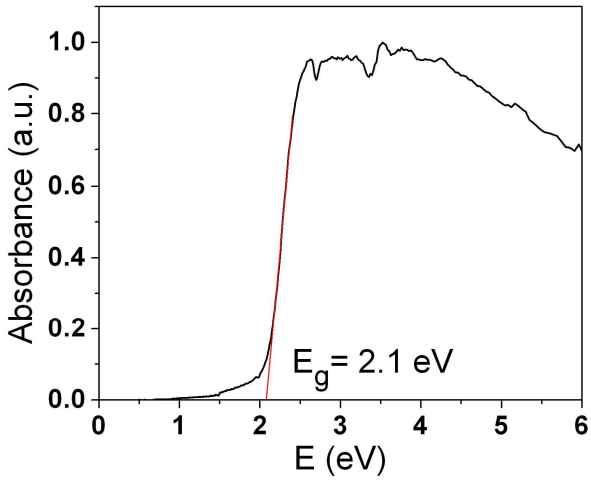

Figure S12. Diffuse reflectance UV-Vis spectrum of $Cs_6As_2(P_2Se_6)_3$.The estimated band gap of 2.1eV matches well with the orange color of the crystals.

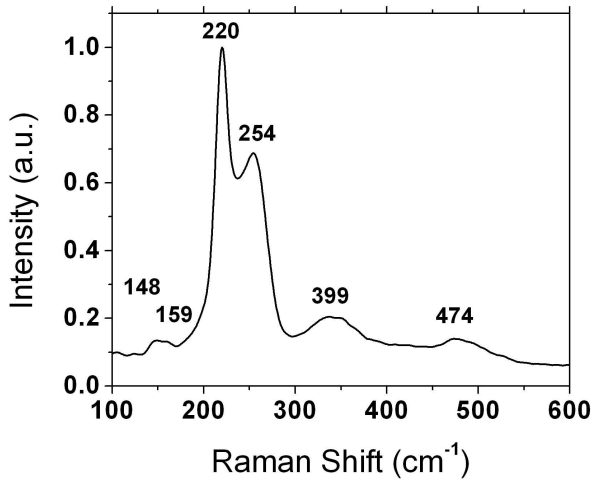

Figure S13. Raman spectrum of $Cs_6As_2(P_2Se_6)_3$. The strongest peak at 220 cm^{-1} is indicative of the totally symmetric stretch of $[P_2Se_6]^{4-}$. All others are also consistent with the anion.

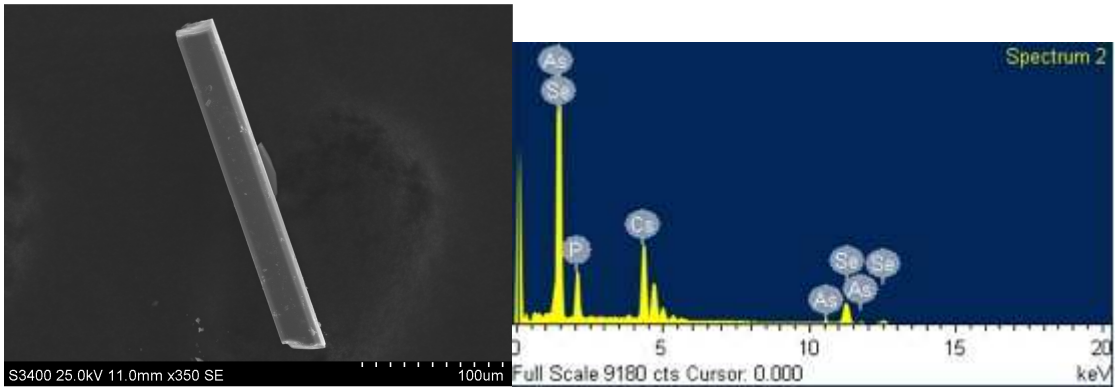

Figure S14. SEM micrograph and corresponding EDS spectrum of a $Cs_5As(P_2Se_6)_2$ crystal. The average composition of multiple scans was $Cs_{4.3}As_{1.0}P_{4.1}Se_{11.1}$.

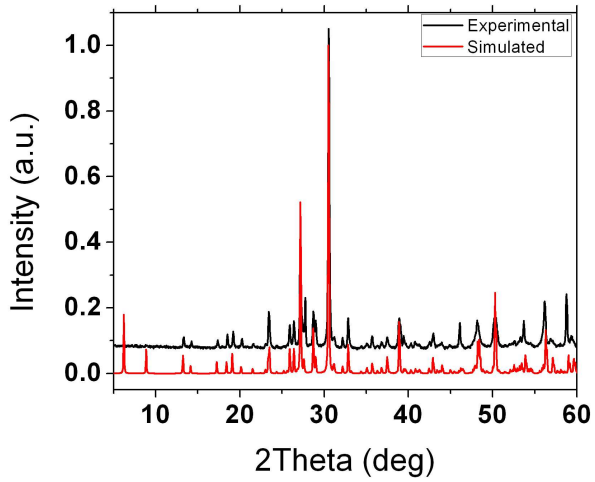

Figure S15. Experimental (black) and simulated (red) PXRD of $Cs_5As(P_2Se_6)_2$. All peaks match between the two patterns.

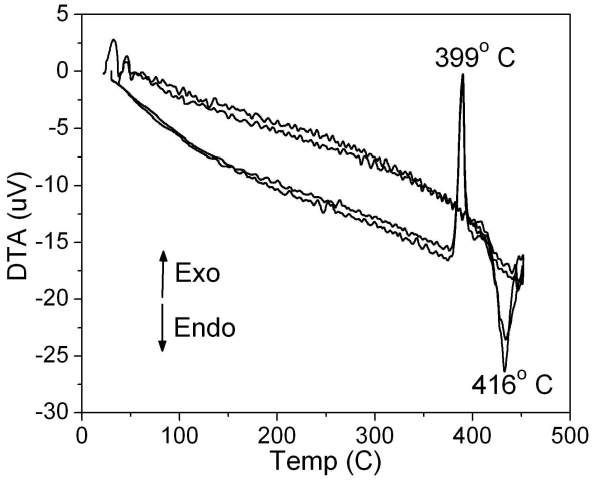

Figure S16. DTA of $Cs_5As(P_2Se_6)_2$. The pure compound melts congruently at 416°C and recrystallizes at 399°C.

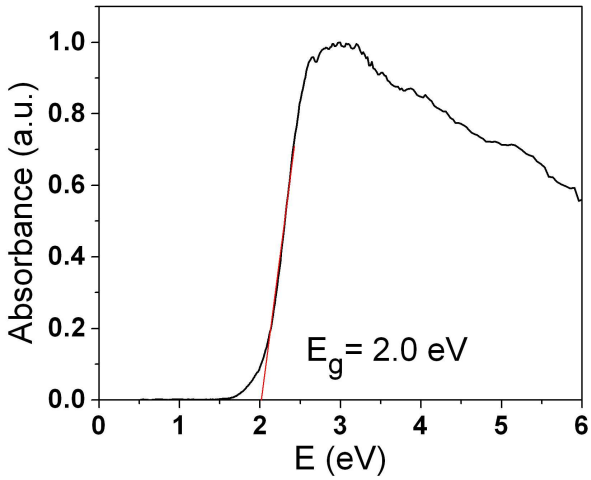

Figure S17. Diffuse reflectance UV-Vis spectrum of $Cs_5As(P_2Se_6)_2$. The estimated band gap of 2.0eV matches well with the red color of the crystals.

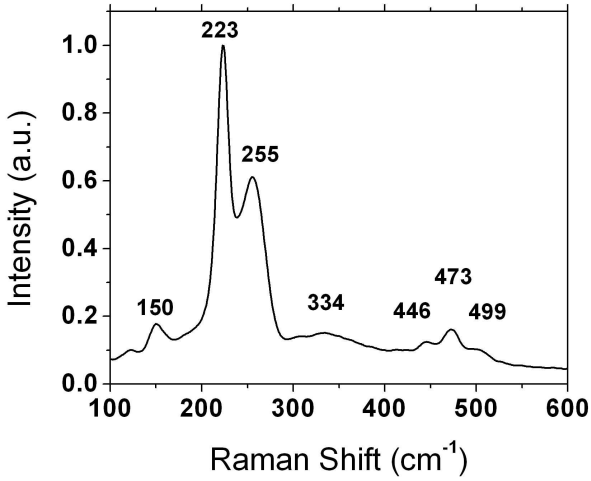

Figure S18. Raman spectrum of $Cs_5As(P_2Se_6)_2$. The strongest peak at 223 cm^{-1} is indicative of the A_{1g} stretch of $[P_2Se_6]^{4-}$. All others are also consistent with the anion.

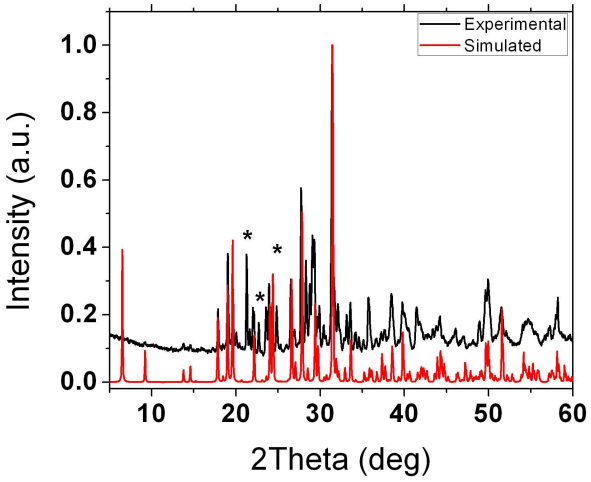

Figure S19. Experimental (black) and simulated (red) PXRD of $Cs_5As(P_2S_6)_2$. Impurity peaks are denoted with an asterisk (*).

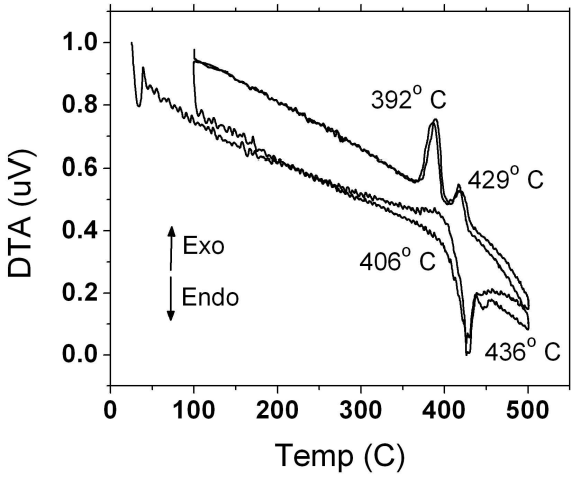

Figure S20. DTA of $Cs_5As(P_2S_6)_2$. The impurity, $Cs_4P_2S_{10}$, is reported to melt congruently at ~420°C, indicating the consistent melting and recrystallization of **4b** at 406°C and 392°C, respectively.

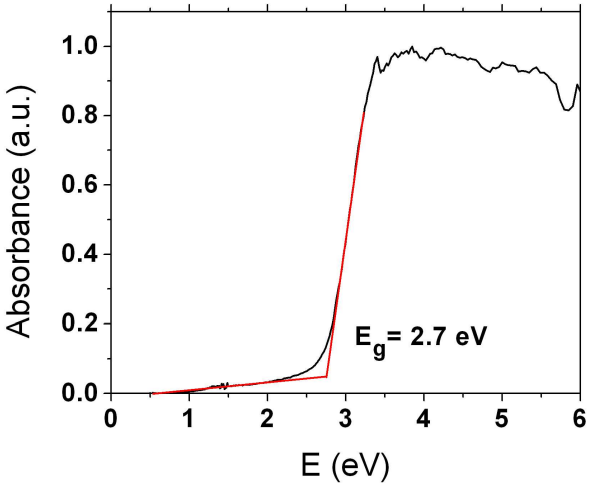

Figure S21. Diffuse reflectance UV-Vis spectrum of $Cs_5As(P_2S_6)_2$. The estimated band gap of 2.7eV matches well with the yellow color of the crystals.

Tables

Table S1. Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for $K_7As_3(P_2Se_6)_4$ (**1**) at 100(2) K.

Label	*x*	*y*	*z*	U_{eq}*
As(1)	0.48469(6)	0.25146(14)	0.07644(2)	0.0206(3)
As(2)	0.37827(6)	0.25574(14)	0.13563(2)	0.0199(3)
As(3)	0.34258(6)	0.23397(14)	0.06170(2)	0.0194(3)
As(4)	0.17321(6)	0.73985(14)	0.24631(2)	0.0203(3)
As(5)	0.68355(6)	0.27867(14)	0.29483(2)	0.0210(3)
As(6)	0.70199(6)	0.26801(14)	0.22130(2)	0.0218(3)
As(7)	0.01474(6)	0.22151(14)	0.39290(2)	0.0197(3)
As(8)	0.04118(6)	0.25106(14)	0.46773(2)	0.0198(3)
As(9)	0.15293(6)	0.24783(14)	0.41298(2)	0.0203(3)
K(1)	0.16810(14)	0.2130(3)	0.04335(6)	0.0293(7)
K(2)	0.18574(16)	0.2624(4)	0.33247(7)	0.0356(8)
K(3)	0.16649(15)	0.7217(4)	0.13269(6)	0.0332(8)
K(4)	0.15732(14)	0.2445(3)	0.14333(6)	0.0309(7)
K(5)	0.02085(13)	0.7625(3)	0.48227(5)	0.0255(7)
K(6)	0.50954(15)	0.2493(4)	0.49452(6)	0.0333(8)
K(7)	0.17813(16)	0.7361(4)	0.03019(8)	0.0412(9)
K(8)	0.63839(13)	0.2761(3)	0.34819(5)	0.0237(6)
K(9)	0.51781(14)	0.2929(3)	0.20845(6)	0.0295(7)
K(10)	0.17884(15)	0.7590(4)	0.34240(6)	0.0335(8)
K(11)	0.33201(14)	0.2785(3)	0.18918(5)	0.0262(7)
K(12)	0.23455(13)	0.2688(3)	0.25522(6)	0.0269(7)
K(13)	0.06594(14)	0.7348(3)	0.40527(6)	0.0276(7)
K(14)	0.01002(14)	0.7302(3)	0.20828(6)	0.0289(7)
K(15)	0.71740(16)	0.2483(4)	0.03446(7)	0.0413(9)
K(16)	0.64498(14)	0.2434(3)	0.11516(6)	0.0286(7)
K(17)	0.60379(14)	0.2426(3)	0.42764(6)	0.0290(7)
K(18)	0.38608(16)	0.2371(4)	0.37714(8)	0.0467(10)
K(19)	0.02773(17)	0.2333(4)	0.20257(7)	0.0387(9)
K(20)	0.30605(14)	0.2430(3)	0.46163(6)	0.0300(7)
K(21)	0.45670(16)	0.2758(4)	0.30435(8)	0.0460(10)
P(1)	0.59244(15)	0.4389(4)	0.05158(6)	0.0222(7)
P(2)	0.47614(15)	0.0537(4)	0.43511(6)	0.0201(7)
P(3)	0.52724(15)	0.4843(3)	0.37693(6)	0.0188(7)
P(4)	0.49061(15)	0.0870(4)	0.15606(6)	0.0212(7)
P(5)	0.29523(15)	0.5267(4)	0.11701(6)	0.0215(7)
P(6)	0.24756(15)	0.3781(4)	0.09565(6)	0.0194(7)
P(7)	0.38025(15)	0.0605(4)	0.01724(6)	0.0204(7)
P(8)	0.30423(15)	0.5520(4)	0.52349(6)	0.0201(7)
P(9)	0.12680(16)	0.5584(4)	0.28791(6)	0.0223(8)
P(10)	0.08891(15)	0.4431(4)	0.25840(6)	0.0206(7)
P(11)	0.15936(14)	0.8906(4)	0.19234(6)	0.0188(7)
P(12)	0.22632(15)	0.0421(4)	0.19246(6)	0.0196(7)
P(13)	0.57037(15)	0.1096(4)	0.27540(6)	0.0222(8)
P(14)	0.36613(15)	0.5046(3)	0.24332(6)	0.0189(7)
P(15)	0.30580(15)	0.0705(4)	0.30009(6)	0.0206(7)
P(16)	0.66635(15)	0.4494(4)	0.16952(6)	0.0212(7)
P(17)	0.05851(15)	0.0425(4)	0.35042(6)	0.0201(7)
P(18)	0.01945(15)	0.4337(4)	0.14528(6)	0.0197(7)
P(19)	0.08591(15)	0.6352(4)	0.57610(6)	0.0203(7)
P(20)	0.04196(14)	0.0156(4)	0.05383(6)	0.0187(7)
P(21)	0.14789(15)	0.0789(4)	0.49056(6)	0.0190(7)
P(22)	0.86445(15)	0.4766(4)	0.04268(6)	0.0203(7)
P(23)	0.19631(15)	0.5485(4)	0.40176(6)	0.0205(7)

P(24)	0.26698(15)	0.4264(4)	0.39189(6)	0.0212(7)
Se(1)	0.59970(6)	0.49352(15)	0.01707(2)	0.0252(3)
Se(2)	0.66223(6)	0.47249(16)	0.07351(3)	0.0263(3)
Se(3)	0.56002(6)	0.21652(14)	0.05325(3)	0.0237(3)
Se(4)	0.45955(6)	0.26835(14)	0.43348(3)	0.0246(3)
Se(5)	0.52094(6)	0.44838(13)	0.09845(2)	0.0197(3)
Se(6)	0.45339(6)	0.47691(15)	0.04550(2)	0.0227(3)
Se(7)	0.53226(6)	0.06305(14)	0.10009(2)	0.0208(3)
Se(8)	0.52452(6)	0.26290(14)	0.37392(3)	0.0235(3)
Se(9)	0.38950(6)	0.05430(13)	0.11157(2)	0.0197(3)
Se(10)	0.57380(6)	0.05933(15)	0.16378(3)	0.0260(3)
Se(11)	0.47246(6)	0.30685(14)	0.14524(2)	0.0202(3)
Se(12)	0.43625(6)	0.01837(15)	0.18032(2)	0.0246(3)
Se(13)	0.37982(6)	0.45534(14)	0.11168(2)	0.0200(3)
Se(14)	0.28903(6)	0.73208(14)	0.10348(3)	0.0230(3)
Se(15)	0.27288(6)	0.49647(15)	0.15090(2)	0.0236(3)
Se(16)	0.16575(6)	0.43926(15)	0.09480(3)	0.0250(3)
Se(17)	0.26976(6)	0.17314(14)	0.10789(2)	0.0210(3)
Se(18)	0.27539(6)	0.41484(14)	0.06087(2)	0.0220(3)
Se(19)	0.29039(6)	0.02027(14)	0.05907(2)	0.0212(3)
Se(20)	0.24037(6)	0.01635(15)	0.00042(3)	0.0240(3)
Se(21)	0.32053(6)	0.72934(14)	0.02406(3)	0.0279(3)
Se(22)	0.35188(6)	0.28041(14)	0.02226(2)	0.0198(3)
Se(23)	0.44067(6)	0.00330(14)	0.04263(3)	0.0244(3)
Se(24)	0.39866(6)	0.46941(16)	0.48312(3)	0.0273(3)
Se(25)	0.08193(7)	0.52304(16)	0.31660(3)	0.0292(3)
Se(26)	0.21111(6)	0.51532(15)	0.29108(3)	0.0257(3)
Se(27)	0.11322(6)	0.77919(14)	0.27578(2)	0.0225(3)
Se(28)	0.10633(6)	0.22713(15)	0.26291(3)	0.0277(3)
Se(29)	0.00703(6)	0.50551(15)	0.25317(3)	0.0262(3)
Se(30)	0.13680(6)	0.52613(14)	0.22990(2)	0.0208(3)
Se(31)	0.12324(6)	0.58131(14)	0.72569(2)	0.0225(3)
Se(32)	0.09919(6)	0.54285(15)	0.66809(3)	0.0246(3)
Se(33)	0.19899(6)	0.69198(14)	0.18980(2)	0.0207(3)
Se(34)	0.26406(6)	0.01600(15)	0.16148(2)	0.0237(3)
Se(35)	0.19957(6)	0.24804(14)	0.20036(2)	0.0234(3)
Se(36)	0.72213(6)	0.47451(14)	0.27691(2)	0.0205(3)
Se(37)	0.59995(6)	0.32818(13)	0.27227(2)	0.0204(3)
Se(38)	0.57567(6)	0.03894(14)	0.30974(2)	0.0222(3)
Se(39)	0.49596(6)	0.08352(16)	0.25682(3)	0.0266(3)
Se(40)	0.28884(6)	0.57354(14)	0.22541(2)	0.0200(3)
Se(41)	0.37286(6)	0.28434(14)	0.24280(2)	0.0235(3)
Se(42)	0.62758(6)	0.08654(14)	0.22193(2)	0.0203(3)
Se(43)	0.64219(6)	0.46708(14)	0.22472(2)	0.0201(3)
Se(44)	0.77435(6)	0.49637(15)	0.20936(3)	0.0248(3)
Se(45)	0.32080(6)	0.28378(14)	0.30560(3)	0.0261(3)
Se(46)	0.69192(6)	0.23280(14)	0.18103(2)	0.0213(3)
Se(47)	0.58147(6)	0.48051(15)	0.16367(3)	0.0250(3)
Se(48)	0.28507(6)	0.00256(15)	0.35754(2)	0.0255(3)
Se(49)	0.88465(6)	0.49183(15)	0.12231(3)	0.0235(3)
Se(50)	0.08353(6)	0.01043(16)	0.31724(3)	0.0270(3)
Se(51)	0.03030(6)	0.26468(14)	0.35387(2)	0.0208(3)
Se(52)	0.00623(6)	0.21369(14)	0.14352(3)	0.0265(3)
Se(53)	0.07913(6)	0.50614(15)	0.16994(3)	0.0251(3)
Se(54)	0.03720(6)	0.50818(14)	0.11031(2)	0.0215(3)
Se(55)	0.05327(6)	0.59996(14)	0.61011(2)	0.0226(3)
Se(56)	0.16749(6)	0.57439(15)	0.57929(3)	0.0269(3)
Se(57)	0.06458(6)	0.66364(14)	0.06219(2)	0.0204(3)
Se(58)	0.04624(6)	0.22067(14)	0.06781(2)	0.0226(3)
Se(59)	0.07005(6)	0.51027(14)	0.52066(2)	0.0223(3)
Se(60)	0.04436(6)	0.44906(14)	0.44346(2)	0.0202(3)

Se(61)	0.13455(6)	0.29932(13)	0.47927(2)	0.0196(3)
Se(62)	0.08593(6)	0.48560(14)	0.01179(2)	0.0235(3)
Se(63)	0.22849(6)	0.45798(15)	0.00171(2)	0.0248(3)
Se(64)	0.05422(6)	0.04837(14)	0.44391(2)	0.0195(3)
Se(65)	0.13935(6)	0.75573(13)	0.46027(3)	0.0224(3)
Se(66)	0.19863(6)	0.05990(13)	0.43653(2)	0.0203(3)
Se(67)	0.18626(6)	0.44650(13)	0.43534(2)	0.0187(3)
Se(68)	0.12872(6)	0.47687(15)	0.38037(3)	0.0248(3)
Se(69)	0.78363(6)	0.26172(14)	0.09640(3)	0.0254(3)
Se(70)	0.33111(6)	0.45321(16)	0.41664(3)	0.0279(3)
Se(71)	0.23020(6)	0.20973(14)	0.39124(3)	0.0240(3)
Se(72)	0.28290(6)	0.48036(15)	0.35799(2)	0.0261(3)

*U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $K_6As_2(P_2Se_6)_3$ (**2**) at 100(2) K.

Label	*x*	*y*	*z*	U_{eq}*
As(1)	0.03926(15)	0.07655(4)	0.23091(9)	0.0366(2)
K(1)	0.1008(5)	0.33330(13)	0.2206(3)	0.0678(8)
K(2)	0.6278(4)	0.19071(11)	0.2467(2)	0.0481(6)
K(3)	0.6590(4)	0.47442(12)	0.2690(3)	0.0715(9)
P(1)	0.0567(3)	0.16571(9)	0.0283(2)	0.0237(4)
P(2)	0.2680(3)	0.82602(9)	0.0480(2)	0.0250(4)
P(3)	0.1224(3)	0.52752(9)	0.0808(2)	0.0282(5)
Se(1)	0.14055(15)	0.25901(4)	0.47391(10)	0.0410(2)
Se(2)	0.11635(15)	0.41572(4)	0.47665(10)	0.0410(2)
Se(3)	0.19395(12)	0.16789(4)	0.24963(8)	0.02971(19)
Se(4)	0.55450(15)	0.33787(5)	0.24039(9)	0.0478(3)
Se(5)	0.68135(15)	0.25203(4)	0.02046(11)	0.0408(2)
Se(6)	0.69541(13)	0.09611(4)	0.05037(8)	0.02873(19)
Se(7)	0.05957(17)	0.10320(4)	0.42726(9)	0.0397(2)
Se(8)	0.24477(16)	0.48214(4)	0.26520(9)	0.0372(2)
Se(9)	0.31242(16)	0.55981(5)	0.02599(12)	0.0518(3)

*U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Table S3. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $Cs_6As_2(P_2Se_6)_3$ (**3**) at 100(2) K.

Label	x	y	z	U_{eq}^*
As(1)	0.17676(5)	0.00161(10)	0.05955(7)	0.0107(2)
Cs(1)	0.08303(3)	0.53130(7)	0.19917(5)	0.01531(15)
Cs(2)	0.25830(3)	0.02663(6)	0.41534(5)	0.01329(15)
Cs(3)	0.56853(3)	0.02221(6)	0.18825(5)	0.01392(15)
P(1)	0.35959(12)	0.1117(2)	0.15539(18)	0.0096(4)
P(2)	0.67405(12)	0.3738(3)	0.43158(18)	0.0100(4)
P(3)	0.01931(12)	0.1162(3)	0.04583(18)	0.0106(4)
Se(1)	0.41223(5)	0.25966(10)	0.05957(7)	0.01242(19)
Se(2)	0.41339(5)	0.03823(11)	0.30737(7)	0.0127(2)
Se(3)	0.25213(5)	0.22487(10)	0.15772(7)	0.01096(19)
Se(4)	0.58695(5)	0.23426(10)	0.45414(8)	0.01326(19)
Se(5)	0.25336(5)	0.53253(10)	0.42358(7)	0.01274(19)
Se(6)	0.25642(5)	0.75208(11)	0.15992(8)	0.01386(19)
Se(7)	0.08807(5)	0.26756(11)	0.45121(8)	0.0148(2)
Se(8)	0.07988(5)	0.02549(11)	0.19498(7)	0.0141(2)
Se(9)	0.06864(5)	0.77011(10)	0.44157(7)	0.01328(19)

*U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Table S4. Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for $Cs_5As(P_2Se_6)_2$ (**4a**) at 100(2) K.

Label	*x*	*y*	*z*	U_{eq}*
As(1)	0.0000	0.5000	0.0000	0.0090(6)
Cs(1)	0.0000	0.0000	0.0000	0.0150(4)
Cs(2)	0.31818(11)	0.65665(11)	0.0000	0.0180(3)
Cs(3)	0.32337(10)	0.03265(11)	0.0000	0.0116(3)
P(1)	0.2030(5)	0.3915(4)	0.0000	0.0129(11)
P(2)	0.1142(4)	0.2555(4)	0.0000	0.0088(10)
Se(1)	0.15093(12)	0.17956(12)	0.24250(19)	0.0130(3)
Se(2)	0.03568(17)	0.69130(17)	0.0000	0.0111(4)
Se(3)	0.3529(2)	0.3651(2)	0.0000	0.0246(6)
Se(4)	0.14851(16)	0.47209(13)	0.2342(3)	0.0252(4)

*U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Table S4. Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for $Cs_5As(P_2S_6)_2$ (**4b**) at 293(2) K.

Label	x	y	z	U_{eq}*
As(1)	0.0000	0.5000	0.0000	0.0255(4)
Cs(1)	0.32396(7)	0.04095(9)	0.0000	0.0360(2)
Cs(2)	0.30806(12)	0.66564(10)	0.0000	0.0560(4)
Cs(3)	0.0000	0.0000	0.0000	0.0702(7)
P(1)	0.1994(3)	0.3944(3)	0.0000	0.0303(8)
P(2)	0.1091(3)	0.2566(3)	0.0000	0.0246(7)
S(1)	0.1410(2)	0.1854(2)	0.2320(4)	0.0371(6)
S(2)	0.0312(3)	0.6885(3)	0.0000	0.0311(7)
S(3)	0.3401(4)	0.3688(5)	0.0000	0.0720(19)
S(4)	0.1477(4)	0.4699(2)	0.2225(6)	0.0686(13)

*U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

Table S5. Selected Bond Distances (Å) and Angles (°) for $Cs_5As(P_2S_6)_2$ (**4b**) at 293(2) K.

S(1)-P(2)	1.997(3)	S(3)-P(1)-P(2)	112.9(3)
S(4)-P(1)	2.045(4)	S(4)-P(1)-P(2)	103.40(17)
S(4)-As(1)	2.614(5)	S(4)#6-P(1)-P(2)	103.40(17)
S(2)-P(2)#4	2.047(5)	S(2)-As(1)-S(2)#4	180.0
S(2)-As(1)	2.596(4)	S(2)-As(1)-S(4)#4	88.32(10)
P(2)-P(1)	2.238(5)	S(2)#4-As(1)-S(4)#4	91.68(10)
P(1)-S(3)	1.943(7)	S(2)-As(1)-S(4)#6	91.68(10)
P(1)-S(4)-As(1)	81.30(18)	S(2)#4-As(1)-S(4)#6	88.32(10)
P(2)#4-S(2)-As(1)	102.00(19)	S(4)#4-As(1)-S(4)#6	103.18(15)
S(1)#6-P(2)-S(1)	115.9(2)	S(2)-As(1)-S(4)#12	88.32(10)
S(1)#6-P(2)-S(2)#4	112.23(15)	S(2)#4-As(1)-S(4)#12	91.68(10)
S(1)-P(2)-S(2)#4	112.23(15)	S(4)#4-As(1)-S(4)#12	76.82(15)
S(1)#6-P(2)-P(1)	106.63(16)	S(4)#6-As(1)-S(4)#12	180.0
S(1)-P(2)-P(1)	106.63(16)	S(2)-As(1)-S(4)	91.68(10)
S(2)#4-P(2)-P(1)	101.82(19)	S(2)#4-As(1)-S(4)	88.32(10)
S(3)-P(1)-S(4)	115.3(2)	S(4)#4-As(1)-S(4)	180.0
S(3)-P(1)-S(4)#6	115.3(2)	S(4)#6-As(1)-S(4)	76.82(15)
S(4)-P(1)-S(4)#6	105.1(3)	S(4)#12-As(1)-S(4)	103.18(15)

Symmetry codes:(1) -y,x,z+1/2 (2) -y+1,x,z+1/2 (3) y,-x+1,-z+1/2 (4) -x,-y+1,-z (5) y,-x+1,-z-1/2 (6) x,y,-z (7) y,-x+1,z-1/2 (8) -y+1,x,z-1/2 (9) y,-x,z-1/2 (10) y,-x,-z+1/2 (11) -y+1,x,-z+1/2 (12) -x,-y+1,z (13) -x,-y,-z (14) -x,-y,z (15) -y,x,z-1/2 (16) -y,x,-z+1/2.