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Table S1. Crystallographic	Details for $K_4Pd(PS_4)_2$.
I. Crystal Data	
Empirical Formula	$K_4Pd(PS_4)_2$
Formula Weight	581.18
Crystal Color, Habit	orange-red, rod
Crystal Dimensions (mm)	$0.19 \times 0.11 \times 0.11$
Crystal System	Triclinic
Lattice Parameters	a = 6.380(1) Å
	b = 6.897(1) Å
	c = 8.999(2) Å
	$\alpha = 87.777(8)^{\circ}$
	$\beta = 81.581(8)^{\circ}$
	$\gamma = 106.61(1)^{\circ}$
	$V = 389.8(2) Å^3$
Space Group	P1 (#2)
Z value	1
D _{calc}	2.469 g/cm ³
μ(μοκα)	17.8 cm^{-1}
II. Intensity Measurements	
Diffractometer	Siemens P4
Radiation	AgK-L _{2,3} (λ = 0.56086 Å)
Temperature	23°C
Scan Type	ω

 $2\theta_{max}$ No. of Reflections measured

Corrections

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AgK-L<sub>2,3</sub> (\lambda = 0.56086 Å)
23°C
\omega
55°
Total : 6814
Unique : 3408 (R<sub>int</sub> = 0.029)
Lorentz-polarization
```

III. Structure Solution and RefinementStructure SolutionDirect MethodsRefinementFull-matrix least squaresFunction minimized $\Sigma \le (|F_0| - |F_c|)^2$ Least-squares Weights $4F_0^2 / \sigma^2 (F_0^2)$ Anomalous DispersionAll non-hydrogen atomsNo. of Observations (I > 3.00σ (I))1541

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No. of Variables	71
Residuals : R; R _w	0.039; 0.050
Goodness of Fit Indicator	1.37
Max Shift / Error in Final Cycle	0.00
Maximum Peak in Final Diff. Map	0.78 e ⁻ / Å ³
Minimum Peak in Final Diff. Map	-0.68 e ⁻ / Å ³

Table S2. Crystallographic	Details for $Cs_4Pd(PSe_4)_2$.
I. Crystal Data	
Empirical Formula	$Cs_4Pd(PSe_4)_2$
Formula Weight	1331.65
Crystal Color, Habit	dark-red, irregular rod
Crystal Dimensions (mm)	0.53 x 0.39 x 0.36
Crystal System	Monoclinic
Lattice Parameters	a = 7.491(2) Å
	b = 13.340(2) Å
	c = 10.030(3) Å
	$\beta = 92.21(2)^{\circ}$
	$V = 1001.6(4) Å^3$
Space Group	P21/c (#14)
Z value	2
D _{calc}	4.415 g/cm ³
μ(Μοκα)	225.64 cm ⁻¹

II. I	Intensity	Measurements	
Diffra Radiat	actometer		Rigaku AFC6S MoK α (λ = 0.71069 Å)
Temper Scan 1	rature Type		-100°C ω-2θ
20 _{max} No. of	E Reflection	ns measured	Total : 1990
Correc	ctions		Lorentz-polarization

Empirical Absorption

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(ψ-scan, DIFABS)
0.748
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min./max. transmission

III. Structure Solution and Refinement Structure Solution Direct Methods Refinement Full-matrix least squares Σ w (|F₀| - |F_c|)² Function minimized $4F_0^2 / \sigma^2 (F_0^2)$ Least-squares Weights Anomalous Dispersion All non-hydrogen atoms No. of Observations (I > 3.00σ (I)) 1391 No. of Variables 70 Residuals : R; Rw 0.029; 0.038 Goodness of Fit Indicator 1.53 Max Shift / Error in Final Cycle 0.00 Maximum Peak in Final Diff. Map $0.95 e^{-} / Å^{3}$ Minimum Peak in Final Diff. Map -1.14 e⁻ / Å³

Table S3. Crystallographic Details for Cs₁₀Pd(PSe₄)₄. I. Crystal Data Empirical Formula Cs₁₀Pd(PSe₄)₄ Formula Weight 2822.71 Crystal Color, Habit red, rod $0.84 \times 0.28 \times 0.28$ Crystal Dimensions (mm) Crystal System Tetragonal Lattice Parameters a = 13.949(2) Å b = 13.949(2) Å c = 11.527(2) Å $V = 2242.7(6) Å^3$ P42c (#112) Space Group Z value 2 4.180 g/cm^{3} D_{calc} 213.61 cm^{-1} μ (MOK α)

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II.	Intensity	Measurements				
Diffr	actometer		Rigaku AFC6S			
Radia	ation		Mok α (λ = 0.71069 Å)			
Tempe	erature		23°C			
Scan	Туре		ω-2θ			
$2\theta_{max}$			55°			
No. of Reflections measured			Total : 1543			
			Unique : 1543			
Corre	ections		Lorentz-polarization			
			Empirical Absorption			
			$(\psi$ -scan, DIFABS)			
min./	'max. transm	ission	0.629			

III. Structure Solution and Re	finement
Structure Solution	Direct Methods
Refinement Function minimized	Full-matrix least squares Σ w (F ₀ - F _c) ²
Least-squares Weights	$4F_o^2$ / $\sigma^2(F_o^2)$
Anomalous Dispersion No. of Observations (I > 3.00σ (I))	All non-hydrogen atoms 830
No. of Variables	73
Residuals : R; R _w	0.038; 0.043
Goodness of Fit Indicator	1.32
Max Shift / Error in Final Cycle	0.00
Maximum Peak in Final Diff. Map	1.77 e ⁻ / Å ³
Minimum Peak in Final Diff. Map	-1.13 e ⁻ / Å ³

Details for $KPdPS_4$.
KPdPS4
304.5
orange-red, rod
$0.23 \times 0.13 \times 0.11$

Crystal System	Tetragonal
Lattice Parameters	a = 8.5337(2) Å
	b = 8.5337(2) Å
	c = 10.5595(5) Å
	$V = 769.0(1) Å^3$
Space Group	P4 ₂ /mmm (#136)
Z value	4
D _{calc}	2.631 g/cm ³
μ(Μοκα)	21.4 cm^{-1}

II. Intensity	Measurements		
Diffractometer		Siemens P4	
Radiation		AgK-L _{2,3} (λ = 0.56086 Å)	
Temperature		23°C	
Scan Type		ω	
$2\theta_{max}$		55°	
No. of Reflection	ns measured	Total : 3366	
		Unique : 1252 (R _{int} = 0.02	24)
Corrections		Lorentz-polarization	

III. Structure Solution and Refinement Structure Solution Direct Methods Refinement Full-matrix least squares Function minimized Σ w (|F₀| - |F_c|)² Least-squares Weights $4F_0^2 / \sigma^2 (F_0^2)$ Anomalous Dispersion All non-hydrogen atoms No. of Observations (I > 3.00σ (I)) 430 No. of Variables 26 Residuals : R; R_w 0.025; 0.030 Goodness of Fit Indicator 0.82 Max Shift / Error in Final Cycle 0.00 Maximum Peak in Final Diff. Map $0.68 e^{-} / Å^{3}$ -0.48 e⁻ / Å³ Minimum Peak in Final Diff. Map

Table S5. Crystallographic Details for K2PdP2S6. I. Crystal Data Empirical Formula K₂PdP₂S₆ 438.9 Formula Weight Crystal Color, Habit red, rod Crystal Dimensions (mm) $0.13 \times 0.04 \times 0.03$ Crystal System Orthorhombic Lattice Parameters a = 15.612(2) Å b = 7.0724(7) Å c = 10.080(1) Å $V = 1113.0(2) Å^3$

 Space Group
 Pnma (#62)

 Z value
 4

 D_{calc}
 2.619 g/cm³

 μ(MoKα)
 30.7 cm⁻¹

II. Intensity Measurements Diffractometer Enraf-Nonius CAD4-F MOK α (λ = 0.71069 Å) Radiation 23°C Temperature Scan Type $\omega - 2\theta$ 350 $2\theta_{max}$ No. of Reflections measured Total : 7674 Unique : 2594 (R_{int} = 0.058) Corrections Lorentz-polarization

III. Structure Solution and Refinement

Structure Solution Direct Methods Refinement Full-matrix least squares Function minimized $\Sigma w (|F_0| - |F_c|)^2$ Least-squares Weights $4F_0^2 / \sigma^2 (F_0^2)$ Anomalous Dispersion All non-hydrogen atoms No. of Observations $(I > 3.00\sigma (I))$ 741 No. of Variables 61 Residuals : R; R_w 0.048; 0.054 Goodness of Fit Indicator 1.29

Max Shift / Error in Final Cycle 0.00 Maximum Peak in Final Diff. Map $1.85 e^{-} / Å^{3}$ Minimum Peak in Final Diff. Map $-1.88 e^{-}$ / Å³

Table S6. Crystallographic Details for Cs2PdP2Se6. I. Crystal Data Empirical Formula Cs₂PdP₂S₆ Formula Weight 907.92 Crystal Color, Habit black, plate Crystal Dimensions (mm) 0.50 x 0.21 x 0.08 Crystal System Monoclinic a = 12.9750 (4) Å Lattice Parameters b = 8.3282 (2) Å c = 13.0568 (1) Å $\beta = 102.940(2)^{\circ}$ V = 1375.07 (5) Å³ C2/c (#15) Space Group Z value 4 4.385 g/cm^{3} Dcalc 226.37 cm^{-1} μ (MOK α)

II. Intensity Measurements

Diffractometer Siemens SMART Platform CCD Radiation Mok α (λ = 0.71073 Å) -141°C Temperature 47° $2\theta_{max}$ No. of Reflections measured Total : 3029 Corrections min./max. transmission 0.125

III. Structure Solution and Refinement Structure Solution Refinement

Unique : 1072 (R_{int} = 0.097) Empirical Absorption SADABS

Direct Methods Full-matrix least squares

 Σ w (|F₀| - |F_c|)² Function minimized $4F_{o}^{2} / \sigma^{2}(F_{o}^{2})$ Least-squares Weights No. of Observations (I > 3.00σ (I)) 650 No. of Variables 80 Residuals : R; R_w 0.067; 0.075 Goodness of Fit Indicator 1.67 Max Shift / Error in Final Cycle 0.00 $1.62 e^{-} / Å^{3}$ 1.62 e / -1.83 e⁻ / Å³ Maximum Peak in Final Diff. Map Minimum Peak in Final Diff. Map

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 Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Pd	0.0199(3)	0.0163(3)	0.0183(3)	-0.0041(2)	-0.0018(2)	0.0039(2)
S (1)	0.0337(8)	0.0216(7)	0.0316(8)	-0.0087(6)	-0.0098(6)	0.0025(6)
S (2)	0.0209(7)	0.0232(6)	0.0284(8)	0.0015(5)	-0.0018(6)	0.0074(5)
S (3)	0.0197(6)	0.0261(7)	0.0224(7)	-0.0053(5)	-0.0037(5)	0.0067(5)
S (4)	0.0294(8)	0.0425(9)	0.0182(7)	-0.0056(6)	0.0002(6)	0.0030(6)
Р	0.01929(7)	0.0201(6)	0.0170(7)	-0.0044(5)	-0.0031(5)	0.0035(5)
K (1)	0.0374(8)	0.0351(7)	0.0299(7)	0.0018(6)	-0.0089(6)	-0.0011(6)
K (2)	0.0348(8)	0.0441(8)	0.0388(8)	-0.0115(6)	-0.0148(6)	0.0114(6)

Table S7. Table of Anisotropic Thermal Parameters for $K_4Pd(PS_4)_2$

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_	Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
_	Cs(1)	0.0159(4)	0.0149(4)	0.0155(4)	-0.0038(3)	-0.0016(3)	0.0010(3)
	Cs(2)	0.0140(4)	0.0145(4)	0.0146(3)	-0.0002(3)	0.0033(3)	-0.0007(3)
	Pd	0.0068(6)	0.0104(6)	0.0081(5)	0.0014(4)	-0.0003(4)	-0.0006(4)
	Se(1)	0.0179(6)	0.0160(6)	0.0085(5)	-0.0011(5)	0.0021(4)	-0.0017(4)
	Se(2)	0.0119(6)	0.0078(5)	0.0124(5)	0.0003(4)	-0.0021(4)	0.0010(4)
	Se(3)	0.0122(6)	0.0115(6)	0.0147(5)	-0.0039(4)	-0.0029(4)	0.0004(4)
	Se(4)	0.0097(6)	0.0165(6)	0.0142(5)	-0.0037(5)	0.0033(4)	0.0014(4)
	Р	0.008(1)	0.006(1)	0.008(1)	0.001(1)	0.001(1)	-0.001(1)

Table S8. Table of Anisotropic Thermal Parameters for $Cs_4Pd(PSe_4)_2$

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Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cs(1)	0.0222(8)	0.031(1)	0.053(2)	0	0	-0.013(4)
Cs(2)	0.064(1)	0.044(1)	0.020(1)	0.005(6)	0	0
Cs(3)	0.041(2)	0.023(2)	0.0261(7)	-0.0003(5)	0.002(2)	0.005(2)
Cs(4)	0.0264(9)	0.0267(9)	0.053(1)	0	0	0.006(4)
Pd(1)	0.0186(8)	0.0186	0.016(1)	0	0	0
Se(1)	0.0186(8)	0.0210(9)	0.036(2)	-0.0015(7)	0.004(3)	0.004(3)
Se(2)	0.036(1)	0.032(1)	0.026(1)	0.014(3)	-0.005(4)	-0.007(1)
Se(3)	0.025(1)	0.031(1)	0.029(1)	-0.0094(8)	0.009(3)	-0.008(3)
Se(4)	0.030(1)	0.028(1)	0.021(1)	-0.001(4)	-0.002(4)	0.005(1)
P(1)	0.019(3)	0.016(3)	0.020(4)	0	0.00(1)	0
P(2)	0.019(3)	0.021(3)	0.015(4)	0	-0.00(1)	0

Table S9. Table of Anisotropic Thermal Parameters for $Cs_{10}Pd(PSe_4)_4$

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	Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
	Pd (1)	0.0246(2)	0.0246(2)	0.0289(3)	-0.0093(2)	0	0
	Pd (2)	0.0279(2)	0.0279(2)	0.0296(3)	0.0127(2)	0	0
	S (1)	0.0423(4)	0.0423(4)	0.0295(5)	0.0204(5)	-0.0005(3)	0.0005(3)
	S (2)	0.0270(5)	0.0324(5)	0.0428(6)	-0.0079(4)	0	0
	Р	0.0309(4)	0.0309(4)	0.0283(7)	0.0128(6)	0	0
	К	0.0533(6)	0.0533(6)	0.0357(7)	0	0	0

Table S10. Table of Anisotropic Thermal Parameters for $RPdPS_4$

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Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Pd	0.0175(6)	0.0171(5)	0.0145(6)	-0.0001(9)	-0.0015(9)	-0.000(1)
S (1)	0.030(2)	0.024(2)	0.015(1)	-0.013(2)	0.003(2)	-0.001(2)
S (2)	0.031(2)	0.025(2)	0.038(2)	0.012(2)	-0.008(2)	-0.006(3)
S (3)	0.016(2)	0.021(2)	0.014(3)	0	-0.002(2)	0
P (4)	0.019(3)	0.015(2)	0.014(3)	0	-0.005(3)	0
P (1)	0.012(3)	0.016(2)	0.016(3)	0	-0.002(2)	0
S (2)	0.033(3)	0.039(3)	0.010(3)	0	-0.007(3)	0
K (1)	0.020(3)	0.040(3)	0.027(3)	0	0.006(2)	0
K (2)	0.038(3)	0.040(3)	0.060(4)	0	-0.010(3)	0

Table S11. Table of Anisotropic Thermal Parameters for K2PdP2S6

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_	Atom	U(1,1)	U(2,2)	U(3,3)	U(1 ,2)	U(1,3)	U(2,3)
	Cs	0.058(1)	0.061(1)	0.045(1)	-0.0165(9)	0.0129(9)	-0.0102(8)
	Pd	0.018(2)	0.054(2)	0.112(3)	0.003(1)	0.001(2)	-0.043(2)
	Se(1)	0.033(2)	0.050(2)	0.073(2)	0.013(1)	-0.007(1)	0.004(1)
	Se(2)	0.058(2)	0.048(2)	0.038(2)	-0.019(1)	-0.001(1)	-0.008(1)
	Se(3)	0.039(2)	0.075(2)	0.065(2)	0.008(2)	0.022(1)	-0.013(1)
	P(1)	0.02(2)	0.06(2)	0.06(2)	0.01(1)	0.00(1)	-0.01(2)
	P(2)	0.04(2)	0.05(2)	0.05(2)	-0.02(2)	0.02(2)	-0.01(2)
	P(3)	0.03(1)	0.04(1)	0.03(1)	0.01(1)	0.01(1)	0.02(1)
	P(4)	0.01(2)	0.04(1)	0.05(2)	0.00(1)	0.00(1)	-0.02(1)

Table S12. Table of Anisotropic Thermal Parameters for Cs2PdP2Se6

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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	<u> </u>	d , $(\dot{\Lambda})$	d . (Å)	I_{1} (\mathcal{O}_{2})
001 $a.8.892$ $a.8.902$ 3002 010 6.8531 6.8624 19100 6.2767 6.2849 44101 5.5158 5.5200 100111 4.4387 4.4351 23-111 3.8414 3.8419 36 012 3.7778 3.7771 100-12 3.6931 3.6919 19112 3.5150 3.5163 20-102 3.4085 3.4088 2021 3.2289 3.2287 710-21 3.1065 3.1062 10-11 2.30900 3.0914 4121 3.0501 3.0493 9-11 2.30900 3.0159 300 3 2.9654 2.9667 4021 2.9424 2.9426 4-20 2.8396 2.8383 81-2 2.6967 2.6987 44-21 2.6967 2.6987 44-21 2.26860 2.6855 320-2 2.3301 2.3303 220 2.4314 2.4321 1620 2.3301 2.3303 220 2.4314 2.4321 1620 2.2334 $2.$	$\frac{11 \text{ K I}}{0 0 1}$	$u_{obs}(A)$	$\frac{u_{calc}(A)}{2}$	$\frac{1_{0bs}(70)}{26}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0.0092	8.9002	30 10
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0.8531	0.8024	19
1015.51585.5200100111 4.5218 4.5200 19110 4.4387 4.4351 23-1113.84143.8419360123.77783.7771100-123.69313.6919191123.51503.516320-1023.40853.408820213.22893.2287710-213.17653.175072003.14193.1425382013.10653.106210-1-123.09003.091441213.05013.04939-1123.01903.015930032.96542.9667402122.7954100222.75002.750790-132.69672.698744-2-112.69672.698744-2-112.69672.698744-2-112.55557-1032.54582.545831-222.68602.6855320-222.68602.6855320-232.3301 <td>1 0 0</td> <td>6.2/6/</td> <td>6.2849</td> <td>44</td>	1 0 0	6.2/6/	6.2849	44
1114.52184.5200191104.43874.435123-1113.84143.8419360123.7778 3.7771 100-123.6931 3.6919 19112 3.5150 3.5163 20-102 3.2289 3.2287 710-21 3.1765 3.1750 7200 3.1419 3.1425 38201 3.1065 3.1062 10-1-12 3.0900 3.0914 4121 3.0501 3.0493 9-112 3.0190 3.0159 3003 2.9654 2.9667 40211 2.9424 2.9426 4-201 2.8396 2.8383 81-21 2.6967 2.6987 44-2-11 2.6967 2.6987 44-2-11 2.5555 7-103 2.5458 2.5458 31-22 2.4816 2.4818 23 -21 2.25555 7-1-13 2.5696 2.5688 13-22 2.3301 2.3303 22 03 2.22725 7-2	1 0 1	5.5158	5.5200	100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 1 1	4.5218	4.5200	19
-1113.84143.8419360123.77783.7771100-123.69313.6919191123.51503.516320-1023.40853.408820213.22893.2287710-213.17653.175072003.14193.1425382013.10653.106210-1123.09003.091441213.05013.04939-1123.01903.015930032.96542.9667402112.94242.94264-2012.83962.838381-212.69672.698744-2-112.69672.698744-2-112.69672.698744-2-112.55512.55557-1032.54582.545831-222.68602.6855320-222.75502.55557-1032.54582.545831-222.48162.481823202.32.27252.77257-21 <td< td=""><td>1 -1 0</td><td>4.4387</td><td>4.4351</td><td>23</td></td<>	1 -1 0	4.4387	4.4351	23
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	-1 1 1	3.8414	3.8419	36
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 1 2	3.7778	3.7771	10
112 3.5150 3.5163 20-102 3.4085 3.4088 2021 3.2289 3.2287 710-21 3.1765 3.1750 7200 3.1419 3.1425 38201 3.1065 3.1062 10-1-12 3.0900 3.0914 4121 3.0501 3.0493 9-112 3.0190 3.0159 3003 2.9654 2.9667 40211 2.9424 2.9426 4-201 2.8396 2.8383 81-21 2.9424 2.9426 4-201 2.8396 2.8383 81-21 2.7948 2.7954 10022 2.7500 2.7507 90-13 2.6967 2.6987 44-2-11 2.5696 2.5688 13-22 2.6860 2.6855 320-22 2.4816 2.4818 2320 2.4314 2.4321 16203 2.2725 2.7725 7-10 2.2234 2.2337 400 4 2.2254 2.2250 62-20 2.2171	0 -1 2	3.6931	3.6919	19
-1023.40853.408820213.22893.2287710 -2 13.17653.175072003.14193.1425382013.10653.106210 -1 123.09003.091441213.05013.04939 -1 123.01903.015930032.96542.9667402112.94242.94264 -2 012.83962.838381 -2 12.79482.7954100222.75002.750790 -1 32.69672.698744 -2 -1 2.69672.698744 -2 -1 2.69672.698744 -2 -1 2.69672.698744 -2 -1 2.69672.698744 -2 -1 2.268602.685532 0 -2 22.68602.685532 0 -2 22.68602.685532 0 -2 22.48162.481823 2 0 232.33012.330322 0 302.28882.28742 0 232.21712.21699 0 <	1 1 2	3.5150	3.5163	20
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-1 0 2	3.4085	3.4088	2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 2 1	3.2289	3.2287	71
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 -2 1	3.1765	3.1750	7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 0	3.1419	3.1425	38
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 1	3.1065	3.1062	10
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-1 -1 2	3.0900	3.0914	4
-1 1 2 3.0190 3.0159 3 0 0 3 2.9654 2.9667 40 2 1 0 2.9654 2.9624 40 2 1 1 2.9424 2.9426 4 -2 0 1 2.8396 2.8383 8 1 -2 1 2.7948 2.7954 10 0 2 2 2.7500 2.7507 9 0 -1 3 2.6967 2.6987 44 -2 -1 1 2.6967 2.6957 44 1 2 2 2.6860 2.6850 32 0 -2 2 2.6860 2.6850 32 1 -1 3 2.5696 2.5688 13 -2 1 1 2.5551 2.5555 7 -1 0 3 2.5458 2.5458 3 1 -2 2.4816 2.4818 23 2 0 2.4314 2.4321 16 2 0 3 2.23301 2.3303 22 0 3 0 2.2888 2.2874 2 0 2 3 2.2725 2.725 7 -2 1 2.2017 2.2022 8 1 1 4 2.1292 2.1296 3 1 -2 3 2.1202 2.1224 6 -1 -3 1	1 2 1	3.0501	3.0493	9
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	-1 1 2	3.0190	3.0159	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\hat{0}$ $\hat{0}$ $\hat{3}$	2 9654	2,9667	40
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 1 0	2 9654	2 9624	40
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 1 0 2 1 1	2.2034	2.9024	40
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-2 0 1	2.2424	2.2420	8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 _2 1	2.0370	2.0505	10
0 -1 3 2.6967 2.6987 44 -2 -1 1 2.6967 2.6957 44 1 2 2 2.6860 2.6855 32 0 -2 2 2.6860 2.6850 32 1 -1 3 2.5696 2.5688 13 -2 1 1 2.5551 2.5555 7 -1 0 3 2.5458 2.5458 3 1 -2 2.4816 2.4818 23 2 2 0 2.4314 2.4321 16 2 0 3 2.3301 2.3303 22 0 3 0 2.2888 2.2874 2 0 2 3 2.2725 2.2725 7 -2 1 2 2.2334 2.2337 4 0 0 4 2.2254 2.2250 6 2 -2 0 2.2171 2.2175 9 0 -3 1 2.2017 2.2022 8 1 1 4 2.1292 2.1296 3 1 -2 3 2.1220 2.1224 6 -1 -3 1 2.1133 2.1140 3 2 -2 2 2.0559 2.0557 24 -2 2 2.0274 2.0273 12 -2 0 3 2.0166 2.0178 13 -1 0 <t< td=""><td>1 - 2 - 1</td><td>2.7500</td><td>2.7507</td><td>0</td></t<>	1 - 2 - 1	2.7500	2.7507	0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 2 2 0 1 3	2.7500	2.7507	4.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 - 1 - 3 2 - 1 - 1	2.0907	2.0907	44
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-2 -1 1 1 2 2	2.0907	2.0957	22
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 2 2	2.0000	2.0033	32
1 -1 3 2.3090 2.3088 13 $-2 1 1$ 2.5551 2.5555 7 $-1 0 3$ 2.5458 2.5458 3 $1 -2 2$ 2.4816 2.4818 23 $2 2 0$ 2.4314 2.4321 16 $2 0 3$ 2.3301 2.3303 22 $0 3 0$ 2.2888 2.2874 2 $0 2 3$ 2.2725 2.725 7 $-2 1 2$ 2.2334 2.2337 4 $0 0 4$ 2.2254 2.2250 6 $2 -2 0$ 2.2171 2.2175 9 $0 -2 3$ 2.2171 2.2169 9 $0 -3 1$ 2.2017 2.2022 8 $1 1 4$ 2.1292 2.1296 3 $1 -2 3$ 2.1220 2.1224 6 $-1 -3 1$ 2.1133 2.1140 3 $2 -2 2$ 2.0559 2.0557 24 $-2 -2 2$ 2.0274 2.0273 12 $-2 0 3$ 2.0166 2.0178 13 $-1 0 4$ 2.0088 2.0089 12	0 - 2 2	2.0600	2.0650	52
-2112.55512.55557 -1 032.54582.54583 1 -2 22.48162.481823 2 202.43142.432116 2 032.33012.330322 0 302.28882.28742 0 232.27252.27257 -2 122.23342.23374 0 042.22542.22506 2 -2 02.21712.21759 0 -2 32.21712.21699 0 -3 12.20172.20228 1 1 4 2.12922.12963 1 -2 32.12202.12246 -1 -3 12.11332.11403 2 -2 22.05592.055724 -2 -2 22.02742.027312 -2 0 3 2.01662.017813 -1 0 4 2.00882.008912		2.3090	2.3088	13
-1 0 3 2.5458 2.5458 3 1 -2 2 2.4816 2.4818 23 2 2 0 2.4314 2.4321 16 2 0 3 2.3301 2.3303 22 0 3 0 2.2888 2.2874 2 0 2 3 2.2725 2.2725 7 -2 1 2 2.2334 2.2337 4 0 0 4 2.2254 2.2250 6 2 -2 0 2.2171 2.2175 9 0 -2 3 2.2171 2.2169 9 0 -3 1 2.2017 2.2022 8 1 1 4 2.1292 2.1296 3 1 -2 3 2.1133 2.1140 3 2 -2 2.0559 2.0557 24 -2 -2 2.0274 2.0273 12 -2 0 3 2.0166 2.0178 13 -1 0 4 2.0088 2.0089 12	-2 1 1	2.5551	2.5555	1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-1 0 3	2.5458	2.5458	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 -2 2	2.4816	2.4818	23
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 2 0	2.4314	2.4321	16
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2 0 3	2.3301	2.3303	22
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 3 0	2.2888	2.2874	2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 2 3	2.2725	2.2725	7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-2 1 2	2.2334	2.2337	4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 0 4	2.2254	2.2250	6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 -2 0	2.2171	2.2175	9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 -2 3	2.2171	2.2169	9
1 1 4 2.1292 2.1296 3 1 -2 3 2.1220 2.1224 6 -1 -3 1 2.1133 2.1140 3 2 -2 2 2.0559 2.0557 24 -2 -2 2 2.0274 2.0273 12 -2 0 3 2.0166 2.0178 13 -1 0 4 2.0088 2.0089 12	0 -3 1	2.2017	2.2022	8
1 -2 3 2.1220 2.1224 6 -1 -3 1 2.1133 2.1140 3 2 -2 2 2.0559 2.0557 24 -2 -2 2 2.0274 2.0273 12 -2 0 3 2.0166 2.0178 13 -1 0 4 2.0088 2.0089 12	1 1 4	2.1292	2.1296	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 -2 3	2.1220	2,1224	6
2 -2 2 2.0559 2.0557 24 -2 -2 2 2.0274 2.0273 12 -2 0 3 2.0166 2.0178 13 -1 0 4 2.0088 2.0089 12	-1 -3 1	2.1133	2,1140	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$	2.0559	2.0557	24
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-2 -2 2	2.0274	2.0273	12
-1 0 4 2.0088 2.0089 12	-2 0 3	2.0274	2 0178	13
	-1 0 4	2 0088	2 0089	12
-3 0 1 19771 19770 4	-3 0 1	1 9771	1 9770	4

Table S13. Calculated and Observed X-ray Powder Pattern of K₄Pd(PS₄)₂.

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-3 -1 1	1.9413	1.9424	7
3 -1 2	1.8792	1.8786	4
2 -1 4	1.8402	1.8400	11
0 3 3	1.8329	1.8338	4
1 0 5	1.7804	1.7809	7
224	1.7576	1.7581	6
040	1.7151	1.7156	13
-1 -3 3	1.7151	1.7152	13
2 0 5	1.6544	1.6537	3
134	1.6326	1.6325	12
3 3 1	1.6326	1.6326	12
1 -4 0	1.6173	1.6175	8
1 -4 1	1.5946	1.5952	6
2 4 1	1.5702	1.5698	3
0 -2 5	1.5638	1.5642	8

Table S14. Calculated and Observed X-ray Powder Pattern of

h k l	d _{obs} (A)	d _{calc} (A)	I_{obs} (%)
0 1 1	8.014	8.035	23
1 1 -1	5.556	5.566	16
1 2 1	4.415	4.417	· 2
1 0 2		4.092	
0 3 1	4.085	4.065	14
1 1 -2		4.042	
200	3.743	3.744	13
1 3 -1	3.595	3.594	36
2 1 -1	3.432	3.435	27
040	3.335	3.332	100
0 1 3	3.241	3.245	24
2 2 -1	3.135	3.136	7
2 2 1	3.073	3.073	4
0 2 3	2.987	2.985	37
202	2.945	2.945	10
1 4 1	2.902	2.909	16
2 1 2	2.876	2.876	13
22-2	2.778	2.776	14
23-1	2.775	2.774	32
2 3 1	2.732	2.735	5
0 3 3	2.671	2.675	40
2 3 2	2.455	2.454	16
2 2 -3	2.375	2.375	20
1 5 -2	2.258	2.257	16
2 4 2	2.207	2.207	30
2 0 -4	2.120	2.119	12
0 5 3	2.085	2.084	16
2 5 -2	2.009	2.009	12
4 0 0	1.871	1.871	10
4 1 0	1.853	1.853	11

Cs₄Pd(PSe₄)₂.

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hkl	d _{obs} (A)	d _{calc} (A)	$I_{obs}(\%)$
1 1 0	6.0226	6.0355	80
0 0 2	5.2764	5.2806	76
$1 \ 1 \ 1$	5.2450	5.2402	68
200	4.2699	4.2677	53
1 1 2	3.9751	3.9742	83
2 1 0	3.8206	3.8172	19
2 1 1	3.5903	3.5899	12
202	3.3200	3.3192	7
103	3.2557	3.2545	15
220	3.0175	3.0177	30
221	2.9013	2.9016	4
3 0 1	2.7471	2.7472	18
3 1 0	2.6986	2.6991	6
0 0 4	2.6411	2.6403	23
222	2.6192	2.6201	3
2 1 3	2.5893	2.5879	7
3 1 2	2.4035	2.4034	100
223	2.2905	2.2912	3
2 0 4	2.2446	2.2453	16
2 1 4	2.1720	2.1715	5
4 0 0	2.1352	2.1339	28
4 1 1	2.0309	2.0315	4
3 3 0	2.0113	2.0118	16
224	1.9869	1.9871	10
4 0 2	1.9780	1.9784	24
4 2 0	1.9084	1.9086	15
3 1 4	1.8872	1.8874	16
3 3 2	1.8797	1.8800	20
422	1.7946	1.7949	2
006	1.7602	1.7602	10
1 1 6	1.6895	1.6898	10
4 0 4	1.6596	1.6596	29
5 1 2	1.5958	1.5957	15
521	1.5677	1.5674	2
424	1.5468	1.5468	7
4 3 3	1.5360	1.5360	6
4 4 0	1.5088	1.5089	22

Table S15. Calculated and Observed X-ray Powder Pattern of KPdPS₄.