

ELECTRONIC SUPPORTING INFORMATION

Unprecedented Layered Coordination Polymers of Dithiolene Group 10 Metals. Magnetic and Electrical Properties

Esther Delgado,^{,a} Carlos J. Gómez-García,^b Diego Hernández,^a Elisa Hernández,^a
Avelino Martín,^c and Félix Zamora^{a,d}*

a) Departamento de Química Inorgánica, Universidad Autónoma de Madrid, 28049 Madrid, Spain. Tel: 34 91 4975268; E-mail: esther.delgado@uam.es.

b) Instituto de Ciencia Molecular. Universidad de Valencia. C/ Catedrático José Beltrán, 2. 46980 Paterna, Valencia, Spain.

c) Departamento de Química Inorgánica, Universidad de Alcalá. Campus Universitario, E-28871, Alcalá de Henares, Spain.

d) Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanociencia), Cantoblanco, 28049 Madrid, Spain.

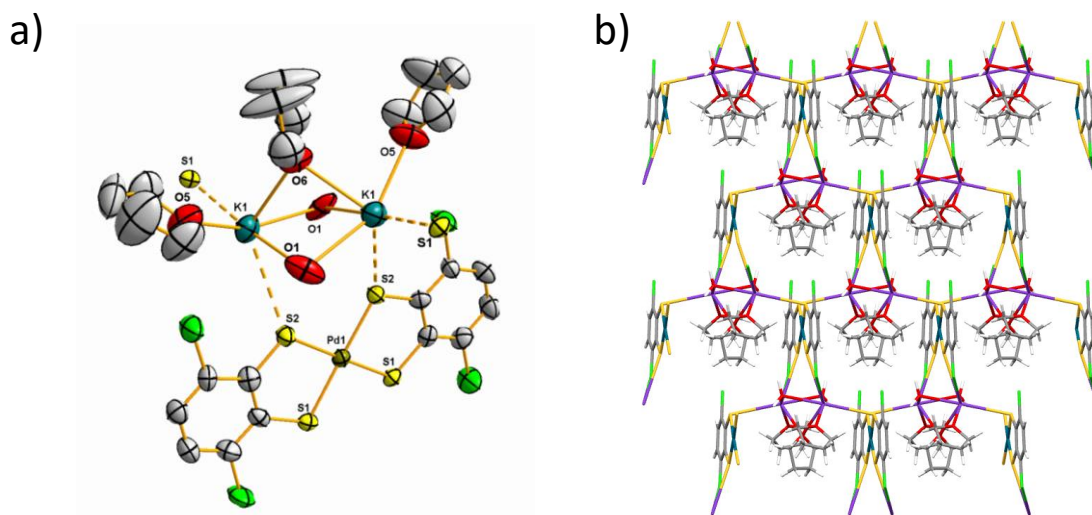


Figure S1. (a) ORTEP of $\{[K_2(\mu-H_2O)_2(\mu-thf)(thf)_2][Pd(SC_6H_2Cl_2S)_2]\}_n$ (**2**). (b) Representation of the bidimensional network of $\{[K_2(\mu-H_2O)_2(\mu-thf)(thf)_2][Pd(SC_6H_2Cl_2S)_2]\}_n$ (**2**).

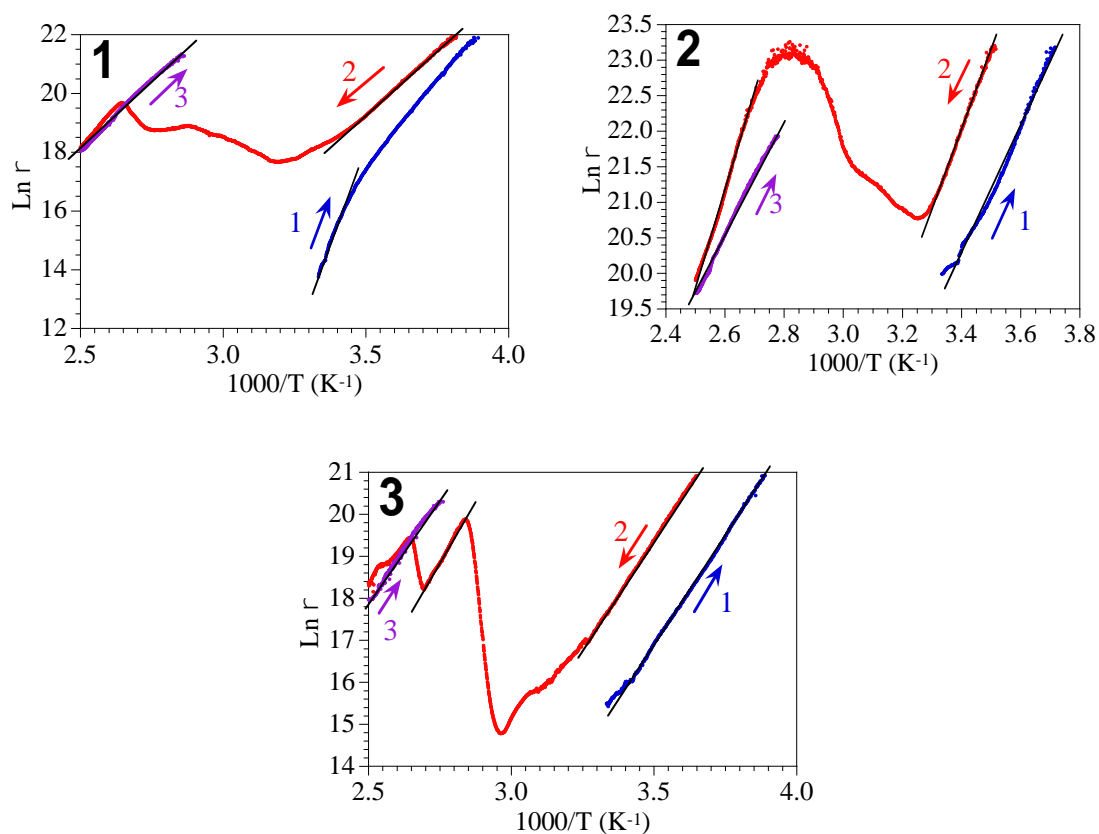


Figure S2. Arrhenius plots of compounds 1-3 showing the semiconducting regimes in the different cooling and heating scans.

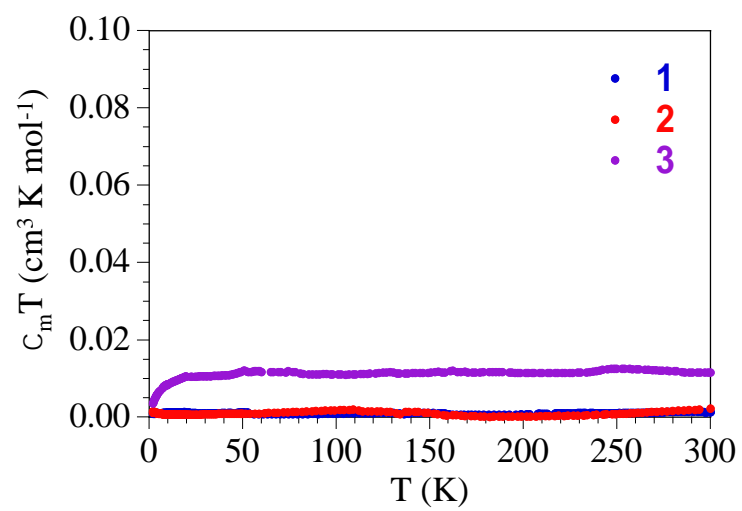


Figure S3. Thermal variation of the $\chi_m T$ product of compounds **1-3**.

Table S1. Crystal data and structure refinement for compounds **1-4**.

Compound	1	2	3	4
<i>moiety formula</i>	C ₂₄ H ₂₈ Cl ₄ K ₂ NiO ₅ S ₄	C ₂₄ H ₃₂ Cl ₄ K ₂ O ₅ PdS ₄	C ₃₆ H ₅₆ Cl ₄ K ₂ O ₈ PtS ₄	C ₂₀ H ₂₂ Cl ₄ K ₂ O ₃ PTs ₄
<i>formula weight</i>	807.44	855.13	1160.13	853.7
<i>temperature [K]</i>	200	200	200	200
<i>wavelength (MoKα) [\AA]</i>	0.71073	0.71073	0.71073	0.71073
<i>crystal system</i>	monoclinic	monoclinic	monoclinic	triclinic
<i>space group</i>	C2/c	C2/c	P2 ₁ /c	P-1
<i>a [\AA]; α($^\circ$)</i>	9.064(3)	9.064(3)	13.933(5)	8.2056(7); 82.782(5)
<i>b [\AA]; β($^\circ$)</i>	14.446(5); 97.27(1)	14.446(5); 97.27(1)	9.234(3); 99.24(2)	12.704(1); 74.848(5)
<i>c [\AA]; γ($^\circ$)</i>	26.473(4)	26.473(4)	18.4983(7)	14.4749(8); 76.633(7)
μ (mm ⁻¹)	1.393	1.365	3.614	5.954
<i>Z ; F(000)</i>	4; 1656	4; 1728	2; 1168	2; 828
<i>crystal size [mm³]</i>	0.26 x 0.24 x 0.14	0.10 x 0.10 x 0.10	0.36 x 0.30 x 0.29	0.38 x 0.26 x 0.13
<i>θ range</i>	3.10 to 27.55 $^\circ$	3.10 to 27.74 $^\circ$	3.14 to 27.62 $^\circ$	3.26 to 27.5 $^\circ$
<i>index ranges</i>	-11 to 11, -18 to 18, -34 to 34	-11 to 11, -18 to 18, -12 to 34	-18 to 17, -11 to 11, 0 to 24	-10 to 10, -16 to 16, -18 to 17
<i>collected reflections</i>	26810	35756	44170	30685
<i>independent reflections</i>	3952 [R _{int} = 0.061]	3939 [R _{int} = 0.144]	5405 [R _{int} = 0.089]	6479 [R _{int} = 0.094]
<i>goodness-of-fit on F²</i>	1.081	1.045	0.948	1.228
<i>final R indices [F > 4σ(F)]</i>	R1=0.081,wR2=0.212	R1=0.095,wR2=0.241	R1=0.042,wR2=0.085	R1=0.064,wR2=0.144
<i>R indices (all data)</i>	R1=0.124,wR2=0.228	R1=0.173,wR2=0.269	R1=0.082,wR2=0.097	R1=0.099,wR2=0.158
<i>largest diff. peak/hole [e\AA⁻³]</i>	1.331 / -1.000	1.693 / -0.995	1.393/-2.331	2.900 / -1.894