Supporting information

Conductive zigzag Pd(III)–Br chain complex realized by multiple-hydrogen-bond approach

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Table S1. Crystallographic data for **2** at 93, 150, 200, 250 and 300 K.

	2				
Radiation type, wave length /Å			MoKα, 0.7107		
Empirical formula			$C_8H_{30}BrN_4O_{11}PdS$		
Formula weight			576.73		
Crystal system			orthorhombic		
Space group			$P2_12_12_1$		
Crystal size /mm^3			0.15 × 0.03 × 0.02		
a/Å	8.4228(3)	8.4341(2)	8.4382(2)	8.4438(3)	8.4409(3)
b/Å	10.2975(3)	10.3131(3)	10.3226(3)	10.3354(3)	10.3431(3)
c/Å	21.9679(6)	21.9665(6)	21.9814(6)	22.0144(6)	22.0437(6)
V/Å^3	1905.36(10)	1910.68(9)	1914.67(9)	1921.20(10)	1924.53(11)
Temperature / K	93	150	200	250	300
Z			4		
Density(calculated) / gcm^{-1}	2.010	2.005	2.001	1.994	1.990
Absorption coefficient /mm^{-1}	3.241	3.232	3.225	3.214	3.209
*R*1, *wR*2 [$I > 2\sigma(I)$]	0.0255, 0.0508	0.0276, 0.0547	0.0269, 0.0536	0.0262, 0.0534	0.0292, 0.0559
*R*1, *wR*2 [all data]	0.0299, 0.0519	0.0321, 0.0558	0.0321, 0.0548	0.0314, 0.0547	0.0374, 0.0578
F(000)			1164		
Goodness of fit on F^2	1.039	1.042	1.062	1.046	1.057
Flack parameter	0.008(5)	0.008(5)	0.015(6)	0.018(6)	0.006(7)

Table S2. Selected interatomic distances, bond lengths and angles of **2** at various temperature.

T/K	*d*(Pd···Pd)/Å	d(Pd–Br)$_{short}$/Å	d(Pd–Br)$_{long}$/Å	(d(Pd–Br)$_{short}$ + d(Pd–Br)$_{long}$)/Å	∠ (Pd–Br–Pd)/°
93	5.1494(2)	2.5757(5)	2.5872(5)	5.1629(10)	171.74
150	5.1571(2)	2.5790(6)	2.5908(6)	5.1698(12)	171.95
200	5.1618(2)	2.5809(5)	2.5929(5)	5.1738(10)	172.19
250	5.1681(2)	2.5838(5)	2.5954(5)	5.1792(10)	172.48
300	5.1719(2)	2.5846(6)	2.5975(6)	5.1821(12)	172.79

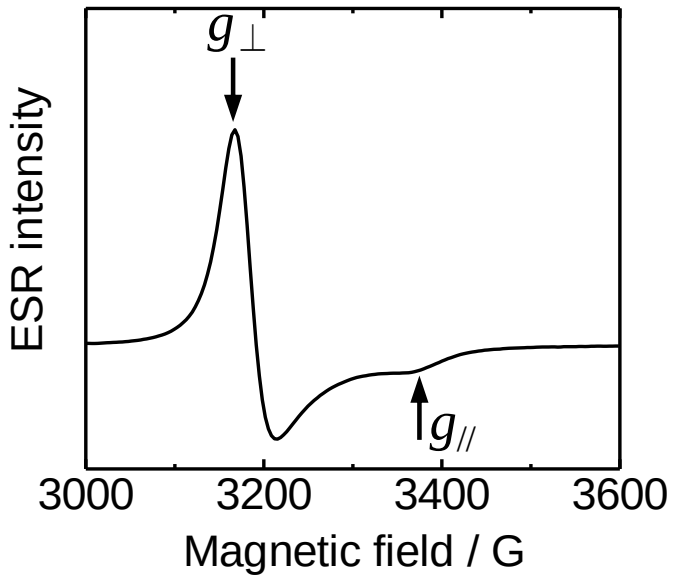

Fig. S1. ESR spectrum of **2** measured at 240 K with the indication of $g_{\perp}$ (= 2.1295) and $g_{||}$ (= 2.0119).