

First platinum(II)–alkaline-earth acetate-bridged complexes $\text{Pt}^{\text{II}}(\mu\text{-OAc})_4\text{M}^{\text{II}}(\text{AcOH})_4$ ($\text{M} = \text{Ca}, \text{Sr}, \text{Ba}$)

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Table S1 Crystal data and structure refinement for **1-6**.

Identification code	1	2	3	4	5	6
Empirical formula	$\text{C}_{16}\text{H}_{28}\text{CaO}_{16}\text{Pt}$	$\text{C}_{16}\text{H}_{28}\text{SrO}_{16}\text{Pt}$	$\text{C}_{16}\text{H}_{28}\text{BaO}_{16}\text{Pt}$	$\text{C}_{16}\text{H}_{28}\text{CaO}_{16}\text{Pd}$	$\text{C}_{16}\text{H}_{28}\text{SrO}_{16}\text{Pd}$	$\text{C}_{16}\text{H}_{28}\text{BaO}_{16}\text{Pd}$
Formula weight	711.54	759.08	808.79	622.86	670.40	720.11
Temperature, K	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Crystal size, mm	$0.10 \times 0.05 \times 0.05$	$0.05 \times 0.05 \times 0.4$	$0.07 \times 0.04 \times 0.03$	$0.15 \times 0.07 \times 0.06$	$0.10 \times 0.05 \times 0.04$	$0.10 \times 0.07 \times 0.04$
Wavelength, Å	0.96990	0.96990	0.96990	0.96990	0.96990	0.96990
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> -1					
<i>a</i> , Å	10.578(2)	10.735(2)	11.427(2)	10.548(2)	10.680(2)	11.341(2)
<i>b</i> , Å	11.655(2)	11.672(2)	11.436(2)	11.622(2)	11.630(2)	11.414(2)
<i>c</i> , Å	11.731(2)	11.823(2)	11.461(2)	11.703(2)	11.780(2)	11.441(2)
α , deg.	88.81(3)	87.33(3)	79.99(3)	88.77(3)	87.45(3)	89.91(3)
β , deg.	69.30(3)	70.81(3)	89.94(3)	69.69(3)	71.22(3)	79.95(3)
γ , deg.	72.72(3)	69.15(3)	61.20(3)	72.56(3)	69.20(3)	61.75(3)
<i>V</i> , Å ³	1286.1(5)	1303.3(6)	1286.5(6)	1278.1(5)	1291.0(5)	1279.0(6)
<i>Z</i>	2	2	2	2	2	2
Density (calc.), Mg/m ³	1.837	1.934	2.088	1.618	1.725	1.870
μ , mm ⁻¹	8.225	8.347	11.160	2.296	2.506	5.250
<i>F</i> (000)	700	736	772	636	672	708

Theta range, deg.	2.509 – 38.435	3.123 – 38.384	2.474 – 38.409	2.518 – 38.498	2.500 – 38.484	3.380 – 38.408
Index ranges	-12 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -14 ≤ <i>l</i> ≤ 14	-13 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -14 ≤ <i>l</i> ≤ 14	-14 ≤ <i>h</i> ≤ 14, -14 ≤ <i>k</i> ≤ 14, -14 ≤ <i>l</i> ≤ 13	-13 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -15 ≤ <i>l</i> ≤ 15	-13 ≤ <i>h</i> ≤ 13, -12 ≤ <i>k</i> ≤ 14, -14 ≤ <i>l</i> ≤ 14	-14 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -13 ≤ <i>l</i> ≤ 13
Reflections collected	31740	21929	27589	19502	16309	21869
Independent reflections	5427 (<i>R</i> _{int} = 0.0865)	5329 (<i>R</i> _{int} = 0.0716)	5158 (<i>R</i> _{int} = 0.0695)	5357 (<i>R</i> _{int} = 0.0823)	5192 (<i>R</i> _{int} = 0.0622)	5078 (<i>R</i> _{int} = 0.0803)
Reflections observed	4744	4439	4641	4164	4432	4416
<i>R</i> ₁ / <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0436 / 0.0976	0.0602 / 0.1333	0.0400 / 0.0942	0.0611 / 0.1349	0.0410 / 0.0949	0.0622 / 0.1485
<i>R</i> ₁ / <i>wR</i> ₂ (all data)	0.0548 / 0.1046	0.0743 / 0.1474	0.0465 / 0.0995	0.0778 / 0.1484	0.0491 / 0.1021	0.0700 / 0.1556
Goodness-of-fit on <i>F</i> ²	1.171	0.983	1.048	0.989	0.860	1.026
Extinction coefficient	0.0030(3)	0.0018(2)	0.0022(2)	0.0056(5)	0.0044(4)	0.0042(4)
<i>T</i> _{min} / <i>T</i> _{max}	0.728 / 0.785	0.660 / 0.700	0.480 / 0.700	0.606 / 0.949	0.730 / 0.900	0.600 / 0.840
Δρ _{max} / Δρ _{min} , e·Å ⁻³	1.530 / -1.857	3.9702 / -3.129	1.690 / -2.057	1.183 / -1.707	0.879 / -1.207	3.707 / -2.018