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Structure and quantum chemical study of crystalline platinum(II) acetate

Alexander A. Markov, Ilya A. Yakushev, Andrey V. Churakov, Victor N. Khrustalev, Natalia V. Cherkashina, Igor P. Stolarov, Alexander E. Gekhman and Michael N. Vargaftik

Table S1 Crystal data and structure refinement for **1** and **2**.

Identification code	**1**	**2**
X-Ray source type	synchrotron	synchrotron
Wavelength, Å	0.78790	0.78700
Empirical formula	$C_{16}H_{24}O_{16}Pt_4$	$C_{158}H_{198}O_{80}Pt_{20}$
Formula weight	1252.71	7278.95
Temperature, K	100(2)	100(2)
Crystal size, mm	0.10 × 0.05 × 0.05	0.15 × 0.12 × 0.08
Color	red	red
Crystal system	Monoclinic	Monoclinic
Space group	$P\ 2_1/c$	$C\ 2/c$
a, Å	11.943(2)	50.081(10)
b, Å	10.607(2)	14.858(3)
c, Å	19.479(4)	29.537(6)
β, deg.	91.92(3)	118.99(3)
V, Å^3	2466.3(9)	19224(8)
Z	4	4
Density (calc.), Mg/mm^3	3.374	2.515
μ, mm^{-1}	29.440	18.847
F(000)	2240	13384
Theta range, deg.	1.891 – 30.767	2.44 – 29.00
Index ranges	$-15 \le h \le 15$, $-13 \le k \le 13$, $-25 \le l \le 25$	$-59 \le h \le 59$, $-17 \le k \le 17$, $-35 \le l \le 35$
Reflections collected	38499	120947
Independent reflections	5633 (R_{int} = 0.0414)	17085 (R_{int} = 0.0687)
Reflections observed	5403	14340
R_1 / wR_2 ($I > 2\sigma(I)$)	0.0303 / 0.0808	0.0299 / 0.0711
R_1 / wR_2 (all data)	0.0315 / 0.0816	0.0398 / 0.0752
Data / restraints / parameters	5633 / 0 / 334	17085 / 43 / 1288

Goodness-of-fit on F^2	1.086	1.074
Extinction coefficient	0.00142(8)	0.0000285(16)
T_{min} / T_{max}	0.157 / 0.321	0.164 / 0.314
$\Delta\rho_{max}$ / $\Delta\rho_{min}$, e·Å^{-3}	1.801 / -2.019	1.509/ -1.838

Table S2 Selected distances (Å) and angles (deg) in **1**.

Selected distances (Å)	
Pt(1)-Pt(2)	2.4970(6)
Pt(1)-Pt(4)	2.4934(5)
Pt(2)-Pt(3)	2.4870(5)
Pt(3)-Pt(4)	2.4915(6)
Pt(1)-O(3)	1.995(5)
Pt(1)-O(16)	2.018(5)
Pt(1)-O(1)	2.184(4)
Pt(1)-O(14)	2.185(5)
Pt(2)-O(4)	2.012(5)
Pt(2)-O(5)	2.014(5)
Pt(2)-O(2)	2.141(4)
Pt(2)-O(7)	2.147(4)
Pt(3)-O(11)	2.006(5)
Pt(3)-O(6)	2.015(5)
Pt(3)-O(9)	2.147(4)
Pt(3)-O(8)	2.164(5)
Pt(4)-O(15)	1.998(4)
Pt(4)-O(12)	2.011(4)
Pt(4)-O(10)	2.154(4)
Pt(4)-O(13)	2.161(4)
Selected angles (deg)	
Pt(4)-Pt(1)-Pt(2)	88.793(18)
Pt(3)-Pt(2)-Pt(1)	89.903(17)
Pt(2)-Pt(3)-Pt(4)	89.059(16)
Pt(3)-Pt(4)-Pt(1)	89.882(18)

Computational levels

NR non-relativistic calculations with all-electron DZP basis for palladium, mDZP basis for platinum, and def2-SVP basis for light atoms

MCP basis IMCP-SR1 with metal core potential and scalar-relativistic corrections

Rel all-electron Sapporo-DKH3-DZP-2012 basis with scalar-relativistic corrections

Rel/sp single point calculations at *Rel* geometry with additional diffuse sp functions

Table S3 Key mean interatomic distances in $Pt_4(\mu\text{-}OOCMe)_8$ **1**: experimental (XRD) and optimised at various computational levels. Standard deviations shown at parenthesis

	XRD	NR	MCP	Rel
<R(Pt-Pt)>, Å	2.492(4)	2.572(3)	2.497(3)	2.505(3)
equatorial <R(Pt-O)>, Å	2.164(14)	2.171(2)	2.171(8)	2.163(1)
axial <R(Pt-O)>, Å	2.009(8)	2.031(7)	2.009(7)	2.009(6)
twisting angle, deg	32.9, 28.9	30.1, 29.1	35.1, 33.6	33.1, 31.6
equatorial <R(C-O)>, Å	1.267(9)	1.262(1)	1.260(1)	1.264(1)
axial <R(C-O)>, Å	1.269(8)	1.262(1)	1.260(1)	1.264(1)
equatorial <R(C-C)>, Å	1.506(11)	1.505	1.503	1.506
axial <R(C-C), Å	1.492(3)	1.495	1.492	1.494

Table S4 Key mean interatomic distances in $Pd_4(\mu\text{-}OOCMe)_8$ **3** optimised at various computational levels. Standard deviations shown at parenthesis

	NR	MCP	Rel
<R(Pd-Pd)>, Å	2.399(4)	2.537(6)	2.484(6)
equatorial $<R_1$(Pd-O)>, Å	2.083(2)	2.019(2)	2.109(4)
equatorial $<R_2$(Pd-O)>, Å	2.091(2)	2.365(4)	2.188(4)
axial <R(Pd-O)>, Å	1.930(8)	1.999(6)	2.001(7)
twisting angle, deg	35.9, 37.2	48.8, 50.3	37.1, 38.5
equatorial $<R_1$(C-O)>, Å	1.263(1)	1.284	1.268(1)
equatorial $<R_2$(C-O)>, Å	1.260	1.223	1.256(1)
axial <R(C-O)>, Å	1.261(1)	1.259	1.262(1)
equatorial <R(C-C)>, Å	1.504	1.506	1.506
axial <R(C-C), Å	1.493	1.493	1.496

Table S5 Key mean interatomic distances (Å) in platinum **1a** and palladium **3a** complexes (with long M-M distances) optimised at various computational levels. Standard deviations shown at parenthesis

	$Pt_4(\mu\text{-}OOCMe)_8$ **1a**			$Pd_4(\mu\text{-}OOCMe)_8$ **3a**		
	NR	MCP	Rel	NR	MCP	Rel
$<R_1(M\text{-}M)>$	3.200	3.328	3.234	3.313	3.210	3.254
$<R_2(M\text{-}M)>$	3.819	3.801	3.727	3.757	3.793	3.766
$<R_3(M\text{-}M)>$	4.785	4.886	4.715	4.863	4.779	4.775
<R(M-O)>	2.043(7)	2.013(5)	2.016(7)	1.930(7)	2.013(6)	2.011(6)
<R(C-O)>	1.258(1)	1.256(1)	1.261(2)	1.258(1)	1.256(1)	1.260(1)
<R(C-C)>	1.501(1)	1.499(1)	1.501(1)	1.502(1)	1.501(1)	1.504

Table S6 Bond critical point data (in atomic units). Standard deviations shown at parenthesis

Complex	ρ_b	$\nabla^2\rho_b$
$Pt_4(\mu\text{-}OOCMe)_8$ **1**		
Pt-Pt	0.098	0.109(1)
equatorial Pt-O	0.081(1)	0.379(3)
axial Pt-O	0.113(2)	0.534(8)
equatorial C-O	0.371(1)	−0.496(16)
axial C-O	0.370(1)	−0.448(10)
equatorial C-C	0.256	−0.569
axial C-C	0.261	−0.591
$Pd_4(\mu\text{-}OOCMe)_8$ **3**		
Pd-Pd	0.077(1)	0.107(2)
equatorial Pd-O	0.076(8)	0.323(3), 0.391(4)
axial Pd-O	0.104(2)	0.524(10)
C-O	0.373(4)	−0.484(31)
equatorial C-C	0.255	−0.567
axial C-C	0.260	−0.587
$Pd_3(\mu\text{-}OOCMe)_6$		
Pd-Pd	0.017(1)	0.039(3)
Pd-O	0.099(2)	0.535(5)
C-O	0.372	−0.427(19)
C-C	0.256	−0.571(1)
$Pt_4(\mu\text{-}OOCMe)_8$ **1a**		
Pt-Pt	0.166(8)	0.034(12)
Pt-O	0.108(2)	0.540(10)
C-O	0.371(1)	−0.427(22)
C-C	0.258	−0.579(2)
$Pd_4(\mu\text{-}OOCMe)_8$ **3a**		
Pd-Pd	0.016	0.037
Pd-O	0.098(2)	0.524(8)
C-O	0.373(1)	−0.454(184)
C-C	0.256	−0.572(2)