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Highly efficient synthesis of mononuclear Pt-based carboxylic complexes *trans*-[$Py_2Pt(OC(O)R)_2$] (R = Me, Bu^t, Ph)

Maria V. Panina, Nadezhda K. Ogarkova, Pavel V. Dorovatovskii, Olesya V. Sulimova, Egor A. Sosunov, Natalia V. Cherkashina, Julia E. Makarevich, Mger A. Navasardyan, Anna S. Popova and Ilya A. Yakushev

IR spectra of the compounds

trans-[$Py_2Pt(OAc)_2$] **2**

IR (ATR, ν/cm^{-1}): 3101 w., 3030 w., 1629 s., 1605 s., 1567 m., 1477 w., 1452 s., 1390 m., 1361 s., 1304 s., 1245 m., 1211 m., 1154 w., 1072 m., 1048 m., 1014 m., 964 w., 929 w., 876 w., 827 w., 764 s., 695 s., 621 m., 533 m., 476 m.

Elemental analysis data:

Found (%): C, 35.79; H, 3.54; N 5.86. Calc. for $C_{14}H_{16}N_2O_4Pt$ (%): C, 35.67; H, 3.42; N, 5.94.

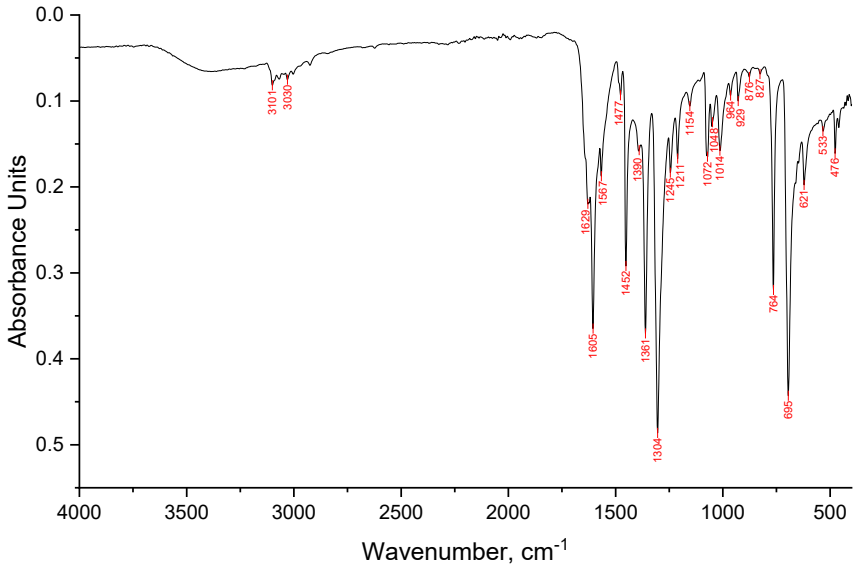

Figure S1. *trans*-[$Py_2Pt(OAc)_2$] **2**

trans-[$Py_2Pt(OC(O)Bu^t)_2$]·2$Bu^tC(O)OH$ **3**

IR (ATR, ν/cm^{-1}): 3390 w., 3111 w., 3081 w., 2955 m., 2926 m., 2901 m., 2867 w., 2823 w., 1702 w., 1630 s., 1605 s., 1558 m., 1476 s., 1452 s., 1391 s., 1361 m., 1346 m., 1306 s., 1244 m., 1199 s., 1149 m., 1114 w., 1073 s., 1031 s., 989 w., 958 m., 936 w., 892 m., 865 w., 805 m., 770 s., 698 s., 659 s., 567 m., 471 m., 445 m.

Elemental analysis data:

Found (%): C, 47.58; H, 6.51; N 3.77. Calc. for $C_{30}H_{48}N_2O_8Pt$ (%): C, 47.42; H, 6.37; N, 3.69.

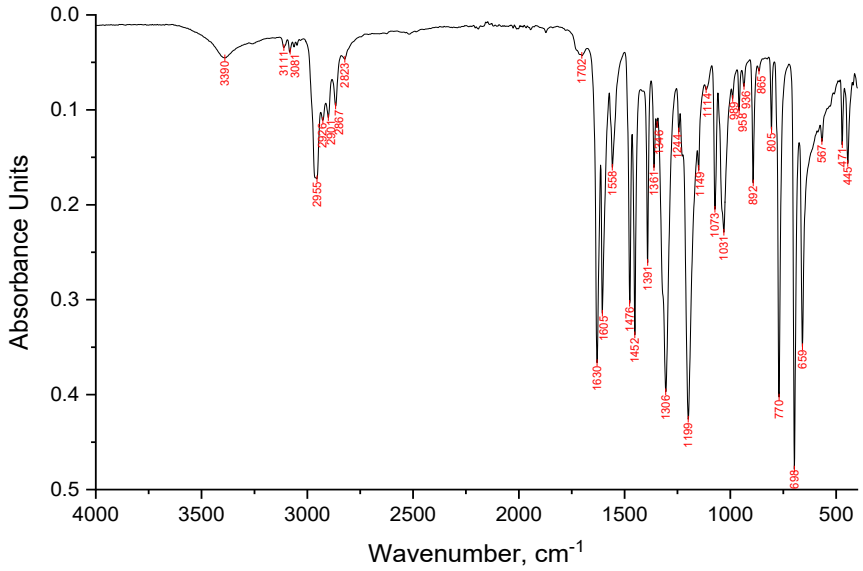

Figure S2. *trans*-[$Py_2Pt(OC(O)Bu^t)_2$]·2$Bu^tC(O)OH$ **3**

trans-[$Py_2Pt(OC(O)Bu^t)_2$]·2MeOH **4**

IR (ATR, ν/cm^{-1}): 3111 w., 3083 w.,2955 m., 2899 w., 2867 w., 1632 s., 1605 s., 1558 m., 1476 s., 1452 s., 1392 s., 1361 m., 1307 s., 1246 m., 1201 s., 1148 m., 1073 m., 1032 m., 990 w., 958 m., 892 m., 805 m., 771 s., 699 s., 661 s., 567 w., 472 m., 445 m.

Elemental analysis data:

Found (%): C, 42.71; H, 5.94; N 4.65. Calc. for $C_{22}H_{36}N_2O_6Pt$ (%): C, 42.65; H, 5.86; N, 4.52.

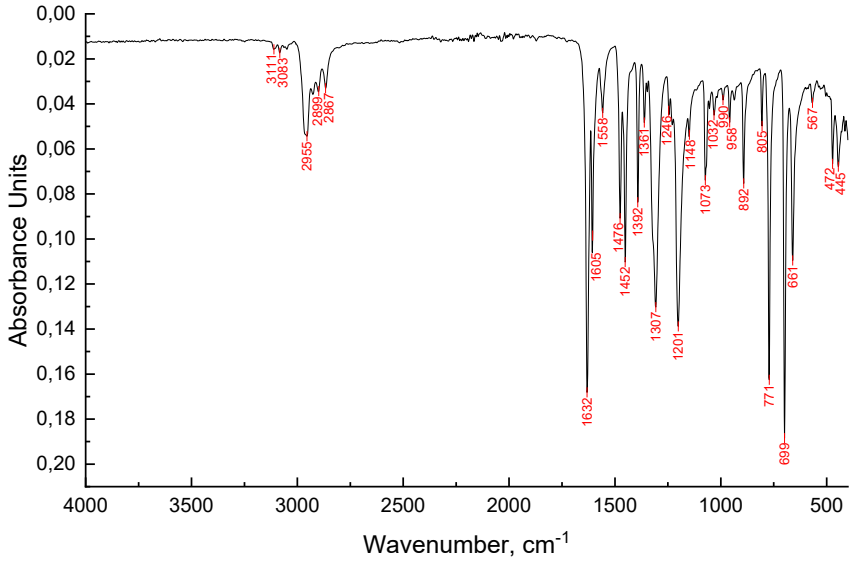

Figure S3. *trans*-[$Py_2Pt(OC(O)Bu^t)_2$]·2MeOH **4**

trans-[$Py_2Pt(OC(O)Ph)_2$] **5**

IR (ATR, ν/cm^{-1}): 3101 w., 3065 w., 3032 w., 1700 m., 1639 m., 1609 m., 1575 m., 1487 w., 1453 s., 1327 s., 1241 s., 1214 m., 1170 m., 1129 m., 1068 m., 1022 m., 937 m., 841 m., 790 m., 766 s., 713 s., 689 s., 656 s., 614 m., 505 m., 475 m. 424 m.

Elemental analysis data:

Found (%): C, 48.56; H, 3.47; N 4.57. Calc. for $C_{24}H_{20}N_2O_4Pt$ (%): C, 48.41; H, 3.39; N, 4.70.

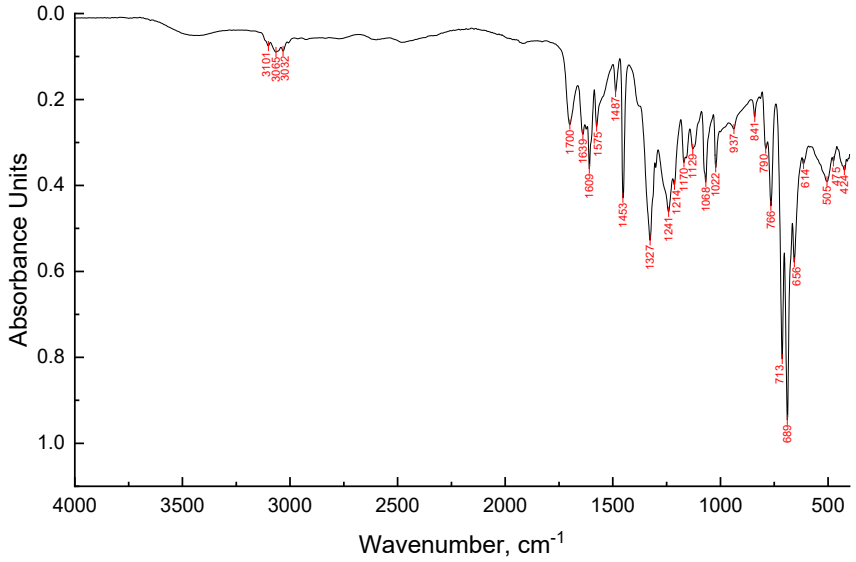

Figure S4. *trans*-[$Py_2Pt(OC(O)Ph)_2$] **5**

Table S1. Crystal Data and Structure Refinement for **2-5**

Identification code	**2**	**3**	**4**	**5**
CCDC No	2162275	2299674	2162276	2263470
Empirical formula	$C_{14}H_{16}N_2O_4Pt$	$C_{30}H_{48}N_2O_8Pt$	$C_{22}H_{36}N_2O_6Pt$	$C_{24}H_{20}N_2O_4Pt$
Formula weight	471.38	759.79	619.62	595.51
Temperature, K	100(2)	100(2)	100(2)	100(2)
Crystal size, mm	0.350×0.050×0.030	0.200×0.060×0.040	0.130×0.110×0.020	0.230×0.150×0.070
Wavelength, Å	0.71073	0.75268	0.71073	0.75268
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	$P2_1/c$	P-1	P-1	$P2_1$
a, Å	7.7617(3)	5.928(2)	5.8821(3)	10.930(3)
b, Å	11.8014(5)	10.8284(18)	8.6827(5)	9.2732(10)
c, Å	8.0673(3)	13.3992(14)	12.9466(7)	11.0814(19)
α, deg.	90	79.606(5)	97.3709(9)	90
β, deg.	91.1421(13)	77.570(6)	96.5006(9)	109.042(12)
γ, deg.	90	83.998(13)	104.9594(8)	90
V, Å^3	738.81(5)	824.2(3)	626.09(6)	1061.7(4)
Z	2	1	1	2
Density (calc.), Mg/m^3	2.119	1.531	1.643	1.863
μ, mm^{-1}	9.513	4.957	5.640	7.651
F(000)	448	384	308	576
Theta range, deg.	2.625 – 30.578	2.831 – 28.922	2.709 – 30.506	2.059 – 29.679
Index ranges	$-11 \le h \le 11$, $-16 \le k \le 16$, $-11 \le l \le 11$	$-7 \le h \le 7$, $-13 \le k \le 13$, $-17 \le l \le 17$	$-8 \le h \le 8$, $-12 \le k \le 12$, $-18 \le l \le 18$	$-14 \le h \le 14$, $-12 \le k \le 12$, $-14 \le l \le 14$
Reflections collected	13066	13290	18313	17463
Independent reflections	2269 (R_{int} = 0.0284)	3616 (R_{int} = 0.0599)	3832 (R_{int} = 0.0370)	5040 (R_{int} = 0.0563)
Data / restraints / parameters	2269 / 0 / 98	3616 / 0 / 197	3832 / 124 / 180	5040 / 1 / 281
R_1 / wR_2 ($I > 2\sigma(I)$)	R_1 = 0.0155 wR_2 = 0.0349	R_1 = 0.0278 wR_2 = 0.0662	R_1 = 0.0227 wR_2 = 0.0560	R_1 = 0.0283 wR_2 = 0.0768
R_1 / wR_2 (all data)	R_1 = 0.0225 wR_2 = 0.0376	R_1 = 0.0278 wR_2 = 0.0662	R_1 = 0.0227 wR_2 = 0.0560	R_1 = 0.0295 wR_2 = 0.0778
Goodness-of-fit on F^2	1.060	1.027	1.043	1.087
Extinction coefficient	n/a	n/a	n/a	0.0126(11)
T_{min} / T_{max}	0.0297 / 0.0739	0.001 / 1.000	0.5646 / 0.7461	0.001 / 1.000
$\Delta\rho_{max}$ / $\Delta\rho_{min}$, e·Å^{-3}	0.836 / –0.777	1.378 / –1.416	1.238 / –1.163	1.083 / –1.631

Table S2. Main interatomic distances [Å] and angles [°] for **2-5**

2		**3**		**4**		**5**	
Pt(1)-N(1)$^{\#1}$	2.014(2)	Pt(1)-N(1)$^{\#1}$	2.023(3)	Pt(1)-O(11)$^{\#1}$	2.003(2)	Pt(1)-N(2)	2.014(5)
Pt(1)-N(1)	2.014(2)	Pt(1)-N(1)	2.023(3)	Pt(1)-O(11)	2.003(2)	Pt(1)-O(11)	2.016(4)
Pt(1)-O(11)$^{\#1}$	2.0148(17)	Pt(1)-O(11)$^{\#1}$	2.028(2)	Pt(1)-N(1)$^{\#1}$	2.029(2)	Pt(1)-N(1)	2.022(5)
Pt(1)-O(11)	2.0148(17)	Pt(1)-O(11)	2.028(2)	Pt(1)-N(1)	2.029(2)	Pt(1)-O(21)	2.026(4)
N(1)$^{\#1}$-Pt(1)-N(1)	180.0	N(1)-Pt(1)-N(1)$^{\#1}$	180.0	O(11)$^{\#1}$-Pt(1)-O(11)	180.0	N(2)-Pt(1)-O(11)	89.67(18)
N(1)$^{\#1}$-Pt(1)-O(11)	91.04(7)	N(1)-Pt(1)-O(11)$^{\#1}$	91.86(11)	O(11)$^{\#1}$-Pt(1)-N(1)$^{\#1}$	90.78(9)	N(2)-Pt(1)-N(1)	178.67(19)
N(1)-Pt(1)-O(11)	88.96(7)	N(1)$^{\#1}$-Pt(1)-O(11)$^{\#1}$	88.14(11)	O(11)-Pt(1)-N(1)$^{\#1}$	89.22(9)	O(11)-Pt(1)-N(1)	91.4(2)
N(1)$^{\#1}$-Pt(1)-O(11)$^{\#1}$	88.96(7)	N(1)-Pt(1)-O(11)	88.14(11)	O(11)$^{\#1}$-Pt(1)-N(1)	89.22(9)	N(2)-Pt(1)-O(21)	87.2(2)
N(1)-Pt(1)-O(11)$^{\#1}$	91.04(7)	N(1)$^{\#1}$-Pt(1)-O(11)	91.86(11)	O(11)-Pt(1)-N(1)	90.78(9)	O(11)-Pt(1)-O(21)	176.7(2)
O(11)-Pt(1)-O(11)$^{\#1}$	180.0	O(11)$^{\#1}$-Pt(1)-O(11)	180.0	N(1)$^{\#1}$-Pt(1)-N(1)	180.0	N(1)-Pt(1)-O(21)	91.76(18)
Symmetry transformations	$^{\#1}$–x+1, –y+1, –z+2	Symmetry transformations	$^{\#1}$–x+1, –y+2, –z+1	Symmetry transformations	$^{\#1}$–x, –y, –z+1		

Table S3. Parameters of hydrogen bonds [Å, °] for **3**, **4**

3				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1S)-H(1S)...O(12)	0.85(6)	1.80(6)	2.638(4)	166(5)
4				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1S)-H(1S)...O(12)	0.89(4)	1.85(4)	2.719(5)	167(9)