Electronic Supplementary Information for Dalton Transactions

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Gold(I) chloride adducts of 1,3-bis(di-2-pyridylphosphino)propane: synthesis, structural studies and antitumour activity

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Supporting Information

Table S1. Torsion Angles in $[Au(d2pypp)_2]Cl.3H_2O$ (**2**)

Atoms	Parameter	Atoms	Parameter
Torsion Angles (°)			
Au(1)-P(1)-C(10)-C(12)	-55.5(6)	C(56)-C(60)-P(6)-Au(2)	50.6(6)
P(1)-C(10)-C(12)-C(20)	80.4(7)	C(50)-C(56)-C(60)-P(6)	-79.1(8)
C(10)-C(12)-C(20)-P(2)	-77.7(7)	P(5)-C(50)-C(56)-C(60)	83.6(8)
C(12)-C(20)-P(2)-Au(1)	50.8(6)	Au(2)-P(5)-C(50)-C(56)	-55.9(7)
P(2)-Au(1)-P(1)-C(10)	30.3(3)	P(5)-Au(2)-P(6)-C(60)	-26.9(3)
P(1)-Au(1)-P(2)-C(20)	-27.9(3)	P(6)-Au(2)-P(5)-C(50)	28.6(3)
Au(1)-P(3)-C(30)-C(34)	-60.5(6)	C(78)-C(80)-P(8)-Au(2)	49.4(6)
P(3)-C(30)-C(34)-C(40)	77.4(8)	C(70)-C(78)-C(80)-P(8)	-74.6(8)
C(30)-C(34)-C(40)-P(4)	-76.5(7)	P(7)-C(70)-C(78)-C(80)	81.2(7)
C(34)-C(40)-P(4)-Au(1)	57.1(6)	Au(2)-P(7)-C(70)-C(78)	-59.5(6)
P(4)-Au(1)-P(3)-C(30)	40.4(3)	P(7)-Au(2)-P(8)-C(80)	-31.9(3)
P(3)-Au(1)-P(4)-C(40)	-37.6(3)	P(8)-Au(2)-P(7)-C(70)	35.2(3)
Au(1)-P(1)-C(111)-N(112)	167.6(5)	Au(2)-P(6)-C(611)-N(612)	176.2(5)
Au(1)-P(1)-C(121)-N(122)	53.1(6)	Au(2)-P(6)-C(621)-N(622)	-43.0(7)
Au(1)-P(2)-C(211)-N(212)	-176.6(5)	Au(2)-P(5)-C(511)-N(512)	166.2(5)-
Au(1)-P(2)-C(221)-N(222)	76.7(6)	Au(2)-P(5)-C(521)-N(522)	84.1(7)
Au(1)-P(3)-C(311)-N(312)	168.5(5)	Au(2)-P(8)-C(811)-N(812)	172.3(4)
Au(1)-P(3)-C(321)-N(322)	-116.2(6)	Au(2)-P(8)-C(821)-N(822)	126.3(6)
Au(1)-P(4)-C(411)-N(412)	-163.2(5)	Au(2)-P(7)-C(711)-C(712)	150.9(5)
Au(1)-P(4)-C(421)-N(422)	-63.0(6)	Au(2)-P(7)-C(721)-C(722)	64.4(6)

Table S2 Torsion Angles in $[Au(d3pype)_2]Cl•5H_2O$ (**3**)

Atoms	Parameter	Atoms	Parameter
Torsion angles (°)			
P(2)-Au-P(1)-C(10)	10.40(9)	C(10)-C(20)-P(20)-Au	-40.2(2)
Au-P(1)-C(10)-C(20)	-38.8(2)	C(20)-P(20)-Au-P(1)	13.03(9)
P(1)-C(10)-C(20)-P(2)	53.8(2)		
Au-P(1)-C(111)-C(116)	56.7(2)	Au-P(2)-C(211)-C(212)	50.2(2)
Au-P(1)-C(121)-C(122)	34.7(3)	Au-P(2)-C(221)-C(222)	-1.7(2)

Transformation of the asymmetric unit: i 1-*x*, ½-*y*, *z*

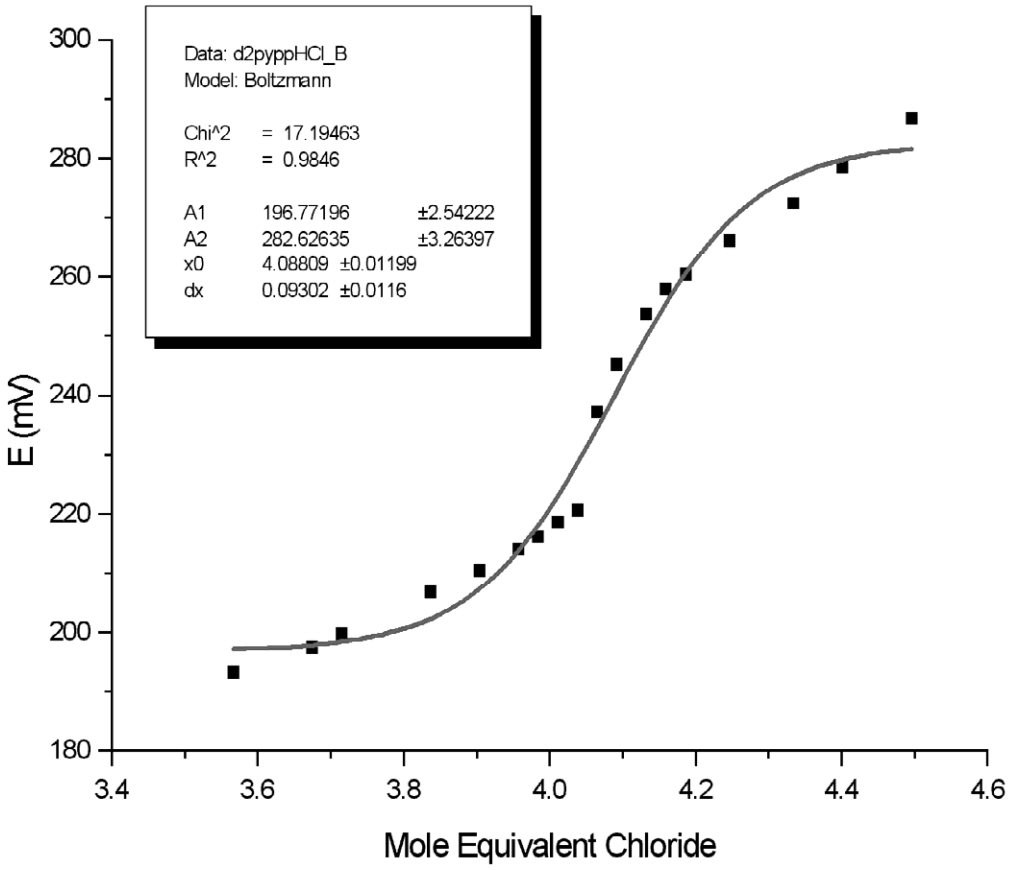

Fig. S1. Potentiometric titration of an aqueous solution of the d2pypp hydrochloride salt

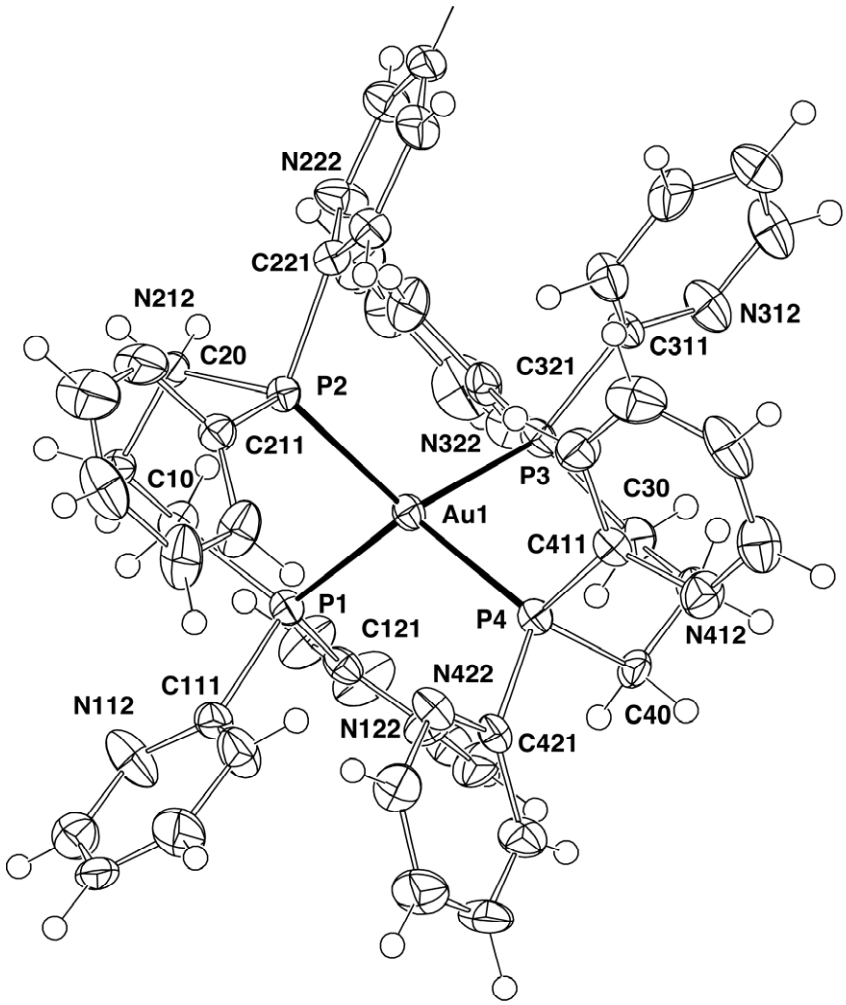

Fig S2. Projection of cation 1 of **2** down the bisector of the largest and smallest P-Au-P angles, which lie trans to each other.

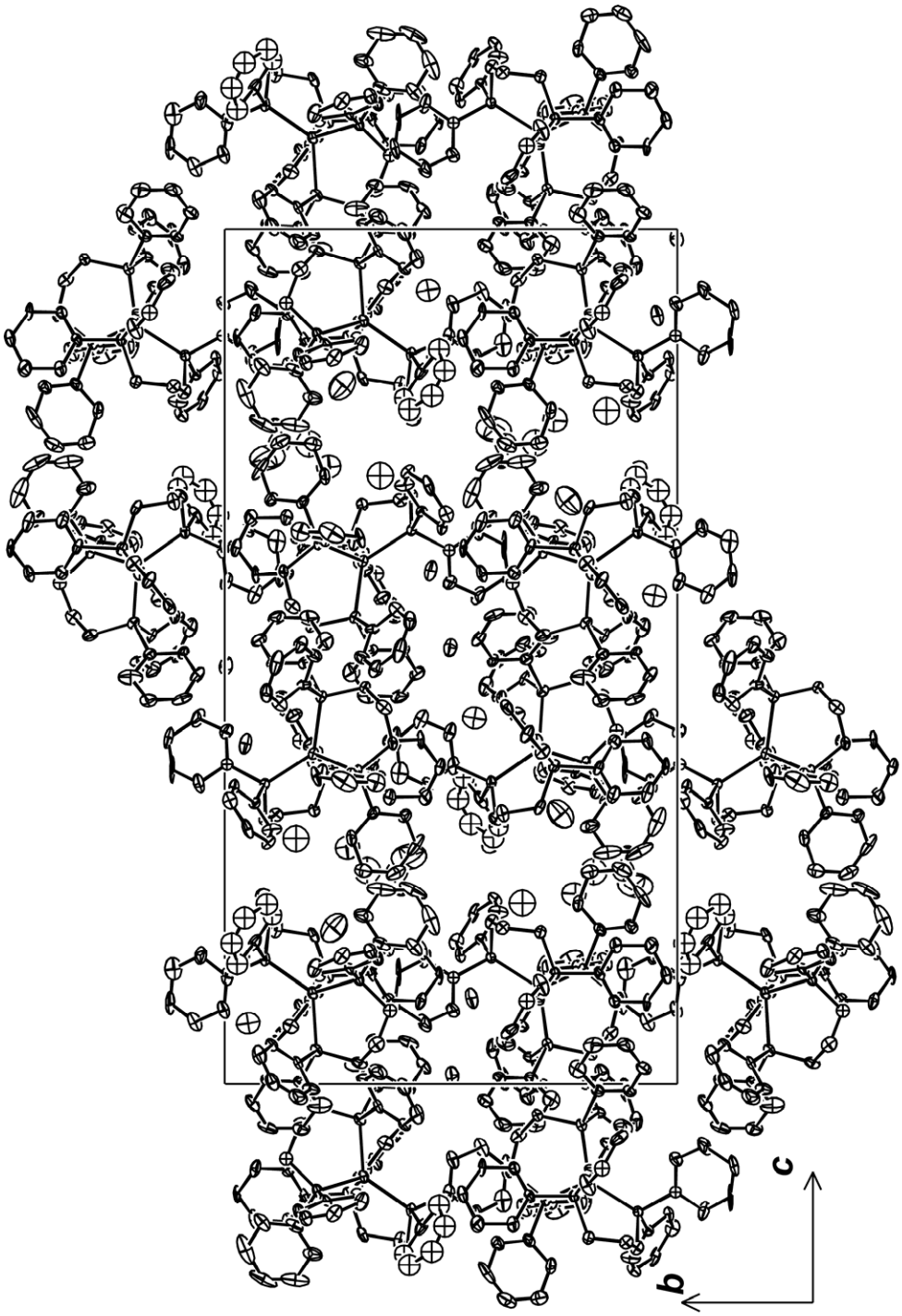

Fig S3. Unit cell contents of **2**, projected down *a*, showing the layering of the structure.

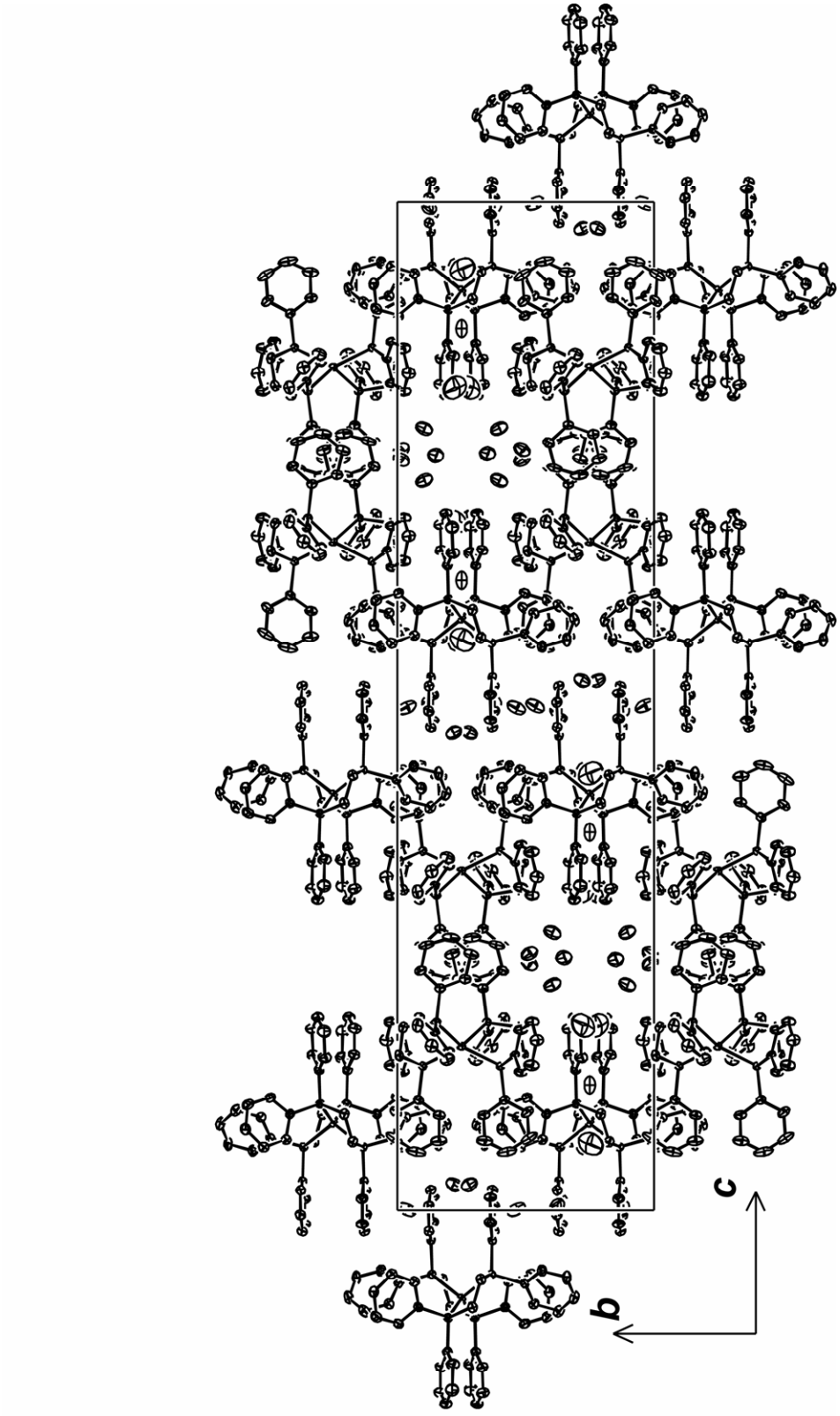

Fig S4. Unit cell contents of **3**, projected down *a*.