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ELECTRONIC SUPPLEMENTARY INFORMATION

Monocationic gold(III) Gly-L-His and L-Ala-L-His dipeptide complexes: crystal structures arising from solvent free and solvent-containing crystal formation and structural modifications tuned by counter-anions

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Abstract

Monocationic gold(III) complexes with histidine-containing peptides, glycyl-L-histidine (Gly-L-His) and L-alanyl-L-histidine (L-Ala-L-His) have been synthesized and characterized by ^{1}H NMR spectroscopy and X-ray crystallography. The crystallized Au(III) complexes, [Au(Gly-L-His-*N,N',N''*)Cl]$NO_3 \cdot 1.25H_2O$ and [Au(L-Ala-L-His-*N,N',N''*)Cl]$NO_3 \cdot 2.5H_2O$, were obtained from water solution at pH < 1.0. The chemical shifts in the ^{1}H NMR spectra of [Au(Gly-L-His-*N,N',N''*)Cl]$NO_3 \cdot 1.25H_2O$ and [Au(L-Ala-L-His-*N,N',N''*)Cl]$NO_3 \cdot 2.5H_2O$ complexes were compared with those for the corresponding Pd(II) complexes and for Pd(II) and Au(III) complexes with Gly-Gly-L-His tripeptide. Crystal data for the hydrated [Au(Gly-L-His-*N,N',N''*)Cl]$NO_3 \cdot 1.25H_2O$ complex and its serendipitously obtained unhydrated form were compared with previously reported X-ray data for the hydrated chloride complex [Au(Gly-L-His-*N,N',N''*)Cl]$Cl \cdot 3H_2O$ and with the analogous, though uncharged, Pd(II) and Pt(II) complexes. Furthermore, in the present study the crystal structure of the nitrate salt of Au(III) complex with L-Ala-L-His dipeptide, [Au(L-Ala-L-His-*N,N',N''*)Cl]$NO_3 \cdot 2.5H_2O$ has been determined.

Keywords: Gold(III) complexes; Glycyl-L-histidine; L-Alanyl-L-histidine; Proton NMR spectroscopy; X-Ray crystallography.

Table 1S Selected bond distances (Å) and bond angles (º) for Au(III) complexes

	[Au(Gly-L-His-*N,N',N''*)Cl]$NO_3 \cdot 1.25H_2O$	[Au(Gly-L-His-*N,N',N''*)Cl]NO_3	[Au(L-Ala-L-His-*N,N',N''*)Cl]$NO_3 \cdot 2.5H_2O$
Au1—N1	1.987(8) 2.026(10)	2.034(13)	2.019(5)
Au1—N2	2.020(10) 2.021(10)	2.010(13)	1.995(5)
Au1—N3	1.996(9) 1.913(10)	1.998(11)	2.001(6)
Au1—Cl1	2.293(3) 2.297(3)	2.294(4)	2.2869(16)
N1—Au1—N2	82.8(4) 82.3(4)	84.1(5)	81.7(2)
N1—Au1—N3	175.3(4) 175.4(4)	174.1(6)	175.8(2)
N3—Au1—N2	92.7(4) 93.2(4)	91.0(5)	94.2(2)
N1—Au1—Cl1	92.5(2) 92.2(3)	94.0(3)	92.93(17)
N2—Au1—Cl1	174.7(3) 174.0(3)	174.2(4)	174.56(17)
N3—Au1—Cl1	92.1(3) 92.4(3)	91.3(3)	91.20(17)

Table 2S Hydrogen bond parameters for Au(III) complexes with Gly-L-His and L-Ala-L-His dipeptides

[Au(Gly-L-His-*N,N',N''*)Cl]NO_3·1.25H_2O

D—H···*A*	*D*—H(Å)	H···*A*(Å)	*D*···*A*(Å)	*D*—H···*A*(º)
N1—H1N···O2W^{i}	0.90	2.07	2.961(15)	171
N1—H2N···O1^{ii}	0.90	2.16	2.876(18)	136
N1'—H1N'···O2W^{i}	0.90	2.05	2.932(15)	166
N1'—H2N'···O5N^{i}	0.90	2.11	2.971(16)	161
N4—H4N···O6N	0.86	2.08	2.90(2)	159
N4'—H4N'···O1N^{iii}	0.86	2.00	2.849(17)	171
O3—H3O···O1N	0.82	2.03	2.680(15)	135
O3'—H3O'···O1W	0.82	1.92	2.709(17)	162
O1W···O3W^{iv}			2.728(17)	
O2W···O2N^{v}			2.770(17)	
O2W···O3N^{v}			3.217(18)	
O2W···O5N^{iv}			2.843(15)	
O3W···O4N^{vi}			2.833(22)	
O3W···O6N			3.064(19)	

Symmetry codes: (i) *x*−1/2, *y*+1/2, *z*; (ii) −*x*+3/2, *y*−1/2, −*z*+2; (iii) −*x*+2, *y*, −*z*+2; (iv) *x*, *y-1, z*; (v) −*x*+2, *y-1*, −*z*+2; (vi) *x*, *y+1, z*.

[Au(Gly-L-His-*N,N',N''*)Cl]NO_3

D—H···*A*	*D*—H(Å)	H···*A*(Å)	*D*···*A*(Å)	*D*—H···*A*(º)
N1—H1NB···O2N^{i}	0.90	2.28	3.074 (19)	146
N1—H1NA···O1^{ii}	0.90	2.22	2.87 (3)	129
N4—H4N···O1N	0.86	1.97	2.815 (18)	166
O3—H3O···O1N^{iii}	0.82	1.76	2.53 (2)	158

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+3/2, *y*+1/2, −*z*; (iii) *x*+1/2, −*y*+3/2, −*z*+1.

[Au(L-Ala-L-His-*N,N',N''*)Cl]NO_3·2.5H_2O

D—H···*A*	*D*—H(Å)	H···*A*(Å)	*D*···*A*(Å)	*D*—H···*A*(º)
O3—H3O···O1W	0.82	1.85	2.653 (14)	168

N1—H1N···O2W	0.90	2.00	2.887 (9)	170
N1—H2N···O3W	0.90	2.26	3.142 (14)	165
N4—H4N···O2N	0.86	1.96	2.808 (19)	170
N4—H4N···O1N'	0.86	2.08	2.89 (3)	157
N4—H4N···O3N'	0.86	2.33	3.07 (4)	144
O1W···O1N'^{i}			2.64 (3)	
O1W···O2N'^{ii}			2.52(2)	
O2W···O3N^{iii}			3.036 (16)	
O2W···O3N^{iv}			3.036 (16)	
O3W···O1^{v}			2.905 (12)	
O3W···O1N^{vi}			3.033 (24)	

Symmetry codes: (i) −*x*+2, *y*−1, *z*; (ii) −*x*−1/2, −*y*+3/2, −*z*+1; (iii) *x*, *y*, *z*−1; (iv) −*x*+2, −*y*+1, *z*−1; (v) −*x*+3/2, *y*−1/2, −*z*; (vi) −*x*+2, −*y*, *z*−1

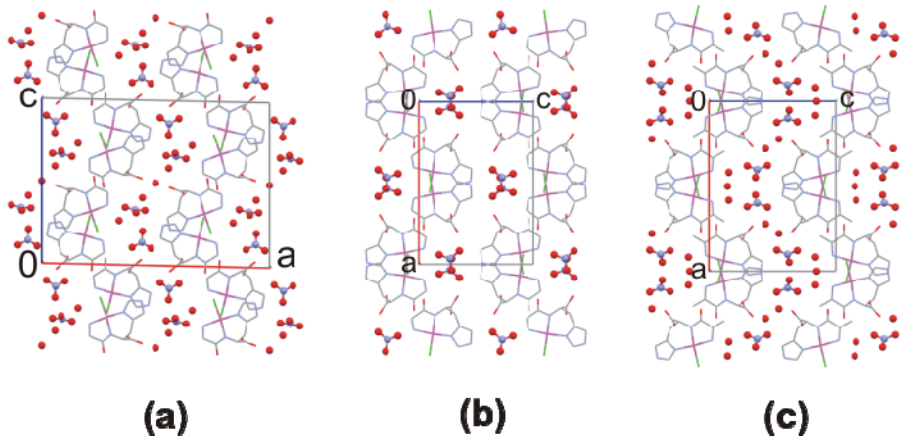

Fig. 1S Arrangement of nitrate anions and water molecules (ball and stick representation) with respect to the complex cations (capped sticks, hydrogen atoms omitted) in hydrated (a) and unhydrated (b) crystal forms of [Au(Gly-L-His-*N,N',N''*)Cl]NO_3, and in [Au(L-Ala-L-His-*N,N',N''*)Cl]$NO_3 \cdot 2.5H_2O$ crystal (c).