

# **Structure and stability of Copper(II) Lactate Complex in Alkaline**

## **Solution: a Case Study by dispersive XAS**

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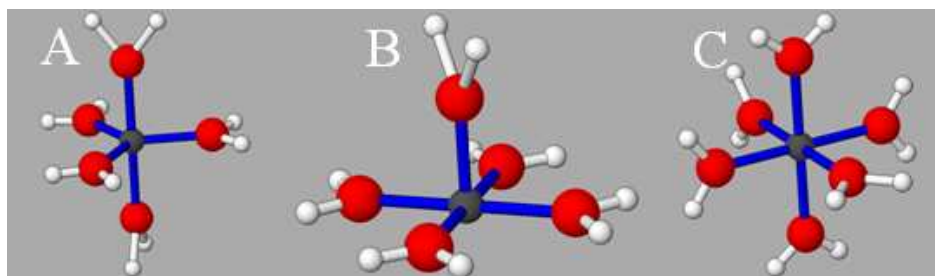
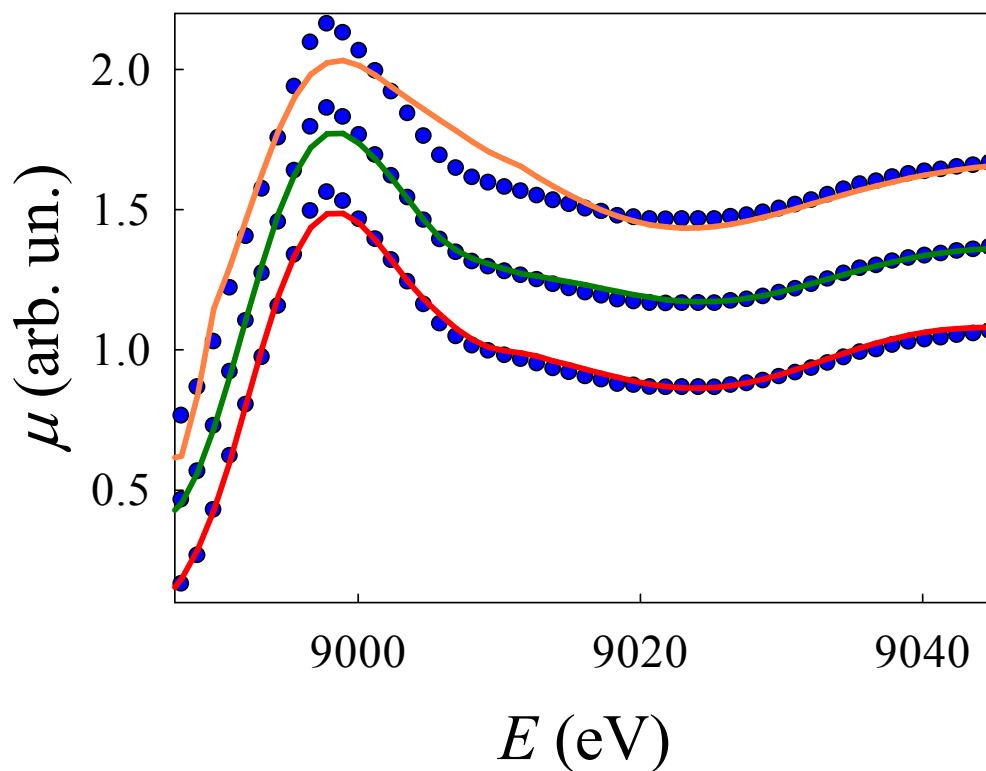
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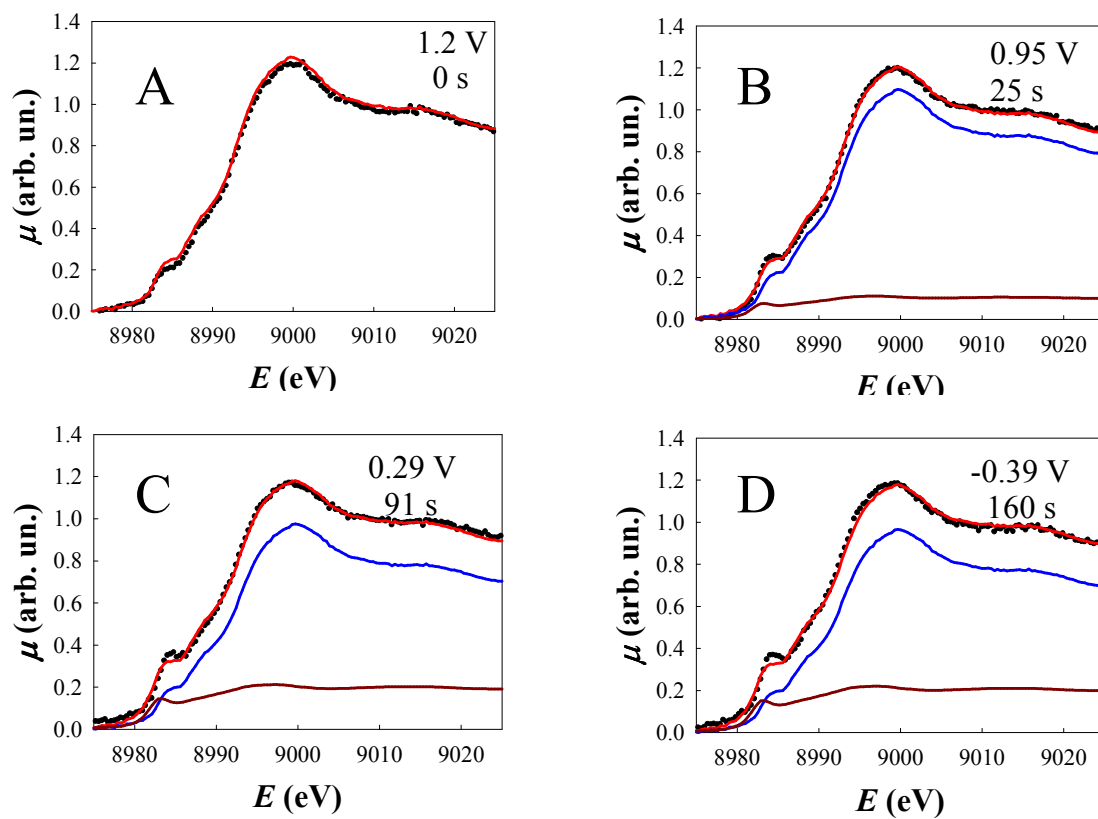
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ASSOCIATED CONTENT

**Supporting Information.**



**Figure S1.** Cu-K edge XANES simulations of Cu(II) aquaion. The blue spots represent the experimental signal while the coloured lines are the theoretical calculations based on a trigonal bipyramidal local arrangement (orange line, A), on a square pyramidal local arrangement (green line, B) and on a distorted octahedral local arrangement (red line, C).



**Figure S2.** Manual linear combination fit of four XANES spectra selected among the entire data set acquired during the LSV program at 1.2 V (A), 0.95 V (B), 0.29 V (C) and -0.39 V (D). The Black spots represent the experimental signal and the red line the theory, the blue line is Copper(II) lactate contribution and the brown line  $\text{Cu}_2\text{O}$  contribution.

**Simulation 1. Distorted Octahedral Arrangement**

Atom	x(Å)	y(Å)	z(Å)
O	1.396	1.396	0.000
O	-1.396	1.396	0.000
O	-1.396	-1.396	0.000
O	1.396	-1.396	0.000
O	0.000	0.000	2.092
O	0.000	0.000	-2.092
H	0.541	0.541	2.952
H	-0.541	-0.541	2.952
H	-0.541	0.541	-2.952
H	0.541	-0.541	-2.952
H	1.264	2.345	0.000
H	-2.345	1.264	0.000
H	-1.264	-2.345	0.000
H	2.345	-1.264	0.000
H	2.345	1.264	0.000
H	-1.264	2.345	0.000
H	-2.345	-1.264	0.000
H	1.264	-2.345	0.000

**Simulation 2. Square Pyramidal Arrangement**

Atom	x(Å)	y(Å)	z(Å)
O	-1.347	1.347	0.000
O	1.347	-1.347	0.000
O	1.347	1.347	0.000
O	-1.347	-1.347	0.000
O	0.000	.0000	1.898
H	-1.264	2.345	0.000
H	1.264	-2.345	0.000
H	1.264	2.345	0.000
H	-1.264	-2.345	0.000
H	-2.345	1.264	0.000
H	2.345	-1.264	0.000
H	2.345	1.264	0.000
H	-2.345	1.264	0.000
H	0.765	0.000	2.952
H	-0.765	0.000	2.952

**Simulation 3. Trigonal Bipyramidal Arrangement**

Atom	x(Å)	y(Å)	z(Å)
O	1.910	0	0
O	-0.956	1.654	0
O	-0.956	-1.654	0
O	0	0	1.967
O	0	0	-1.967

H	-0.603	2.573	0
H	-1.927	-1.808	0
H	2.529	-0.765	0
H	2.529	0.765	0
H	-1.927	1.808	0
H	-0.603	-2.573	0
H	0.541	0.541	2.952
H	-0.541	0.541	2.952
H	-0.541	0.541	-2.952
H	0.541	-0.541	-2.952

**Table S1.** Coordinates referred to the three different geometries employed in the simulation of the spectrum of Cu(II) aquaion.

<i>Simulation 1. Distorted Octahedral Arrangement</i>					
Shell	Coordination Number	Type of atom	Distance from Cu(II) (Å)	$\sigma^2$ (Å <sup>2</sup> )	$\beta$ (Å <sup>3</sup> )
1	4	O	1.97(2)*	4(2) x 10 <sup>-3</sup> *	--
2	2	O	2.09(3)*	7(7) x 10 <sup>-3</sup> *	-1.1(3)*
3	8	H	2.664	5.0 x 10 <sup>-3</sup>	--
4	4	H	3.050	5.0 x 10 <sup>-3</sup>	--
Goodness of Fit <i>F</i> : 2.8 %					
<i>Simulation 2. Square Pyramidal Arrangement</i>					
Shell	Coordination Number	Type of atom	Distance from Cu(II) (Å)	$\sigma^2$ (Å <sup>2</sup> )	$\beta$ (Å <sup>3</sup> )
1	4	O	1.90(3) *	3(4) x 10 <sup>-3</sup> *	-0.4(2)
2	1	O	1.90(8)*	1(1) x 10 <sup>-2</sup> *	-2(1)
3	8	H	2.664	5.0 x 10 <sup>-3</sup>	--
4	2	H	3.050	5.0 x 10 <sup>-3</sup>	--
Goodness of Fit <i>F</i> : 2.8 %					
<i>Simulation 3. Trigonal Bipyramidal Arrangement</i>					
Shell	Coordination Number	Type of atom	Distance from Cu(II) (Å)	$\sigma^2$ (Å <sup>2</sup> )	$\beta$ (Å <sup>3</sup> )
1	3	O	1.91(5)*	1(1) x 10 <sup>-2</sup> *	--
2	2	O	1.97(6)*	1(2) x 10 <sup>-2</sup> *	--
3	6	H	2.642	5.0 x 10 <sup>-3</sup>	--
4	4	H	3.050	5.0 x 10 <sup>-3</sup>	--
Goodness of Fit <i>F</i> : 13.9 %					
* Fitted values					

**Table S2.** XANES Calculation parameters of the simulations obtained for the three different geometries. For each shell is reported the coordination number, the type of atom, the distance from the photo-absorber, the thermal disorder ( $\sigma^2$ ) and the skewness ( $\beta$ ) when different from zero.

<i>Coordinates of all atoms in Model D</i>			
Atom	x(Å)	y(Å)	z(Å)
O <sub>1</sub>	-1.071	1.071	1.071
O <sub>1</sub>	1.071	-1.071	1.071
O <sub>1</sub>	1.071	1.071	-1.071
O <sub>1</sub>	-1.071	-1.071	-1.071
H <sub>2</sub>	0.750	2.795	0.698
H <sub>2</sub>	-0.750	-2.795	0.698
H <sub>2</sub>	-2.795	0.750	-0.698
H <sub>2</sub>	2.795	-0.750	-0.698
C <sub>3</sub>	-1.238	1.762	2.088
C <sub>3</sub>	1.238	-1.762	2.088
C <sub>3</sub>	1.762	1.238	-2.088
C <sub>3</sub>	-1.762	-1.238	-2.088
O <sub>4</sub>	0.951	2.627	1.629
O <sub>4</sub>	-0.951	-2.627	1.629
O <sub>4</sub>	-2.627	0.951	-1.629
O <sub>4</sub>	2.627	-0.951	-1.629
C <sub>5</sub>	-0.177	2.751	2.498
C <sub>5</sub>	0.177	-2.751	2.498
C <sub>5</sub>	2.751	0.177	-2.498
C <sub>5</sub>	-2.751	-0.177	-2.498
O <sub>6</sub>	-2.249	1.640	2.758
O <sub>6</sub>	2.249	-1.640	2.758
O <sub>6</sub>	1.640	2.249	-2.758
O <sub>6</sub>	-1.640	-2.248	-2.758
H <sub>7</sub>	0.131	2.548	3.524
H <sub>7</sub>	-0.131	-2.548	3.524
H <sub>7</sub>	-2.548	0.131	-3.524
H <sub>7</sub>	2.548	-0.131	-3.524
H <sub>8</sub>	-1.047	4.373	1.380
H <sub>8</sub>	1.047	-4.373	1.380
H <sub>8</sub>	4.373	1.047	-1.380
H <sub>8</sub>	-4.373	-1.047	-1.380
C <sub>9</sub>	-0.739	4.171	2.406
C <sub>9</sub>	0.739	-4.171	2.406
C <sub>9</sub>	4.171	0.739	-2.406
C <sub>9</sub>	-4.171	-0.739	-2.406
H <sub>10</sub>	-1.599	4.265	3.069
H <sub>10</sub>	1.599	-4.265	3.069
H <sub>10</sub>	4.265	1.599	-3.069
H <sub>10</sub>	-4.265	-1.599	-3.069
H <sub>11</sub>	0.028	4.885	2.703
H <sub>11</sub>	-0.028	-4.885	2.703
H <sub>11</sub>	-4.885	0.028	-2.703
H <sub>11</sub>	4.885	-0.028	-2.703

**Table S3.** Coordinates referred to the cluster indicated in Fig. 3 E.