Supporting Information for Copper (II) Complexes of Bis(amino amide) Ligands: Effect of Changes in the Amino Acid Residue

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Supplementary material

S1. Species distribution curves for the different protonated forms.

S2. Species distribution curves for the different Cu (II) complexes.

S3. UV/Vis absorption spectra in methanol for the different Cu (II) complexes for the ligands at different pH values.

S4. ESI-MS spectra for the different Cu (II) complexes at several pH values.

S5. Species distribution curves for the compound AlaA3 (1d, n=1) and for Cu (II) complexes. UV/Vis absorption spectra and ESI-MS spectra for the Cu (II) complexes at several pH values.
S1. Species distribution curves for the different protonated forms.

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**PheA2**

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**PheA3**

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**PheA4**

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**PheA5**

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**PheA6**

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S2. Species distribution curves for the different Cu (II) complexes.

CuPheA2

CuPheA3

CuPheA4

CuPheA5

CuPheA6
S3. UV/Vis absorption spectra in methanol for the different Cu (II) complexes for the ligands at different pH values

CuPhglyA2

CuPhglyA6

CuProA2

CuProA6

CuGlyA2

CuGlyA6
CuAlaA2  CuAlaA6

![Graph of CuAlaA2 absorbance against pH](image1)

- pH=2.04
- pH=3.92
- pH=5.29
- pH=6.71
- pH=11.48

![Graph of CuAlaA6 absorbance against pH](image2)

- pH=8.94
- pH=6.78
- pH=4.69
- pH=1.68

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S4. ESI-MS spectra for the different Cu (II) complexes at several pH values.
CuPheA3 pH = 3.7

CuPheA3 pH = 4.66

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CuPheA3 pH = 5.98

CuPheA3 pH = 9.4

[Electronic Supplementary Material (ESI) for Dalton Transactions]
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CuPheA4 pH = 3.8

CuPheA4 pH = 5.2
CuPheA6 pH=5.30

CuPheA6 pH=7.8

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CuPhglyA2 pH=11.37

CuPhglyA6 pH=2.06
CuPhglyA6 pH=5.75

CuPhglyA6 pH=8.85
CuPhglyA6 pH=10.92

CuProA2 pH=1.70
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CuProA2 pH=6.20

[\text{[CuLH}}^{-1})^+\text{]+[CuL}^+\text{+Cl}^{-}\text{]+[L}^+\text{+H}^+\text{]+[(CuLH}}^{-2})^2\text{+K}^+\text{]}

CuProA2 pH=11.56

[\text{[CuLH}}^{-2})^+\text{+Na}^+\text{]+[(CuLH}}^{-2})^+\text{+Na}^+\text{]}

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CuProA6 pH=6.45

[CuL+Cl]^+

[CuLH\textsubscript{1}]^+

CuProA6 pH=8.35

[CuL+Cl]^+

[CuLH\textsubscript{1}]^+
CuAlaA2 pH=5.29

CuAlaA2 pH=6.71
CuAlaA2 pH = 11.48

CuAlaA6 pH = 1.68
CuAlaA6 pH=8.49

CuAlaA6 pH=11.13
**CuGlyA2** pH=12.33

\([\text{CuLH}]^+\)

**CuGlyA6** pH=1.04

\([\text{CuL}+\text{Cl}]^+\)

\([\text{CuL}+\text{H}]^+\)
**S5. Species distribution curves for the compound AlaA3 (1d, n=1) and for Cu (II) complexes. UV/Vis absorption spectra and ESI-MS spectra for the Cu (II) complexes at several pH values.**

**Table 1.** Logarithms of the cumulative and stepwise basicity constants of AlaA3 determined in 0.1 M NaCl at 298.1 ± 0.1 K.

<table>
<thead>
<tr>
<th>Reaction[a],[c]</th>
<th>AlaA3</th>
</tr>
</thead>
<tbody>
<tr>
<td>H + L = HL</td>
<td>8.40(6)[b]</td>
</tr>
<tr>
<td>2H + L = H₂L</td>
<td>15.56(7)</td>
</tr>
<tr>
<td>H + HL = H₂L</td>
<td>7.16(7)</td>
</tr>
</tbody>
</table>

[a] Charges omitted for clarity. [b] All values in parentheses have the standard deviations in the last significant figure. [c] Determined in an aqueous solution 0.1 M NaCl using 0.1 mmol of ligand.

**Table 2.** Logarithms of the formation constants for the Cu²⁺ complexes of the ligand AlaA3 determined in 0.1 M NaCl at 298.1 ± 0.1 K.

<table>
<thead>
<tr>
<th>Reaction[a],[c]</th>
<th>AlaA3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu⁺ + L = CuL</td>
<td>---</td>
</tr>
<tr>
<td>Cu + L + H = CuHL</td>
<td>13.74(5)[b]</td>
</tr>
<tr>
<td>Cu + L = CuH⁺L + H</td>
<td>2.37(3)</td>
</tr>
<tr>
<td>Cu + L = CuH₂L + 2H</td>
<td>-3.69(4)</td>
</tr>
<tr>
<td>Cu + L = CuH₃+ + 3H</td>
<td>---</td>
</tr>
<tr>
<td>CuL + H = CuHL</td>
<td>---</td>
</tr>
<tr>
<td>CuL = CuH⁺L + H</td>
<td>---</td>
</tr>
<tr>
<td>CuH⁺L = CuH₂L + H</td>
<td>-6.06(4)</td>
</tr>
</tbody>
</table>

[a] Charges omitted for clarity. [b] All values in parentheses have the standard deviations in the last significant figure. [c] Determined in an aqueous solution 0.1M NaCl using 0.1 mmol of ligand and 0.1 mmol of the copper (II) salt.

**DISTRIBUTION DIAGRAMS**

![Species distribution curves for AlaA3 and CuAlaA3](image)
UV/VIS ABSORPTION SPECTRA FOR THE Cu (II) COMPLEXES AT SEVERAL pH VALUES.

![UV/VIS Absorption Spectra](image1)

ESI-MS SPECTRA FOR THE Cu (II) COMPLEXES AT SEVERAL pH VALUES.

![ESI-MS Spectra](image2)
CuAlaA3 pH=3.68

CuAlaA3 pH=4.87
CuAlA$^3$ pH=9.37

$\left[(\text{CuLH}_2)^+ \text{Na}^+\right]^+$