

SUPPORTING INFORMATION

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Title: Speciation Behavior of Copper(II) Acetate in Simple Organic Solvents – Revealing the Effect of Trace Water

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High-resolution mass measurements of some complexes

In order to support the assignments made to the various species measured with the ion trap mass spectrometer, additional exploratory experiments were performed with a SYNAPT G2 ion mobility instrument (WATERS, Manchester, U.K.). Accurate masses were determined via internal calibration with reference compounds with known mass-to-charge ratios. In most cases, the differences are below ± 0.0002 amu obtained (Table S1) which fully supports the assignments made on the basis of the IT-MS experiments.

Table S1. Measured and calculated masses of complexes discussed in the text.

	calculated	experimental	Δm , milliamu
$[\text{Cu}(\text{CH}_3\text{CN})]^+$	103.9561	103.8662	-0.4
$[\text{Cu}(\text{CH}_3\text{CN})(\text{H}_2\text{O})]^+$	121.9667	121.8727	-0.1
$[\text{Cu}(\text{OAc})(\text{CH}_3\text{CN})]^+$	162.9694	162.8677	-0.1
$[\text{Cu}(\text{CH}_3\text{CN})_2]^+$	144.9827	144.8841	0.0
$[\text{Cu}(\text{OAc})(\text{CH}_3\text{OH})_2]^+$	185.9953	185.8898	0.7
$[\text{CuOAc}(\text{CH}_3\text{OH})]^+$	153.9691	153.8688	-0.1
$[\text{Cu}_2(\text{OAc})_2]^+$	243.8857	243.7778	-1.3
$[\text{Cu}_3(\text{OAc})_4(\text{OMe})]^+$	455.8604	455.7526	-0.2
$[\text{Cu}_4(\text{OAc})_5(\text{MeO})_2]^+$	608.8216	608.7198	-1.8
$[\text{Cu}_5(\text{OAc})_5(\text{MeO})_4]^+$	733.7880	733.6918	1.9
$[\text{Cu}_5(\text{OAc})_6(\text{MeO})_3]^+$	761.7829	761.6938	-1.0
$[\text{Cu}_4(\text{OAc})_4(\text{MeO})_3]^+$	580.8267	580.7202	1.9
$[\text{Cu}(\text{CH}_3\text{CN})(\text{H}_2\text{O})]^+$	121.9667	121.8724	-0.1
$[\text{NaCu}(\text{OAc})_2]$	203.9459	203.8387	0.0
$[\text{Cu}_2(\text{OAc})_3(\text{CH}_3\text{CN})]^+$	343.9256	343.8116	0.5
$[\text{NaCu}_2(\text{OAc})_4]^+$	384.9021	384.7883	-0.4
$[\text{Cu}_3(\text{OAc})_5]^+$	483.8553	483.7443	0.2
$[\text{NaCu}_3(\text{OAc})_6]^+$	565.8583	565.7516	0.9
$[\text{Cu}_4(\text{OAc})_7]^+$	664.8115	664.7136	-0.3
$[\text{NaCu}_4(\text{OAc})_8]^+$	746.8145	746.7238	0.0
$[\text{Cu}_5(\text{OAc})_9]^+$	845.7677	845.6882	-0.4

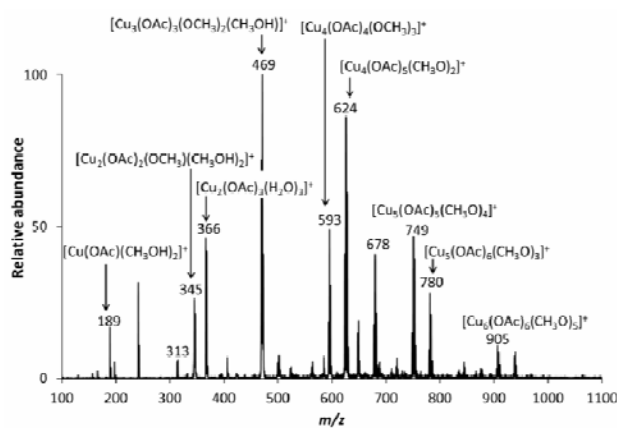


Figure S1. Positive-mode ESI-MS of $\text{Cu}(\text{OOCCD}_3)_2$ (10^{-3} M) in pure methanol.

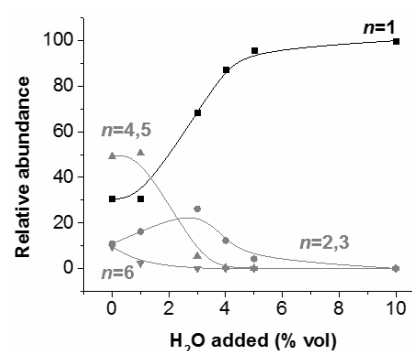


Figure S2. Normalized abundances ($\Sigma I_i = 100$) of $[\text{Cu}_n(\text{OAc})_{2n-1}(\text{CH}_3\text{CN})_n]^+$ cations with various cluster sizes n as a function of the water content of the feed solution of $\text{Cu}(\text{OAc})_2$ (1 mM) in acetonitrile.

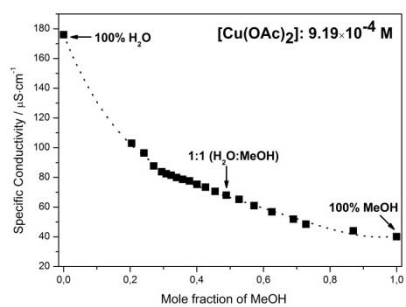


Figure S3. Specific conductivity of a ca. mM solution of $\text{Cu}(\text{OAc})_2$ in water/methanol mixtures.

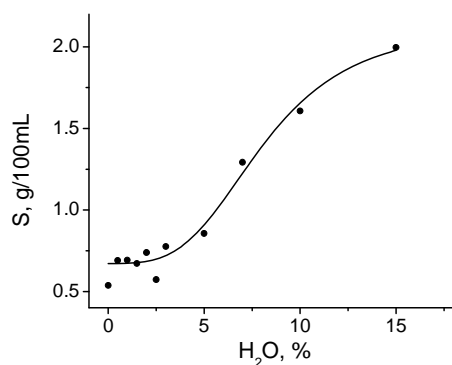


Figure S4. The effect of H_2O addition on the solubility of $\text{Cu}(\text{OAc})_2$ in methanol.

CID spectra

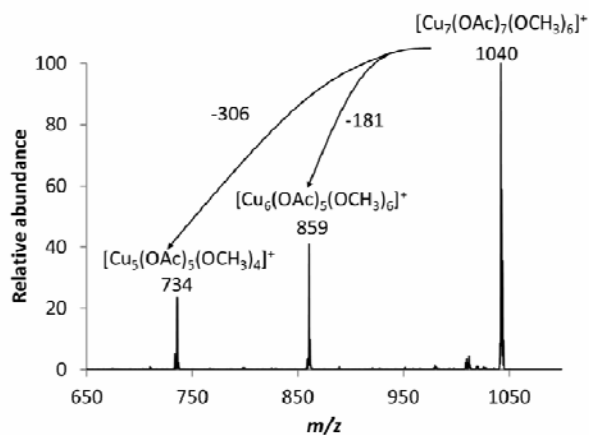


Figure S5. CID spectrum of mass-selected m/z 1040

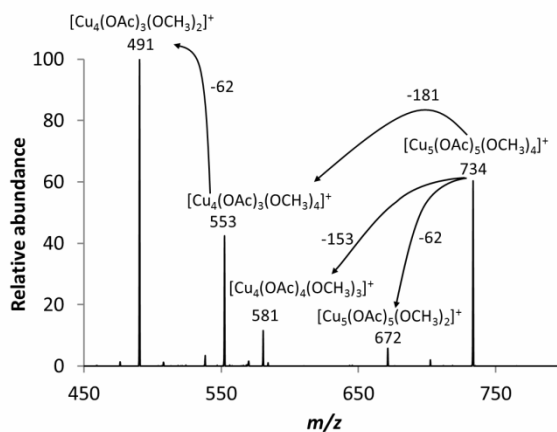


Figure S6. CID spectrum of mass-selected m/z 734

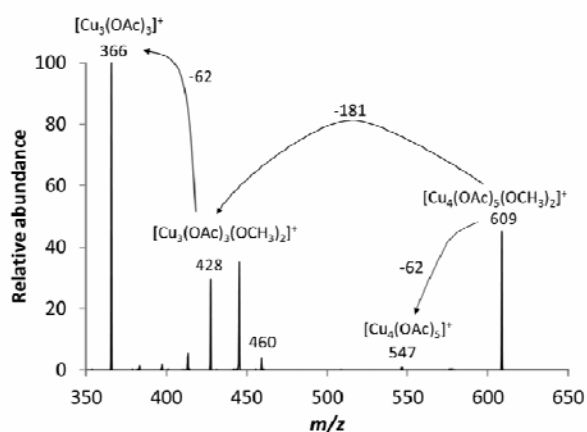


Figure S7. CID spectrum of mass-selected m/z 609

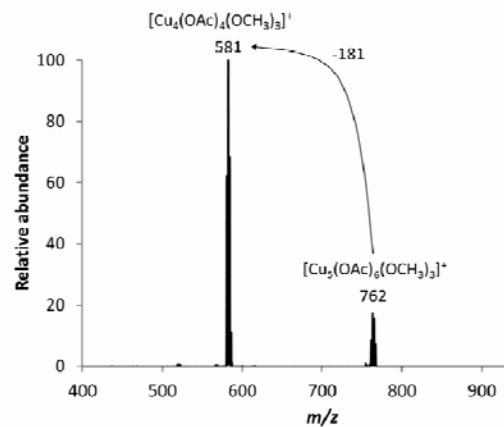


Figure S8. CID spectrum of mass-selected m/z 762

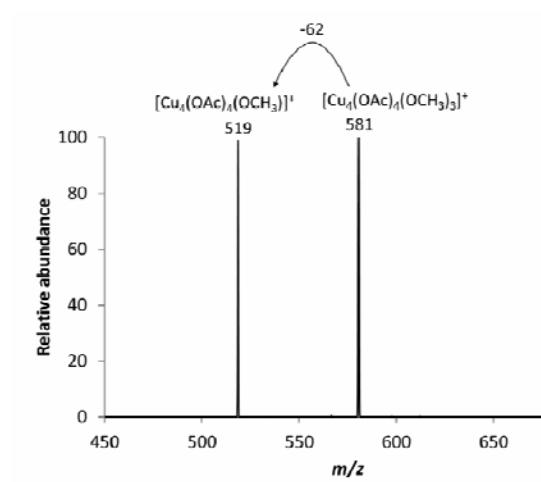


Figure S9. CID spectrum of mass-selected m/z 581