

A Sugar Discriminating Binuclear Copper(II) Complex

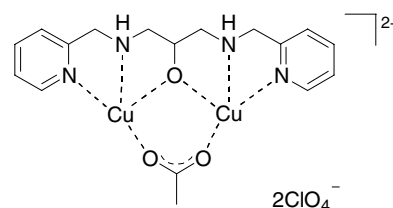
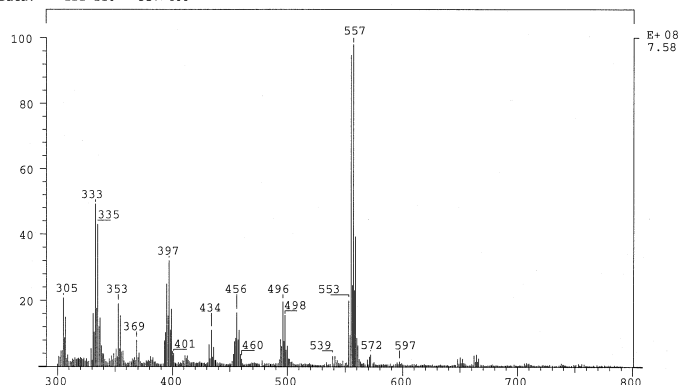
Susanne Striegler,* Michael Dittel

Images of the spectra for characterization of

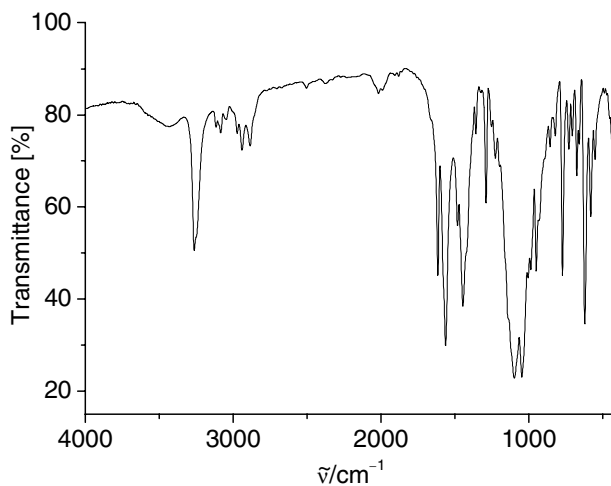
(A) *N,N'*-{1,3-bis[(pyridin-2-ylmethyl)amino]propan-2-ol}ato dicopper(II) (μ -acetato) diperchlorate (**1**), $\text{Cu}_2(\text{bpdpo})$.

FAB mass spectrum

SPEC: dittel25 24-APR-07 DERIVED SPECTRUM #9
 Samp: ppcu I Start : 15:11:10 455
 Comm: Matrix: m-NBA
 Mode: FAB +QIMS LMR UP LR
 Oper: Schmidtberg Client: AC II Inlet :
 Base: 556.7 Inten : 757694144 Masses: 300 > 800
 Norm: 556.7 RIC : 9911780142 #peaks: 619
 Peak: 1000.00 mmu Defect: 0 @ 1, 204 @ 1000
 Data: + 121>220 - 357>400

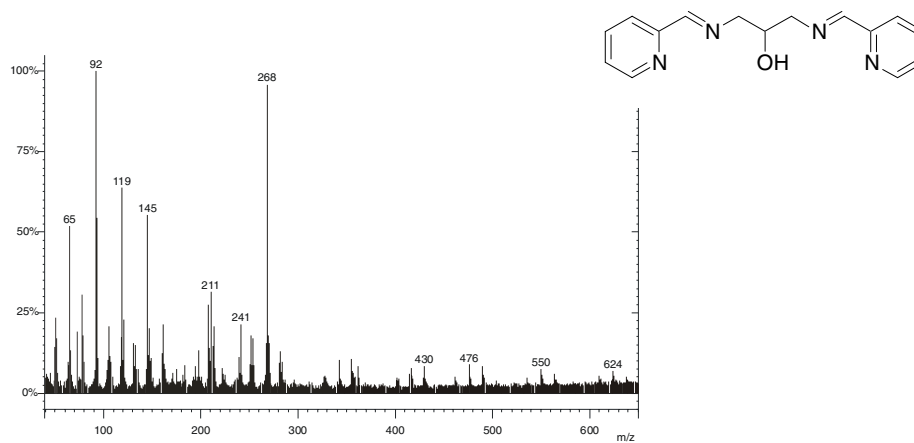
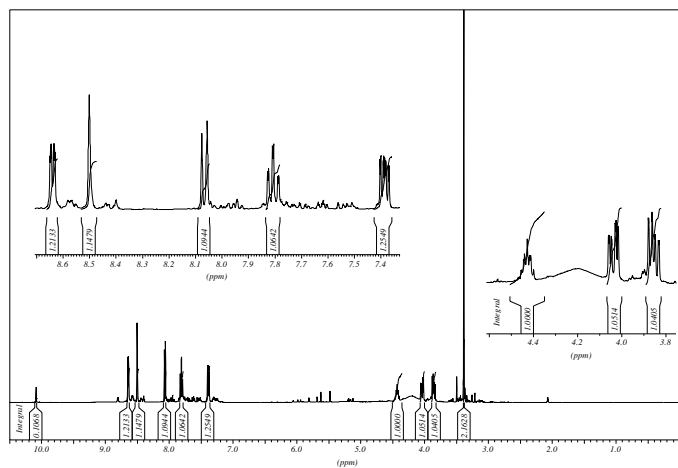
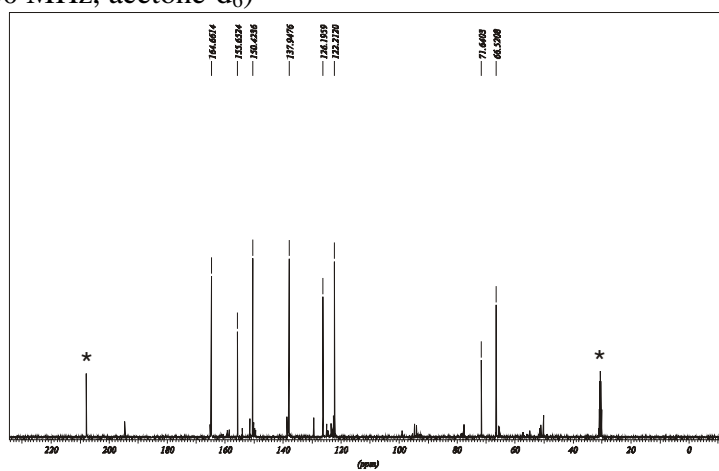


Infra red spectrum (KBr)

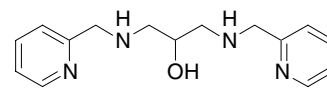


(B) 1,3-bis[(pyridin-2-ylmethylene)amino]propan-2-ol

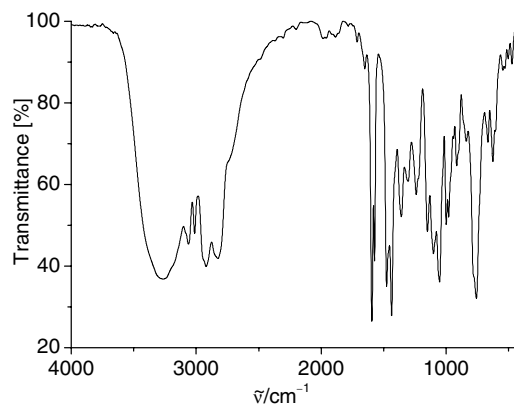
EI mass spectrum

 ^1H NMR spectrum (400 MHz, acetone- d_6) ^{13}C NMR spectrum (100 MHz, acetone- d_6)

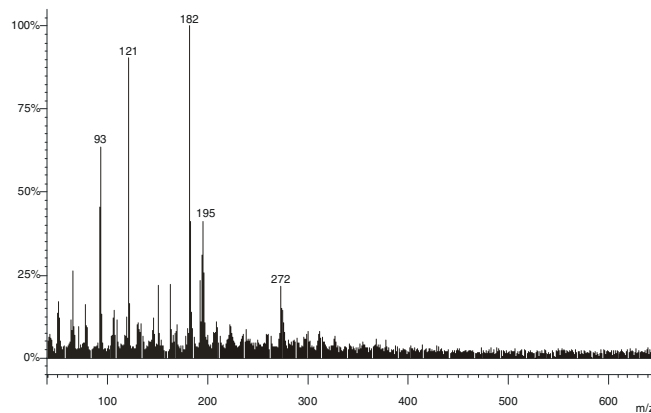
(C) 1,3-bis[(pyridin-2-ylmethyl)amino]propan-2-ol, bdpdo



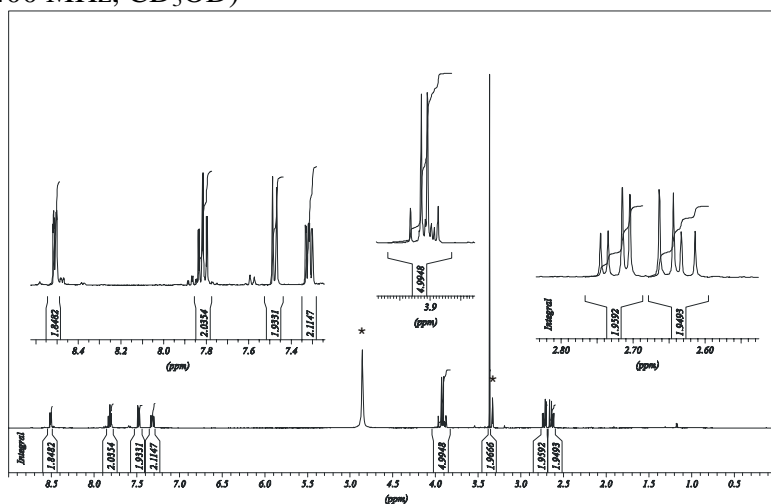
IR spectrum



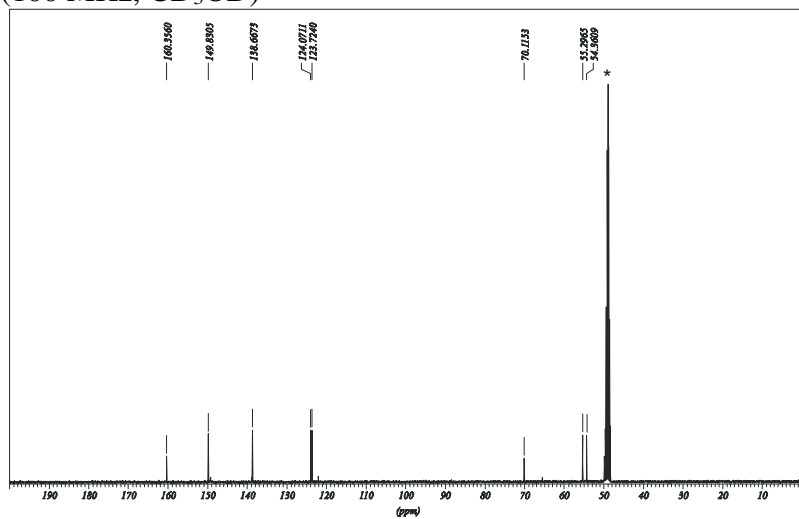
EI mass spectrum



^1H NMR spectrum (400 MHz, CD_3OD)



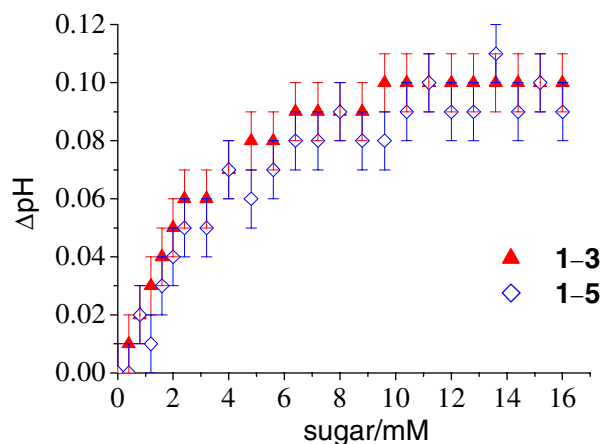
^{13}C NMR spectrum (100 MHz, CD_3OD)



The asterisk corresponds to residual non-deuterated solvent

pH measurements during complex formation

The binuclear copper(II) complex **1** ($M_t = 2\text{mM}$) was titrated with mannose (**3**) or glucose (**5**) solutions, which were separately prepared at pH 12.40. The pH of the resulting solution was measured immediately after mixing.

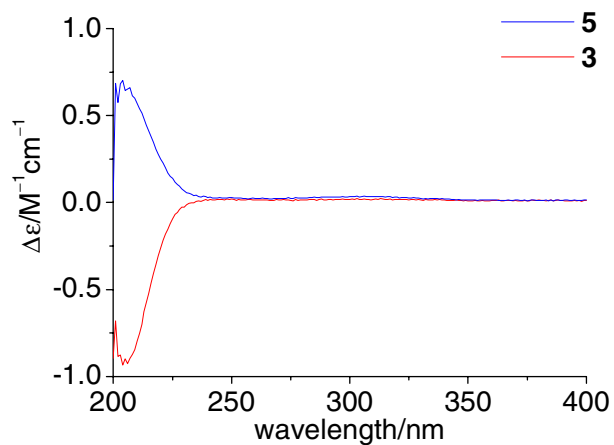


Measured and calculated pH drop during formation of a 1–3 complex

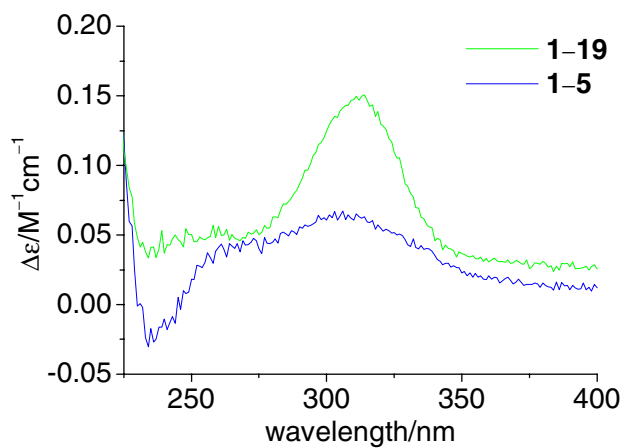
solution	number of protons released	proton release [mM]	pH of the resulting solution
<i>measured</i>			
3	--	--	12.40
1–3	--	--	12.30
<i>calculated</i>			
1–3	--	--	12.31
1–3	1	2	12.05
1–3	2	4	11.79
1–3	3	6	11.47

CD spectra in aqueous solution at pH 12.40 of

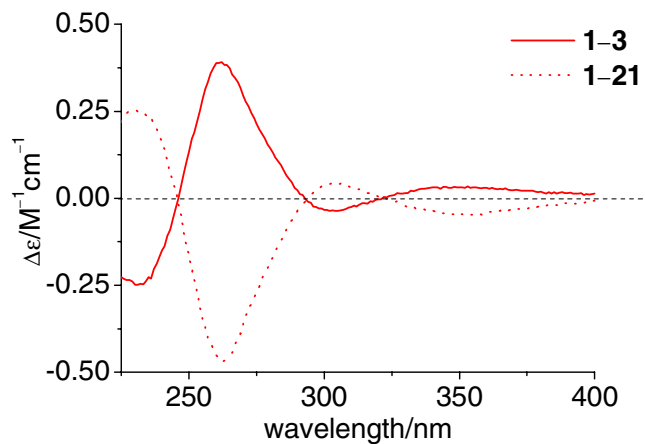
(A) the carbohydrates D-mannose (**3**) and D-glucose (**5**)



(B) the complexes **1-5** and **1-19**



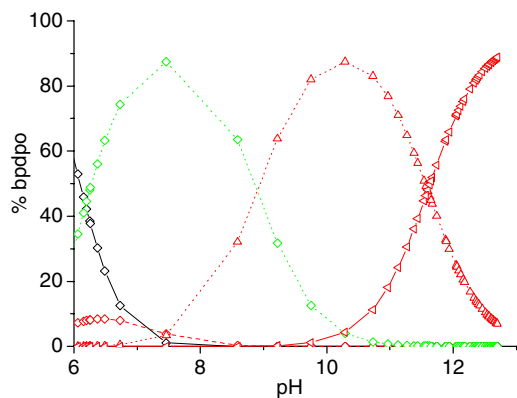
(C) the complexes **1-3** and **1-21** derived from epimeric D-mannose (**3**) and L-mannose (**21**)



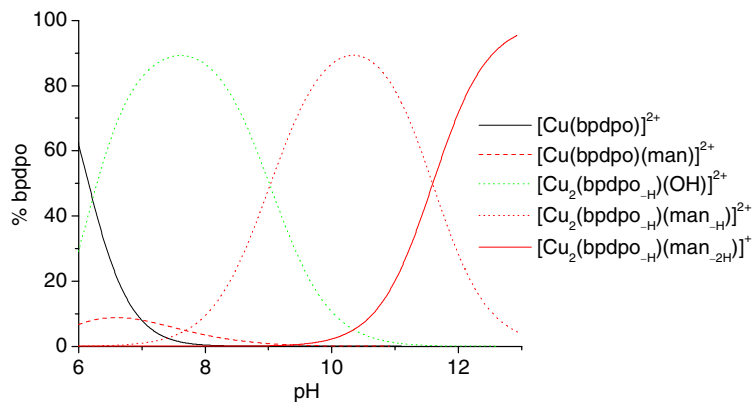
Distribution of species between pH 6 and 13 for

(A) the formation of complexes derived from $\text{Cu}_2(\text{bpdpo})$ (**1**) and mannose (**3**) in a 1:5 molar ratio.

measured:

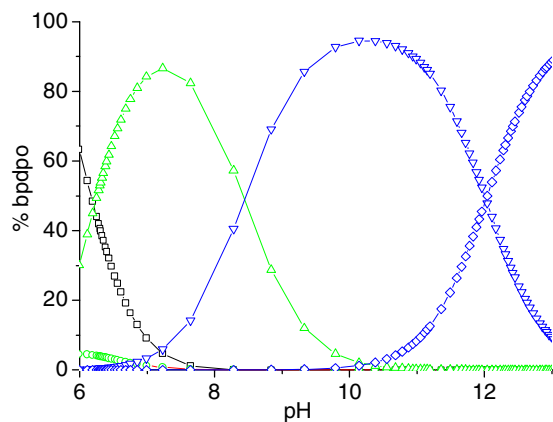


calculated:

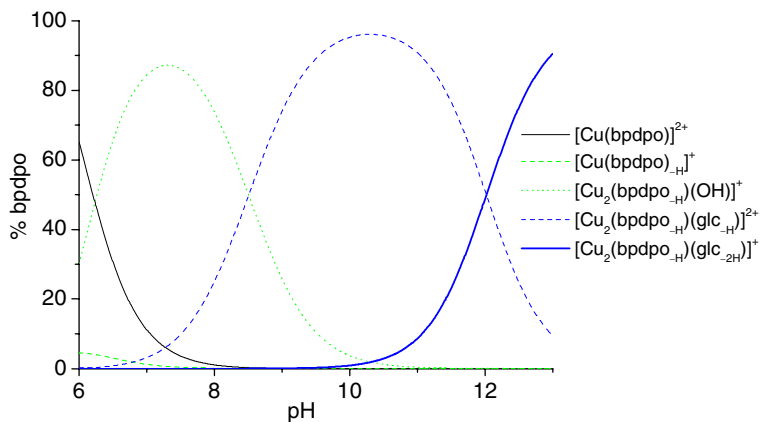


(B) the formation of complexes derived from $\text{Cu}_2(\text{bpdpo})$ (**1**) and glucose (**5**) in a 1:5 molar ratio.

measured:



calculated:



The distributions of species are given in relation to the percentage of bpdpo ligand. Complexes with an amount remaining below 5 % are not shown. Excess of non-bound carbohydrate is omitted for clarity.