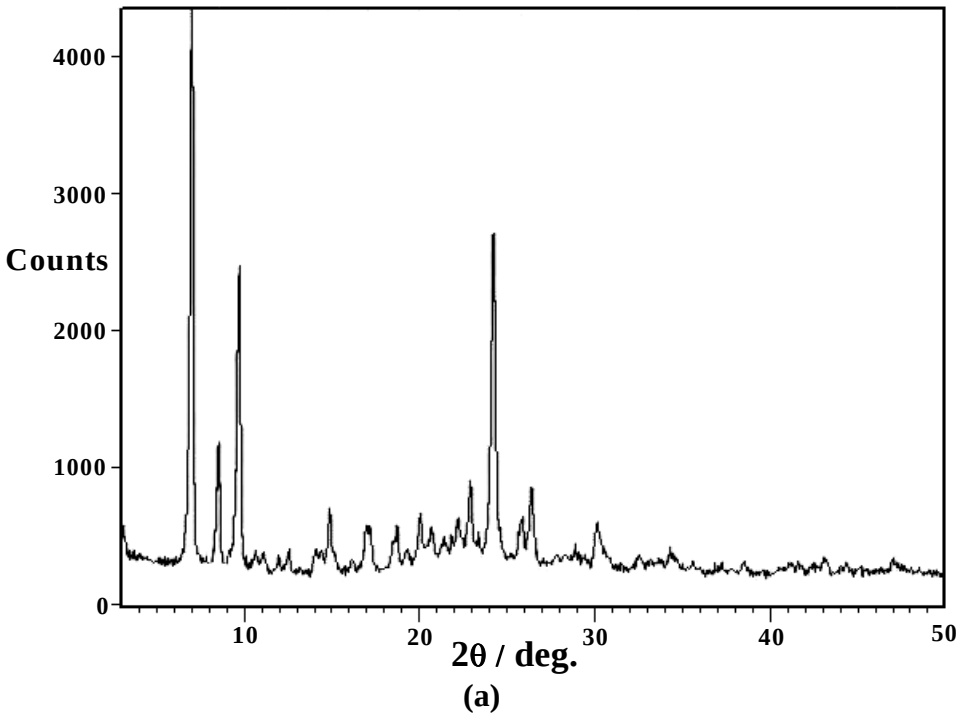
Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supplementary Information

For

Metal complex analogues of crown ethers as the preorganized motif to stabilize aquated proton in solid state

Arpita Jana, Thomas Weyhermueller and Sasankasekhar Mohanta*



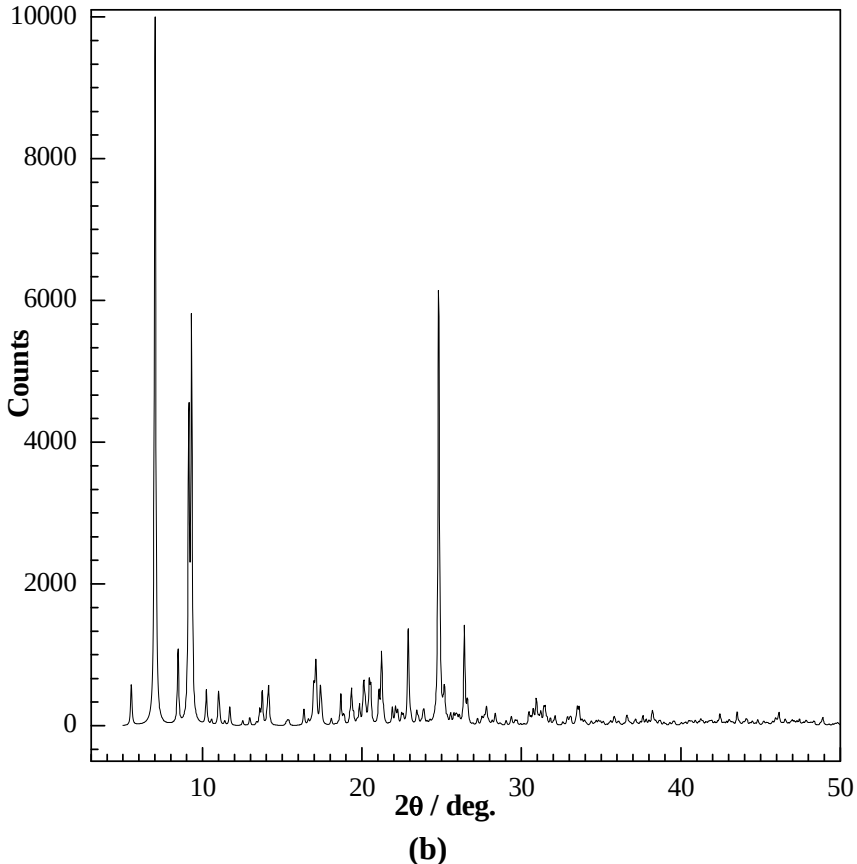
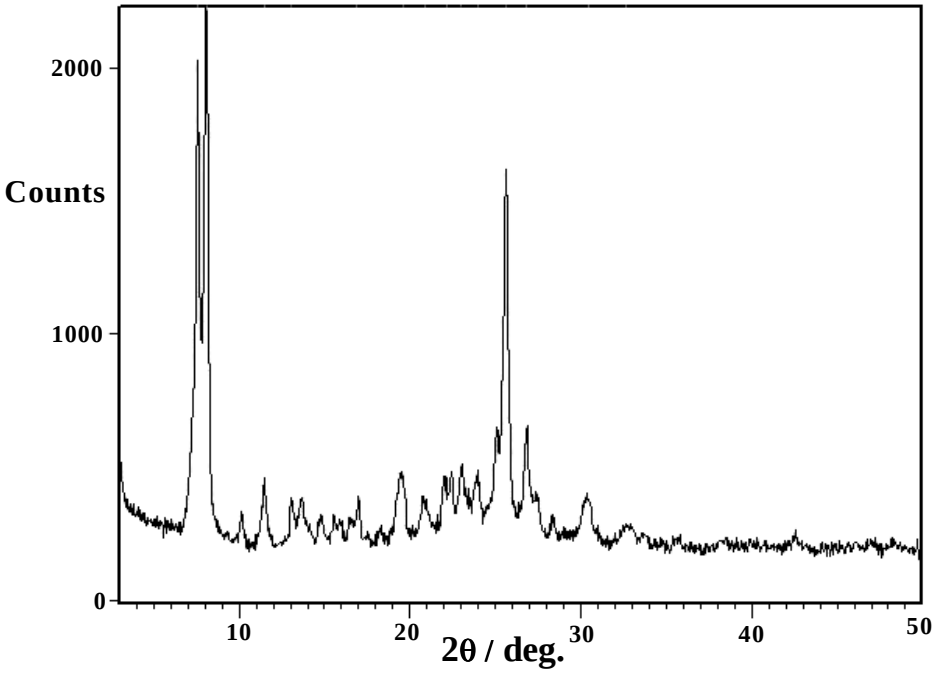
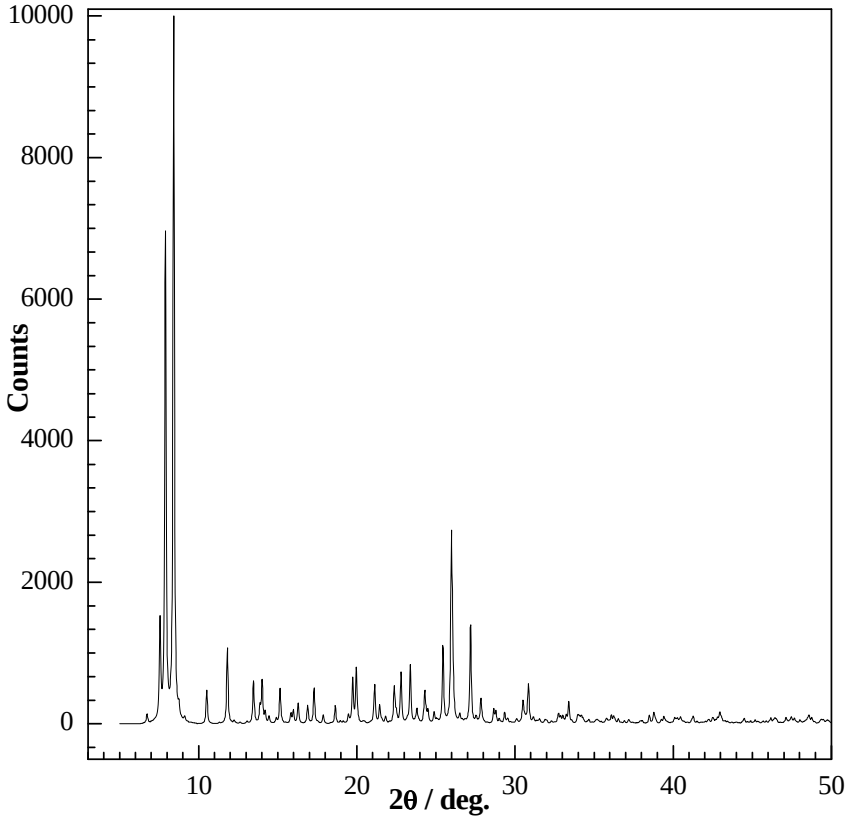


Fig. S1. Powder XRD pattern of $[\{Cu^{II}L^{hex}\}_2(H_5O_2)](ClO_4)$ (**2**): (a) Observed; (b) Simulated (using MERCURY Program) on the basis of single crystal diffraction data.



(a)



(b)

Fig. S2. Powder XRD pattern of $[\{Cu^{II}L^{en}\}_2(H_5O_2)](ClO_4)$ (**3**): (a) Observed; (b) Simulated (using MERCURY Program) on the basis of single crystal diffraction data.

Table S1

Bond lengths (Å) and bond angles (°) for the copper(II) centres of **1** and **2**

Bond lengths			Bond angles		
	1	**2**		**1**	**2**
Cu(1)–O(1)	1.914(2)	1.924(3)	N(1)–Cu(1)–O(2)	177.78(10)	172.86(16)
Cu(1)–O(2)	1.920(2)	1.910(3)	N(2)–Cu(1)–O(1)	177.50(10)	174.74(16)
Cu(1)–N(1)	1.949(3)	1.936(4)	N(1)–Cu(1)–N(2)	84.19(11)	84.11(18)
Cu(1)–N(2)	1.946(3)	1.934(4)	N(1)–Cu(1)–O(1)	93.32(11)	93.73(17)
			N(2)–Cu(1)–O(2)	93.60(10)	92.84(16)
			O(1)–Cu(1)–O(2)	88.90(9)	89.84(14)
Cu(2)–O(5)	1.898(2)	1.893(3)	N(3)–Cu(2)–O(6)	175.39(11)	171.50(15)
Cu(2)–O(6)	1.902(2)	1.889(3)	N(4)–Cu(2)–O(5)	173.19(11)	168.73(16)
Cu(2)–N(3)	1.937(3)	1.913(4)	N(3)–Cu(2)–N(4)	84.16(11)	84.47(17)
Cu(2)–N(4)	1.946(3)	1.935(4)	N(3)–Cu(2)–O(5)	94.04(10)	93.53(15)
			N(4)–Cu(2)–O(6)	93.60(10)	93.55(15)
			O(5)–Cu(2)–O(6)	88.65(9)	89.99(13)

Table S2

Bond lengths (Å) and bond angles (°) for the copper(II) centres of **3**

Unit-I		**Unit-II**	
Cu(1)–O(1)	1.914(2)	Cu(3)–O(9)	1.920(2)
Cu(1)–O(2)	1.941(2)	Cu(3)–O(10)	1.931(2)
Cu(1)–N(1)	1.947(3)	Cu(3)–N(5)	1.940(3)
Cu(1)–N(2)	1.931(3)	Cu(3)–N(6)	1.937(3)
Cu(2)–O(5)	1.924(2)	Cu(4)–O(13)	1.934(2)
Cu(2)–O(6)	1.902(2)	Cu(4)–O(14)	1.903(2)
Cu(2)–N(3)	1.930(3)	Cu(4)–N(7)	1.933(3)
Cu(2)–N(4)	1.938(3)	Cu(4)–N(8)	1.941(3)
N(1)–Cu(1)–O(2)	175.41(11)	N(5)–Cu(3)–O(10)	174.83(11)
N(2)–Cu(1)–O(1)	176.44(11)	N(6)–Cu(3)–O(9)	176.65(11)
N(1)–Cu(1)–N(2)	84.00(12)	N(5)–Cu(3)–N(6)	84.17(12)
N(1)–Cu(1)–O(1)	92.48(11)	N(5)–Cu(3)–O(9)	92.49(11)
N(2)–Cu(1)–O(2)	92.44(11)	N(6)–Cu(3)–O(10)	92.14(11)
O(1)–Cu(1)–O(2)	91.10(9)	O(9)–Cu(3)–O(10)	91.20(9)
N(3)–Cu(2)–O(6)	176.95(12)	N(7)–Cu(4)–O(14)	177.01(13)
N(4)–Cu(2)–O(5)	173.75(12)	N(8)–Cu(4)–O(13)	172.94(12)
N(3)–Cu(2)–N(4)	84.69(13)	N(7)–Cu(4)–N(8)	84.19(15)
N(3)–Cu(2)–O(5)	92.06(11)	N(7)–Cu(4)–O(13)	92.21(13)
N(4)–Cu(2)–O(6)	92.95(12)	N(8)–Cu(4)–O(14)	92.91(13)
O(5)–Cu(2)–O(6)	90.46(10)	O(13)–Cu(4)–O(14)	90.75(10)

Table S3

The O–H distances (Å) in $H_5O_2^+$ moiety involving the central hydrogen atom in **1**–**3**

	1	**2**	**3, Unit-I**	**3, Unit-II**
O(1W)–H(1WC)	0.82(5)	1.11(8)	1.132	
O(2W)···H(1WC)	1.66(5)	1.40(8)	1.352	
O(3W)–H(3WC)				1.019
O(4W)···H(3WC)				1.446