

ESI-Tab-1 Cremer & Pople puckering and asymmetry parameters* for all the complexes. The puckering parameters are denoted by Q (Å⁰), θ(°) and φ(°). In each case (i) represents the saccharide six membered ring and (ii) represents the 4,6-O-protected six membered ring..

	Six membered rings	Q(Å ⁰), θ(°), φ(°)
1a (i)	O10-C36-C30-C29-C28-C38	0.580, 176.21, 55.27
	O5-C9-C3-C2-C1-C11	0.568A, 179.21, 85.59
(ii)	C36-C30-O11-C31-O12-C35	0.548, 5.12, 69.088
	C3-C9-C8-O8-C4-O7	0.532, 3.23, 117.063
2a (ii)	O6-C30-C39-C38-C37-C31	0.593A, 3.10, 2.13
	O3-C9-C3-C2-C1-C10	0.587A, 175.97, 87.93
(ii)	C37-C31-C32-O9-C33-O10	0.568, 175.82, 46.28
	C3-C9-C8-O8-C4-O7	0.594, 2.99, 83.33
3a (i)	O8-C12-C13-C14-C15-C16	0.613, 5.17, 87.78
	O3-C31-C32-C33-C34-C35	0.587, 1.83, 1.07
(ii)	C15-C16-C17-O7-C18-O6	0.590, 1.98, 112.97
	C35-C36-O2-C37-O1-C34	0.564, 1.47, 30.17
4a (A) (i)	O11C-C10C-C16C-C14C-C13C-C12C	0.617, 2.55, 331.83
	O11D-C10D-C16D-C14D-C13D-C12D	0.590, 3.58°, 347.75
(ii)	C13D-C12D-C22D-O21D-C19D-O18D	0.602, 1.29, 174.50
	C13C-C12C-C22C-O21C-C19C-O18C	0.588, 3.07, 300.65
(B) (i)	O11A-C10A-C16A-C14A-C13A-C12A	0.616, 1.59, 335.72
	O11B-C10B-C16B-C14B-C13B-C12B	0.596, 2.60, 355.71°
(ii)	C12B-C13B-O18B-C19B-O21B-C22B	0.596, 1.25, 15.68
	C12A-C13A-O18A-C19A-O21A-C22A	0.583, 2.57, 36.65
4b (i)	O11B-C10B-C16B-C14B-C13B-C12B	0.579, 4.63, 351.42
	O11A-C10A-C16A-C14A-C13A-C12A	0.590, 3.90°, 304.97
(ii)	C12A-C13A-O18A-C19A-O21A-C22A	0.584, 3.11, 308.09
	C12A-C13A-O18A-C19A-O21A-C22A	0.587, 1.55, 92.54
5a (i)	O12A-C11A-C17A-C15A-C14A-C13A	0.604, 1.20, 357.63
	O12B-C11B-C17B-C15B-C14B-C13B	0.611, 1.87, 28.42
(ii)	C14A-C13A-C23A-O22A-C20A-O19A	0.601, 3.85, 31.73
	C14B-C13B-C23B-O22B-C20B-O19B	0.593, 1.64, 162.21
5b (i)	O12B-C11B-C17B-C15B-C14B-C13B	0.573, 6.97, 359.05
	O12A-C11A-C17A-C15A-C14A-C13A	0.579, 1.95, 29.54
(ii)	C14A-C13A-C23A-O22A-C20A-O19A	0.579, 2.14, 341.27
	C14B-C13B-C23B-O22B-C20B-O19B	0.562, 6.39, 92.18

*ΔCs(I-J) are Asymmetry parameters for bond I-J and it is found to be zero for the atoms separated by two atoms. A refers to **4a-2** and B refers to **4a-1**

ESI-Tab-2 The torsional angles (Å) for one of the dimeric copper complex unit **4a-1**

O(1A)-Cu(1)-Cu(2)-O(1B)	160.4(3)	N(9A)-Cu(1)-O(1A)-C(2A)	1.2(4)
N(9A)-Cu(1)-Cu(2)-O(1B)	-7.8(2)	O(17B)-Cu(1)-O(1A)-C(2A)	-177.8(4)
O(17B)-Cu(1)-Cu(2)-O(17A)	-173.7(2)	O(17A)-Cu(1)-O(1A)-C(2A)	-97.4(16)
O(1A)-Cu(1)-Cu(2)-N(9B)	-6.7(2)	C(7B)-C(2B)-O(1B)-Cu(2)	-10.0(7)
N(9A)-Cu(1)-Cu(2)-N(9B)	-174.9(2)	O(17A)-Cu(2)-O(1B)-C(2B)	-164.5(4)
O(1A)-C(2A)-C(7A)-C(6A)	-179.4(5)	N(9B)-Cu(2)-O(1B)-C(2B)	13.2(4)
O(1A)-C(2A)-C(7A)-C(8A)	1.8(9)	O(17B)-Cu(2)-O(1B)-C(2B)	-70.2(19)
O(1B)-C(2B)-C(7B)-C(6B)	176.5(5)	C(10A)-C(16A)-O(17A)-Cu(2)	178.5(3)
O(1B)-C(2B)-C(7B)-C(8B)	-0.5(8)	C(10A)-C(16A)-O(17A)-Cu(1)	46.4(4)
C(2A)-C(7A)-C(8A)-N(9A)	-1.5(9)	O(1B)-Cu(2)-O(17A)-C(16A)	37.4(5)
C(2B)-C(7B)-C(8B)-N(9B)	3.6(8)	N(9B)-Cu(2)-O(17A)-C(16A)	-133.6(6)
N(9A)-C(10A)-C(16A)-O(17A)	-50.4(5)	O(17B)-Cu(2)-O(17A)-C(16A)	-138.5(5)
N(9B)-C(10B)-C(16B)-O(17B)	-54.1(5)	Cu(1)-Cu(2)-O(17A)-C(16A)	-134.3(5)
C(7A)-C(8A)-N(9A)-Cu(1)	1.2(8)	O(1B)-Cu(2)-O(17A)-Cu(1)	171.71(16)
C(16A)-C(10A)-N(9A)-C(8A)	-148.6(5)	N(9B)-Cu(2)-O(17A)-Cu(1)	0.8(7)
C(16A)-C(10A)-N(9A)-Cu(1)	30.4(4)	O(17B)-Cu(2)-O(17A)-Cu(1)	-4.14(16)
O(1A)-Cu(1)-N(9A)-C(8A)	-0.9(5)	O(1A)-Cu(1)-O(17A)-C(16A)	74.2(17)
O(17B)-Cu(1)-N(9A)-C(8A)	175.2(6)	N(9A)-Cu(1)-O(17A)-C(16A)	-24.8(3)
O(17A)-Cu(1)-N(9A)-C(8A)	174.5(4)	O(17B)-Cu(1)-O(17A)-C(16A)	155.4(3)
Cu(2)-Cu(1)-N(9A)-C(8A)	171.3(4)	O(1A)-Cu(1)-O(17A)-Cu(2)	-77.0(16)
O(1A)-Cu(1)-N(9A)-C(10A)	-179.9(3)	N(9A)-Cu(1)-O(17A)-Cu(2)	-176.02(18)
O(17B)-Cu(1)-N(9A)-C(10A)	-3.7(9)	O(17B)-Cu(1)-O(17A)-Cu(2)	4.17(16)
O(17A)-Cu(1)-N(9A)-C(10A)	-4.5(3)	C(10B)-C(16B)-O(17B)-Cu(1)	179.1(3)
Cu(2)-Cu(1)-N(9A)-C(10A)	-7.6(4)	C(10B)-C(16B)-O(17B)-Cu(2)	47.9(4)
C(7B)-C(8B)-N(9B)-C(10B)	176.8(5)	O(1A)-Cu(1)-O(17B)-C(16B)	37.7(5)
C(7B)-C(8B)-N(9B)-Cu(2)	3.9(7)	N(9A)-Cu(1)-O(17B)-C(16B)	-138.4(6)
C(16B)-C(10B)-N(9B)-C(8B)	-139.0(5)	O(17A)-Cu(1)-O(17B)-C(16B)	-137.6(5)
C(16B)-C(10B)-N(9B)-Cu(2)	34.8(5)	O(1A)-Cu(1)-O(17B)-Cu(2)	171.22(17)
O(1B)-Cu(2)-N(9B)-C(8B)	-10.3(5)	N(9A)-Cu(1)-O(17B)-Cu(2)	-4.9(8)
O(17A)-Cu(2)-N(9B)-C(8B)	160.7(5)	O(17A)-Cu(1)-O(17B)-Cu(2)	-4.12(16)
O(17B)-Cu(2)-N(9B)-C(8B)	165.6(5)	O(1B)-Cu(2)-O(17B)-C(16B)	60.1(18)
O(1B)-Cu(2)-N(9B)-C(10B)	176.1(3)	O(17A)-Cu(2)-O(17B)-C(16B)	155.1(3)
O(17A)-Cu(2)-N(9B)-C(10B)	-12.9(9)	N(9B)-Cu(2)-O(17B)-C(16B)	-23.7(3)
O(17B)-Cu(2)-N(9B)-C(10B)	-8.0(3)	O(1B)-Cu(2)-O(17B)-Cu(1)	-90.8(18)
C(7A)-C(2A)-O(1A)-Cu(1)	-1.8(7)	O(17A)-Cu(2)-O(17B)-Cu(1)	4.17(16)

ESI-Tab-3 Conformation of the chelates formed in the dinuclear copper complexes.

Complex	Chelate	Conformation
1a	Cu2-N4-C49-C48-C39-O4	Skew-Boat
	Cu1-N3-C22-C21-C12-O3	<i>B</i>
	Cu2-O1-C28-C38-N4	<i>C₂</i>
	Cu1-O2-C1-C11-N3	<i>C₂</i>
2a	Cu2-O12-C11-C16-C17-N1	<i>B</i>
	Cu1-O11-C23-C28-C29-N2	<i>B</i>
	Cu2-N1-C10-C1-O1	<i>C₂</i>
	Cu1-N2-C30-C39-O2	<i>C₂</i>
3a	Cu1-N2-C30-C26-C27-O12	<i>B</i>
	Cu2-N1-C11-C10-C9-O11	<i>B</i>
	Cu1-O5-C32-C31-N2	<i>C₂</i>
	Cu2-O10-C13-C12-N1	<i>C₂</i>
4a	Cu3-O1c-C2c-C7c-C8c-N9c	Chair
	Cu3-N9c-C10c-C16c-O17c	<i>C_s</i>
	Cu4-O1d-C2d-C7d-C8d-N9d	Skew-Boat
	Cu4-N9d-C10d-C16d-O17d	<i>C_s</i>
	Cu1-O1a-C2a-C7a-C8a-N9a	Chair
	Cu1-N9a-C10a-C16a-O17a	<i>C_s</i>
	Cu2-N9b-C10b-C16b-O17b	<i>C_s</i>
	Cu2-O1b-C2b-C7b-C8b-N9b	Skew-Boat
4b	Cu1-N9a-C8a-C7a-C2a-O1a	Skew-Boat
	Cu2-N9b-C8b-C7b-C2b-O1b	<i>B</i>
	Cu1-O17a-C16a-C10a-N9a	<i>C_s</i>
	Cu2-O17b-C16b-C10b-N9b	<i>C₂</i>
5a	Cu2-O1b-C2b-C8b-C9b-N10b	<i>B</i>
	Cu2-N10b-C11b-C17b-O18b	<i>C_s</i>
	Cu1-O18a-C17a-C11a-N10a	<i>C_s</i>
	Cu1-N10a-C9a-C8a-C2a-O1a	Skew-Boat
5b	Cu1-N10a-C9a-C8a-C2a-O1a	<i>B</i>
	Cu2-O18b-C17b-C11b-N10b	<i>C_s</i>
	Cu2-N10b-C9b-C8b-C2b-O1b	Skew-Boat
	Cu1-O18a-C17a-C11a-N10a	<i>C_s</i>

[#]*C₂* = half-chair form; *C_s* = envelop form; *B* = Boat

ESI-Tab-4 Deviation of the copper centers from the coordinated plane in the dinuclear copper complexes.

Complex	Deviation (Å) of the copper center from the mean plane $O_{Sacch}-O_{Sacch}-$ $O_{Phen}-N_{Imine}$
1a	(Cu1) = -0.2785(0.0043) (Cu2) = +0.331(0.0045)
2a	(Cu1) = +0.2941(0.0048) (Cu2) = -0.3060(0.0050)
3a	(Cu1) = -0.0209(0.0025) (Cu2) = +0.0377(0.0023)
4a	(Cu1) = -0.0418(0.0020) (Cu2) = -0.0492(0.0021) (Cu3) = 0.0138(0.0021) (Cu4) = 0.1281(0.0020)
4b	(Cu1) = -0.2304(0.0038) (Cu2) = -0.2221(0.0040)
5a	(Cu1) = 0.0227(0.0020) (Cu2) = 0.1271(0.0022)
5b	(Cu1) = 0.2931(0.0047) (Cu2) = -0.2052(0.0044)

ESI-Tab-5 Hydrogen bond data for dinuclear copper complexes. D and A refer to the donor and acceptor of hydrogen respectively.

D-H...A	d(H..A)(Å)	d(D..A) (Å)	<(DHA) ^o	Symmetry
1a				
O(6)-H(6)...O(2)	2.594	2.993	111.4	
O(6)-H(6)...O(4)	1.972	2.763	161.7	
O(9)-H(9A)...O(3)	1.995	2.807	170.4	
C(25)-H(25)...O(6)	2.552	3.228	129.8	1+x,y,z
2a				
O(5)-H(50)...O(12)	2.017	2.703	170.9	
C(18)-H(18)#...O(12)	2.588	3.192	116.8	
C(17)-H(17)...O(3)	2.344	2.773	106.6	
O(4)-H(40)...O(11)	1.97	2.717	165.0	
3a				
O(13)-H(131)...O(4)	2.570	2.896	121.0	
O(13)-H(131)...O(14)	2.210	2.641	137.0	
O(13)-H(132)...O(14)	1.840	2.839	162.0	-1+x, y, z
O(9)-H(90)...O(12)	1.982	2.703	146.4	
C(4)-H(4)...O(7)	2.541	3.465	172.0	2-x,1/2+y,-z
C(12)-H(12)...O(9)	2.446	3.394	162.4	1+x,y,z
C(16)-H(16)...O(9)	2.597	3.475	149.1	1+x,y,z
4a				
O(15a)-H(15a)...O(1b)	1.851	2.685	173.0	.
O(15b)-H(15b)...O(1a)	1.853	2.675	165.5	.
O(15c)-H(15c)...O(1d)	1.881	2.708	166.8	.
O(15d)-H(15d)...O(1c)	1.842	2.680	173.3	.
C(10c)-H(10c)...O(15b)	2.389	3.376	169.2	1-x, -1/2+y, 1/2-z
C(12b)-H(12b)-O(18a)	2.505	3.496	170.8	1/2+x, 3/2-y, -z
C(16a)-H(16a)...O(18d)	2.594	3.585	170.7	-x, 1/2+y, 1/2-z
C(19b)-H(19b)...O(18c)	2.597	3.570	164.3	1-z, 1/2+y, 1/2-z
C(32)-H(32b)...O(15d)	2.493	3.409	155.4	-x, -1/2+y, 1/2-z
4b				
O(15a)-H(15a)...O(1b)	1.834	2.672	179.5	.
O(15b)-H(15b)...O(1a)	1.870	2.678	162.9	.
C(6b)-H(6b)...O(21a)	2.518	3.410	156.3	x, -1+y, z
C(12b)-H(12b)...N(60)	2.529	3.471	156.8	-1/2+x, 1/2-y, -z
5a				
O(16a)-H(16a)...O(1b)	1.903	2.728	167.3	.
O(16b)-H(16b)...O(1a)	1.886	2.690	160.1	.
O(16c)-H(16c)...O(1d)	1.875	2.661	156.1	.
O(16d)-H(16d)...O(1c)	1.882	2.691	163.1	.
O(41)-H(41)...O(51)	2.208	2.772	124.6	x, -1+y, z
O(51)-H(51)...O(41)	1.955	2.772	163.9	x, 1+y, z
O(61)-H(61)...O(71)	1.962	2.782	164.8	1+x, y, z
O(71)-H(71)...O(16b)	1.858	2.692	171.7	-1+x, -1+y, z
C(9c)-H(9c)...Br(6d)	2.776	3.619	148.4	x, y, -1+z
C(11b)-H(11b)-O(16d)	2.243	3.229	168.4	.
C(15a)-H(15a)...O(12c)	2.576	3.559	167.3	.
C(23c)-H(23e)...O(19a)	2.524	3.505	171.0	.
C(60)-H(60a)...O(19a)	2.551	3.349	138.5	1+x, y, z
C(70)-H(70c)...O(19b)	2.586	3.304	130.2	-1+x, -1+y, z
5b				
O(16a)-H(16a)...O(1b)	1.961	2.760	158.8	.
O(16b)-H(16b)...O(1a)	1.886	2.705	164.3	.
O(16c)-H(16c)...O(1d)	1.891	2.694	159.2	.
C(16d)-H(16d)...O(1c)	1.960	2.762	159.2	.

FIGURE CAPTIONS FOR ESI

ESI-Fig-1 (a) ^1H NMR spectra for the ligand H_3L^2 and (b) its copper complex **2**.

ESI-Fig-2 (a) Circular dichroism spectra for $\text{H}_3\text{L}^2(10^{-3}\text{M})$, (i) and **2** (10^{-3}M), (ii). (b) The corresponding UV-Visible absorption spectra for $\text{H}_3\text{L}^2(10^{-4}\text{M})$, (iii), and **2** (10^{-4}M and 10^{-3}M), (iv). The spectrum labeled as (v) is an expanded version for **2** in the visible region.

ESI-Fig-3 ORTEP structures for **4a**. The structure is one of the dinuclear copper complex **4a-1** present in the asymmetric unit. The copper center in this structure is square planar. No fifth ligand is present on any copper centers.

ESI-Fig-4 ORTEP structures for, **4a** The structure is one of the dinuclear copper complex **4a-2** present in the asymmetric unit. One of the copper center has the square pyramidal geometry and the other has the square planar geometry, DMSO acts as the fifth ligand.

ESI-Fig-5 Molecular structure of, **2a** is drawn using ORTEP. In the structure the coordination geometry around copper center is square pyramidal and the pyridine molecules are oriented in a direction opposite to each other with respect to the Cu_2O_2 core.

ESI-Fig-6 Molecular structure of, **4b** as drawn using ORTEP. In the complex the coordination geometry around copper center is square pyramidal. The pyridine molecules are oriented in syn-orientation with respect to the Cu_2O_2 core

ESI-Fig-7 Molecular structure of, **5b** as drawn using ORTEP. In the complex the coordination geometry around copper center is square pyramidal. The pyridine molecules are oriented in an opposite direction with respect to Cu_2O_2 core.

ESI-Fig-8 Stereo view of one of the dinuclear copper complex units **4a-1** present in the asymmetric unit cell of **4a** as prepared by ORTEP using 50% ellipsoid probability.

ESI-Fig-9 Correlation between the $\text{Cu}\dots\text{Cu}$ (\AA) distance and $\text{Cu}\dots\text{O}_{\text{sacch}}\dots\text{Cu}$ angle ($^\circ$) observed in case of the complexes reported in this paper.

ESI-Fig-10 Hydrogen bond data correlations in the dinuclear copper complexes reported in this paper: triangles represent $\text{O-H}\dots\text{O}$ and squares represent $\text{C-H}\dots\text{O}$ interactions. The $d-\theta$ scatter plot for the hydrogen bond interactions is shown.

ESI-Fig-11 The lattice structure for **3a**, showing the intermolecular $\text{C-H}\dots\text{O}$ interactions, where the cavity formed between the adjacent molecules is filled with water molecules. One of the water molecules is interacting with the C-3-O of the glyco-unit. The two water molecules are shown as filled circle.