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Direct Evidence of Oxygen Vacancies in a New Family of BICUWOX Compounds

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Crystallographic data in CIF format for $Bi_4Cu_{1/3}W_{2/3}O_{8-\delta}Cl$; table with relations between the point group, the zone axis and the ideal symmetry in the tetragonal system (Table S1); table of measured coordinates from the ESW-phase image along [100] for $[Bi_2O_2Cl][Bi_2W/CuO_{6-\delta}]_2$ phase (Table S2); plot of the magnetic susceptibility vs temperature for $Bi_4Cu_{1/3}W_{2/3}O_{8-\delta}Cl$. This material is available free of charge via the Internet at http://pubs.acs.org.

Table S1. Relations between the point group, the zone axis and the ideal symmetry in the tetragonal system after ref. [25]. The BF (Bright Field) symmetry is indicated between brackets.

	[001]	**<100>**	**<110>**	**[0vw]**	**[uv0]**	**[uuw]**	**[uvw]**
4/mmm	4mm (4mm)	2mm (2mm)	2mm (2mm)	m (2mm)	m (2mm)	m (2mm)	1 (2)
-42m	2mm (4mm)	2 (2mm)	m (m)	1 (m)	1 (m)	m (m)	1 (1)
4mm	4mm (4mm)	m (m)	m (m)	m (m)	1 (m)	m (m)	1 (1)
422	4 (4)	2 (2mm)	2 (2mm)	1 (m)	1 (m)	1 (m)	1 (1)
4/m	2 (4)				m (2mm)		1 (2)
-4	2 (4)				1 (m)		1 (1)
4	4 (4)				1 (m)		1 (1)

Table S2. Measured coordinates from the ESW-phase image along [100] for $[Bi_2O_2Cl][Bi_2W/CuO_{6-\delta}]_2$ phase (see Figure 5a).

Atom	Wyckoff	x	y	z
Cl1	1*a*	0	0	0
Cl2	1*d*	1/2	1/2	1/2
W1/Cu1	2*h*	1/2	1/2	0.15
W2/Cu2	2*g*	0	0	0.33
Bi1	2*h*	1/2	1/2	0.04
Bi2	2*g*	0	0	0.09
Bi3	2*g*	0	0	0.22
Bi4	2*h*	1/2	1/2	0.26
Bi5	2*h*	1/2	1/2	0.39
Bi6	2*g*	0	0	0.45
O1	4*i*	1/2	0	0.15
O2	2*h*	1/2	1/2	0.18
O3	2*h*	1/2	1/2	0.12
O4	4*i*	1/2	0	0.33
O5	2*g*	0	0	0.36
O6	2*g*	0	0	0.29
O7	4*i*	1/2	0	0.06
O8	4*i*	0	1/2	0.24
O9	4*i*	1/2	0	0.42
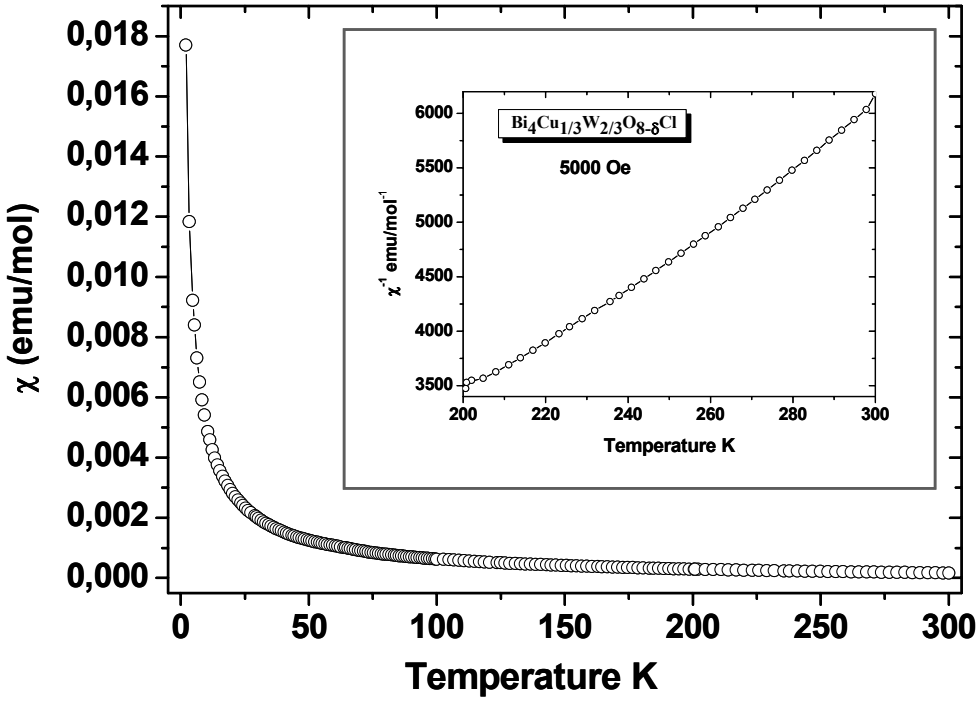
Figure S1 Plot of the magnetic susceptibility vs temperature. The inset shows the linear part of the χ^{-1} curve for the sample.