Supporting material

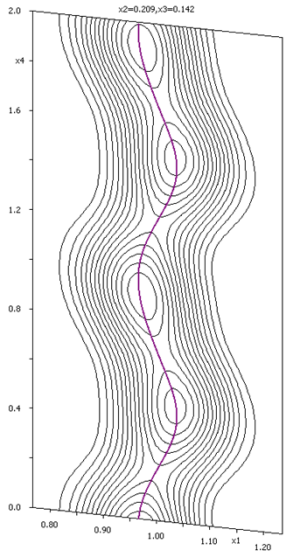
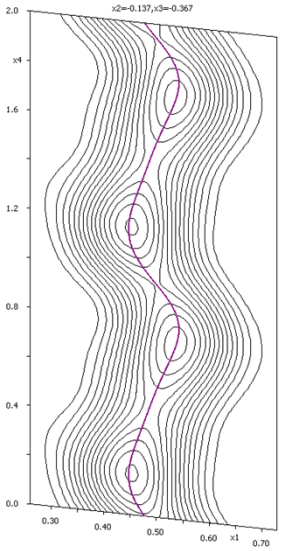
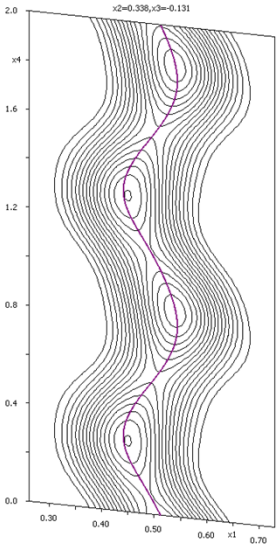
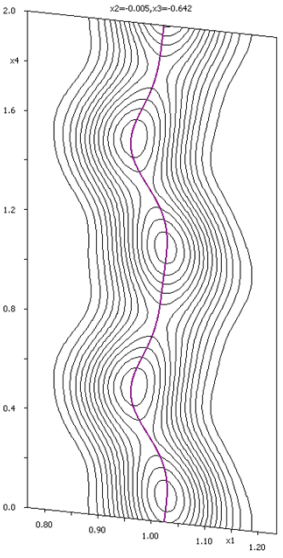
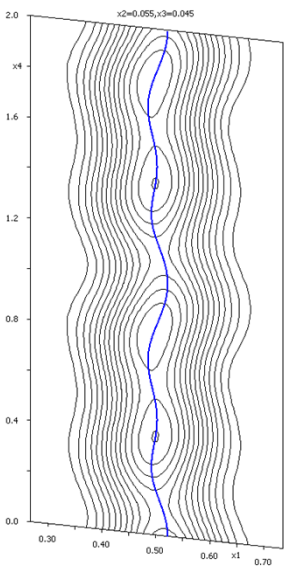
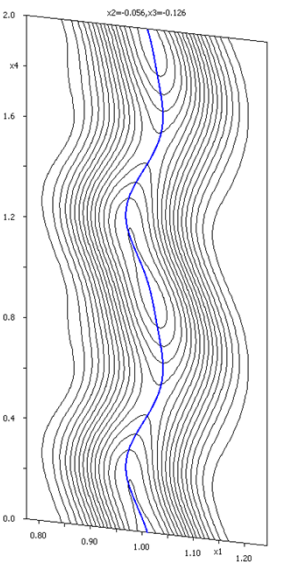
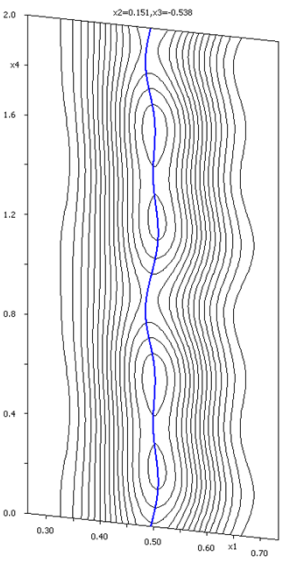
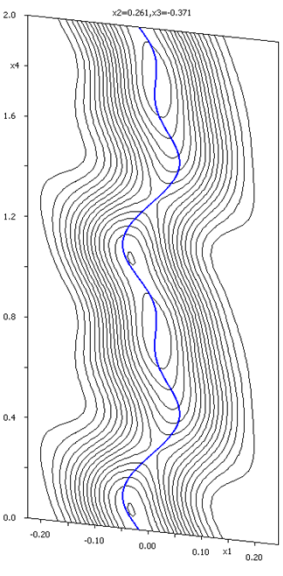
Synthesis and crystal structure of a series of incommensurately modulated composite oxohalide compounds

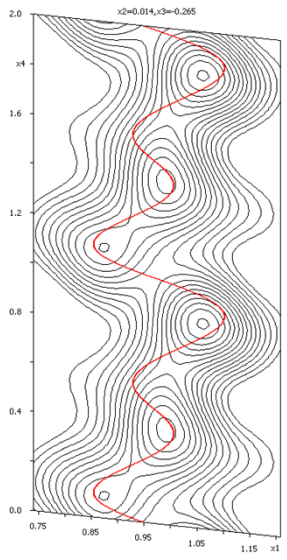
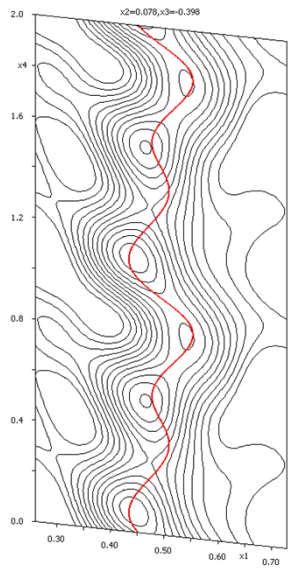
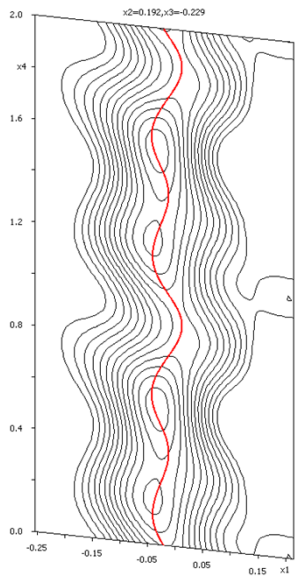
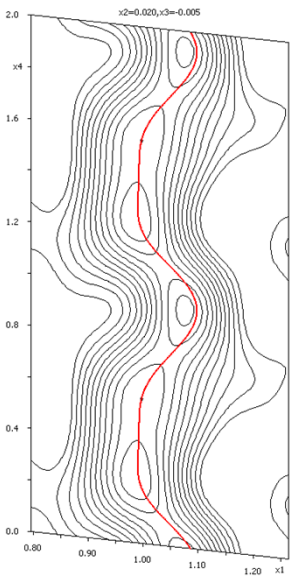
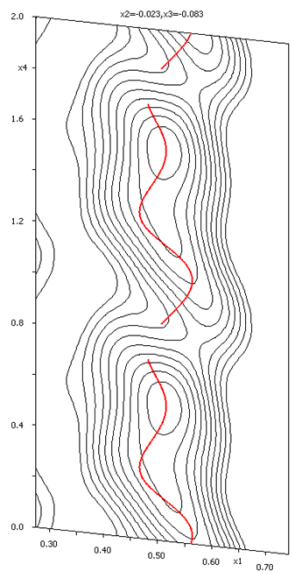
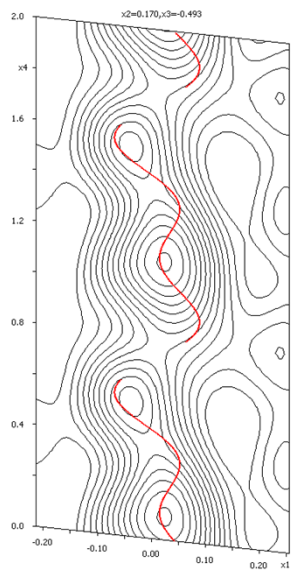
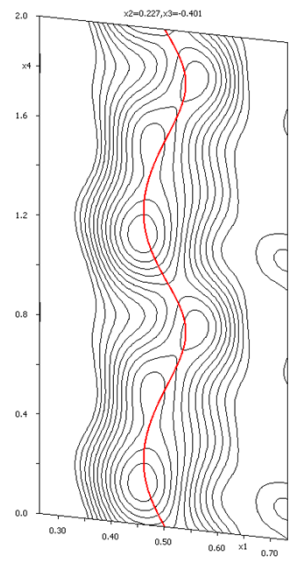
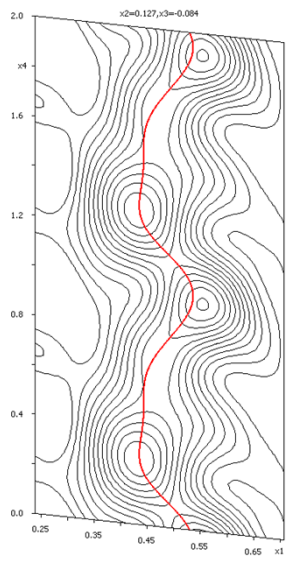
Iwan Zimmermann[a], Alexis Corgnet[a], Mats Johnsson[a*], Sven Lidin[b]

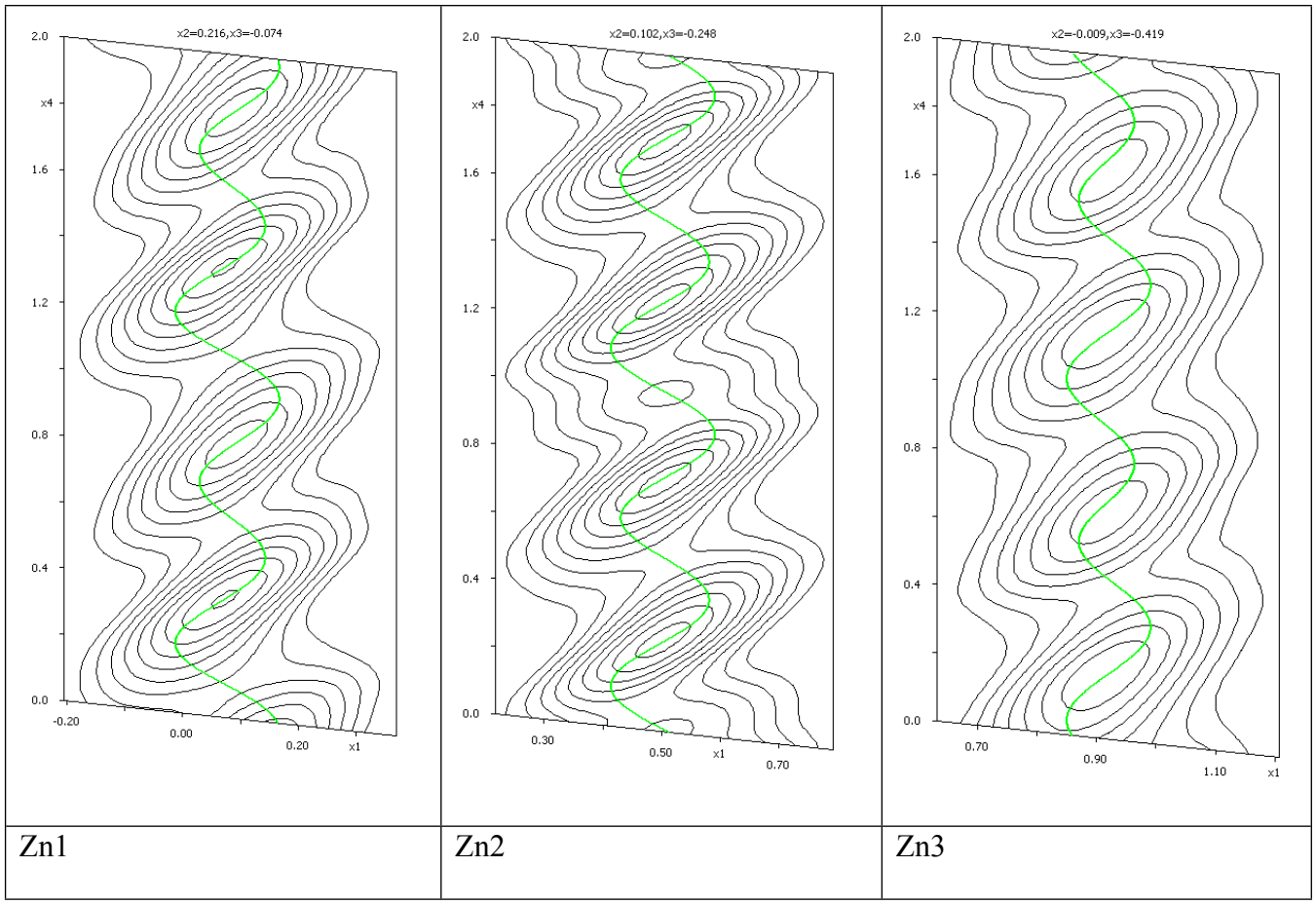
a) Department of Materials and Environmental Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden

b) Department of Chemistry, Division of Polymer & Materials Chemistry, Lund University, Box 124, SE-221 00 Lund, Sweden

* Corresponding author, Email: mats.johnsson@mmk.su.se, tel: +46-8-162169, fax: +46-8-152187

			
I1	I2	I3	I4
			
Sb1	Sb2	Sb3	Sb4

			
O1	O2	O3	O4
			
O5	O6	O7	O8



Zn1 | Zn2 | Zn3

Figure S-1 Selected sections of electron density maps of the various atomic species in the structure. The Zn atoms are located in a second composite unit cell. All sections show the same section of the structure, the position in x1 as a function of x4. All maps are summed over 0.5Å in x2 and x3. The levels of electron density are different in the different images.

ZnCl	O	Cl	Zn	Sb
Spectrum 1	63.4	9.05	12.6	14.9
Spectrum 2	66.4	9.12	12.5	12
Spectrum 3	58.7	11.7	14.3	15.4
Spectrum 4	63.3	10.4	13.1	13.2
Spectrum 5	66.4	8.75	12.8	12
Spectrum 6	57.7	11.6	14.4	16.3
Spectrum 7	58	11.4	14.4	16.3
Mean	**62.0**	**10.3**	**13.4**	**14.3**
Std. deviation	3.83	1.31	0.87	1.87

Table S-1 EDS data for $[Sb_4O_{7+3\delta}Cl_4][Zn_3]_{1+\delta}$, $\delta \approx 0.2$

ZnBr	O	Zn	Br	Sb
Spectrum 1	54.5	16.9	13.4	15.2
Spectrum 2	53.8	14.8	13.7	17.7
Spectrum 3	49.7	17.3	14.6	18.5
Spectrum 4	56.3	14.8	12.9	16.0
Spectrum 5	49.6	17.5	14.3	18.6
Spectrum 6	47.6	18.1	17.2	17.2
Spectrum 7	46.9	18.4	17.2	17.5
Mean	**51.2**	**16.8**	**14.8**	**17.3**
Std. deviation	3.65	1.47	1.76	1.25

Table S-2 EDS data for $[Sb_4O_{7+3\delta}Br_4][Zn_3]_{1+\delta}$, $\delta \approx 0.2$

ZnI	O	Zn	I	Sb
Spectrum 1	49.8	15	14.7	20.5
Spectrum 2	52.3	17.4	12.8	17.5
Spectrum 3	50	12.9	15.5	21.5
Spectrum 4	54	12.7	13.6	19.7
Spectrum 5	53.8	19.5	12.6	14.2
Spectrum 6	52.7	19.2	13.4	14.7
Spectrum 7	49.4	16.3	16.6	17.7
Mean	**51.7**	**16.2**	**14.2**	**18.0**
Std. deviation	1.94	2.75	1.49	2.78

Table S-3 EDS data for $[Sb_4O_{7+3\delta}I_4][Zn_3]_{1+\delta}$, $\delta \approx 0.2$

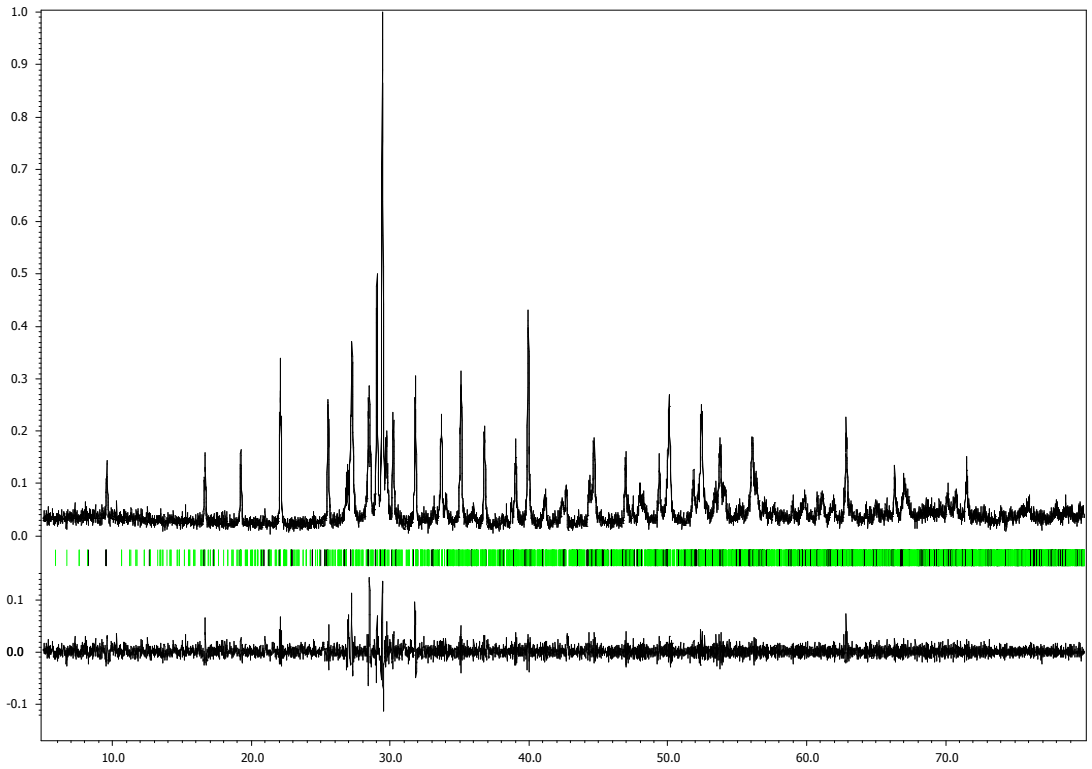


Figure S-2 The powder diffractogram of $[Sb_4O_{7+3\delta}I_4][Zn_3]_{1+\delta}$, $\delta \approx 0.2$ was analyzed using the Le Bail fitting algorithm. GOF = 1.07, Rp = 15.63 %, Rwp = 20.74 %.