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Supporting information for article:

Synthesis, crystal structure and phase transitions of novel hybrid perovskite: bis(1,2diaminepropane) di-μ-chloro-bis[diaquadichloro-manganate(II)] dichloride

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Supplementary materials

The crystallographic information for the structure reported in this work can be obtained free of charge via Cambridge Crystallographic Data Centre as supplementary publication, deposit number. CCDC 2087833 Copies of the data can be obtained on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44 1223 336 033; e-mail: deposit@ccdc.cam.ac.uk).

Simulated powder XRD patterns

hkl=001
$F(001)=0.41*f_{mn}-0.2*f_{cl}+0.93f_{cl4}+0.85f_{O}$

$F(011)=0.64f_{Mn}+0.41f_{cl}-0.58f_{cl4}+0.98f_{O}$

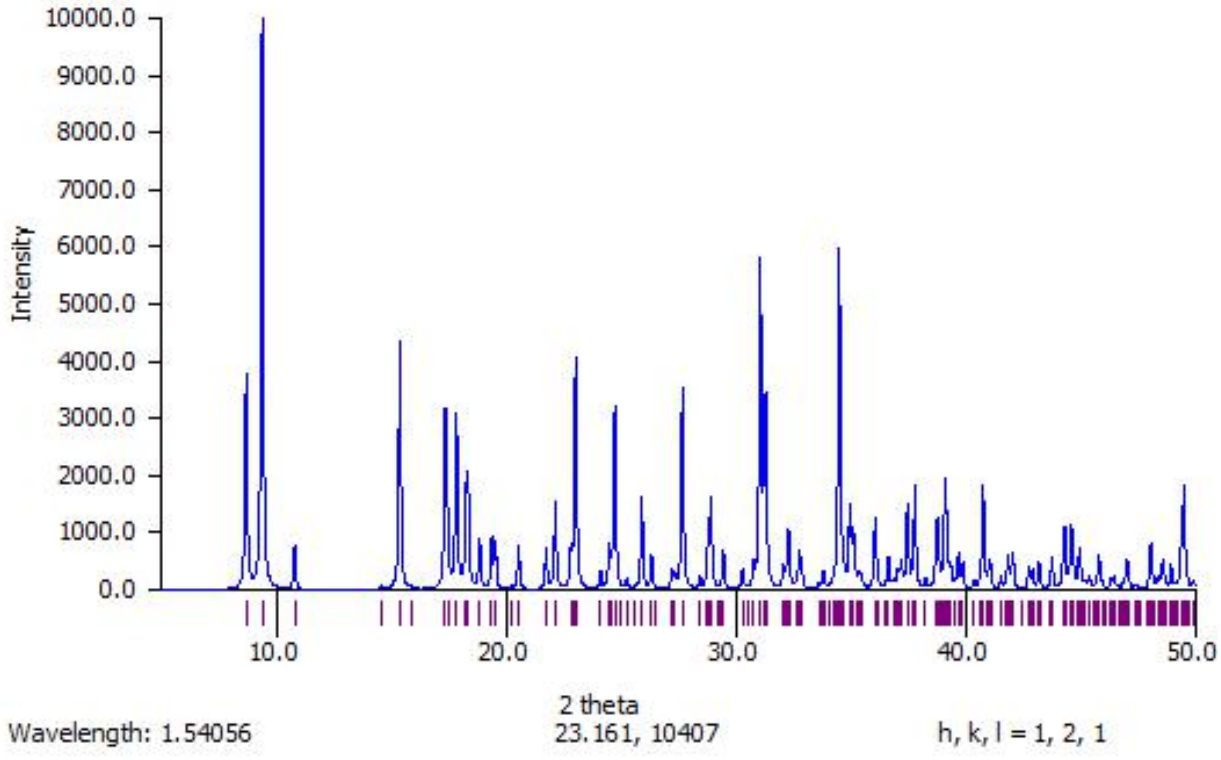

Figure S1: Simulated XRD powder diffraction pattern (original)

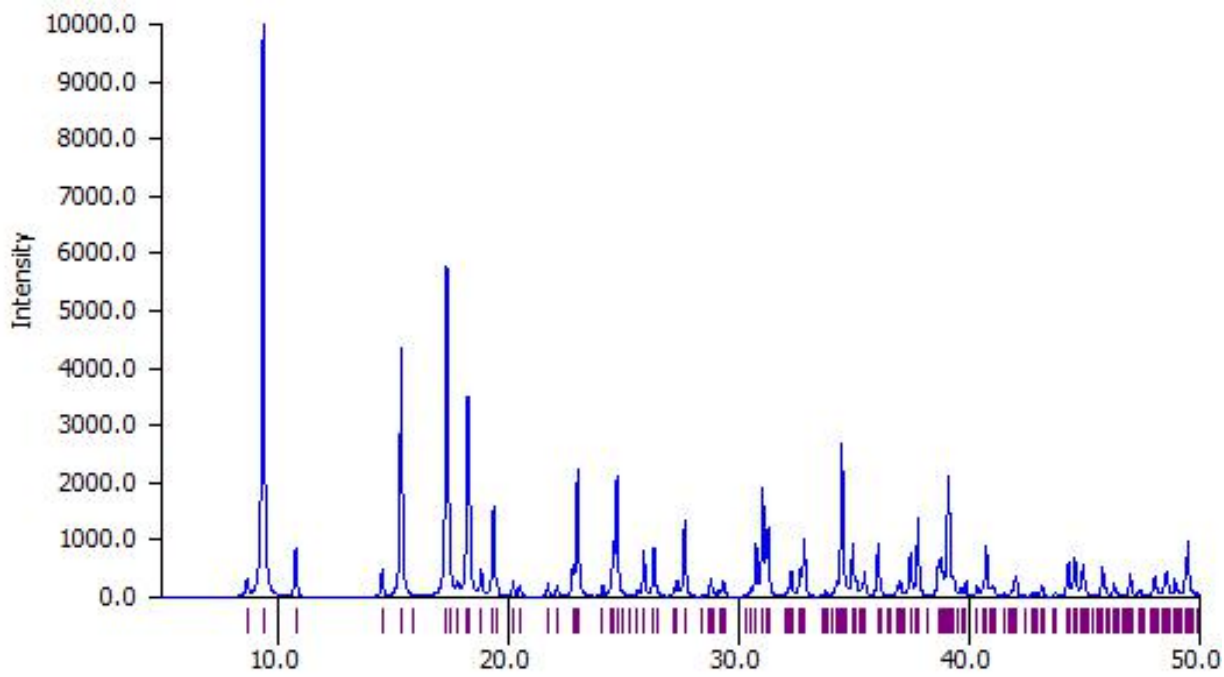

Figure S2: Simulated XRD powder diffraction pattern without O1, O2 and Cl4

Table S1: peak indexation for the high temperature phase

The best unit cell parameters refined for the new phase is monoclinic C, **a** = 15.676(3)Å, **b** = 15.959(3)Å, **c** = 12.769(3)Å, β= 109.03(1)º, V= 3020(2)Å^3.

Wavelength : 1.540598
Number of accepted peaks : 45
2Theta window : 0.100
2Theta zeropoint : 0.0362 (refineable)
Symmetry : Monoclinic_B C

Initial cell parameters :
Cell_A : 15.6300
Cell_B : 15.9630
Cell_C : 12.7400
Cell_Beta : 109.070

Refined cell parameters :
Cell_A : 15.676(3)
Cell_B : 15.959(3)
Cell_C : 12.769(3)
Cell_Beta : 109.026(13)
Cell_Volume: 3019.9(16)

Number of single indexed lines : 34
Number of unindexed lines : 0
2Theta zeropoint : 0.036(4)

Final 2Theta window : 0.0300

N	2Th[obs]	H	K	L	2Th[calc]	obs-calc	Int.	d[obs]	d[calc]
1	8.132	1	1	0	8.135	-0.0034	3.4	10.8640	10.8594
2	9.555	-1	1	1	9.558	-0.0024	42.1	9.2483	9.2460
3	11.935	2	0	0	11.934	0.0005	100.0	7.4095	7.4098
4	12.187	1	1	1	12.186	0.0013	26.9	7.2566	7.2573
5	13.286	0	2	1	13.290	-0.0047	43.2	6.6589	6.6566
6	14.669	0	0	2	14.664	0.0050	2.5	6.0338	6.0358
7	14.981	-1	1	2	14.981	0.0001	9.2	5.9090	5.9090
8	15.610	-2	0	2	15.611	-0.0006	6.7	5.6721	5.6719
9	16.208	-2	2	1	16.208	-0.0000	8.3	5.4642	5.4642
10	16.327	2	2	0	16.312	0.0157	2.9	5.4245	5.4297
11	17.695	1	3	0	17.700	-0.0053	2.3	5.0083	5.0068
12	17.909	-3	1	1	17.910	-0.0008	19.0	4.9488	4.9486
13	18.423	-1	3	1	18.406	0.0167	29.2	4.8120	4.8163
		0	2	2	18.416	0.0069		4.8138	
		1	1	2	18.430	-0.0067		4.8103	
14	19.180	-2	2	2	19.183	-0.0031	10.8	4.6237	4.6230
15	19.444	2	2	1	19.446	-0.0019	14.5	4.5615	4.5610
16	19.933	1	3	1	19.916	0.0166	8.3	4.4508	4.4544
		-3	1	2	19.934	-0.0014		4.4504	
17	21.764	-1	3	2	21.761	0.0029	7.9	4.0802	4.0807
18	22.246	3	1	1	22.242	0.0037	7.2	3.9929	3.9935
		0	4	0	22.264	-0.0181		3.9897	
19	23.904	-3	3	1	23.899	0.0057	2.7	3.7195	3.7204
20	24.162	-2	2	3	24.160	0.0021	9.9	3.6804	3.6807
		-3	1	3	24.169	-0.0068		3.6794	
21	24.292	1	3	2	24.296	-0.0034	15.0	3.6610	3.6605
22	24.515	2	2	2	24.512	0.0029	3.6	3.6282	3.6287
23	25.301	-4	2	1	25.303	-0.0022	47.9	3.5173	3.5170
24	26.240	-4	2	2	26.243	-0.0021	5.8	3.3935	3.3932
25	26.506	4	2	0	26.504	0.0026	1.9	3.3600	3.3603
26	27.357	3	3	1	27.338	0.0186	11.9	3.2575	3.2597
		3	1	2	27.354	0.0026		3.2578	
		4	0	1	27.365	-0.0080		3.2566	
27	27.502	2	4	1	27.497	0.0056	6.4	3.2406	3.2412
28	28.726	-1	1	4	28.725	0.0013	27.8	3.1052	3.1054
29	29.037	-1	5	1	29.039	-0.0022	6.5	3.0727	3.0725
30	29.428	-5	1	2	29.433	-0.0051	10.3	3.0327	3.0322
31	29.589	0	0	4	29.576	0.0132	15.0	3.0166	3.0179

		4	2	1	29.604	-0.0147		3.0151	
32	30.030	1	5	1	30.044	-0.0148	32.5	2.9733	2.9719
33	30.660	5	1	0	30.655	0.0048	5.0	2.9136	2.9141
34	31.066	-2	4	3	31.075	-0.0088	22.5	2.8764	2.8756
35	31.341	-1	5	2	31.331	0.0105	4.2	2.8518	2.8528
		2	4	2	31.355	-0.0141		2.8506	
36	31.585	-5	1	3	31.588	-0.0032	10.0	2.8304	2.8301
37	32.618	1	1	4	32.612	0.0056	38.8	2.7431	2.7435
38	32.781	-4	4	2	32.753	0.0289	13.0	2.7298	2.7321
39	33.496	-4	2	4	33.508	-0.0119	24.3	2.6731	2.6722
		-5	3	2	33.524	-0.0281		2.6709	
40	34.123	4	2	2	34.134	-0.0109	23.1	2.6255	2.6246
41	34.424	-6	0	2	34.432	-0.0082	7.0	2.6032	2.6026
42	35.540	3	5	1	35.535	0.0052	15.6	2.5239	2.5243
		4	4	1	35.556	-0.0158		2.5228	
		2	0	4	35.562	-0.0216		2.5224	
43	35.795	-2	6	1	35.792	0.0033	25.4	2.5065	2.5068
44	36.101	-2	4	4	36.086	0.0154	6.4	2.4860	2.4870
		-3	1	5	36.100	0.0017		2.4861	
		-1	1	5	36.102	-0.0004		2.4859	
45	36.418	-6	2	1	36.424	-0.0059	43.3	2.4650	2.4647
		2	4	3	36.429	-0.0109		2.4643	

Average delta(2Theta) = 0.005
Maximum delta(2Theta) = 0.029 (peak 38) = 5.6 * average

Figure of Merit F(30) = 139.9 (0.003, 66)

Durbin-Watson serial correlation = 2.389 (not significant)

Sqrt[sum(w * delta(q)^2) / (Nobs - Nvar)] = 6.0208e-005