Crystal and magnetic structures of the high pressure RMnMnTaO₆ (R = Rare earth) double (double) perovskites

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Perovskites ABO₃ are of great interest due to their large variety of electronic and magnetic properties. Their compositions can be modified to induce different cation orderings giving double perovskites AA'B₂O₆ or A₂BB'O₆, and even more complex double double perovskites (AA'BB'O₆) [1]. Recently, by using high-pressure and high-temperature (HPHT) techniques, we reported a new type of double double perovskite derivatives (DDPv) where columnar ordering at A-site and rock-salt ordering at B site are combined [2]. These crystallise with space group $P4_2/n$ and two families have been established; those with R (= rare earth) cations at A sites in RMnMnSbO₆ [2]; and those with Ca e.g. CaMnMReO₆ (M = Mn, Fe) [3].

We have successfully synthesised a new R-based series of HPHT perovskites, RMnMnTaO₆. Large R cations (R = La-Sm) result in a DDPv structure with space group $P4_2/n$; whereas a disordered A-site DPv structure has been observed for the smaller R =Eu-Y, with space group $P2_1/n$. By increasing the temperature, a structural transition from DDPv to DPv was observed for the very first time (**Fig.** 1), confirming the structural phase boundary for the RMnMnTaO₆.

Magnetic measurements show a ferrimagnetic ordering for the DDPv and a ferromagnetic ordering for the DPv. Two magnetic transitions with spin reorientation have been found for the DDPv Nd-compound. All information above indicates a very rich structural and magnetic behaviour for the RMnMnTaO₆ family.



Figure 1. Phase diagram for RMnMnTaO₆ showing the boundary between DDPvs and DPvs. The grey region refers to a mixture of DDPvs and DPvs.

[1] King, G., Woodward, P. M. (2010). J. Mater. Chem. 20, 5785.

[2] Solana-Madruga, E., Arévalo-López, Á. M., Dos Santos-García, A. J., Urones-Garrote, E., Ávila-Brande, D., Sáez-Puche, R. & Attfield, J. P. (2016). Angew. Chem. Int. Ed. 55, 9340.

[3] McNally, G. M., Arévalo-López, Á. M., Kearins, P., Orlandi, F., Manuel, P., & Attfield, J. P. (2017). Chem. Mater. 29, 8870.

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