Perovzalates: a family of perovskite-related oxalates

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Perovskites are one of the most prevalent classes of functional materials and are already known to exhibit a wide range of properties, including ferroelectricity, superconductivity and magnetism amongst others [1]. Many traditional perovskites have poor toxicity and sustainability; however, the inclusion of organic components could help alleviate these issues and provide greater structural diversity. Several examples of hybrid perovskites with interesting properties have already been reported with the inclusion of complex anions such as cyanides, formates and azides on the X site of the perovskite [2]. Whilst the oxalate ligand has already been extensively used in coordination polymers, its use in perovskite materials has only recently been reported in the compound $KLi_3Fe(C_2O_4)_3$ [3], the compound exhibits simultaneous 1:3 ordering on both the A and B sites of the perovskite Fig 1. In order to gain a more detailed understanding of this structure type, a series of compounds with the general formula $A^{I}Li_3M^{II}(C_2O_4)_3$ where A = K^+, Rb^+, Cs^+ and M = Fe^{2+}, Co^{2+}, Ni^{2+} have been synthesised and characterised [4].

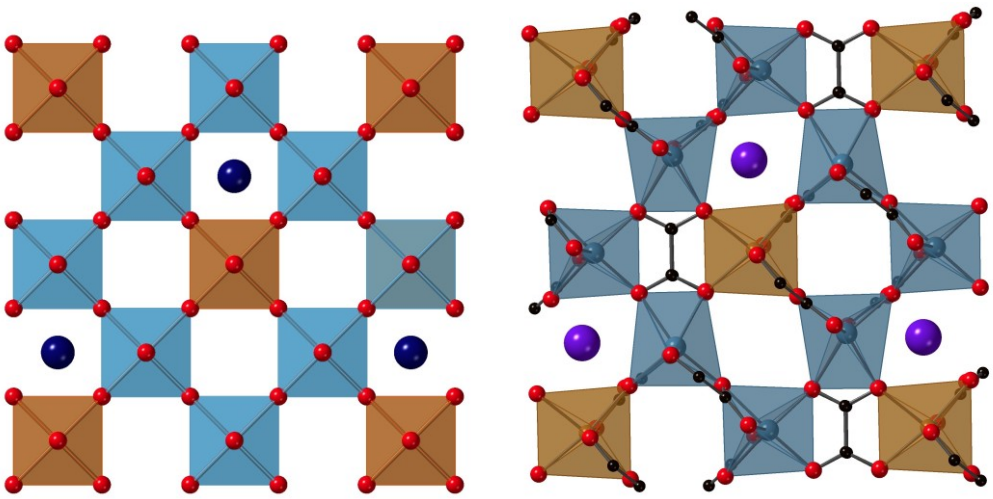

Figure 1. Comparison of hypothetical cubic perovskite with 1:3 cation ordering at the A and B site (left) and the corresponding crystal structure of the perovzalates (right). Li octahedra blue, M octahedra brown and A cation purple.

1 J. P. Attfield, P. Lightfoot and R. E. Morris, *Dalt. Trans.*, 2015, **44**, 10541–10542.

2 G. Kieslich and A. L. Goodwin, *Mater. Horizons*, 2017, **4**, 362–366.

3 W. Yao, Y. Guo and P. Lightfoot, *Dalt. Trans.*, 2017, **46**, 13349–13351.

4 R. Clulow, A. J. Bradford, S. L. Lee and P. Lightfoot, *Dalt. Trans.*, 2019, **48**, 14461–14466.

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