



Correction: Density functional theory study of superoxide ions as impurities in alkali halides

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Correction for 'Density functional theory study of superoxide ions as impurities in alkali halides' by Alexander S. Tygesen *et al.*, *Phys. Chem. Chem. Phys.*, 2020, DOI: 10.1039/d0cp00719f.

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In the right-hand column of the eighth page of the manuscript, all occurrences of the squared vibronic constant, F , should not be squared. Thus, the text should read: "The magnitude of the Q_1 distortion can be written in the first approximation as $Q_1^{\min} = F/K$, where F and K are the vibronic coupling constant and the force constant for the Q_1 mode, respectively.²⁷ In general, both F and K decrease as the lattice parameter is increased. It can be seen from Table 4 that the magnitude of the Q_1 distortion decreases as we move from sodium halides to potassium halides and from alkali bromides to alkali chlorides, which indicates that F decreases faster than K with the increase in lattice parameter."

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

