



## 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.<sup>27</sup> 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.

