

1. In Section V.C.2, we have included an explanation of the 'MAGMOM' term and removed the term 'paramagnetic' and replaced it with non-magnetic as per referee's suggestion.
2. In Section V.C.3, we have added a description of the way the calculations were carried out as per referee's recommendations.
3. In Section V.B.1, we have added a description of how the phonon calculations were carried out as per referee's recommendations.
4. In Section V, on page 15, an equation and its description have been added to describe how volumetric strain energy was calculated.
5. A typographical error was corrected in the title of Table II, meV/atom was changed to meV/f.u