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REPLY

Reply to comment on 'Calculated chiral and magneto-electric dichroic signals for copper metaborate (CuB_2O_4) in an applied magnetic field'

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Abstract
From the dawn of modern electromagnetism it has been known that a magnetic field is not handed (chiral). Arima and Saito (2009 *J. Phys.: Condens. Matter* **21** 498001) persist with unwisdom in their repeated claim to have observed control of chirality using a magnetic field by and in itself. In our reply to their claim, we demonstrate damning errors in all challenges in the comment levelled at our analysis of the observation reported by Saito *et al* (2008 *Phys. Rev. Lett.* **101** 117402) and made on a crystal of copper metaborate.

Lord Kelvin knew that a magnetic field intrinsically has neither left-handed nor right-handed quality, i.e., no chirality, as Faraday also realized [1]. Unlike Pasteur in the middle of the 19th century who attempted—in vain—to use magnetism to grow homochiral crystals, followed by many other searches for magnetically induced chirality that were similarly destined to fail [2, 3]. It is beyond doubt that enantioselectivity induced by magnetic fields *per se* is not allowed [4], whereupon a magnetic field by or in itself does not resolve an achiral (racemic) mixture [5].

Notwithstanding this well-documented, established wisdom Saito *et al* [6] and Arima and Saito [7] now claim that a magnetic field by or in itself can control the chirality of a single crystal of copper metaborate. We addressed the erroneous claim and, additionally, proposed a most plausible alternative interpretation of the experimental data on which the error is founded [5]. To this end, we found that the experimental method used by Saito *et al* [6] to measure a dichroic signal from the crystal is misreported, while their favoured atomic model is inconsistent with a required parity-odd absorption event. With style set by Saito *et al* [6], Arima and Saito's comment [7] on our paper [5] is a tissue of false claims that dents not one jot the validity of the analysis we reported.

We examine principal false claims in the comment [7].

(a) Bulk properties of a crystal are constrained by symmetry operations in the appropriate point group [8]. These operations do not include translational elements such as glide planes, of course, and the d-glide in the paramagnetic structure of copper metaborate, space group # 122 ($I\bar{4}2d$), is not relevant in establishing properties of a dichroic signal. In consequence, the comment's supposedly damning criticism of our work, expressed by Arima and Saito [7] in the statement '... a serious error in their treatment of crystallographic symmetry', is patently false.

(b) Physical properties of paramagnetic copper metaborate do not distinguish between the crystal a-axis and b-axis, contrary to the statement on this matter in the comment [7]. The false claim permeates the comment and, notably, it contributes to the erroneous conclusion, given in a discussion of figure 1(b) [7], that the paramagnetic structure can support an enantiomorphic pair of units. The fact that the crystal structure superficially looks different viewed down the a-axis from down the b-axis is simply that the tetrad element in the point group is reflection–rotation $S_{4z} = IC_{4z}$ and not proper rotation C_{4z}. Using the appropriate proper transformation, the view down the b-axis is identical to that down the a-axis. It is important in an analysis of data gathered on a tetragonal

crystal to choose axes and to adhere consistently to the choice. However, the choice of axes is no more than convention which ultimately has no bearing on material quantities [8].

(c) Another false claim by Arima and Saito [7] is that optical activity (rotation) and chirality are synonymous. Optical activity is allowed in 15 crystal classes of which 11 are chiral (enantiomorphic) [8]. Paramagnetic copper metaborate belongs to one of the four classes that are not enantiomorphic yet permit optical activity.

(d) Space group #23 (I222) employed by Arima and Saito [7] is unlikely to accommodate ions in copper metaborate [9]. If properties of the crystal evolve continuously with the applied field the space group will descend from # 122 to a maximal non-isomorphic subgroup. Of these subgroups, # 24 ($I2_12_12_1$) belongs to the enantiomorphic crystal-class 222 we deduced for the crystal structure with a field applied parallel to the *a*-axis or *b*-axis [5]. The space group # 23 is not an isotropy subgroup of # 122 at the gamma point whereas # 24 is. Since the transition to # 24 satisfies both the Landau and the Lifshitz condition it is potentially continuous, and also potentially a proper ferroelastic [10]. Copper ions in copper metaborate use sites 4(a), 4(b) and 4(c) in structure # 24, and we find the corresponding natural circular dichroism (NCD) is independent of the direction of an applied magnetic field, as expected.

(e) The paramagnetic crystal structure, # 122, is not enantiomorphous [8, 10]. Space group diagram # 122 contains points that are enantiomorphs of each other, i.e., the space group # 122 contains both hands. Arima and Saito say in the second paragraph of their comment that space group # 122 ($I\bar{4}2d$) is 'non-enantiomorphic' yet thereafter ignore the fact. Instead, with the help of figure 1, they falsely argue that the paramagnetic crystal structure can support enantiomorphic units. Cartoons on the top left and bottom left of figure 2 in [7] represent equivalent systems.

(f) In the presence of a magnetic field normal to the beam of light, we already have shown that rotation of the crystal by 90° about the beam changes the sign of linear dichroism (LD) [5] (We see no value in repeating here the calculation given in our paper [5].) This finding is contrary to the false conclusion obtained by Arima and Saito [7]. LD is a prime candidate for the signal reported by Saito *et al* [6], which indeed changes sign on rotation of the crystal by 90° about the beam. In their original paper, Saito *et al* [6] report that they rotated the magnetic field by 90° around the beam of light. Subsequently we learned from Professor Arima that the crystal, and not the field, was rotated about the beam, and Arima and Saito [7] confirm that this procedure was implemented in the experiment [6].

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