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Ab Initio Calculation of Chirality in Crystals

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ABSTRACT

The chirality of a free molecule in solution is relatively easy to determineby measuring its optical activity or rotatory power, but this is not the case in the solid state. Indeed, the absolute structure of tartaric acid, for example, as obtained from the magnitude and sign of the chirality, χ, did not become available until 150 years after the discovery of Pasteur. This is due to the fact that, in solids, χ is a small quantity thatcontributes weakly to the refractive index *n* of crystal, and its circular birefringence, according to the expression: $n \sim \varepsilon^{1/2} \pm \varepsilon\, \omega\, \chi$ (for a non-magnetic material), where ϵ is the relative dielectric matrix and ω is the light frequency.

On the other hand, the quantum mechanical calculation of optical rotatory power as other magnetic response properties has its own issues due in particular to the choice ofthe gauge origin, R, in the angular momentum expression: $L = (r - R) \times \nabla_r / i$. If the gauge invariance is well solved for the magnetic properties of molecules, the appropriate form of the angular momentum operator is not a straightforward matter forperiodic systems (see Ref.: Rérat and Kirtman, JCTC 17, 4063, 2021, https://doi.org/10.1021/acs.jctc.1c00243).

This theoretical work will be detailed in my presentation, with applications on minerals and molecular crystals.

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