































where  $R$  is a parameter selected to ensure convergence. The optical rotation  $\rho(\mathbf{k})$  and optical dielectric constants  $\varepsilon_{ij}$  are derived as follows:

$$\rho(\mathbf{k}) = \frac{-e_{rij}k_r}{2n\nu} \text{Im} \sum_{ss'} (C_{ss'})_{ij} \quad (\text{A5})$$

$$\varepsilon_{ij} = \delta_{ij} + \frac{1}{\nu} \sum_{ss'} (C_{ss'})_{ij} \quad (\text{A6})$$

where ( $e_{rij}$  = Levi-Civita symbol,  $\mathbf{k}$  = wave vector,  $n$  = average refractive indices,  $\nu$  = unit volume and  $\delta_{ij}$  = Kronecker delta). The Levi-Civita operation  $e_{rij}$  accomplishes the cross product between the spatial coordinates of  $C_{ss'}$  and the wave vector.

The rotatory power  $\rho_{ij}$  is defined as the *clockwise* rotation of linear polarized light passing through a non-birefringent sample of 1 mm thickness as observed when looking towards the light source. This theoretical model reliably calculates optical rotation on the basis of the interacting forces in inorganic structures. It was further applied successfully to molecular crystals where the interacting fields within a molecule are more significant than those between the molecules [61].

*Sample Availability:* Samples of the compounds **1-3** are available from MDPI.

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