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A Tip for Non-Cyclical Crystallographic Axis Interchanges Verified by a Chiral Compound $[C_{24}H_{22}N_4O_4S]_2 \cdot HCl$

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If a non-cyclical crystallographic axis interchange should be performed unavoidably, a transformation matrix P with each matrix element having minus sign must be operated to the three axes in order to obtain same type of unit cell as the initial one and a matrix $[P^T]^{-1}$ must be operated to atomic coordinates of a non-centrosymmetric crystal as well to keep up the absolute configuration unchanged, and intensity data must be also transformed by the matrix P with each matrix element having minus sign if the crystal structure refinement is required. As the centrosymmetric crystal has the general positions ±x, ±y, ±z, the transformation matrix for the atomic coordinates does not necessarily have to include the minus sign.
The behaviour of absolute configuration caused by crystallographic axis interchanges is examined theoretically and experimentally on a compound (S)-(+)-4-phenyl-1-[1-(4-aminobenzoyl) indoline-5-sulfonyl]-4,5-dihydro-2-imidazolone hydrochloride.