

17O and 14N quadrupole coupling and the mechanism of the ferroelectric transition in diglycine nitrate

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Abstract: The 14N and 17O quadrupole couplings in diglycine nitrate have been determined by proton- 14N and proton-17O double resonance. The O—H—O bonded proton is moving between two off-centre sites in the H—bond above TC and is frozen out in an off-centre site below TC. The results show that the basic phase transition mechanism is a biasing of the flipping of the —NH3 groups around the C—N bond between two equilibrium orientations separated by $\sim 60^\circ$ connected with a corresponding rotation of the NO3[−] ions, an exchange of the ionic character of the two glycine molecules and a transfer of the O—H—O bonded proton.

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