

# Phase Transformation and Structure of N-chlorocarbonylisocyanide Dichloride\*

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The  $^{35}\text{Cl}$  nuclear quadrupole resonances in N-chlorocarbonylisocyanide dichloride show that it exists in two polymorphic forms. The metastable  $\alpha$  phase has six  $^{35}\text{Cl}$  NQR lines and the stable  $\beta$  phase has three. The latter is obtained irreversibly by annealing the  $\alpha$  phase at 179 K. The temperature dependences of the  $^{35}\text{Cl}$  NQR frequencies, spin-lattice and spin-spin relaxation times are obtained in both phases. The results of the  $^{35}\text{Cl}$  NQR studies are discussed together with calculated MNDO level data and other physical properties (IR frequencies, dipole moments) of this compound.

*Key words:* N-Chlorocarbonylisocyanide Dichloride; Structure; Phase Transformation;  $^{35}\text{Cl}$  NQR Parameters; MNDO calculation.

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