characterized by two angles $\Theta_2$ ($\angle{X_1-X_2-X_3}$) = 90° and $\Theta_2$ ($\angle{X_1-X_2-X_3}$) = 120° and (b) Type II (X1 $\cdots$ X2) interactions persist. A plot of the number of $X \cdots X$ interactions and divalent S and Se in their S$\cdots$S and Se$\cdots$Se interactions show the "electrophile-nucleophile" pairing and Type III contacts.

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C13 H11 N2 O3, orthorhombic, Pna21, Z=4, a=11.841(3), b=9.820(3), c=12.917(3) A., V=1312(1) A.$^3$. Dc=1.415 g cm$^{-3}$. $\mu$(MoK$\alpha$) = 2.33 cm$^{-1}$. R=0.037, $\omega R=0.034$ for 1070 observed reflections.

Fig. 1 shows the Newman projections of the chain in both a) solution and b) solid state. Fig. 2 represents the molecular structure. The diastereotropic effect of the methylene protons of the chain, occurring in solution, can be improved with the results in solid state: 1) a rigid anchorage of H91 to O1 prevents free rotation of the chain, 2) a dipolar stabilization effect of the sauche sl conformation occurs between dipole moments of -Cl at N2 and -NI-C9-, this fact leads Cl at N2 close to N1-C9, but only to the gauche conformation. Because the steric hindrance would prevent the eclipsed conformation, 3) the o-substitution obliges to a rigid repositionment of the -C9N function, which cannot rotate closer to the o-group. Rotation in opposite sense is prevented by the diple charse enhancement mentioned above.


Some N-p-cyanoethyl-o-substituted anilides in solution, show a diastereotropic coupling effect in the H-nmr spectra, due to the methylene protons of the N-p-cyanoethyl chain. An X-ray analysis of the title compound has been carried out to investigate this effect. C13 H11 N2 O3 Cl, orthorhomic. Pna21, Z=4, a=11.841(3), b=9.820(3), c=12.917(3) A., V=1312(1) A.$^3$. Dc=1.415 g cm$^{-3}$. $\mu$(MoK$\alpha$) = 2.33 cm$^{-1}$. R=0.037, $\omega R=0.034$ for 1070 observed reflections.

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