The isomerisation process involves, in essence, the formation of a new bond between the amide nitrogen and the acetyl carbon atom. The conformation of the reactant molecule (I) is such that the amide group and the acetyl group make angles of 40° and 77° respectively with the plane of the benzene ring. The product molecule (II), on the other hand, is virtually planar. Thus the process involves, in addition to the migration of the acetyl group, large conformational changes. This may explain why a single crystal of the reactant breaks up into a polycrystalline product. Within the reactant molecule (I) there is a short contact of 3.27 Å between the reactant centres. Between screw-related molecules of (I) the N...C distance is 3.68 Å, while between glide-related molecules it is 3.91 Å. Thus, while the inter-molecular separation is the smallest, even the inter-molecular separations are within the range in which solid state reactions are known to take place (see for example, Paul and Curtin, Acc. Chem. Res. (1973) 2086). An intramolecular process seems to involve the least movement of the atoms, followed by the intermolecular process involving glide-related molecules. Thus, from structural considerations, while other processes cannot be entirely ruled out, the intramolecular mechanism appears most likely.

The isomerisation process has been studied in the solid state, and in solution, employing spectroscopic and thermal techniques (Gordon, Tetrahedron (1967) 23, 863) and this is the first example for such a process. Yet, there is a clear evidence that the transformation occurs in the solid state, and the possibility of surface melting and transformation in the liquid state can not be excluded.

The crystal data are: (I) Monoclinic, a=15.156(5), b=15.857(2), c=15.956(2)Å, β=95.64 (6°), space group P2₁/c, Z=4. (II) Triclinic, a=4.596(9), b=10.943(8), c=9.340(9)Å, α=94.45 (7°), β=94.28(7), γ=97.22(6°), space group P1, Z=2. The structures were solved by direct methods and refined by least-squares procedures using 1604 and 1148 diffractometer data to R-values of 0.076 and 0.052 respectively.