The isomerisation process involves, in essence, the breaking of a single 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 79° 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 3.86 Å; while between glide-related molecules it is 3.91 Å. Thus, while the intra-molecular separation is the smallest, even the inter-molecular separations are within the range in which solid state reactions are known to take place (Sear for example, Paul and Curtin, Acc. Chem. Res. (1973) 6). In an attempt to understand the mechanism of the process, the isomerisation occurs in the solid state, and the possibility of surface melting and transformation in the liquid state can not be excluded.

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