

Single-Crystal-to-Single-Crystal Photochemistry in Inclusion Compounds Tali Lavy, Yana Sheynin, Moshe Kapon and Menahem Kaftory *Department of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel*

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In heterogeneous photochemical reactions, at certain extent of conversion, phase separation occurs. In contrast, homogeneous photochemical reactions are characterized by the persistence of the crystal throughout the whole conversion range. In a specific example it was shown that when the wavelength of the absorption maximum was used, heterogeneous reaction took place. However, a single-crystal-to-single-crystal photodimerization was observed when the wavelength of the flank of the absorption was chosen [1]. We have found that homogeneous reaction takes place when we irradiated inclusion compounds with a regular Xe lamp. For example, benzylideneacetophenone (a), or pyridone (c) undergo solid-state photodimerization under irradiation of its inclusion compound with (I) as the host, with no destruction of the crystallinity of these compounds. The case of inclusion compound (I-c) was of special interest. At a certain stage of the reaction it became apparent that a foreign molecule was penetrating the crystal, as shown by an additional electron density that was found in the difference Fourier map, without destroying the crystal. This electron density is suspected to be the oxygen of a water molecule. Enantioselective Ring closure of (e) to (f) was observed while its inclusion compound with the chiral host compound (II) was irradiated. In all cases the effect of the geometry change, imposed on the guest molecules by the reaction, on the host molecules was severe and no damage to the crystal was observed. Therefore the crystal structures at different conversions and at the end of the reaction could be determined. In contrary to the above cases, the guest molecule tropolone methyl ether (g) in the inclusion compound with the chiral host (III) undergoes heterogeneous enantioselective photoreaction to yield (h). The disability to undergo homogeneous photoreaction is explained in terms of the space needed for this reaction.

[1] Enkelmann, V.; Wegner, G. *J. Am. Chem. Soc.* **1993**, *115*, 10390.

