

Solid-Solid Reactions of Xanthenols with Unsaturated Hydrocarbons

Luigi R Nassimbeni^a, Mino R Caira^a, Elizabeth Curtis^a, Hong Su^a and Benjamin Taljaard^b, ^a*Department of Chemistry, University of Cape Town, Rondebosch, 7701, South Africa.* ^b*Department of Chemistry, University of Port Elizabeth, Port Elizabeth, 6000, South Africa.* E-mail: xrayluig@science.uct.ac.za

The structures of the inclusion compounds of the host H = 9-(4-methoxyphenyl)-9H-xanthen-9-ol with a series of aromatic guests: naphthalene, anthracene, phenanthrene, pyrene and α -naphthol have been elucidated. The structures are similar, crystallise in the space group P(-1), and are characterised by pairs of hydrogen-bonded host molecules, with the guests located at centres of inversion.

The kinetics of the solid-solid reactions between the host, H, and naphthalene and α -naphthol were monitored by X-Ray powder diffraction at 25°C and their rate constants established.

Linear relationships were derived for unit cell volumes versus the number of guest atoms in this series as well as from the structures containing benzene, toluene and the isomers of xylene as guests.

Lattice energy calculations for the naphthalene and α -naphthol structures were reconciled with the results of thermal analysis obtained by DSC.

Keywords: solid-solid reaction, clathrate, kinetics