Inclusion Compounds of Isomeric Xanthenol Hosts with Aniline

Ayesha Jacobs[a], Luigi R. Nassimbeni[a], Benjamin Taljaard[b], [a]*Faculty of Applied Sciences, Cape Town Campus, Cape Peninsula University of Technology, Cape Town.* [b]*Nelson Mandela Metropolitan University, South Campus, Port Elizabeth, South Africa.* E-mail: jacobsa@cput.ac.za

Two isomeric xanthenol host compounds have been found to form inclusion compounds with aniline. These hosts are H1 = 9-(4-methoxyphenyl)-9H-xanthen-9-ol and H2 = 9-(3-methoxyphenyl)-9H-xanthen-9-ol. We have elucidated the structures of the inclusion compounds and determined their kinetics of desolvation. H1•½aniline crystallises in the triclinic space group P(1 bar) with the host in general positions and the aniline guest on a centre of symmetry. H2•aniline was solved successfully in the monoclinic space group $P2_1/c$ with both the host and guest molecules in general positions. For H1•½aniline there is (Host)─OH•••O─(Host) hydrogen bonding whereas in H2•aniline (Host)─OH•••N─(Guest) hydrogen bonding occurs. We have correlated the structures with the thermal stabilities of the compounds.

Keywords: isomeric hosts, aniline, desolvation