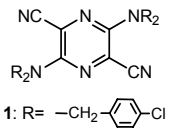
Phase Relationship of Two Polymorphs of a Diaminodicyanopyrazine Dye

Yoko Uchida[a], Shinya Matsumoto[a], Mitsuhiro Yanagita[b], [a]*Department of Environmental Sciences, Faculty of Education and Human Sciences, Yokohama, National University, Yokohama Japan.* [b]*R&D Laboratory for High-Performance Materials, Nippon Soda Co. Ltd., Chiba, Japan.* E-mail: d04ha011@ynu.ac.jp

2,5-Diamino-3,6-dicyanopyrazine dyes are novel fluorescent dyes for opto-electronic applications [1]. These dyes have been found to have crystal polymorphs with different colours depending on the amino substituents. The colour difference is considered to be ascribed to the different molecular conformation among the polymorphs. In this study, the stability relationship of two polymorphs (red and yellow) of **1** were determined by melting data and correlated with their molecular and crystal structures.



The red phase was found to transform to the yellow phase at room temperature. DSC measurement showed that the yellow phase has a higher melting point than that of the red phase. The heat capacities were also determined by DSC measurement. These results suggest that the red phase and the yellow phase are a monotropic relationship. The phase relationship will be also discussed on the basis of their molecular and crystal structures.

[1] Matsuoka M., in *Colorants for Non-textile Applications,* Freeman H. S. and Peters A. T. Ed., Elsevier Science, 2000, 339.

Keywords: polymorphism, phase stability, properties and strutcures relationship