Poster Presentation

MS07.P02

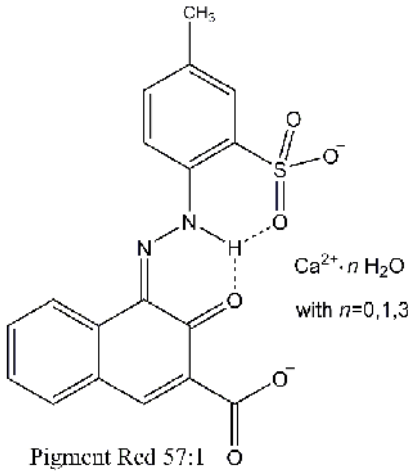
Crystal Structures of Pigment Red 57:1

S. Hammer[1], S. Bekö[1], J. Glinnemann[1], M. Schmidt[1]

[1]*Goethe University, Institute of Inorganic and Analytical Chemistry, Frankfurt am Main, Germany*

Zeitschrift für Kristallographie, Angewandte Chemie, The New York Times, The Sun, El Pais, La Republica, Le Monde, Shanghai Daily, and many more journals and newspapers are printed with Pigment Red 57:1. P.R.57:1 (C18H12CaN2O6S · n H2O, n = 0,1,3) is the most important organic red pigment with a production of more than 50,000 tons per year and an annual sales volume of more than 200 million Euro.[1] In printing ink the pigment is not dissolved, but finely dispersed. Consequently its solid-state properties are maintained. Like most pigments, P.R.57:1 occurs in different crystal phases with different colours. Upon synthesis a trihydrate is formed. Drying at 50 °C generates a monohydrate with magenta shade, which is used for printing inks. The monohydrate is thermally stable up to temperatures higher than 190 °C before it releases water to yield a hygroscopic anhydrous phase with dull dark magenta shade. For all three phases the growth of single crystals is impeded by the low solubility of the pigment in most media. The crystal structures of all three forms were determined from in-house X-ray powder data.[2] The structures were solved by real-space methods with simulated annealing. Subsequently a Rietveld refinement with restraints on bond lengths, bond angles and planar groups was performed. All three phases crystallize in space-group type P21/c, Z = 4. The trihydrate and the monohydrate show eightfold coordination of the Ca ions, the anhydrate a sevenfold one. Apparently the increasing anion-cation interactions lead to the observed colour shift. The arrangement of cations and anions is similar in all three forms. The crystal structures exhibit double layers, one polar, one nonpolar. The polar layer consists of water molecules, calcium ions, sulfonate, keto and carboxylate groups, held together mostly by hydrogen bonds and Coulomb interactions. The nonpolar layer contains naphthalene and toluene moieties.

[1] *W. Herbst, K. Hunger, Industrial Organic Pigments, 3rd ed., Wiley-VCH, Weinheim, 2004.,* ***[2]*** *S. L. Bekö, S. M. Hammer, M. U. Schmidt, Angew. Chem. 2012, 124, 4814-4818, Angew. Chem. Int. Ed. 2012, 51, 4735-4738.*



Pigment Red 57:1

Keywords: X-ray powder diffraction, organic pigments, crystal structure