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Crystal Structures of Six Industrial Benzimidazolone Pigments from X-ray Powder Data. Svetlana N. Ivashevskaya^a, Jacco van de Streek^b, Martin U. Schmidt^c, Jürgen Brüning^c, Martin Ermrich^d. ^a*Institute of Geology Karelian Research Centre RAS, Petrozavodsk, Russia.* ^b*Avant-garde Materials Simulation, Freiburg, Germany.* ^c*Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, Frankfurt am Main, Germany.* ^d*Röntgenlabor Dr. Ermrich, Am Kandelborn 7, D-64354 Reinheim, Germany.*
E-mail: ivashevskaja@yahoo.com

Solving the crystal structures of organic pigments is not just an academic exercise: the majority of organic pigments are polymorphic, and the polymorphic form determines the colouristic properties. Pigments are practically insoluble in their application media; their crystal structures are maintained and the properties of the final product depend on the solid state structure.

Benzimidazolone pigments cover the spectrum from greenish yellow to orange and are produced industrially on a large scale. They have an excellent fastness to light and weathering and good hiding power. They are used in the automobile industry, to colour plastics and as high grade printing inks [1].

On account of very low solubility of pigments in all solvents, it was impossible to grow single crystals suitable for X-ray analysis. For a better understanding of the pigments' properties, their crystal structures were determined from laboratory X-ray powder diffraction data.

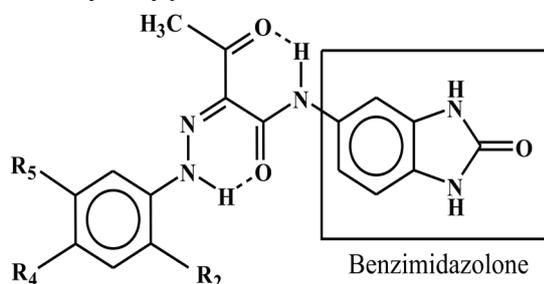


Fig. 1 The general framework of the benzimidazolone pigments.

The crystal structures of six benzimidazolone pigments were determined from laboratory X-ray powder diffraction data by real-space methods using the programs *DASH* [2] and *MRIA* [3]. Powder patterns were indexed by the program *DICVOL91* [4]. Rietveld refinements were carried out with *TOPAS* [5].

All crystal structures are different and exhibit five different hydrogen-bond topologies. Apparently, the good application properties of the benzimidazolone pigments are the result of a combination of efficient molecular packing and strong intermolecular hydrogen bonds.

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In situ X-ray Diffraction Study of Titanium Sesquioxide. Afir Arezki. *Université des sciences et de la technologie USTHB, Faculté de chimie - BP 32 El-Alia, Bab Ezzouar - Alger, Algeria.*
E-mail: houriachikh@yahoo.fr

High-temperature X-rays diffractometry is used to study Ti_2O_3 rhombohedral oxide formed by reduction of titanium dioxide, under vacuum and in the presence of graphite or metallic titanium. The sesquioxide is characterized by a homogeneous field of very low oxygen pressure, both boundary phase appearing independently from one another between 800 and 1715°C. The $c/a = 2.660$ value for $Ti_{2-x}O_3$ oxidized from of the equivalent hexagonal cell reaches $c/a = 2.735$ for Ti_2O_3 reduced form, which does not undergo quenching ($c/a = 2.640$ at room temperature)

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Synthesis and Crystal Structures of the Hole-doped Oxy-chlorides $(Ba,Sr)_2Cu_3O_4Cl_2$. Abderrahim Benabbas. *L.I.M.E Laboratory. University Of Jijel. B.P. 98 Ouled-Aissa 18000 Jijel. Algeria.*
E-mail: Abderrahim.benabbas@gmail.com

There is still no general microscopic model for superconductivity, particularly for high- T_c cuprates both in their normal, pseudo-gap and superconductor states. Any proposition of such mechanisms should need the knowledge of accurate details of the crystal structures and their evolution with doping, temperature, pressure... The crystal structures of high- T_c cuprates are composed of the so-called charge-reservoir blocks and CuO_2 planes where the superconductivity is thought to take place. In the undoped compositions, these materials are antiferromagnetic insulators. The long-range magnetic order is destroyed upon doping and is replaced by superconductivity. $(Ba,Sr)_2Cu_3O_4Cl_2$ oxychloride [1-2] noted 2342 is a prototype of these undoped compounds since it is an antiferromagnet with a layered body-centred tetragonal structure which presents great similarities either to that of La_2CuO_4 or to an anion-ordered perovskite one. However, this phase is slightly different since it has a Cu_3O_4 planes with two independent Cu-sites. The Two-thirds of these sites (A-sites) are surrounded by four equatorial oxygen and two apical chlorine anions and the rest (B-sites) are coordinated by four oxygen. These sites interact by super-exchange along Cu_A-O-Cu_A or along Cu_A-O-Cu_B [3-5]. Magnetization measurements show two transitions at $T \approx 380$ K and $T \approx 40$ K corresponding to the ordering of moments in the sub-lattices indicated before. In order to obtain superconductivity, several attempts were