High-Frequency and -Field Electron Paramagnetic Resonance Studies of Yellow/ Orange/ Red Pigments Based on Iron^{3+}

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The starting material of this work was $YInO_3$, which is amenable to doping of its trigonal bipyramidal (TBP) indium^{3+} site by a wide range of metal ions. Among these are manganese^{3+} (spin number S = 2) and iron^{3+} (S = 5/2). The former, $YIn_{1-x}Mn_xO_3$, was the subject of an earlier investigation at the MagLab (Ref. 1) and has been successfully commercialized as a novel and attractive blue pigment in a variety of applications including paints and heat-reflective roof covers. Unlike manganese^{3+} which produces a bright blue color, iron^{3+} ion imparts a color on the otherwise colorless (off-white) indium compound varying from pale yellow to orange to intense red depending on its concentration (see Fig. 1).

The $YIn_{1-x}Fe_xO_3$ (x = 0.1 to 0.3) series of materials was synthesized in the group of Prof. Subramanian at Oregon State University. Since the optical properties (color) of the materials depend on the electronic structure of iron^{3+}, which is paramagnetic, these properties are correlated with the magnetic properties of that ion. For that reason, they were studied by EPR, and in particular its high-frequency and -field version (HFEPR) at the National MagLab in Tallahassee.

Like their manganese-based analogs, the current class of iron-based pigments offers a non-toxic alternative to more conventional pigments in a variety of applications.

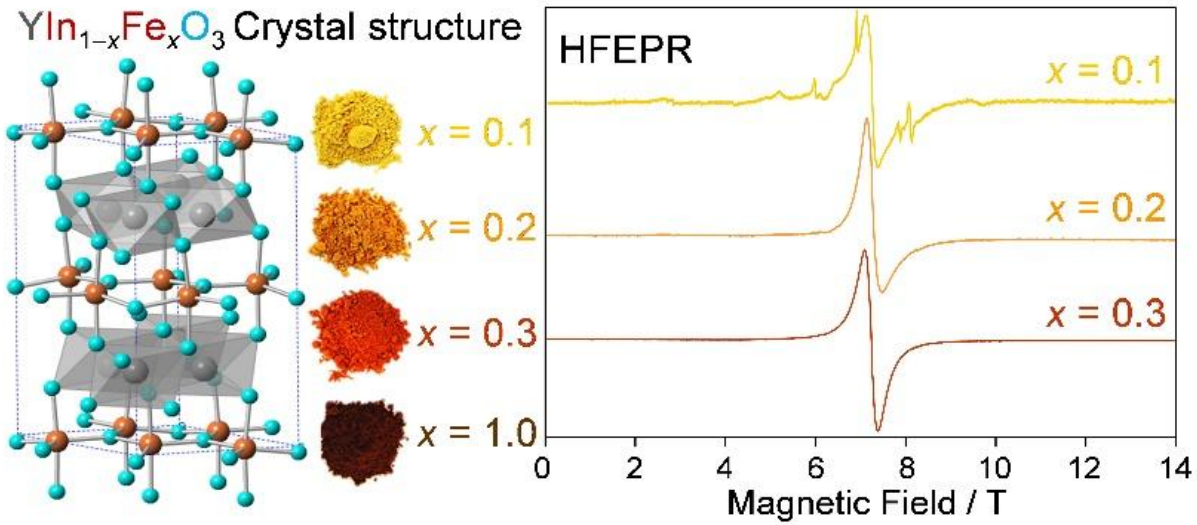

Figure 1. (Left) Crystal structure of $YIn_{1-x}Fe_xO_3$ showing layers of MO_5 (M = In, Fe) trigonal bipyramids (TBP) interspersed with layers of YO_6 octahedra (Y, gray spheres; In/Fe, orange spheres; O, turquoise spheres). (Center) Colors of $YIn_{1-x}Fe_xO_3$ samples varying from yellow to orange and red/brown with increasing Fe content (x = 0 is off-white). (Right) HFEPR spectra of $YIn_{1-x}Fe_xO_3$ for different doping levels of iron at 203.2 GHz and 10 K.

Facilities and instrumentation used: The EMR Facility at the NHMFL / Tallahassee was used including its 15/17 T superconducting magnet.
Citations: (1) Krzystek, J.; Telser, J.; Li, J.; Subramanian, M.A., Magnetic properties and electronic structure of manganese-based blue pigments: a high-frequency and -field EPR study, Inorganic Chemistry, 54, 9040-9045 (2015) doi.org/10.1021/acs.inorgchem.5b01306; **(2)** Krzystek, J.; Telser, J.; Jiang, P.; Gopakumar, G.M.; Subramanian, M.A., High-Frequency and -Field Electron Paramagnetic Resonance Studies of Yellow/Orange/Red Pigments Based on Fe3+ in Trigonal Bipyramidal Coordination, Inorganic Chemistry, 65, 12524-12531 (2026) doi.org/10.1021/acs.inorgchem.6c01324.