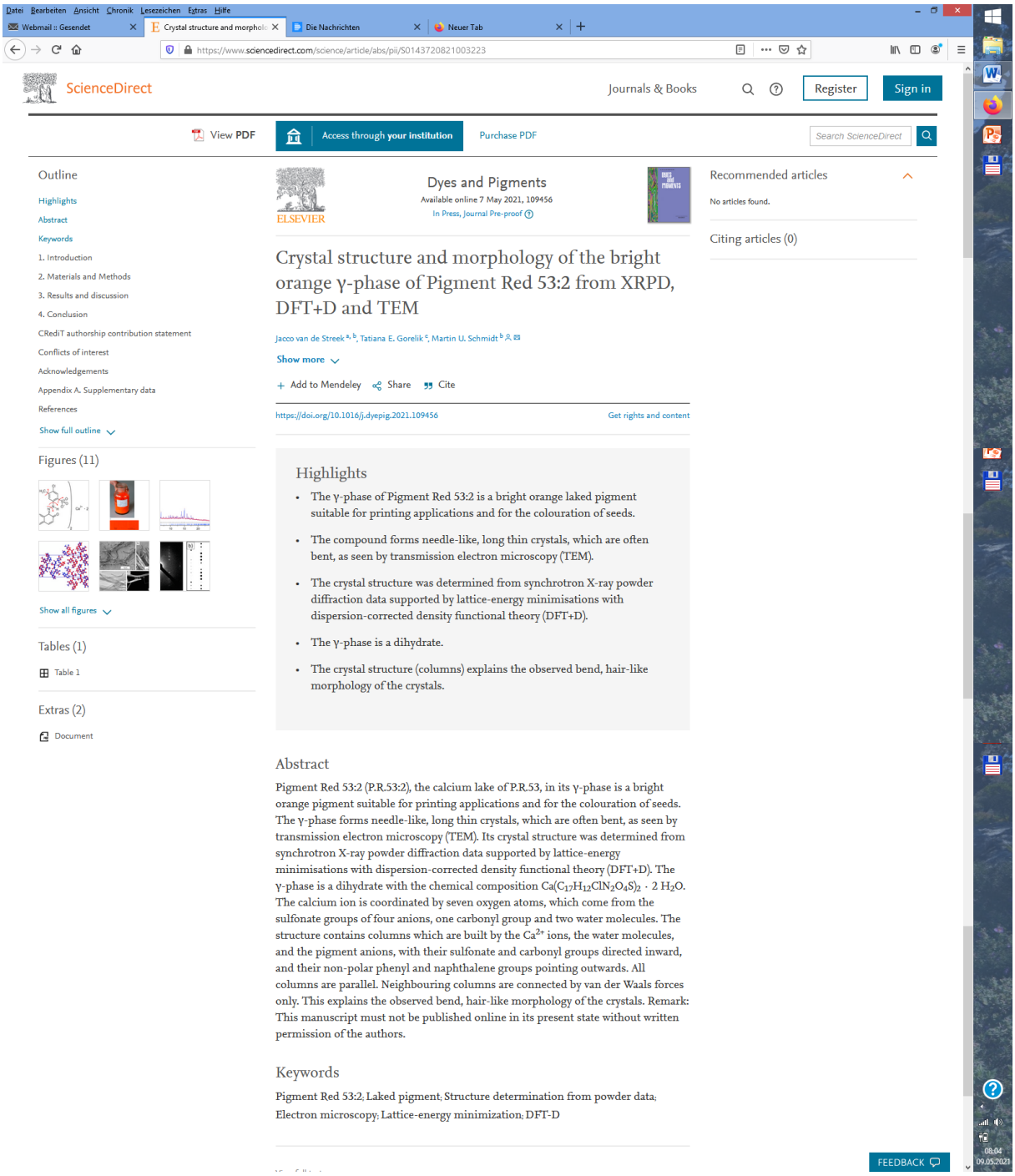
Elsevier publishes manuscripts in bad layout state against the explicit statements of the authors

Manuscript available online on 9 May 2021:



See what is written in the last line of the abstract!

The layout was not done carefully. This can be seen, e.g., in the figure caption of Figure 2 of the published manuscript:

Like most pigments, P.R.53:2 is hardly soluble in water or any other solvent. Melting results in decomposition. Sublimation is not possible, either. Consequently, it is difficult to grow single crystals. We managed to grow single crystals by recrystallisation from large amounts of hot DMSO. However, the crystals turned out to contain DMSO in their crystal lattice (π-phase) [11], which makes this phase commercially useless.

Similar difficulties have been experienced also for other laked pigments. Consequently, despite the commercial importance of laked red pigments, only a very small number of crystal structures of industrial laked pigments could be solved by single-crystal X-ray analysis. This includes P.R.49 lakes [12,13], the β-phase of Pigment Yellow 183 (P.Y.183) [14], a non-commercial dichloro-derivative of P.R.57:1 [15], and several solvates.

If no single crystals can be grown, three methods remain to determine the crystal structures:

- Structure determination by powder diffraction (SDPD) [16].
- Single-crystal electron diffraction (ED) [10,17–19].
- Crystal structure prediction (CSP) [20].

The first two methods were applied on P.R.53:2.

From 2004 to 2006, we tried to determine the crystal structure of the commercially promising γ-phase of P.R.53:2 using electron diffraction. However, the recorded ED data disagreed with the X-ray powder data of the γ-phase. It turned out that during the preparation of the sample for ED a polymorph transition took place. Upon suspending the sample in ethanol, the γ-phase transformed into the ζ-phase. The crystal structure of the ζ-phase was then solved from the ED patterns of a twinned crystal. This was one of the first structure determinations of an organic compound solely from ED data [10].

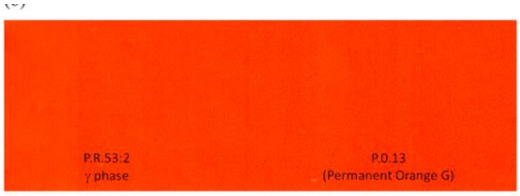


Fig. 1. The γ-phase of P.R.53:2. (a) Pigment powder; (b) Offset printing, in comparison with Pigment Orange 13. Note for the layout: Both images should be printed with sufficient size.

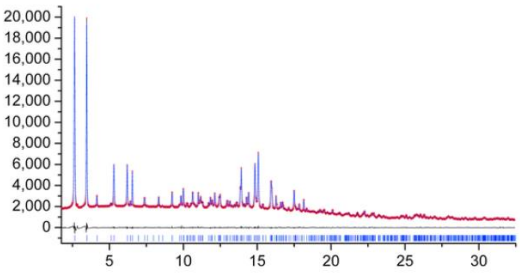
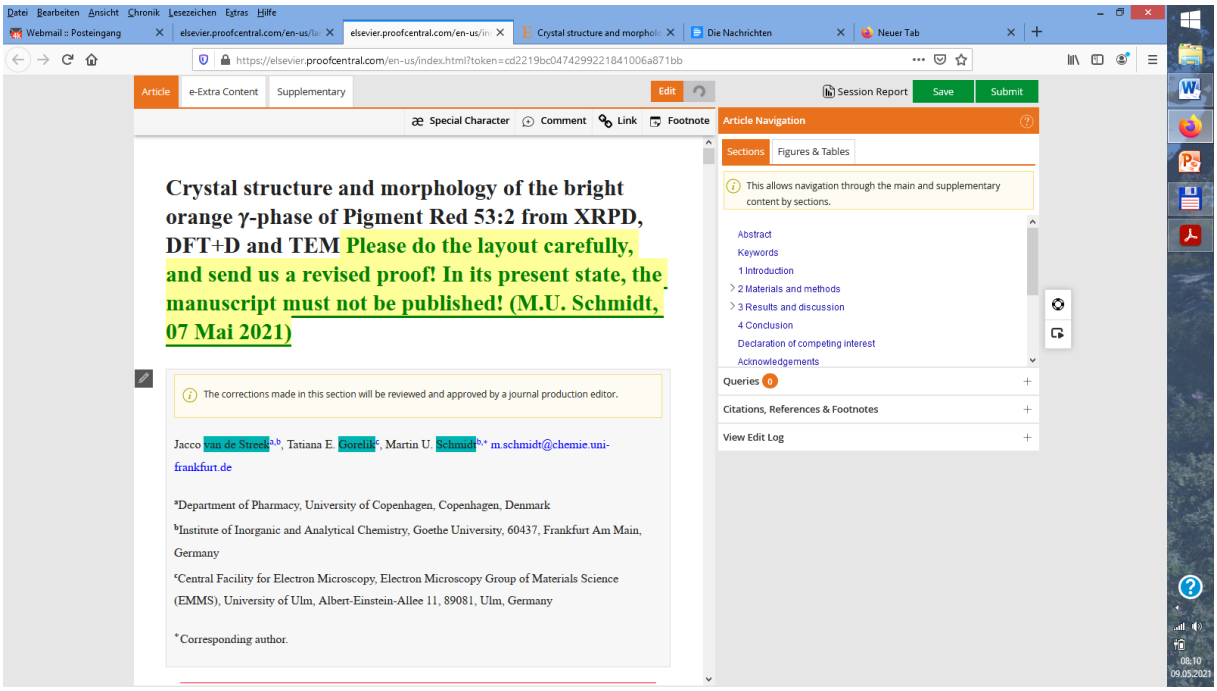


Fig. 2. Rietveld refinement fit for the γ-phase of P.R.53:2: red crosses, measured data points; blue line, calculated profile; black line, difference curve; blue tickmarks, calculated reflection positions. *Note for the layout: This figure should be printed with full page width.*

My correction of the proofs on 7 May 2021:



My mail to the head of the Indian production office on 6 May 2021:

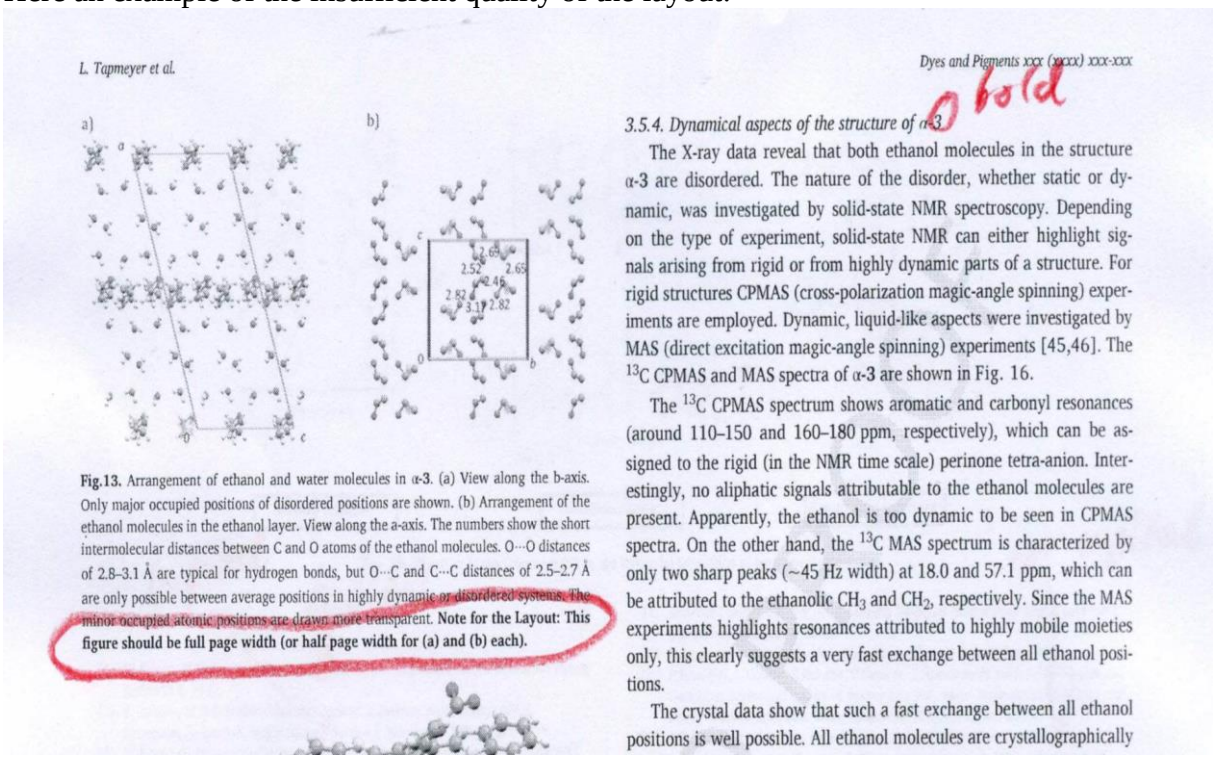
>Dear Antony J C Nathanial,

please prepare the proofs carefully.

Yours sincerely
Martin Schmidt
<
Remark: I did not receive any reply to this mail.

This is already the second case that Elsevier publishes a manuscript in bad layout state violating explicit statements of the authors.

The first case was a paper in *Dyes and Pigments*, **2020**, *181*, 108442, doi.org/10.1016/j.dyepig.2020.108442
Also there, the manuscript was published online, before the layout was done carefully, and against the explicit statement of the authors.
Here an example of the insufficient quality of the layout:



L. Tapmeyer et al.

Dyes and Pigments xxx (xxxx) xxx-xxx

bold

a)

b)

Fig.13. Arrangement of ethanol and water molecules in α-3. (a) View along the b-axis. Only major occupied positions of disordered positions are shown. (b) Arrangement of the ethanol molecules in the ethanol layer. View along the a-axis. The numbers show the short intermolecular distances between C and O atoms of the ethanol molecules. O···O distances of 2.8–3.1 Å are typical for hydrogen bonds, but O···C and C···C distances of 2.5–2.7 Å are only possible between average positions in highly dynamic or disordered systems. The minor occupied atomic positions are drawn more transparent. **Note for the Layout: This figure should be full page width (or half page width for (a) and (b) each).**

3.5.4. Dynamical aspects of the structure of α-3

The X-ray data reveal that both ethanol molecules in the structure α-**3** are disordered. The nature of the disorder, whether static or dynamic, was investigated by solid-state NMR spectroscopy. Depending on the type of experiment, solid-state NMR can either highlight signals arising from rigid or from highly dynamic parts of a structure. For rigid structures CPMAS (cross-polarization magic-angle spinning) experiments are employed. Dynamic, liquid-like aspects were investigated by MAS (direct excitation magic-angle spinning) experiments [45,46]. The ^{13}C CPMAS and MAS spectra of α-**3** are shown in Fig. 16.

The ^{13}C CPMAS spectrum shows aromatic and carbonyl resonances (around 110–150 and 160–180 ppm, respectively), which can be assigned to the rigid (in the NMR time scale) perinone tetra-anion. Interestingly, no aliphatic signals attributable to the ethanol molecules are present. Apparently, the ethanol is too dynamic to be seen in CPMAS spectra. On the other hand, the ^{13}C MAS spectrum is characterized by only two sharp peaks (~45 Hz width) at 18.0 and 57.1 ppm, which can be attributed to the ethanolic CH_3 and CH_2, respectively. Since the MAS experiments highlights resonances attributed to highly mobile moieties only, this clearly suggests a very fast exchange between all ethanol positions.

The crystal data show that such a fast exchange between all ethanol positions is well possible. All ethanol molecules are crystallographically

In this state, the paper was published online.

This is a shame for the journal Dyes and Pigments, and especially for the Elsevier production site in India.

Conclusion:
I advise all colleagues not to publish in Elsevier journals.

Martin Schmidt
May 9th, 2021