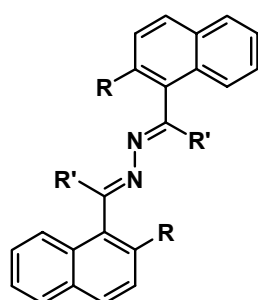


Unexpected Solid State Fluorescence of an Organic Pigment. Martin U. Schmidt ^a, Juste E. Djanhan ^a, Thomas Metz ^b, Michael Bolte ^a; (a) *Institute for Inorganic and Analytical Chemistry, University of Frankfurt, Marie-Curie-Str. 11, D-60439 Frankfurt am Main, Germany*; (b) *Clariant GmbH, Div. Pigments and Additives, SU-TIM, Research, G834, D-65931 Frankfurt am Main, Germany*.

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According to theory, organic compounds can show fluorescence in the solid state only if the chromophor-chromophor distances are large (6 - 8 Å, for $\pi - \pi^*$ transitions) [1]; otherwise the vibrational coupling between neighbouring molecules leads to enhanced electron-phonon coupling, and the fluorescence is quenched.

To prove this theory the compounds **1** - **4** were synthesized, crystallized, and their crystal structures and fluorescence behaviour were determined. Surprisingly, compound **3** shows strong solid state fluorescence, although the chromophor-chromophor distance between the centres of molecules is 3.863 Å only, the interplanar distance between neighbouring molecules being 3.548 Å only. The reason for this unexpected fluorescence is not understood yet.



- 1: R= OH, R'= H
(C.I. Pigment Yellow 101)
- 2: R= OCH₃, R'= H
- 3: R= OH, R'= CH₃
- 4: R= H, R'= H

Compound No.	1	2	3	4
Fluorescence in solution:	strong	no	strong	no
Solid state fluorescence:	strong	no	strong	no
Chromophor-chromophor distance ^a [Å]:	6,114	7,007	3,863	6,085
Space group:	<i>P</i> 2 ₁ / <i>c</i> ^b	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i> ^b
<i>Z</i>	2	2	4	2

a) Distance between the centres of neighbouring molecules
b) **1** and **4** are isostructural.

[1] H. Langhals, T. Potrawa, H. Nöth, G. Linti, *Angew. Chem.* **101** (1989), 497-499; *Angew. Chem. Int. Ed. Engl.* **28** (1989), 478-480.