University of Groningen

Blue Luminescence of Facial Tris(quinolin-8-olato)aluminum(III) in Solution, Crystals, and Thin Films

Muccini, Michele; Loi, Maria Antonietta; Kenevey, Kester; Zamboni, Roberto; Masciocchi, Norberto; Sironi, Angelo

Published in:
Advanced materials

DOI:
[10.1002/adma.200305421](https://doi.org/10.1002/adma.200305421)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2004

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Muccini, M., Loi, M. A., Kenevey, K., Zamboni, R., Masciocchi, N., & Sironi, A. (2004). Blue Luminescence of Facial Tris(quinolin-8-olato)aluminum(III) in Solution, Crystals, and Thin Films. *Advanced materials*, 16(11), 861 - 864. <https://doi.org/10.1002/adma.200305421>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

ADVANCED MATERIALS

Supporting Information

for

Advanced Materials, adma.200305421

© Wiley-VCH 2004
69451 Weinheim, Germany

Supporting Information

Figure SF1: Entire ^1H NMR spectra (0-10 ppm, Bruker DRX 300) of $\delta\text{-Alq}_3$ at -10°C in CDCl_3 : as prepared (see text, *fac*- Alq_3 , bottom) and after 2 hrs. (*mer*- Alq_3 , top). Apart from the signals of the oxyquinoline ligands of the *fac*- and *mer*- Alq_3 molecules (in the 7 - 9 ppm range), only strong resonances due to contaminating CHCl_3 (δ 7.28, s), H_2O in CHCl_3 (δ 1.7, s) and of traces of cyclohexane (δ 1.3, s) and silicone can be seen, thus excluding the presence of other Al(III) oxyquinoline derivatives.

Figure SF2: ^1H NMR spectra of $\delta\text{-Alq}_3$ (dissolved in CDCl_3 at -50°C), normalized to the CDCl_3 peak. Spectra are measured *isothermally* (-10°C) at the indicated interval time.

Figure SF3: Rietveld refinement plot for the Γ dataset ($\gamma\text{-Alq}_3/\delta\text{-Alq}_3 = 89/11$, see text), with peak markers and difference plot at the bottom.

$$R_{wp} = 0.133;$$

$$R_p = 0.102;$$

$$R_{Bragg}(\gamma) = 0.037$$

Table ST1. Fractional atomic coordinates for $\gamma\text{-Alq}_3$ (from rigid body refinement on the Γ dataset).

site	AlG	x	0.33333	y	0.66667	z	0.24108
site	N1G	x	0.57240	y	0.36772	z	-0.03477
site	C2G	x	0.58693	y	0.42476	z	0.15586
site	C3G	x	0.49961	y	0.42469	z	0.25399
site	C4G	x	0.39776	y	0.36757	z	0.16149
site	C5G	x	0.38323	y	0.31052	z	-0.02914
site	C6G	x	0.47055	y	0.31060	z	-0.12727
site	C7G	x	0.28137	y	0.25340	z	-0.12165
site	C8G	x	0.26684	y	0.19635	z	-0.31228
site	C9G	x	0.35417	y	0.19643	z	-0.41041
site	C10G	x	0.45602	y	0.25355	z	-0.31790
site	O1G	x	0.54315	y	0.25362	z	-0.41582
site	H2G	x	0.66563	y	0.46890	z	0.22734
site	H3G	x	0.51084	y	0.46877	z	0.40129
site	H4G	x	0.33029	y	0.36751	z	0.23731
site	H6G	x	0.21390	y	0.25334	z	-0.04582
site	H7G	x	0.18815	y	0.15222	z	-0.38375
site	H8G	x	0.34294	y	0.15235	z	-0.55770