Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supporting Information

Crystal structure determination of ANTBD

Measurements were made at 150 K on an Oxford Diffraction Gemini A Ultra diffractometer using graphite-monochromated Mo-Kα radiation (λ = 0.71073 A˚). Cell parameters were refined from the observed positions of all strong reflections. Intensities were corrected semiempirically for absorption, based on symmetry-equivalent and repeated reflections. The structures were solved by direct method and refined on *F*2 values for all unique data. More information can be found in the supplementary information. All non-hydrogen atoms were refined anisotropically, and C-bound H atoms were constrained with a riding model; *U*(H) was set at 1.2 (1.5 for methyl groups) times *U*eq for the parent C atom. Programs were Oxford Diffraction CrysAlisPro[1], and SHELXTL for structure solution and refinement,[2] and Mercury for molecular graphics.

1 *CrysAlisPro* Oxford Diffraction Ltd, Oxford, UK, 2008;
2: Y: G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 2008, **64**, 112.

Crystal data. $C_{23}H_{15}BF_2N_2$, *M* = 368.18, orthorhombic, *a* = 13.0065(7), *b* = 12.4226(6), *c* = 21.835(1) Å, *U* = 3528.0(3) Å3, *T* = 150 K, space group *Pbca* (no. 61), *Z* = 8, 13782 reflections measured, 4207 unique (*R*int = 0.0368) which were used in all calculations. The final *wR*(*F*2) was0.0972 (all data).
Fluorine atoms were found to be positionally disordered and successfully modelled in a 60:40 ratio.

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_publ_contact_author_name   'Andrew C. Benniston'
_publ_contact_author_address

Molecular Photonics Laboratory
School of Chemistry
Newcastle University
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NE1 7RU
UK

_publ_contact_author_phone     '44 191 222 5706'
_publ_contact_author_fax       '44 191 222 6929'
_publ_contact_author_email      a.c.benniston@ncl.ac.uk
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Exciplex-like emission from a closely-spaced,
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C8 C 0.33395(11) 0.23616(11) 0.27881(6) 0.0309(3) Uani 1 1 d . A .
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C9 C 0.28353(10) 0.26377(11) 0.22487(6) 0.0295(3) Uani 1 1 d . . .

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C15 C -0.03849(10) 0.23124(10) 0.51897(6) 0.0245(3) Uani 1 1 d . . .
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C1 N1 B1 N2 177.03(12) . . . . ?
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C4 N1 B1 F1A -135.2(5) . . . . ?
C4 N1 B1 F2 124.6(9) . . . . ?
C4 N1 B1 F2A 107.8(3) . . . . ?
C4 N1 B1 N2 -3.7(2) . . . . ?
B1 N1 C1 C2 179.57(14) . . . . ?
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N1 C1 C2 C3 -0.43(16) . . . . ?
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B1 N1 C4 C5 2.9(2) . . . . ?
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C3 C4 C5 C10 4.8(2) . . . . ?
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C16 C11 C12 C13 0.34(18) . . . . ?
C11 C12 C13 C14 0.12(19) . . . . ?
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C11 C16 C17 C18 -0.60(18) . . . . ?
C15 C16 C17 C18 177.71(11) . . . . ?
C16 C17 C18 C19 -179.40(12) . . . . ?
C16 C17 C18 C23 -0.79(17) . . . . ?
C17 C18 C19 C20 176.78(12) . . . . ?
C23 C18 C19 C20 -1.83(18) . . . . ?
C18 C19 C20 C21 0.70(19) . . . . ?
C19 C20 C21 C22 1.0(2) . . . . ?
C20 C21 C22 C23 -1.5(2) . . . . ?
C5 C10 C23 C18 -178.73(10) . . . . ?
C5 C10 C23 C22 0.13(17) . . . . ?
C11 C10 C23 C18 -0.99(17) . . . . ?
C11 C10 C23 C22 177.87(11) . . . . ?
C21 C22 C23 C10 -178.59(12) . . . . ?
C21 C22 C23 C18 0.29(18) . . . . ?
C17 C18 C23 C10 1.58(17) . . . . ?
C17 C18 C23 C22 -177.34(11) . . . . ?
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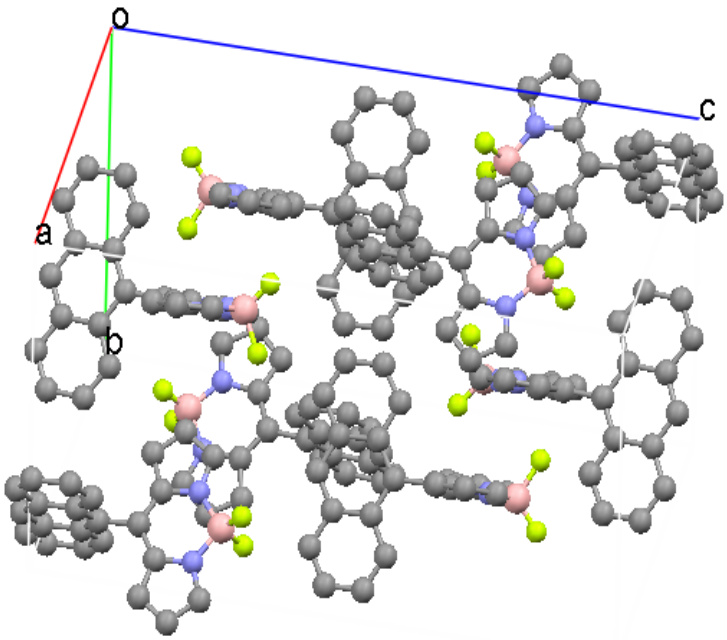

Figure S1. Crystal packing diagram for **ANTBD**.