Supporting information file

Implementing fluorescent MOFs as down-converting layers in hybrid light-emitting diodes

Enrico Angioni,[a] Ross J. Marshall,[b] Neil J. Findlay,[b] Jochen Bruckbauer,[c] Ben Breig,[a] David J. Wallis,[de] Robert W. Martin,[c] Ross S. Forgan[b]* and Peter J. Skabara[b]*

[a] WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde, G1 1XL, UK

[b] WestCHEM, School of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK

[c] Department of Physics, SUPA, University of Strathclyde, Glasgow, G4 0NG, UK

[d] Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, CB3 0FS, UK

[e] Centre for High Frequency Engineering, University of Cardiff, Cardiff, CF24 3AA, UK

Email: ross.forgan@glasgow.ac.uk or peter.skabara@glasgow.ac.uk

Contents

Figure S1: ^{1}H NMR spectrum of **BTBMBA** in DMSO-d_6.
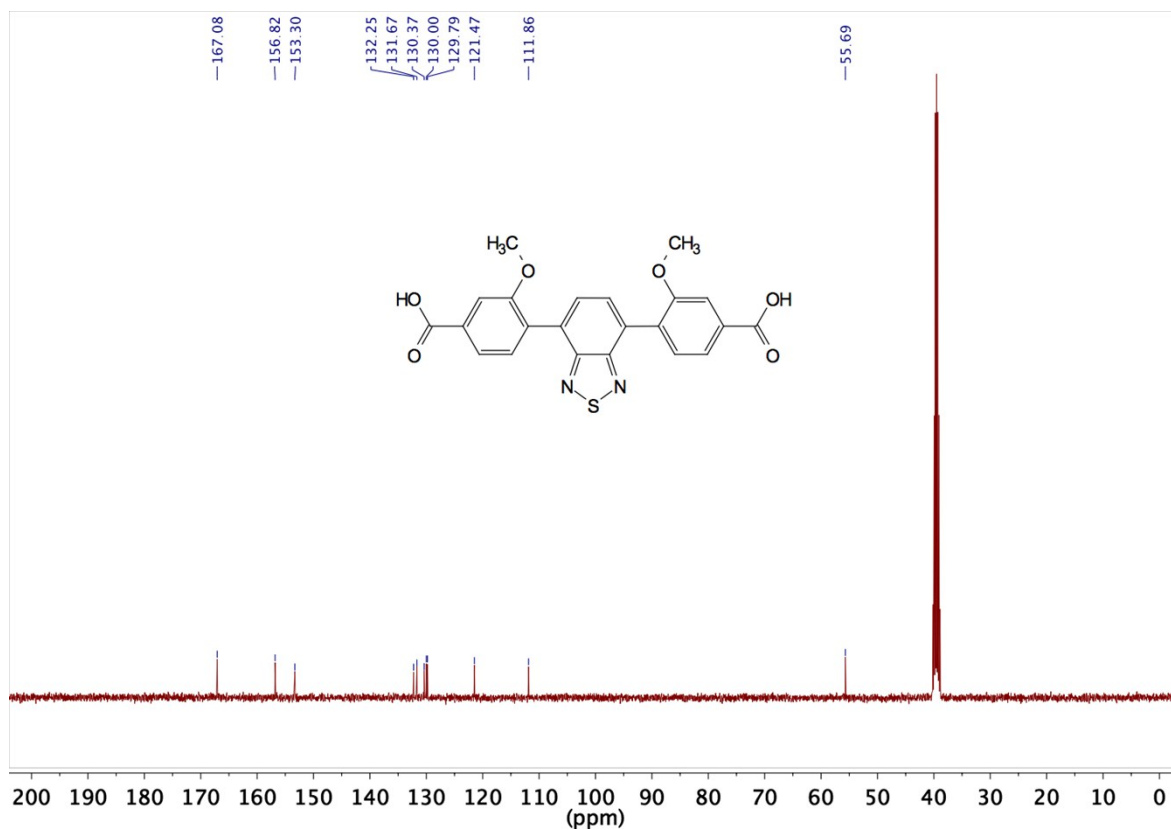
Figure S2: ^{13}C NMR spectrum of **BTBMBA** in DMSO-d_6.

EA082 MW=436?
(DCM)/MeOH+DEA
C22H16N2O6S

EPSRC National Facility Swansea
LTQ Orbitrap XL

Dr Neil Findlay
15/06/2015 15:10:12

Observed Data

435.0649
z=1

436.0678
z=1

435.5668
z=2

437.0605
z=1
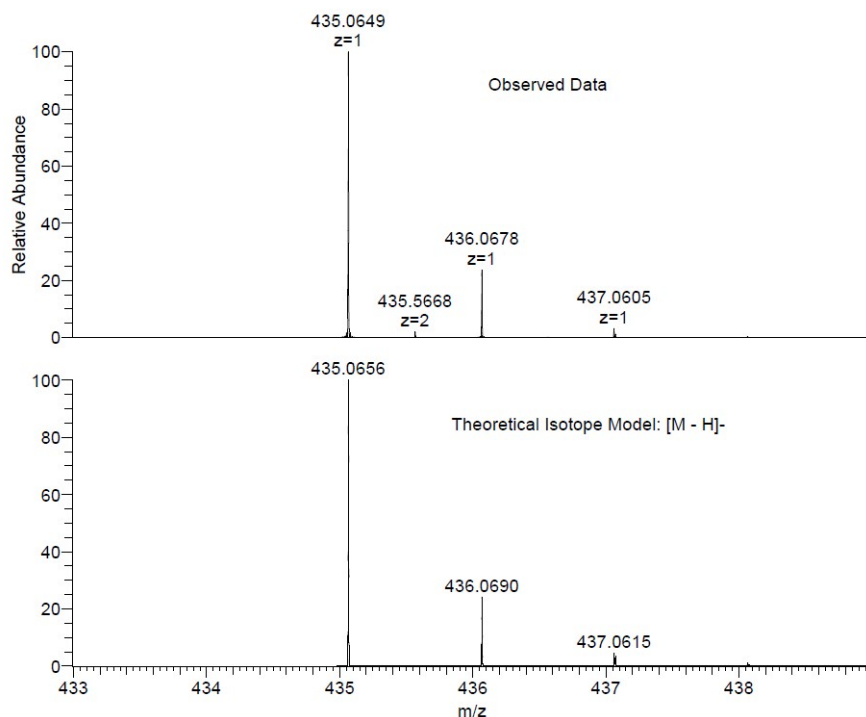
NL:
2.78E7
STRSKA046-OJ-HNESN#45-
77 RT: 0.72-0.93 AV: 8 T:
FTMS - p NSI Full ms
[120.00-615.00]

Theoretical Isotope Model: [M - H]-

435.0656

436.0690

437.0615

NL:
1.72E4

$C_{22} H_{15} N_2 O_6 S$:
$C_{22} H_{15} N_2 O_6 S_1$
p (gss, s /p:40) Chrg -1
R: 100000 Res .Pwr . @FWHM

STRSKA046-OJ-HNESN #45-77 RT: 0.72-0.93 AV: 8 SM: 7G NL: 3.01E7
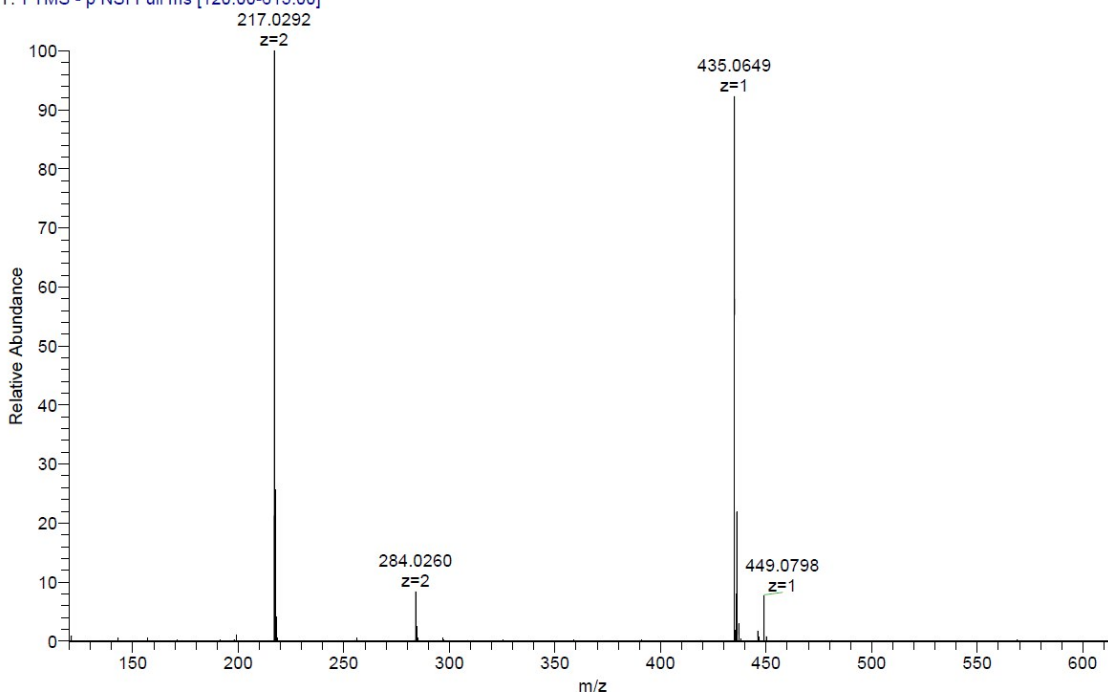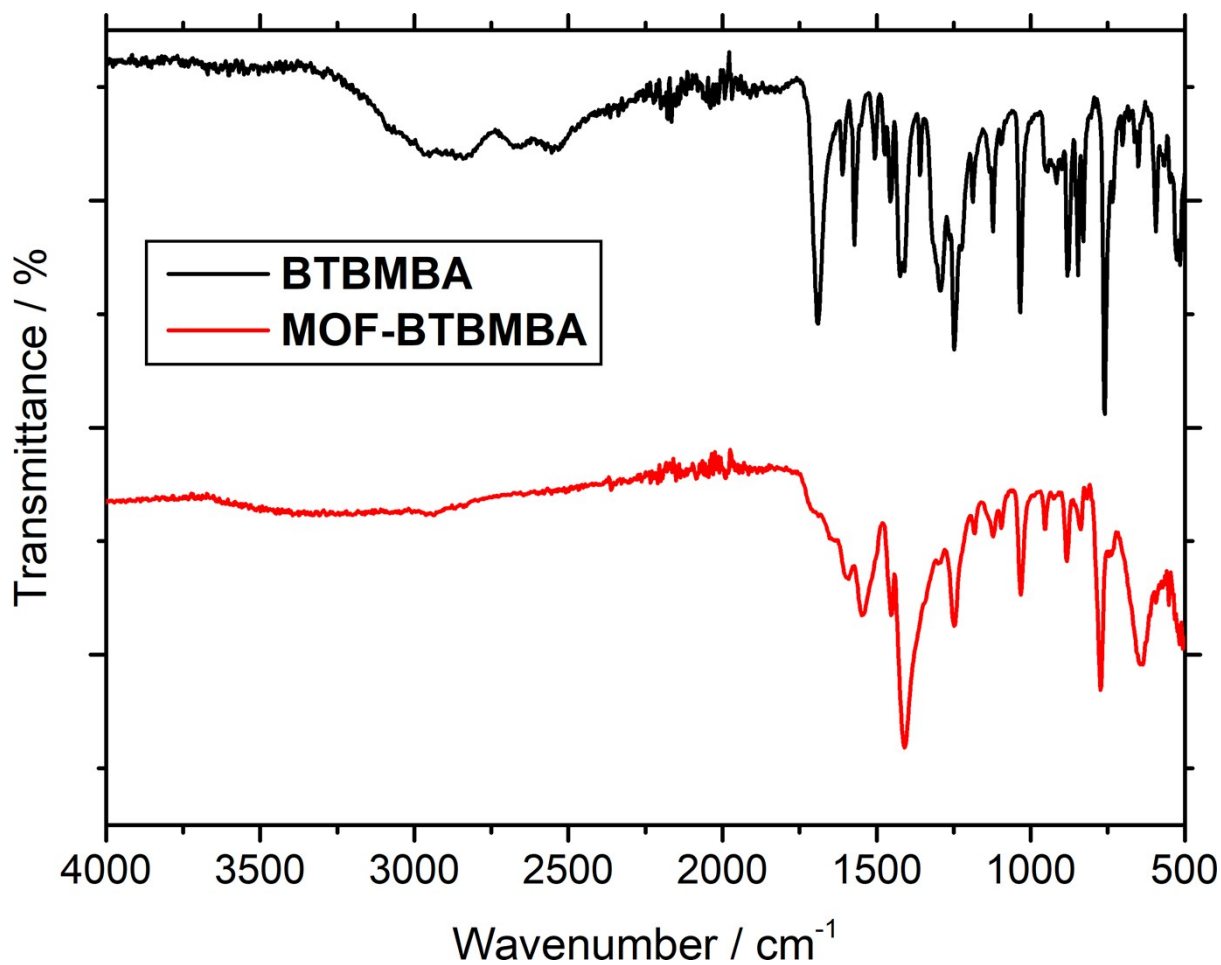T: FTMS - p NSI Full ms [120.00-615.00]

217.0292
z=2

435.0649
z=1

284.0260
z=2

449.0798
z=1

Figure S3: HRMS data of **BTBMBA**.

Figure S4: Stacked FTIR spectrum of **BTBMBA** (top) and **MOF-BTBMBA** (bottom). Peaks for **BTBMBA** are tentatively assigned as C=O (1692 cm^{-1}); C=N (1572 cm^{-1}); N-S (750 cm^{-1}). Coordination to the Zr^{4+} cations has shifted the C=O stretch in **MOF-BTBMBA** to lower frequency, which is suggestive of MOF formation, and it now overlaps with the C=N signals. Characteristic stretches in the fingerprint region of the ligand are retained.
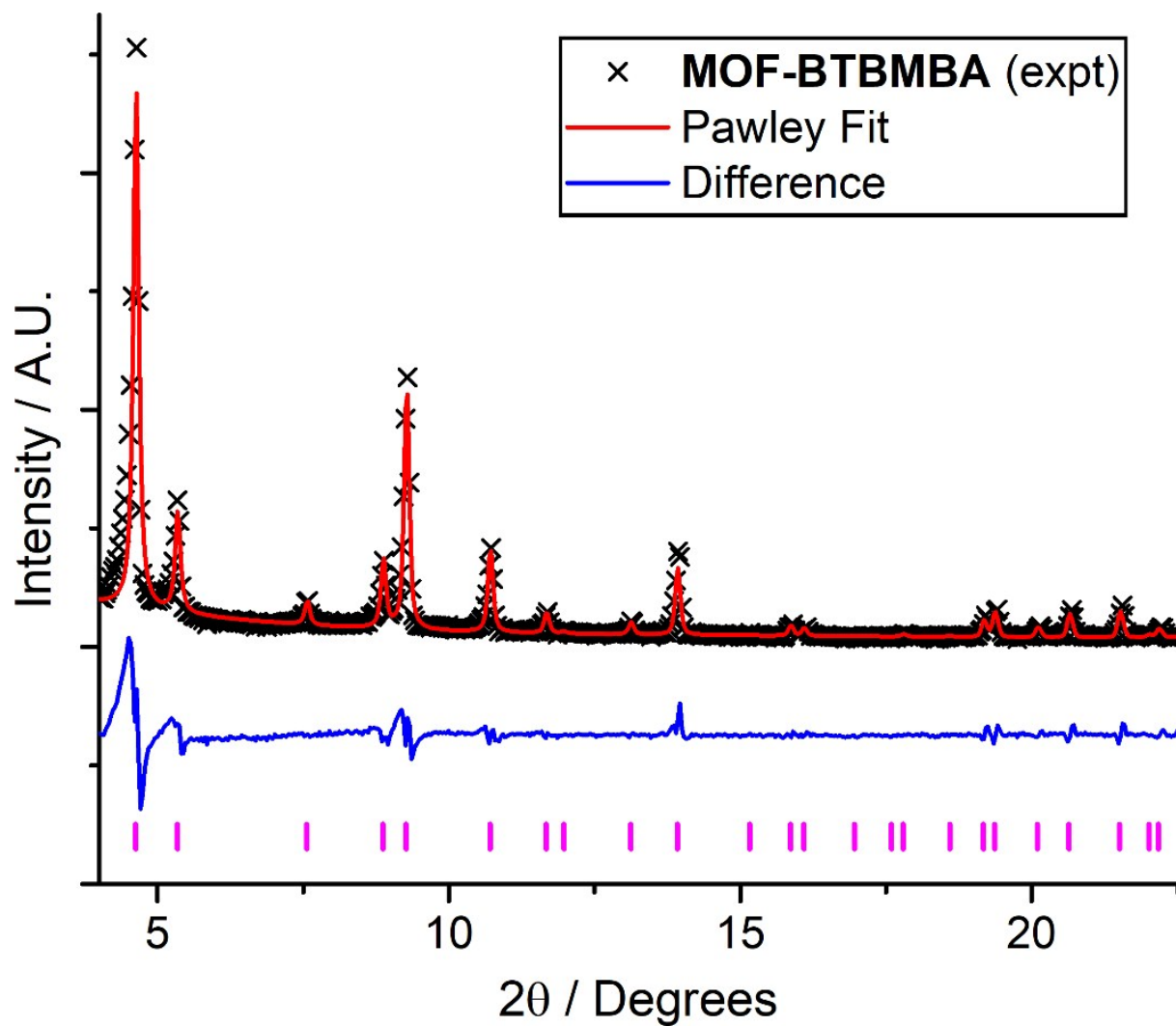
Figure S5: Pawley fit of the PXRD data for **MOF-BTBMBA**. The data fit a cubic unit cell of *a* = 33.02947 Å in the *Fm3m* space group, with wR = 20.4%. Some discrepancies from the model are expected as the sample was collected on a lab source with the sample on a flat plate and not spun.