Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Non-aggregated Zn(II)octa(2,6-diphenylphenoxy) phthalocyanine as a Hole Transporting Material for efficient Perovskite Solar cells

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Table S1. Photovoltaic parameters, standard deviation, and average values, obtained for the perovskite solar cells employing phthalocyanine **TT80** as hole-transporting material. P_{in}, incident intensity of simulated AM1.5G solar light.[a]

Cell	Solvent	Additives[b]	J_{SC} [mA·cm^{-2}]	V_{OC} [mV]	Fill Factor	P_{in} [mW.cm^{-2}]	PCE [%]
1	PhCl	NO	11.903	578.352	0.362	96.98	2.5697
2			11.890	550.080	0.349	96.29	2.3706
Average			11.897	564.22	0.3555	–	2.470
Standard deviation			0.006	14.14	0.0065	–	0.100
Relative error			–	–	–	–	4.0%
Average rounded			11.897±0.006	564±14	0.356±0.007	–	**2.5±0.1**
1	PhCl	YES	16.354	797.414	0.503	97.37	6.7368
2			16.694	821.913	0.484	99.05	6.7047
3			15.693	814.042	0.505	98.19	6.5702
4			17.056	786.684	0.478	98.20	6.5312
Average			16.449	805.01	0.4925	–	6.630
Standard deviation			0.502	13.79	0.0117	–	0.091
Relative error			–	–	–	–	1.4%
Average Rounded			16.4±0.5	805±14	0.493±0.01	–	**6.6±0.1**
1	$PhCH_3$	YES	16.914	795.603	0.450	0.974	6.2147
2			16.190	797.372	0.464	0.977	6.1329
3			17.401	803.157	0.408	0.972	5.8694
4			16.333	812.572	0.408	0.980	5.5271
Average			16.710	802.18	0.4325	–	5.870
Standard deviation			0.483	6.62	0.0250	–	0.364
Relative error			–	–	–	–	6.2%
Average Rounded			16.7±0.5	802±7	0.433±0.03	–	**5.9±0.4**

[a]For 1 sun irradiation, P_{in} = 100 mW·cm^{-2}. [b]Additives: LiTFSI +TBP.

Table S2. Effect of the spin-coating speed on the photovoltaic parameters obtained for the perovskite solar cells devices employing phthalocyanine **TT80** as hole-transporting material.

Additives	Solvent	Spin-coating speed (rpm)	P_{in} [mW·cm^{-2}]	J_{SC} (mA·cm^{-2})	V_{OC} (mV)	F.F. (%)	η (%)
LiTFSI +TBP	PhCl	2000	97.4	16.35	797	50.3	6.7
		500	98.2	11.82	378	25.1	2.35
LiTFSI +TBP	$PhCH_3$	2000	97.4	16.91	796	45.0	6.2
		500	96.9	16.49	815	35.2	4.88

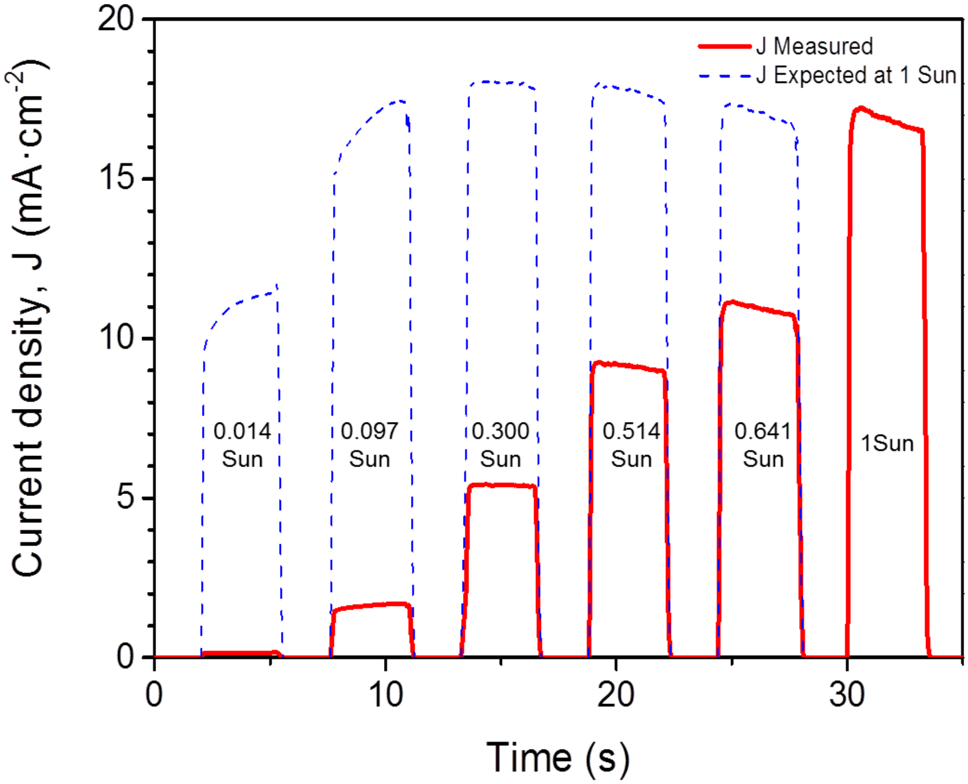

Figure S1. Current dynamics spectrum for the best PSC/**TT80** cell (**TT80**+LiTFSI+TBP in PhCl).[S1, S2] Shutter was closed for 2s and then automatically opened during 3.5s with different sun filters to tune the incidence sun intensity. The expected photocurrent at 1Sun was calculated multiplying the measured photocurrent at each sun by the factor 1/incidence sun. Except in the case of 0.014 Sun, where the very small incidence light in comparison with 1 Sun can conduct bigger errors, a linear behavior was observed, thus the total J_{SC} at 1 sun can be calculated at any diffuse light only multiplying by the conversion factor ($I_{1Sun}/I_{incidence}$). At medium sun intensities (0.3 and 0.514 Sun), the response of the transient photocurrent was while at high sun intensities a very small discharge in current was observed. The latter phenomena can be attributed to small saturation where some of the created charges were not collected properly until the stationary state is reached. If this behavior is not taken in consideration, higher currents can be recorded in the *J-V* curve providing slightly higher values in power conversion efficiency. For this reason, we illuminated the perovskite solar cell during 5s before recording the *J-V* curve and we have controlled the sweeping rate during the experiment (around 0.1V/s).

S1 Q. Jiang, X. Sheng, Y. Li, X. Feng and T. Xu, *Chem. Commun.*, 2014, **50**, 14720-14723.

S2 B. C. O'Regan, K. Bakker, J. Kroeze, H. Smit, P. Sommeling and J. R. Durrant, *J. Phys. Chem. B*, 2006, **110**, 17155-17160.

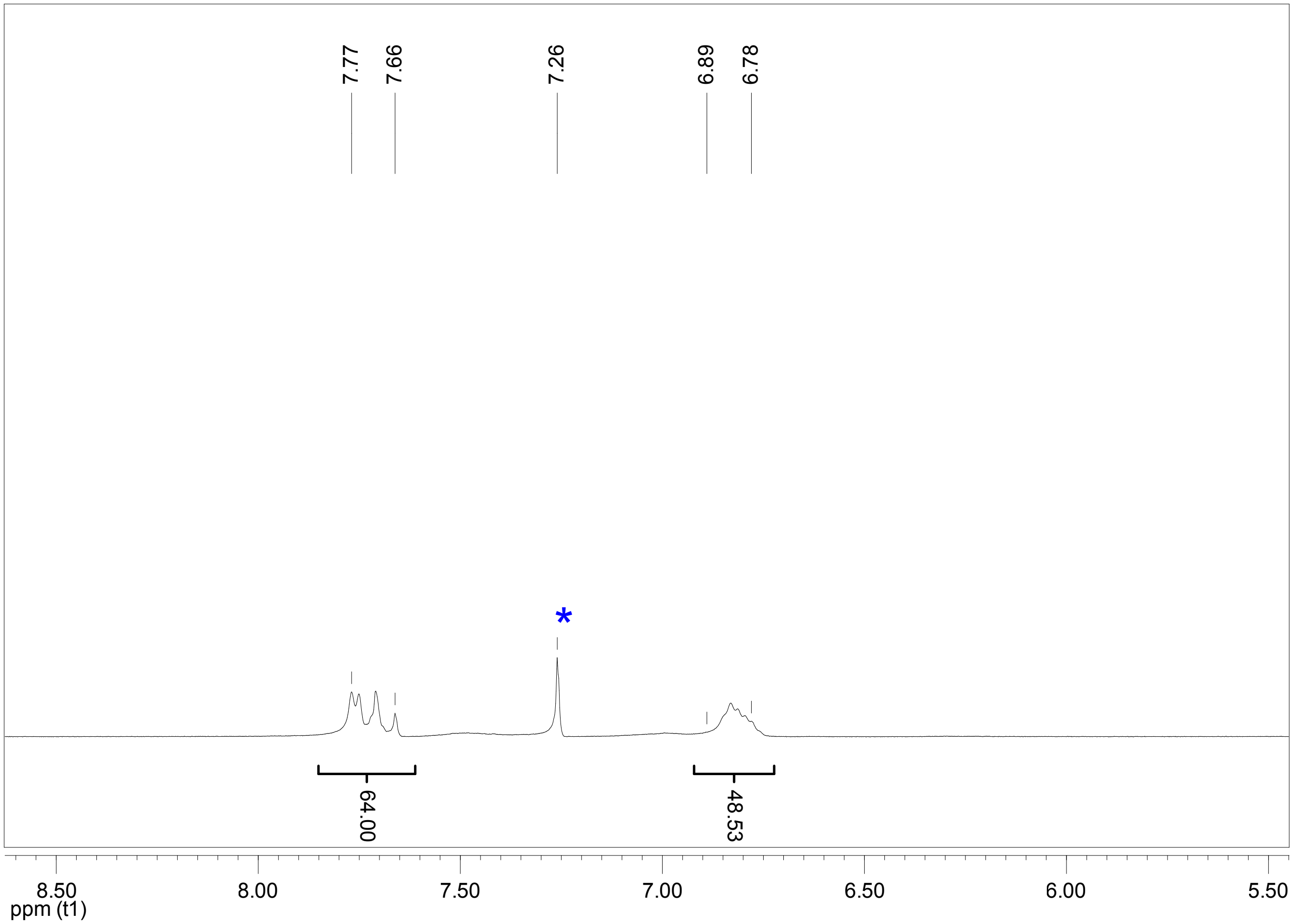

Figure S2. ^{1}H NMR spectrum ($CDCl_3$; 400 MHz) of **TT80** (* denotes the residual solvent peak of the $CDCl_3$ solvent).

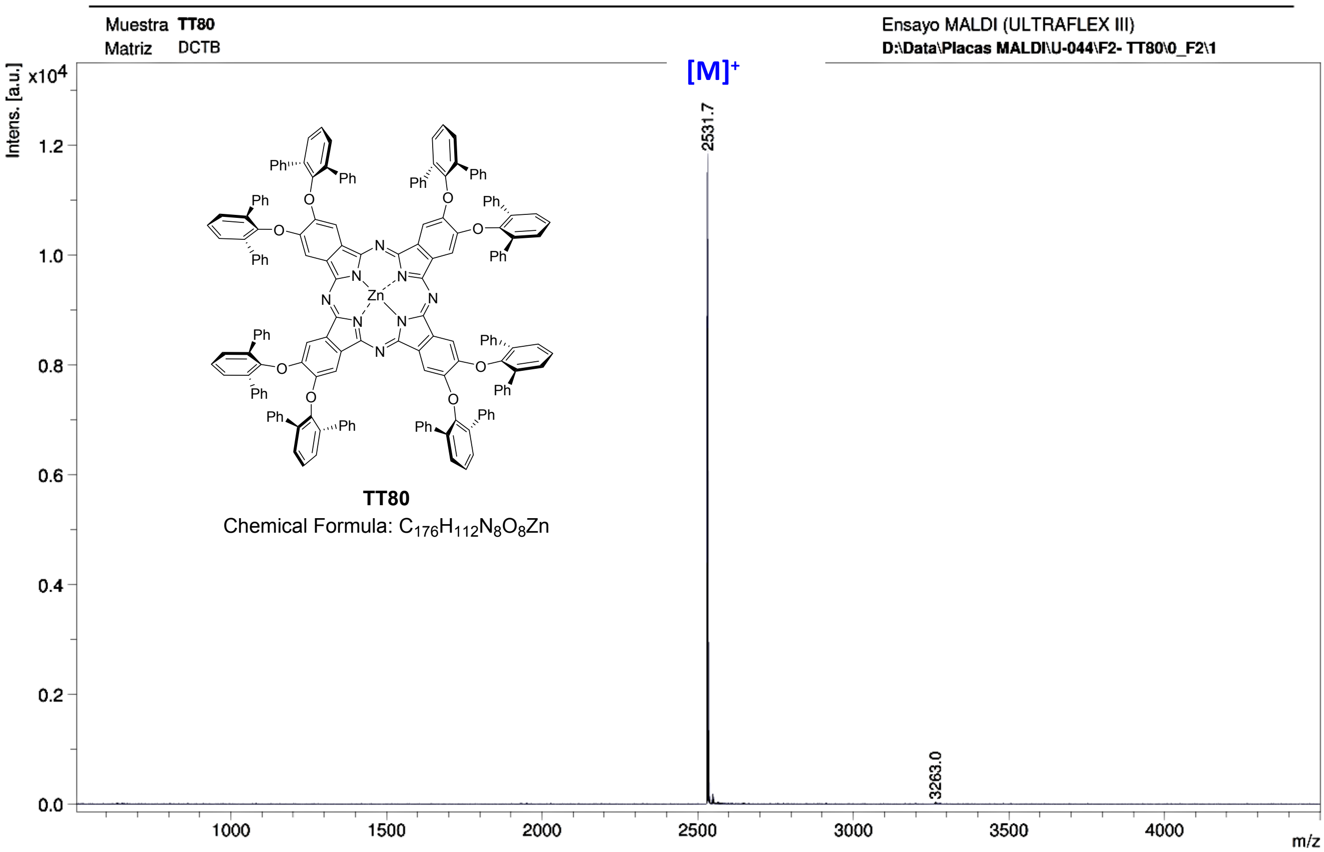

Figure S3. MALDI-TOF mass spectrum of **TT80** (matrix: DCTB); the most abundant peak is denoted.

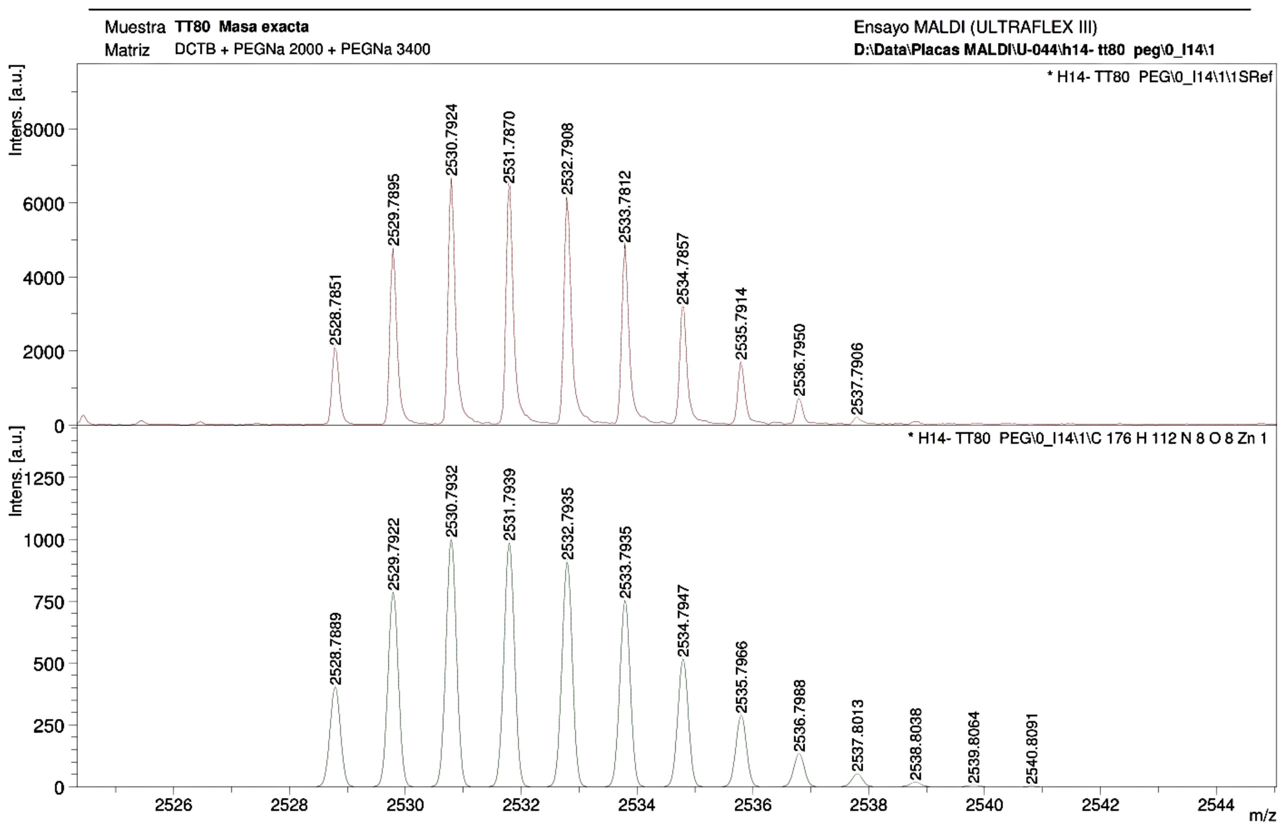

Figure S4: HRMS (MALDI-TOF) spectrum of **TT80** (matrix: DCTB + PEGNa 2000+PEGNa 3400). Top inset: experimental; bottom inset: theoretical isotopic distribution simulated for $[M]^+$ ($C_{176}H_{112}N_8O_8Zn_1$).

Generated Molecular Formulas

Formula	Mass	Error	DblEq	N rule	Electron Configuration
C 171 H 112 N 10 O 10 Zn 1	2,528.7849	0.0839	121.00	ok	odd
C 176 H 112 N 8 O 8 Zn 1	2,528.7889	1.5069	125.00	ok	odd
C 180 H 110 N 7 O 6 Zn 1	2,528.7804	1.8755	129.50	ok	even
C 177 H 112 N 6 O 9 Zn 1	2,528.7777	2.9353	125.00	ok	odd
C 181 H 112 N 6 O 6 Zn 1	2,528.7929	3.0977	129.00	ok	odd
C 175 H 110 N 9 O 8 Zn 1	2,528.7763	3.4663	125.50	ok	even
C 172 H 114 N 9 O 10 Zn 1	2,528.7975	4.8893	120.50	ok	even
C 175 H 112 N 10 O 7 Zn 1	2,528.8001	5.9491	125.00	ok	odd
C 177 H 114 N 7 O 8 Zn 1	2,528.8015	6.4801	124.50	ok	even
C 179 H 108 N 8 O 6 Zn 1	2,528.7678	6.8486	130.00	ok	odd
C 176 H 110 N 7 O 9 Zn 1	2,528.7651	7.9085	125.50	ok	even
C 174 H 108 N 10 O 8 Zn 1	2,528.7638	8.4394	126.00	ok	odd
C 173 H 116 N 8 O 10 Zn 1	2,528.8100	9.8624	120.00	ok	odd

Figure S5: Single mass analysis of **TT80** (Mass expressed in Da; Error expressed in mDa).