Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Efficient Blue Phosphorescent Host through Nonbonded Conformational Locking Interactions

Jongchul Kwon,[a] Tae-Hyuk Kwon,[a] Hyo Soon Cho,[a] Myoung Ki Kim,[a] Ik-Soo Shin,[a] Su-Jin Park,[b] Dae Yeup Shin,[b] Jong-In Hong[a,*]

[a]*Department of Chemistry, College of Natural Sciences, Seoul National University, Seoul 151-747, Korea, and* [b]*Corporate R&D Center, Samsung SDI, Yongin 449-902, Korea.*

Contents

Electrochemical Study

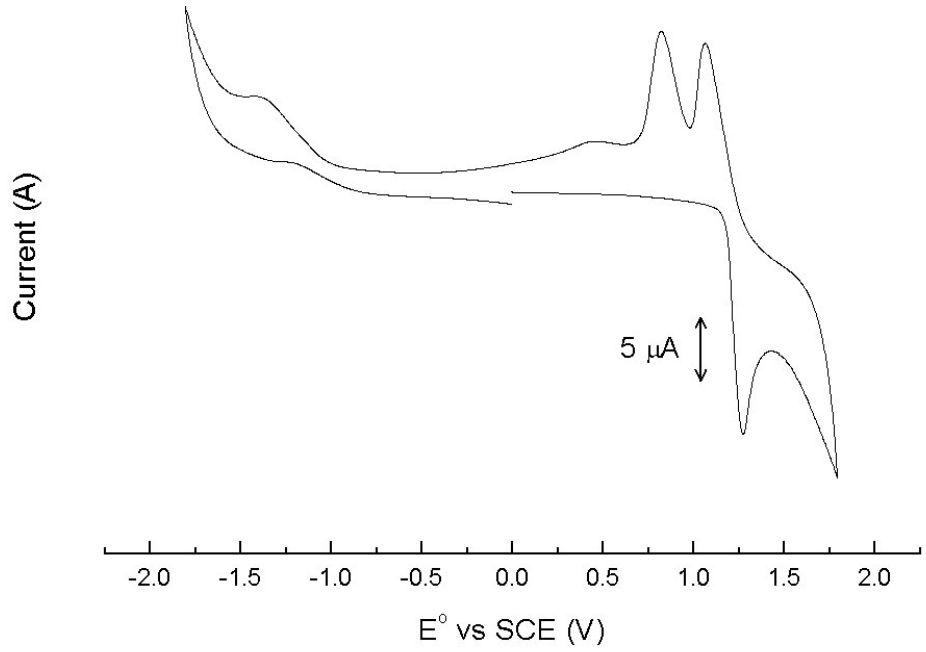


Figure S1. Cyclic voltammogram of 0.5 mM TCTEB in MeCN solution. Scan rate is 0.2 V/s (Pt working electrode, Pt counter electrode, silver wire quasi-reference electrode, and 0.1 M $TBAPF_6$ supporting electrolyte).

The oxidation half-wave potential of TCTEB is observed at $E_{1/2}$ = 1.50 V vs SHE. The HOMO energy level of TCTEB (-5.99 eV) is calculated from $E_{1/2}$ after correction of the vacuum energy level (4.49 eV). The anodic oxidation of TCTEB showed irreversible redox electrochemistry and we could only determine the first oxidation potential ($E_{1/2}$) of TCTEB from repetitive batch test. Cyclic voltammetry (CV) was performed using a CH Instruments 660 Electrochemical Analyzer (CH Instruments, Inc., Texas). The electrochemical experiment was referenced with respect to a Ag wire quasireference electrode (AgQRE). All potential values were calibrated against the standard calomel electrode (SCE) by adding ferrocene as an internal reference (E^0 (Fc/Fc^+) = 0.424 V vs SCE) and calculated to standard hydrogen electrode (SHE).[1,2] A platinum (Pt) disk (diameter: 2 mm) working electrode was used for electrochemical study. It was polished with 0.05 μM alumina (Buehler, Lake Bluff, Illinois) on a felt pad and sonicated in absolute

ethanol for 5 min. Then the electrode was heated at 70 °C for 15 min before each experiment. Solutions were prepared in a dry box incorporating a N_2 atmosphere or were prepared in air, purged with N_2.

Device Study

Organic layers were fabricated by high-vacuum (10^{-7} torr) thermal evaporation onto a patterned ITO glass pre-cleaned by a UV-ozone chamber. The 10 nm-thick film of copper phthalocyanine (CuPc) and 30 nm-thick film of 4, 4`-bis[*N*-(naphthyl-*N*-phenylamino)biphenyl (α-NPD) served as a hole injection layer (HIL) and a hole transport layer, respectively. The EML was prepared by co-evaporating a TCTEB or TCTMB host and *x* wt % FIrpic dopant. Dopant concentration is in the 6 – 11 wt % range. Next, a 30 nm-thick 4-biphenyloxolatoaluminium(III)bis(2-methyl-8-quinolinato)4-phenylphenolate (BAlq) layer, as both a hole blocking layer (HBL) and electron transporting layer (ETL), was deposited, which was then followed by deposition of LiF as an electron injection layer. Finally, after changing the metal mask, a 100 nm thick aluminum film was deposited on the EIL and then encapped. The Keithly 2400 as a source meter with a computer was used to operate the device. The EL spectra were obtained from PR 650 spectroradiometer.

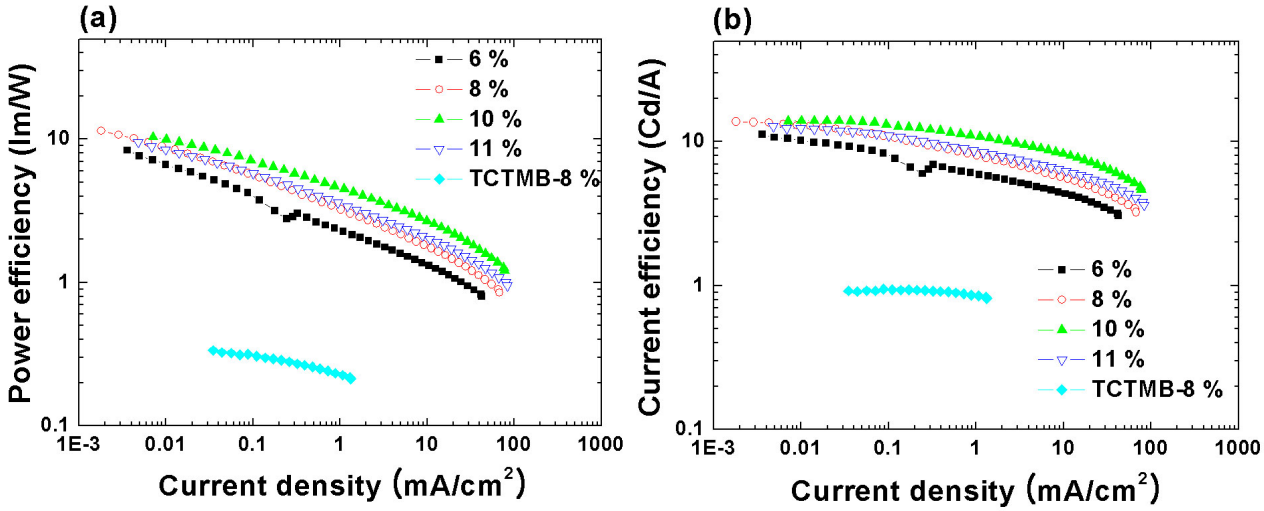


Figure S2. EL device data. (a) Current density J(mA/cm^2) vs Power efficiency (lm/W) (b) Current density J(mA/cm^2) vs Current efficiency I(cd/A)

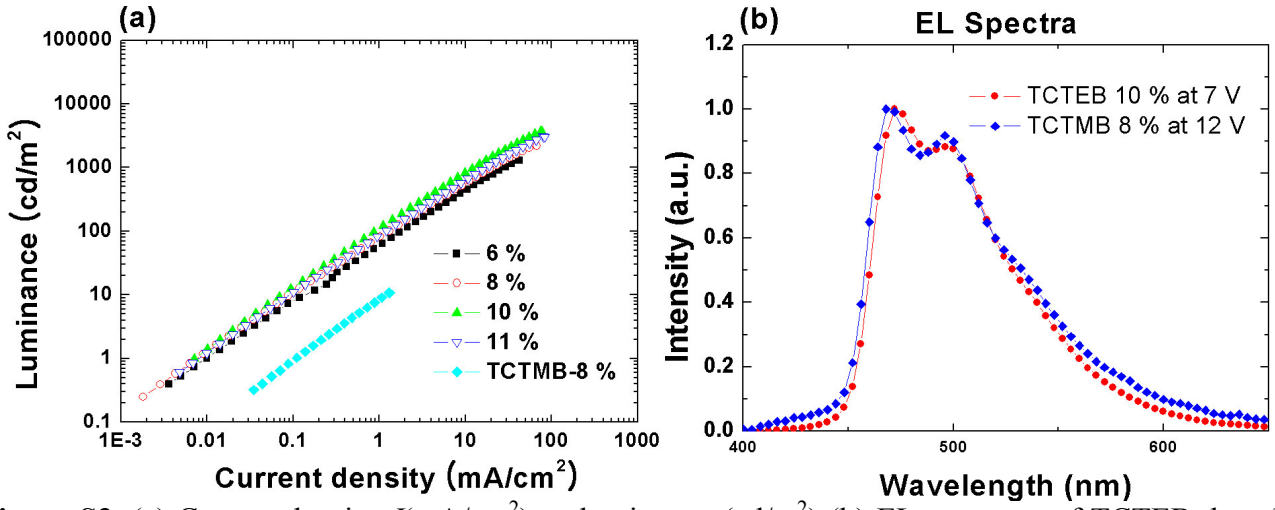


Figure S3. (a) Current density J(mA/cm^2) vs luminance (cd/m^2) (b) EL spectrum of TCTEB doped 10 wt % FIrpic at 7 V and TCTMB doped with 8 wt % at 12 V.

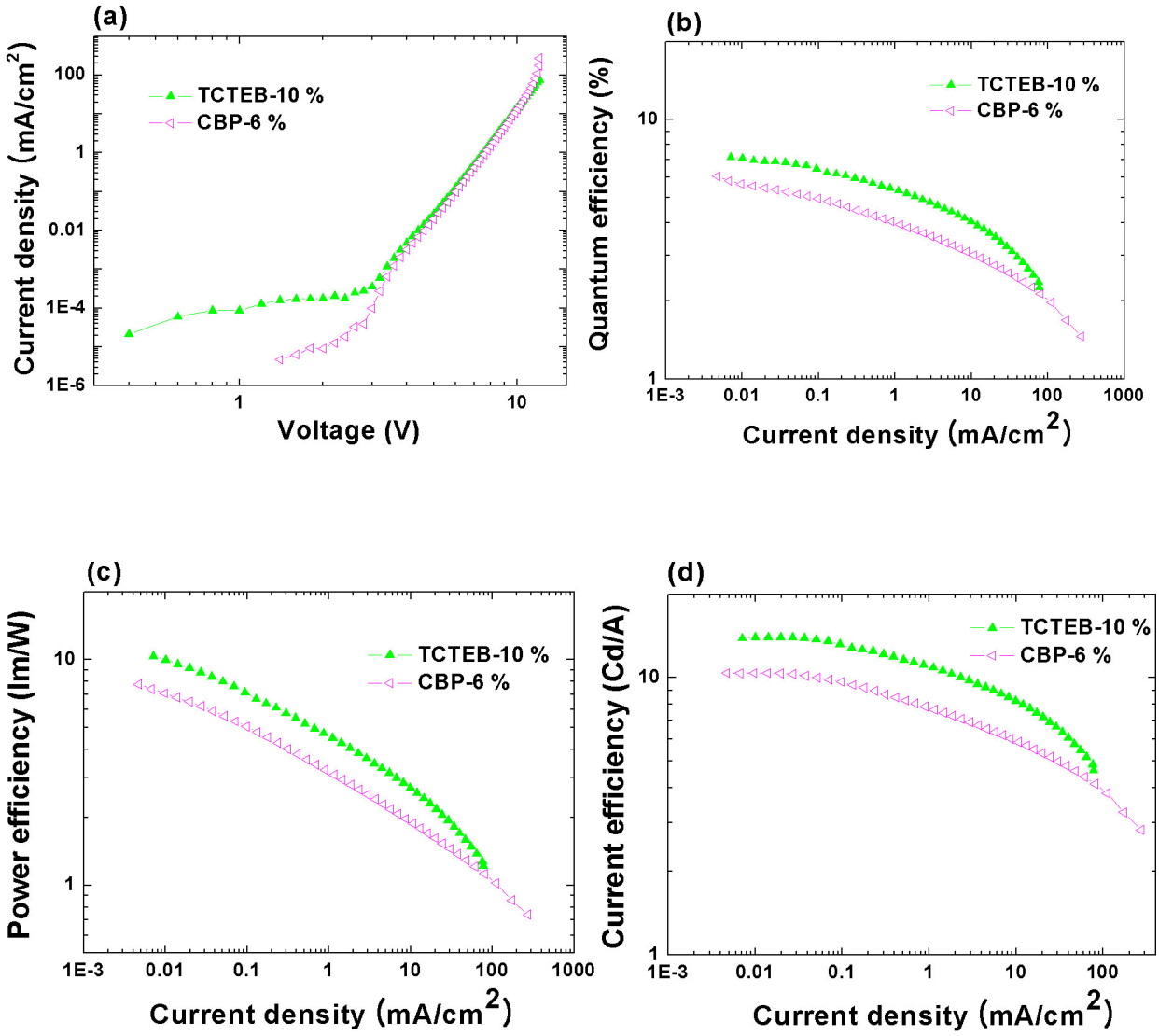


Figure S4. EL device data for ITO/CuPC (10 nm)/NPD (30 nm)/EML (30 nm) TCTEB or CBP doped with FIrpic 10 wt % and 6 wt %, respectively /BAlq (30 nm)/LiF (1 nm)/Al (100 nm). (a) Voltage vs Current density J(mA/cm^2) (b) Current density J(mA/cm^2) vs Quantum efficiency (%) (c) Current density J(mA/cm^2) vs Power efficiency (lm/W) (d) Current density J(mA/cm^2) vs Current efficiency I(cd/A)

TGA and DSC

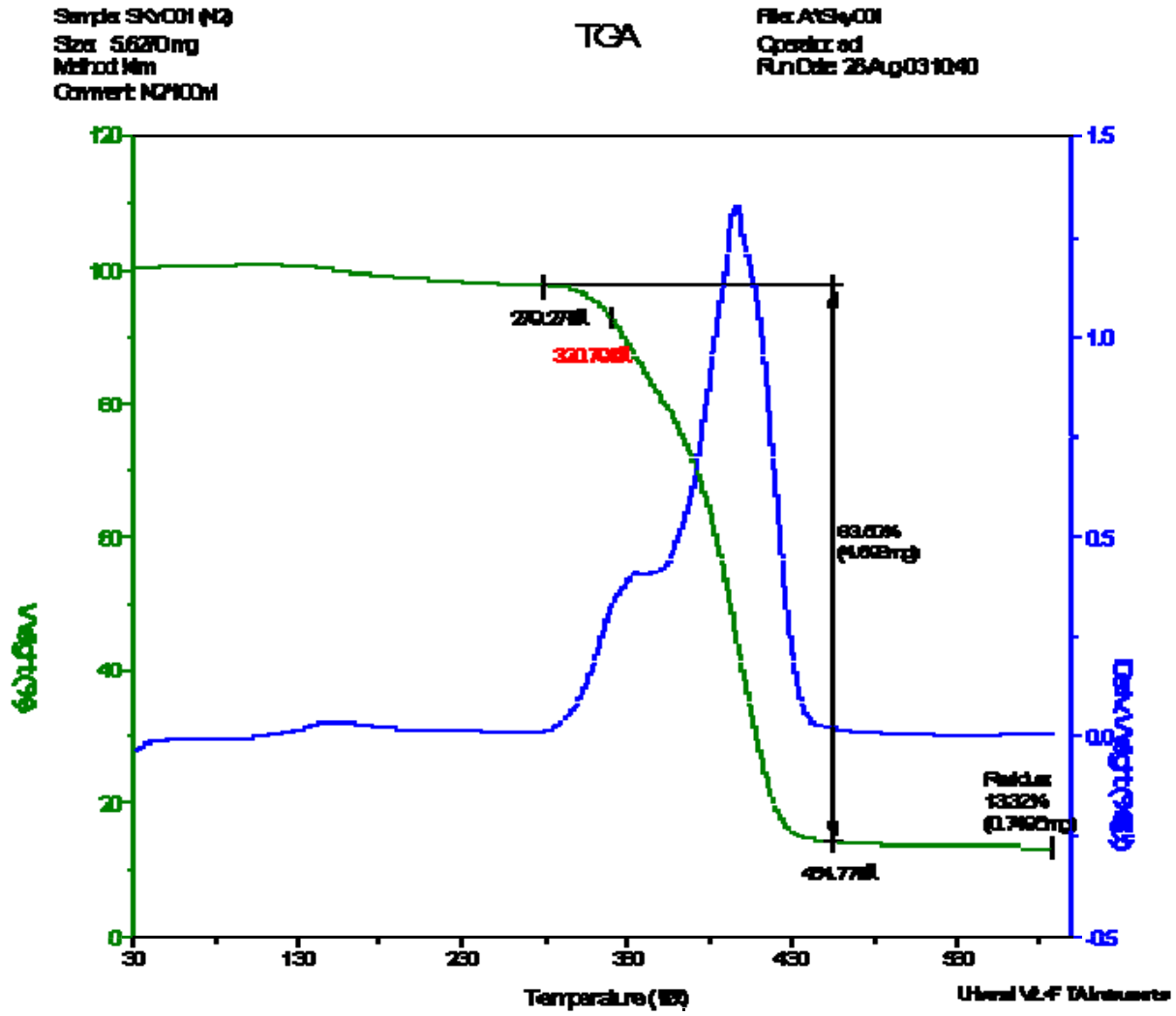


Figure S5. TGA data of TCTEB.

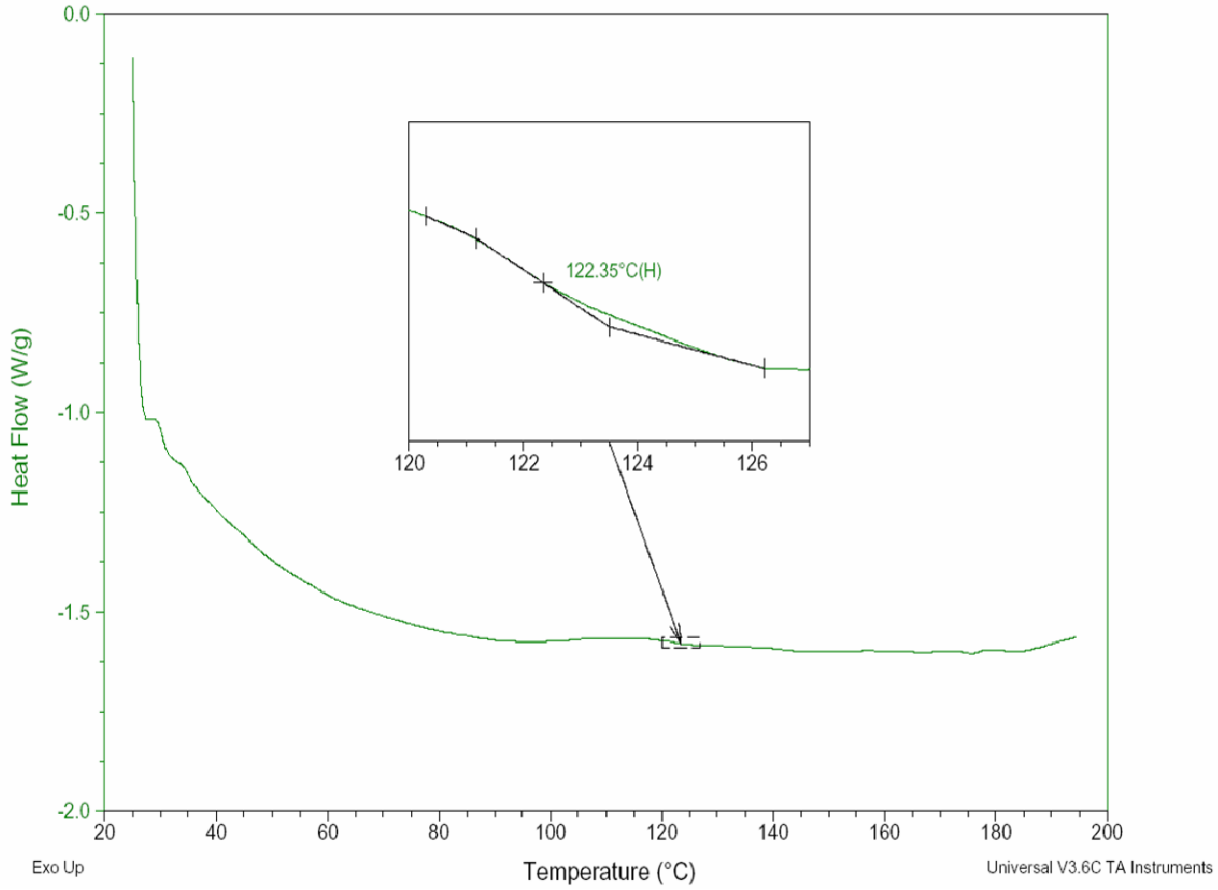


Figure S6. DSC data of TCTEB.

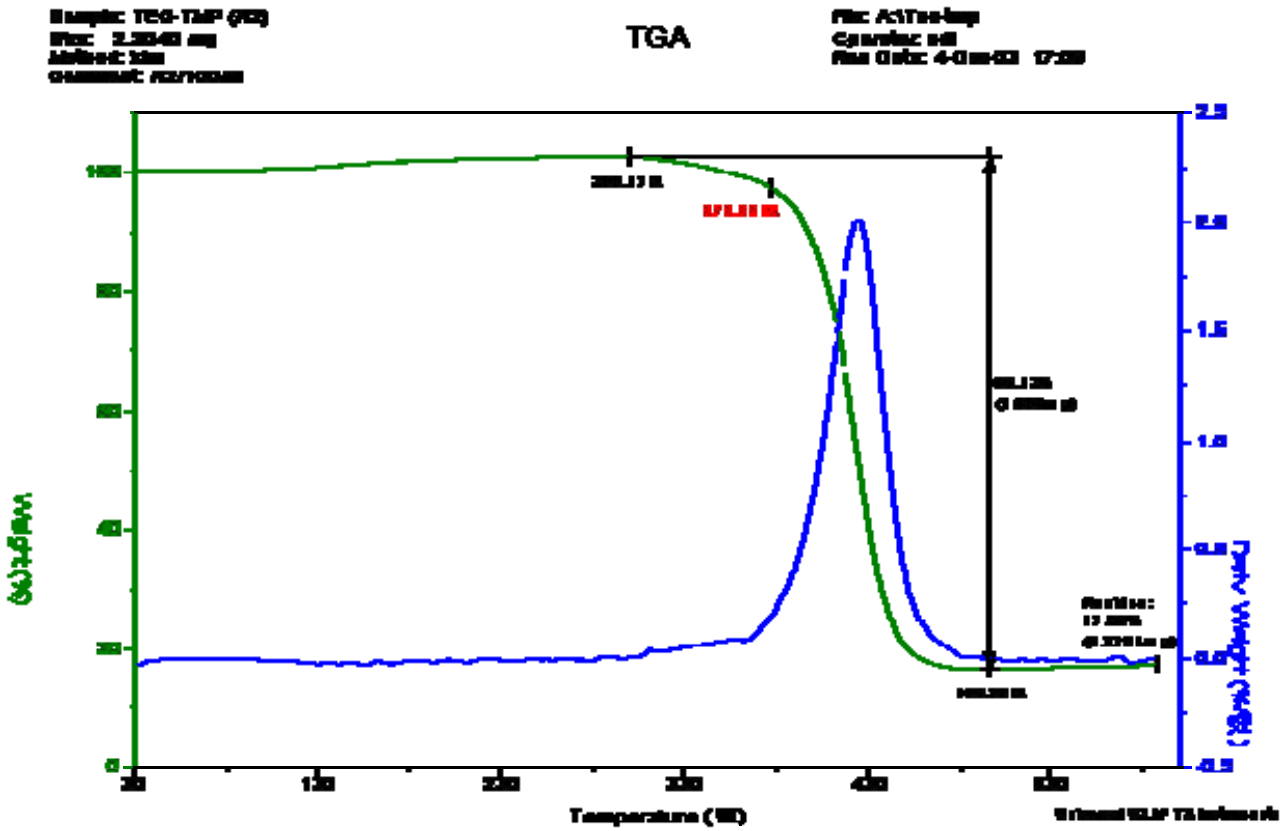


Figure S7. TGA (top) data of TCTMB.

Table S1. TGA analysis of TCTMB and TCTEB.

Sample name	First step decomposed temperature & reduced weight	T_d (5% reduced weight)	Final residue (at 600°C)
TCTEB	279~455 °C	321 °C	13.32%
	83.50%		
TCTMB	299~496 °C	377 °C	17.20%
	86.12%		

DFT Calculations

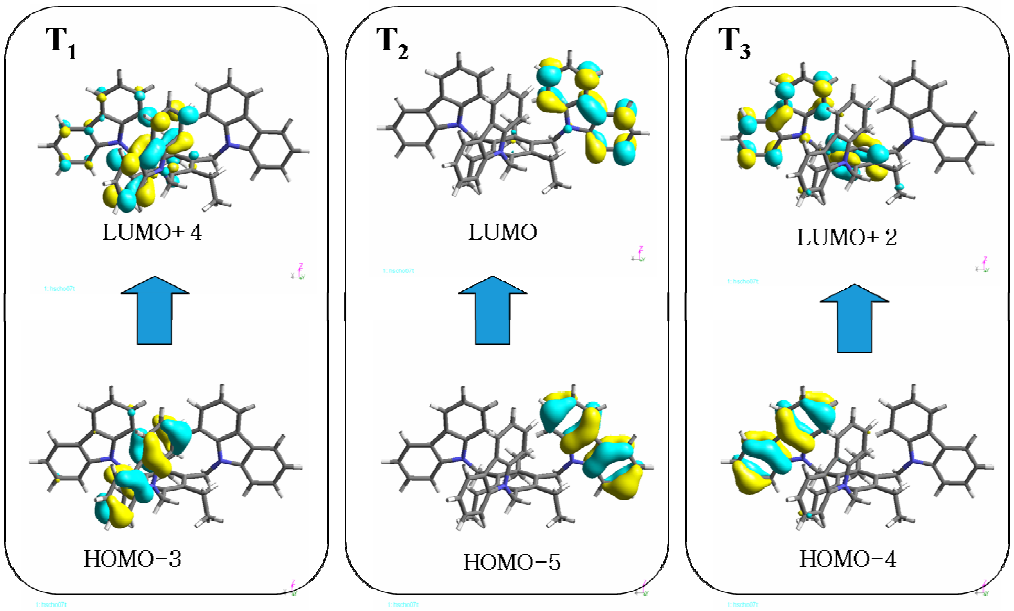


Figure S8. Contour plot of HOMO and LUMO orbital for TCTEB.

DFT calculations for TCTEB and TCTMB were carried out using the B3LYP functional with the 6-31G(*) basis set. Contour plot of HOMO and LUMO orbital for TCTEB and energy level are shown in Figure S8 and Table S2. All triplet state, T_1, T_2, and T_3 are degenerated.

Table S2. Calculated Energy Level for TCTEB.

state	eV	nm	f	Origin
1st Triplet	3.1401	395	0.000	HOMO-3 → LUMO+4
2nd Triplet	3.1411	395	0.000	HOMO-5 →LUMO
3rd Triplet	3.1445	394	0.000	HOMO-4 → LUMO+2
1st Singlet	3.3455	371	0.0015	HOMO → LUMO+1
2nd Singlet	3.3474	370	0.0147	HOMO-2 → LUMO HOMO →LUMO+2

3rd Singlet	3.3858	366	0.0237	HOMO-2 →LUMO

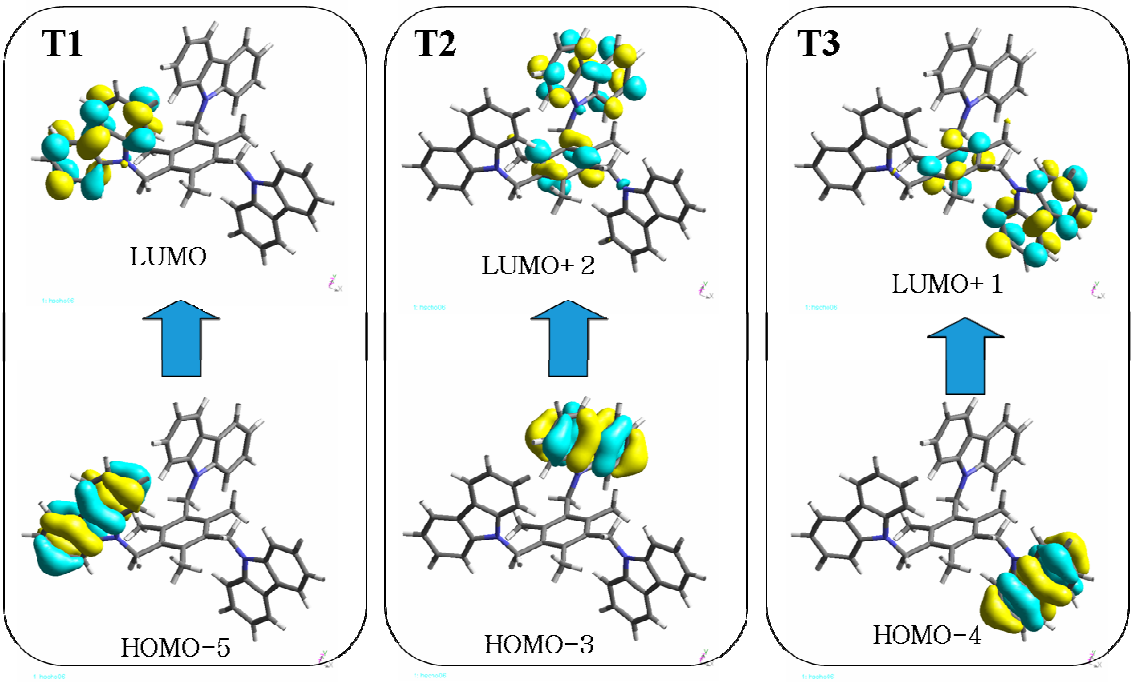


Figure S9. Contour plot of HOMO and LUMO orbital for TCTMB.

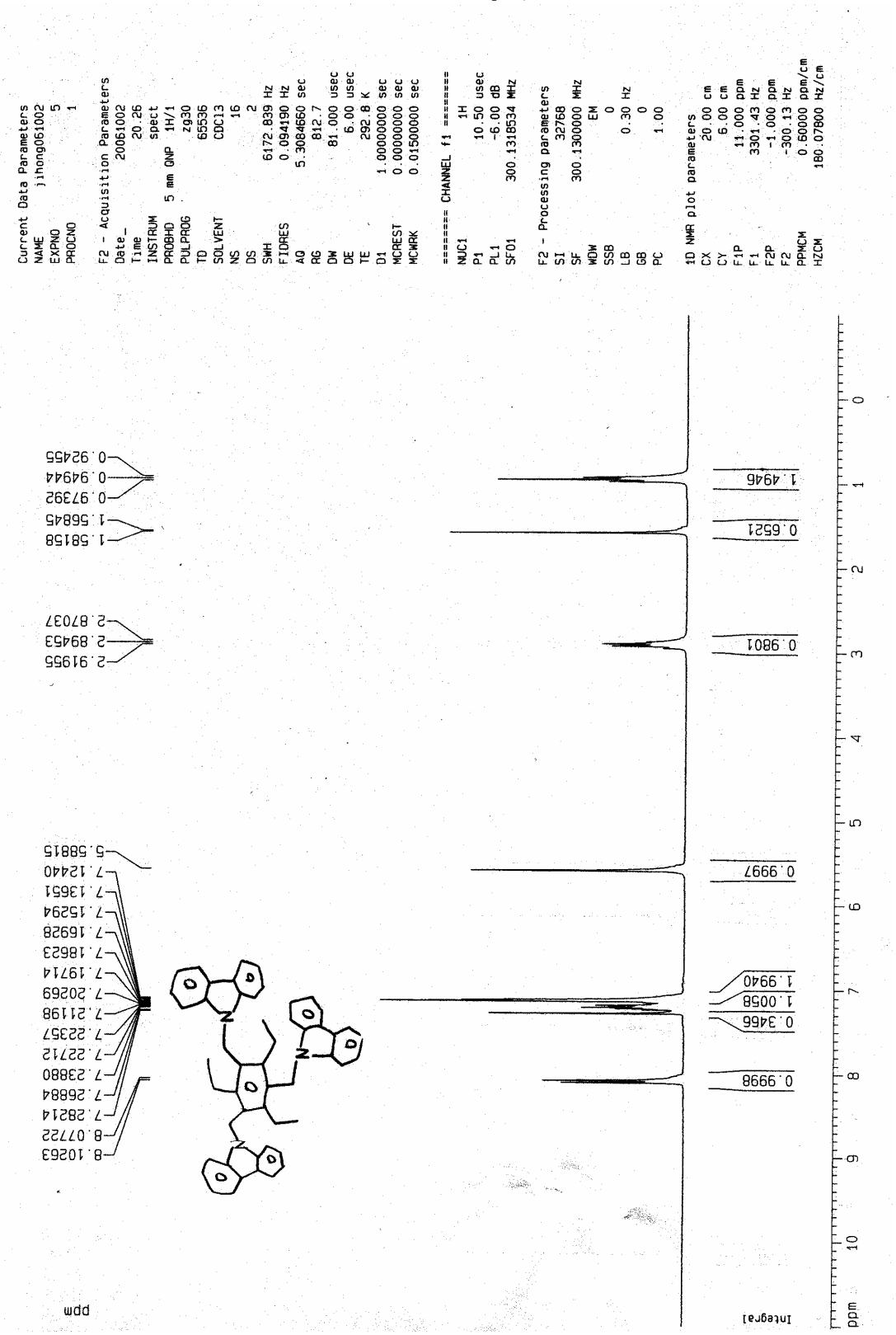
Contour plot of HOMO and LUMO orbital for TCTMB and energy level are shown in Figure S9 and Table S3. All triplet state, T_1, T_2, and T_3 are degenerated.

Table S3. Calculated Energy Level for TCTMB.

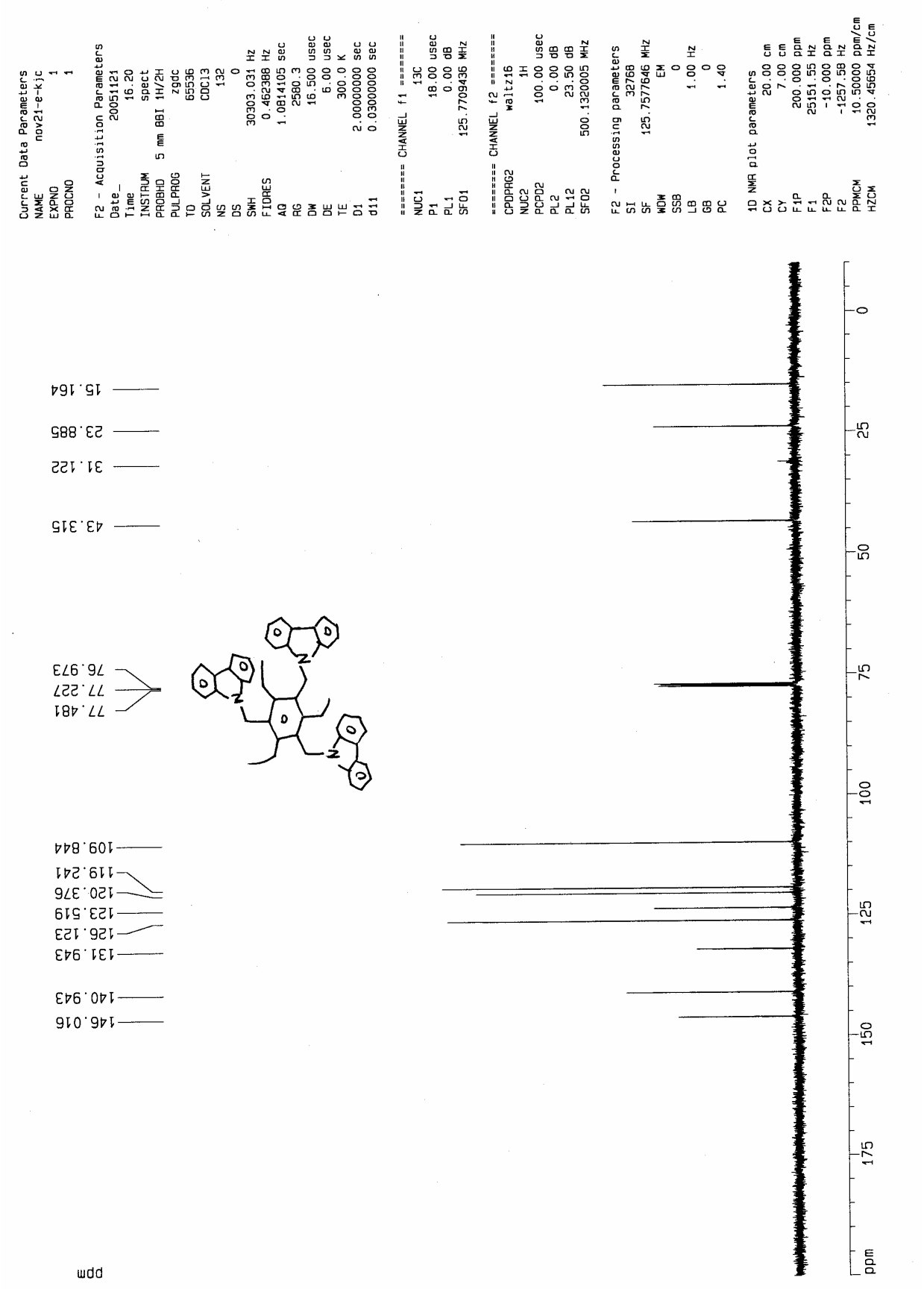
state	eV	nm	f	Origin
1st Triplet	3.1406	395	0.000	HOMO-5 → LUMO
2nd Triplet	3.1443	394	0.000	HOMO-3 → LUMO+2
3rd Triplet	3.1443	394	0.000	HOMO-4 →LUMO+1
1st Singlet	3.3438	371	0.0185	HOMO-2 →LUMO

2nd Singlet	3.3443	371	0.0417	HOMO-1 → LUMO+1
3rd Singlet	3.4042	364	0.0116	HOMO-2 → LUMO

^{1}H NMR-TCTEB



^{13}C NMR-TCTEB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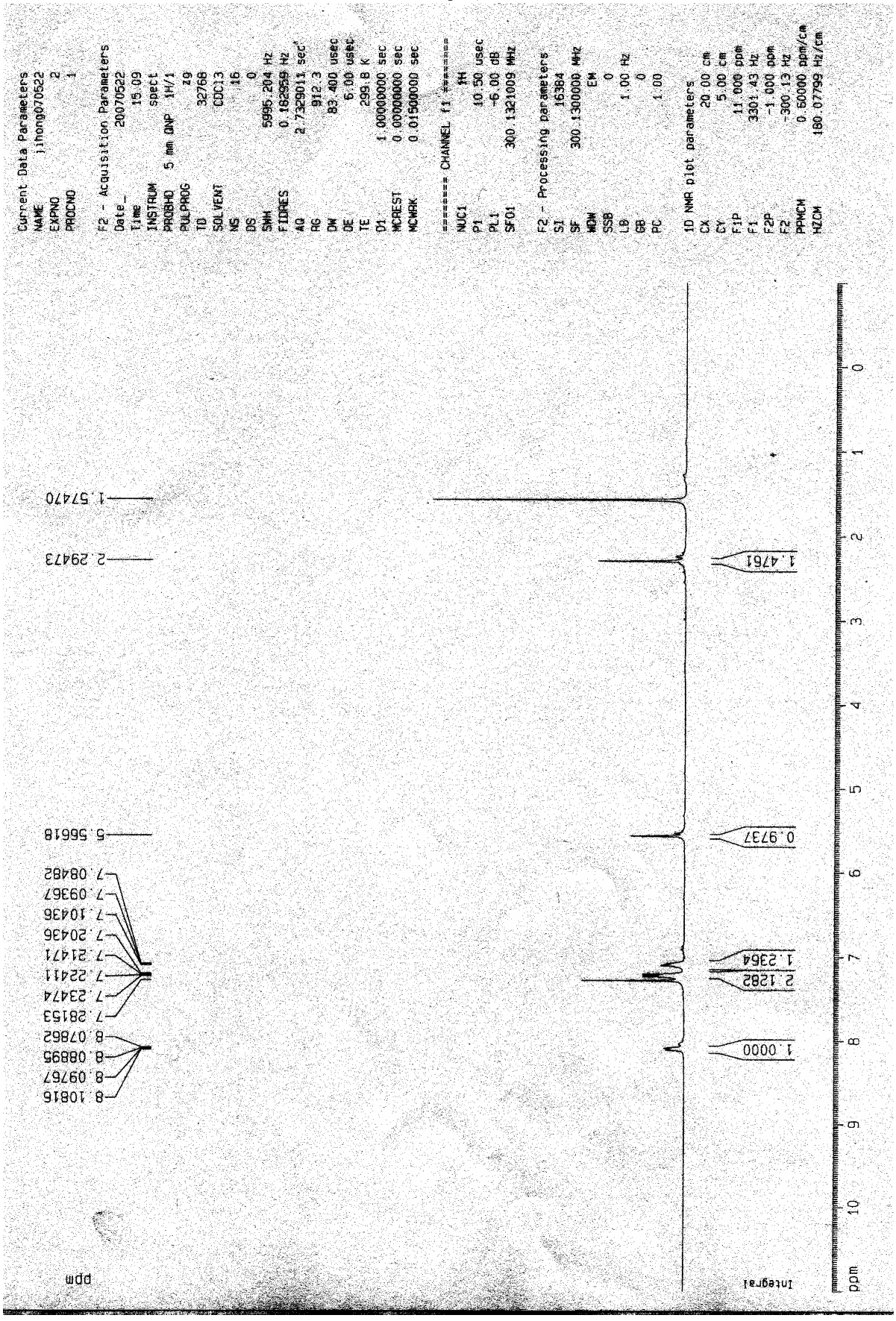
^{1}H NMR-TCTMB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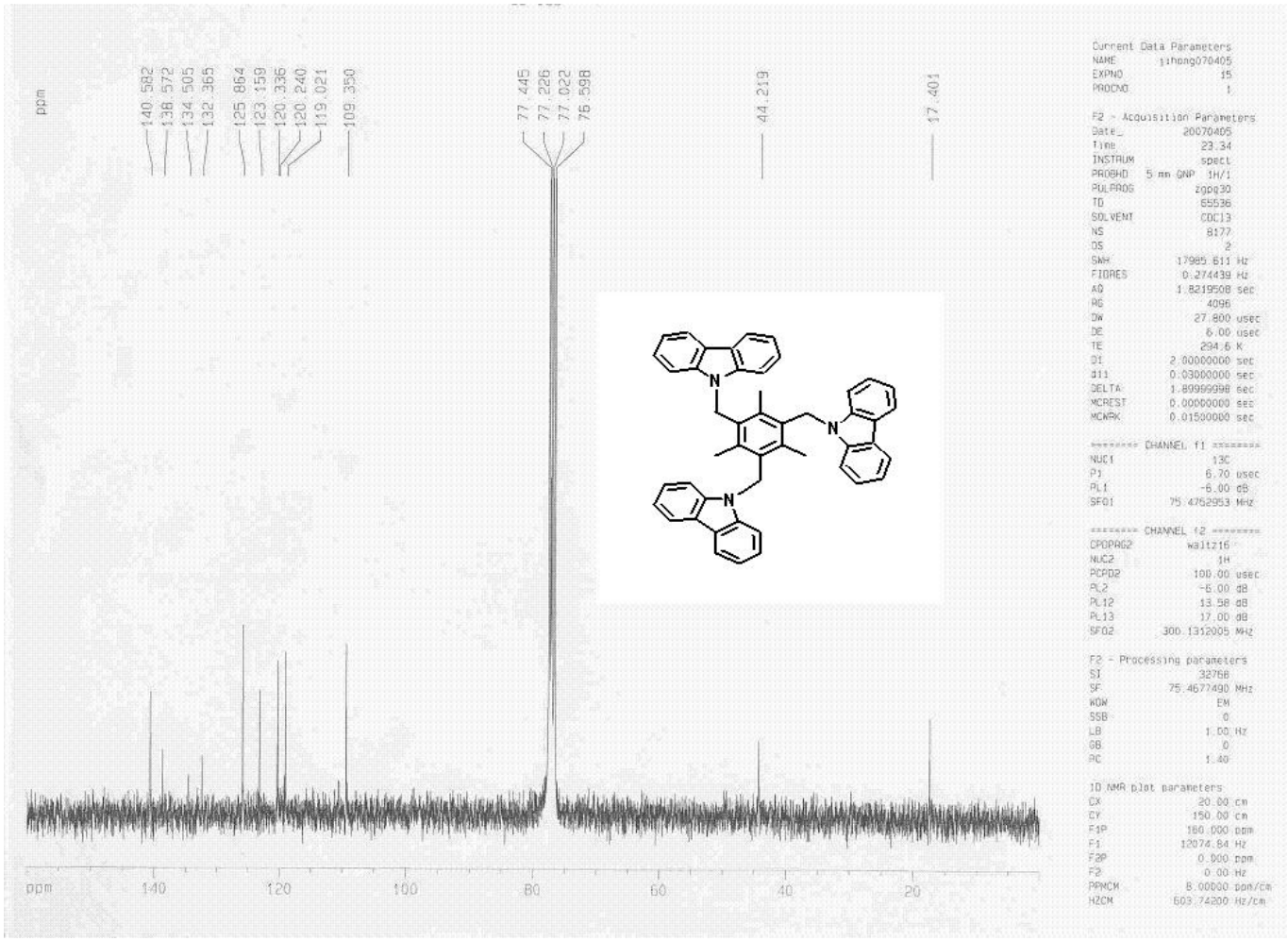
^{13}C NMR-TCTMB



Reference

1. M. Masui, H. Sayo and Y. Tsuda, *J. Chem. Soc. B* 1968, 973.

2. A. J. Bard and L. R. Faulkner, *Electrochemical Methods; Fundamentals and applications*, 2nd ed.; John Wiley & Sons, Inc.: New York, **2001**.