Electronic Supplementary Material (ESI) for RSC Advances.

A bluish – green emitting organic compound Methyl 3–[(E)–(2–hydroxy–1-naphthyl)methylidene]carbazate: Spectroscopic, thermal, fluorescence, antimicrobial and molecular docking studies

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Single crystal and Powder X – ray diffraction studies

Single crystal X – ray diffraction results confirm that MNMC crystallizes in orthorhombic crystal system with cell parameters a = 5.204 (8) Å, b = 9.727 (14) Å, c = 23.67 (4) Å, α = β = γ = 90°, V = 1142 (4) Å^3, with non centrosymmetric space group $P2_12_12_1$. The values of the cell parameters obtained in the present investigation agree well with the already reported values.[10] Table 1 shows the results of the present investigation with the reported literature data.

Table S1. Cell parameters of MNMC single crystal

Crystal Parameters	Present Values	Reported Values[10]
Crystal system, Space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
a (Å)	5.204 (8)	5.1754 (3)
b (Å)	9.727 (14)	9.2787(5)
c (Å)	23.67 (4)	23.6766 (12)
α = β = γ (°)	90	90
V (Å^3)	1142 (4)	1136.97 (11)

Powder X-ray diffraction measurement was carried out for the MNMC compound and the powder X-ray diffraction pattern (Fig. S1a) drawn by using Powder X software. Mercury software was used to get the powder X-ray diffraction pattern of the reported compound (Fig. S1b). (hkl) planes and cell parameters obtained for the title compound were compared with the alredy reported values.

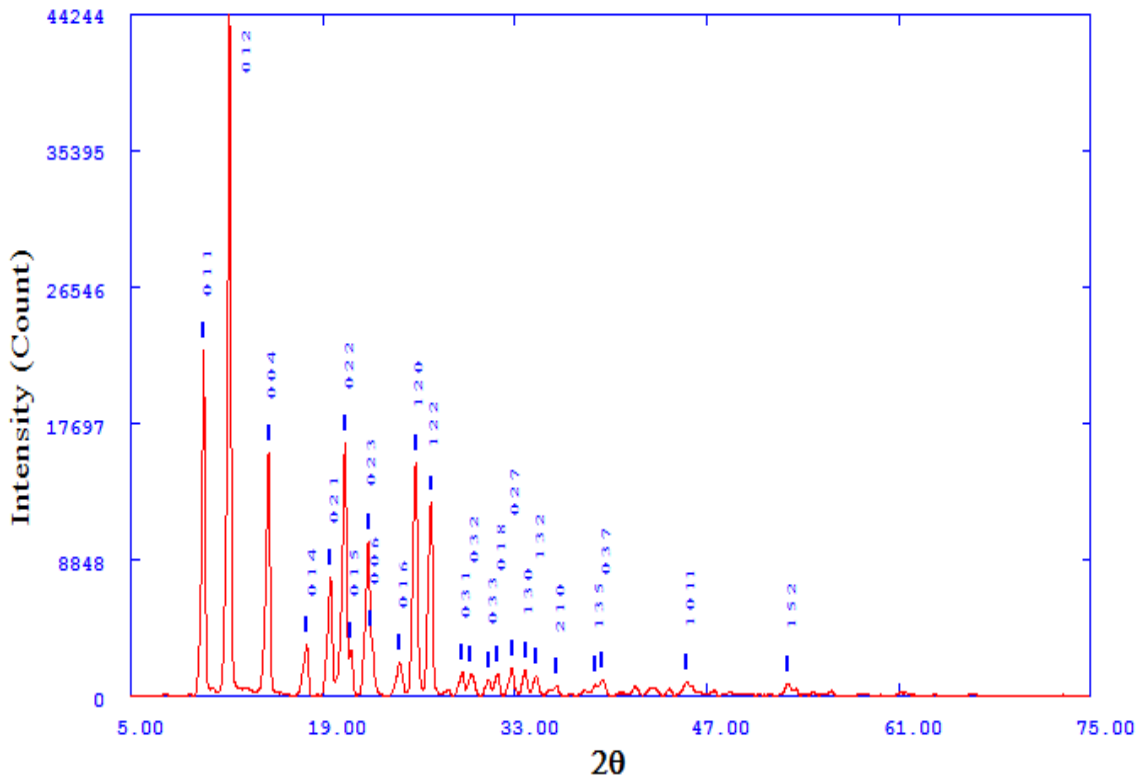

Fig. S1a. Powder X-ray pattern of MNMC compound (Powder X software)

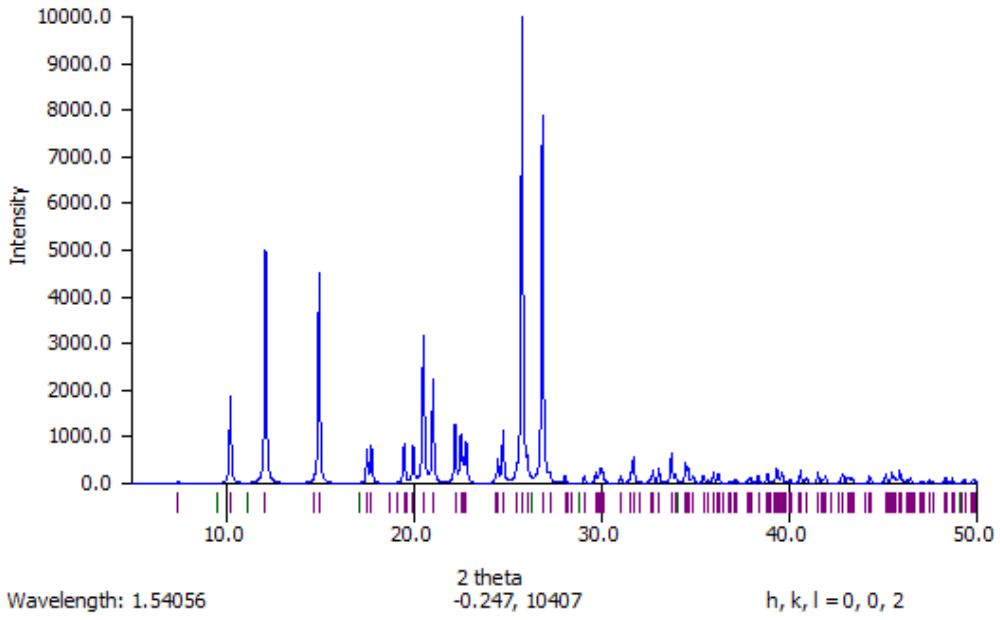

Fig.S1b. Powder X-ray diffraction pattern of MNMC compound (Mercury software)

Table S2. FT - IR and FT - RAMAN spectral assignments

IR	RAMAN	ASSIGNMENTS
3749		O – H stretching
3362, 3246		N – H stretching
	3077	Aromatic C-H symmetric stretching
3068, 3168		Aromatic C – H stretching
	2962	Symmetric and asymmetric stretching of C-H out of
2960		CH_3 symmetric and asymmetric stretching
1701		C = O stretching
1669		C = N Stretching
	1669, 1623	O = C – N stretching, C = O stretching
1622, 1596		Ring quadrant stretching
	1604, 1576	C = N stretching
	1532	Asymmetric C – N stretching
1528		C = C stretching
1503		CH_3 asymmetric stretching, NH_2 scissoring
	1470	CH_3 asymmetric deformation
1449		CH_3 in phase bending
1420	1420	C-OH bending, C – H deformation
	1398	CH_3 asymmetric deformation
	1379	CH_3 asymmetric deformation, C - H symmetric
1358, 1236		C-OH stretching vibration of phenol
	1239, 1195	Ar – O – H stretching
1188, 1147, 1092		Aromatic C-H in plane bending
1060		C-O-C out of phase vibration
	1037	C – H in plane bending
950		C-H wagging
896, 859, 819, 767, 737		Aromatic C-H out of bending
715		N – H wagging
672		N-H out of plane bending
577		O = C – N bending
	169, 100, 81,	Lattice vibrations of crystal

Thermal analysis

The TG-DTA-DSC analysis was performed to study the thermal stability of MNMC compound. It can be observed from TG, two stages of weight loss which is also very clear from the DTA with two sharp inflections. First stage of weight loss occurs between 200 to 259 °C with mass change of 26.62%.

The sharp melting of the MNMC compound was found at 205° C. There was no visible weight loss before the melting and hence it proves the absence of water molecules in the crystal lattice. Second stage of weight loss obtained between 266 to 450° C where the mass change is of 60.48%. The mass of final residue 12.27% was left out at a temperature above 450° C (Fig. S2a).

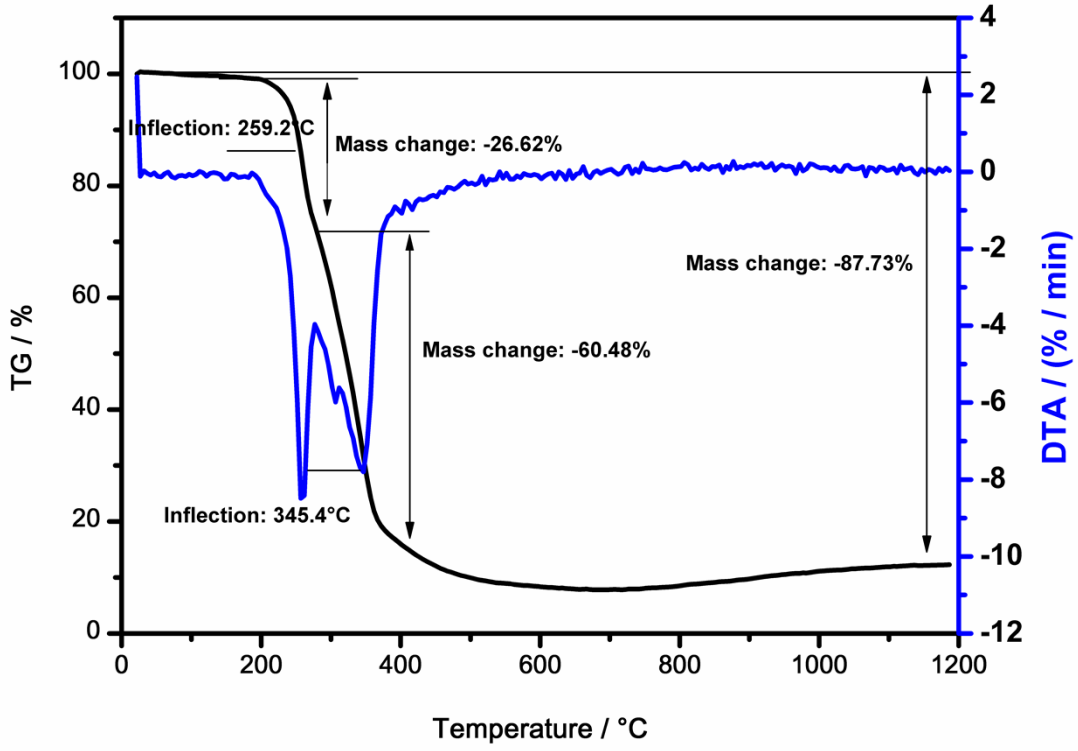

Figure S2a. TG – DTA analysis of MNMC compound

The DSC trace plot has been represented with an downward arrow for exothermic process. From the DSC trace (Fig. S2b), it is observed that there is a sharp endothermic peak at 205° C, which is the melting point of the material. The sharp peak represents the high purity of the compound. The exothermic peak at 268° C and another endothermic peak at 368° C indicate two stages of decomposition of the compound. The MNMC compound can be utilized well below 205° C in optical application.

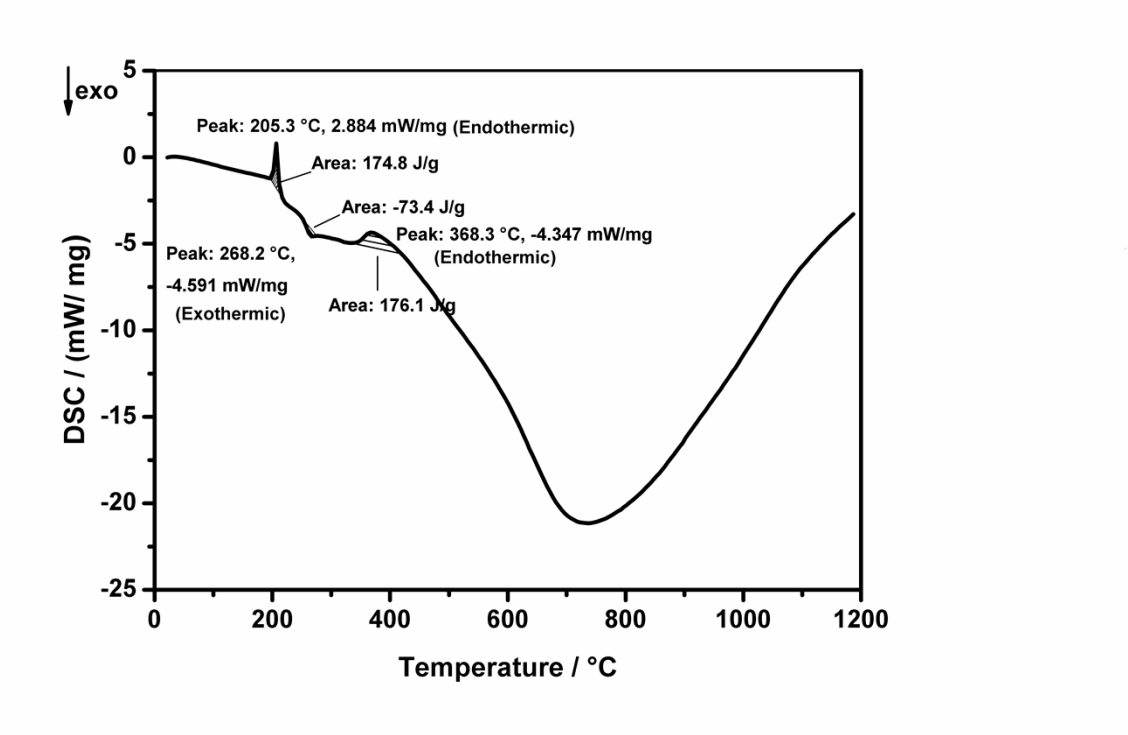

Figure S2b. DSC trace of MNMC compound

Second harmonic generation efficiency

The Kurtz – Perry powder technique20 was employed to screen the second harmonic generation efficiency of the material. The output voltage obtained for MNMC, KDP and Urea are 36, 34.7, 45.3 mV, respectively. The second harmonic generation efficiency of MNMC is found to be 1.04 and 0.8 times as that of KDP and Urea, respectively.