Novel organic solar thermal energy storage materials: efficient visible light-driven reversible solid–liquid phase transition †

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Innovation In novel OPTCMs, the dye was used as a photon antenna that served as an effective ‘‘photon capture and molecular heater’’ of light-to-heat conversion, and phase change material stored heat energy by phase transition with high energy storage density. The light-to-heat conversion and thermal storage efficiency (η) of the OPTCM turns out to be over 0.94. The dye of OPTCMs can absorb different wavelengths of sunlight. So the new material can achieve a high efficiency of the sunlight to heat conversion and efficient heat storage.

Structural analysis 1H NMR spectra were recorded employing a Varian INOVA 400 MHz NMR spectrometer at 400 MHz, using solutions of the compounds in 0.5 ml of CDCl3 or DMSO-d6 containing TMS (tetramethylsilane) as the internal standard. Mass spectra were recorded on MALDI micro MX.

Compound 4 1H NMR spectrum was recorded on a VARIAN INOVA 400 MHz NMR spectrometer. 1H NMR (400 MHz, CDCl3, 25 ºC, TMS): δ=2.61-2.67 (d, 2H, CH2), 2.78-2.81 (m, 1H, CH), 3.41-3.48 (m, 2H, CH2), 3.54-3.56 (t, 2H, CH2), 3.65 (s, 70H, CH2), 3.81-3.82 (t, 2H, CH2); IR (KBr pellet): 3480 (δ H2O), 2882 (ν C-H aliphatic), 1466 (δ CH2), 1359 (δ CH3), 1279 (ν C-O-C exopy), 1112 (νs C-O-C ployether), 1060 (νs C-O-C ployether); MS (ESI, positive) ([M+K]+): 699.4, 743.4, 787.4, 831.4, ΔM= 44 (CH2CH2O).

Compound 5 Dye-Yellow 1H NMR spectrum was recorded on a VARIAN INOVA 400 MHz NMR spectrometer. 1H NMR (400 MHz, CDCl3, 25 ºC, TMS): δ= 8.05 (d, 2H, Ar-H), 7.92 (d, 2H, Ar-H), 7.54 (d, 2H, Ar-H), 7.42 (t, 2H, Ar-H), 7.22 (t, 1H, Ar-H), 2.38 (s, 3H, -CH3). MS (ESI, positive) [M+H]+ measured: m/z=376.7.

Compound 5 Dye-Red 1H NMR spectrum was recorded on a VARIAN INOVA 400 MHz NMR spectrometer. 1H NMR (400 MHz, DMSO-d6, 25 ºC, TMS): δ= 0.88-0.91 (t, 3H, CH3), 1.19-1.23 (t, 6H, CH3), 1.31-1.38 (m, 2H, CH2), 1.47-1.57 (m, 2H, CH2), 3.27-3.29 (d, 2H, CH2), 3.53-3.54 (d, 4H, CH2), 6.65-6.67 (d, 1H, Ar-H), 7.75-7.77 (d, 1H, Ar-H), 7.81 (s, 1H, Ar-H), 7.88-7.90 (d, 2H, Ar-H), 8.36-8.38 (d, 2H, Ar-H), 10.46 (s, 0.28H, NH), 10.75 (s, 0.63H, NH); Q-TOFMS: [M+H]+ measured: m/z=498.2928.

Compound 5 Dye-Blue 1H NMR spectrum was recorded on a VARIAN INOVA 400 MHz NMR spectrometer. 1H NMR (400 MHz, DMSO-d6, 25 ºC, TMS): δ= 0.88-0.93 (t, 3H, CH3), 1.17-1.23 (m, 6H, CH2), 1.47-1.52 (m, 2H, CH2), 1.61-1.68 (m, 2H, CH2), 3.54-3.59 (d, 4H, CH2),
3.83 (s, 3H, CH₃), 4.20-4.24 (t, 3H, CH₃), 7.38 (s, 1H, Ar-H), 7.88 (s, 1H, Ar-H), 8.32-8.35 (d, 1H, Ar-H), 8.54-8.57 (d, 1H, Ar-H), 8.80 (s, 1H, Ar-H), 9.62 (s, 0.12H, NH), 9.85 (s, 0.45H, NH); Q-TOFMS: [M+H]+ measured: m/z=553.2488.

OPTCM 3 ¹H NMR spectrum was recorded on a VARIAN INOVA 400 MHz NMR spectrometer. ¹H NMR (400 MHz, DMSO-d₆, 25 °C, TMS): δ=1.26-1.30 (t, CH₂), 1.63 (s, H, NH), 1.26-1.30 (t, 2H, CH₂), 1.88-1.94 (t, 2H, CH₂), 2.07 (s, H, NH), 2.20 (s, H, CH), 2.66-2.68 (d, 4H, CH₂), 2.46 (s, 3H, CH₃), 3.54-3.57 (t, 14H, CH₂), 3.67 (s, 1H, OH), 3.95-3.96 (d, 2H, CH₂), 4.05-4.09 (t, H, CH), 4.12-4.17 (m, H, CH), 4.37 (s, H, NH), 4.38 (s, H, NH), 7.33-7.38 (t, 1H, CH), 7.57-7.61 (t, 2H, CH), 7.76-7.78 (d, 2H, CH), 7.98-8.00 (d, 2H, CH), 8.02-8.03 (d, 2H, CH), 8.12-1.14 (d, 1H, CH); IR (KBr pellet): 3348 (ν N-H), 2882 (ν C-H aliphatic), 1667 (ν C=O Pyrazolone), 1466 (δ CH₂), 1359 (δ CH₂), 1344 (νₛ S=O), 1280 (ν C-N), 1147 (ν, S=O), 1112 (νₐs C-O-C ployether), 1060 (νₛ C-O-C ployether).

OPTCM 9 ¹H NMR spectrum was recorded on a VARIAN INOVA 400 MHz NMR spectrometer. ¹H NMR (400 MHz, DMSO-d₆, 25 °C, TMS): δ=0.79-0.94 (s, H, CH₃), 1.20 (s, H, CH₂), 1.55 (s, H, NH), 2.41 (s, 3H, CH₃), 2.75 (d, 4H, CH₂), 3.27 (s, 2H, NH), 3.54 (t, 13H, CH₂), 3.68 (s, 1H, OH), 4.12-4.17 (m, H, CH), 5.43 (s, H, NH), 6.60-8.37 (m, 8H, Ar-H); IR (KBr pellet): 3345 (ν N-H), 2883 (ν C-H aliphatic), 1609 (ν C-C), 1540 (ν C=N S-triazine), 1465 (δ CH₂), 1359 (δ CH₂), 1279 (ν C=N aromatic), 1198 (ν C-N aliphatic), 1103 (νₐs C-O-C ployether), 1059 (νₛ C-O-C ployether).

OPTCM 10 ¹H NMR (400 MHz, DMSO-d₆, 25 °C, TMS): δ=0.79-0.03 (s, H, CH₃), 1.17-1.22 (s, H, CH₂), 1.50 (s, H, NH), 2.40 (s, 3H, CH₃), 2.73 (d, 4H, CH₂), 3.25 (s, 2H, NH), 3.52 (t, 14H, CH₂), 3.80 (s, 1H, OH), 4.12-4.17 (m, H, CH), 5.43 (s, H, NH), 6.96-9.12 (m, 6H, Ar-H); IR (KBr pellet): 3332 (ν N-H), 2883 (ν C-H aliphatic), 1607 (ν C-C aromatic), 1540 (ν C=N S-triazine), 1465 (δ CH₂), 1359 (δ CH₂), 1279 (ν C-N), 1103 (νₐs C-O-C ployether), 1059 (νₛ C-O-C ployether).