*Electronic Supplementary Information for*

# Tandem generation of isocoumarins in the hollow microporous organic networks: Nitrophenols sensing based on visible light

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## *Experimental Sections*

Transmission (TEM) and scanning electron microscopy (SEM) images were obtained using a JEOL 2100F unit and a FE-SEM (JSM6700F), respectively. The $N_2$ adsorption-desorption isotherms were measured at 77K using a BELSORP II-mini equipment. The pore size analysis was conducted based on the DFT method. PXRD patterns were obtained using a Rigaku MAX-2200 (filtered Cu-Ka radiation). Infrared absorption spectra were obtained using a Bruker VERTEX 70 FT-IR spectrometer. The absorption spectra of solid MON materials were obtained through the conversion of diffuse reflectance spectra which were obtained using a SHIMADZU UN-3600. The UV/vis absorption and emission spectra were obtained using a JASCO V-630 and JASCO FP-6200 spectrofluorometers, respectively. The solid phase $^{13}$C-NMR spectroscopy was conducted using a Bruker 400 MHz solid state DSX NMR spectrometer at the Korea Basic Science Institute (KBSI). $^{1}$H and $^{13}$C NMR spectra were obtained by a 500 MHz Varian spectrometer. Elemental analysis was conducted using a CE EA1110 instrument. High resolution mass spectrum was obtained using a JEOL JMS 700 high resolution mass spectrometer at the KBSI. The TGA curve was obtained by Seiko Exstar 7300.

## *Synthetic procedure for hollow (H-IC-MON) and non-hollow (IC-MON) microporous organic networks*

To use as the templates, silica spheres with a 250 ± 26 nm average diameter were prepared by the Stöber method reported in the literature.[1] In this study, the following synthetic procedure was applied to prepare silica templates. Ethanol (200 mL), water (18 mL), and ammonia solution (4 mL, 28% aqueous solution) were added to a 250 mL round-bottomed flask at room temperature. The reaction mixture was stirred for 30 min. Then, tetraethyl orthosilicate (TEOS, 14 mL, 63 mmol) in ethanol (56 mL) was added slowly to the solution. The reaction mixture was stirred for 2 h at room temperature. The silica spheres were collected by centrifugation, washed with methylene chloride, hexane, and acetone, and dried under vacuum. Tris(4-ethynylphenyl)amine was prepared by the procedure reported in the literature.[2] 5-Bromo-2-iodobenzoic acid is commercially available (Aldrich. Chem. Co.). For the preparation of H-IC-MONs, silica spheres (0.70 g, 300 nm diameter), $Pd(PPh_3)_4$ (14 mg, 0.012 mmol), $PPh_3$ (6.3 mg, 0.024 mmol), and $ZnCl_2$ (98 mg, 0.72 mmol) were added to a flame-dried 100 mL Schlenk flask under argon. DMF (20 mL) and triethylamine (30 mL) were added to the reaction mixture and was stirred at room temperature for 1 h. Then, tris(4-ethynylphenyl)amine (76 mg, 0.24 mmol) and 5-bromo-2-iodobenzoic acid (0.12 g, 0.36 mmol) in DMF (10 mL) were added to the reaction mixture and stirred at 100 °C for 48 h. After the solution being cooled to room temperature, the precipitate was isolated by centrifugation. After being washed with DMSO, methanol, dichloromethane, and acetone two

times, respectively, the solid was dried under vacuum. The $SiO_2$@IC-MON (0.75 g) was added to the mixture of HF solution (20 mL, 48% aqueous solution) and methanol (5 mL) in a Falcon tube. *Caution: the HF solution is extremely dangerous to touch and to be inhaled. Thus, it should be handled with the utmost caution and specific gloves in hood. Before using the HF solution, please read thoroughly the MSDS sheets.* The reaction mixture was stirred for 1 h at room temperature. After adding 20 mL methanol, the resultant H-IC-MONs were retrieved by centrifugation, washed with a 1:1 mixture of $H_2O$/methanol, methanol, and acetone, and dried under vacuum. For the preparation of non-hollow IC-MONs, the same synthetic procedure used for H-IC-MONs was applied without using the silica spheres.

***Synthetic procedure for hollow model materials, hollow MON without isocoumarins (H- MON)***

Interestingly, the H-MONs could not be obtained under the synthetic conditions used for the synthesis of H-IC-MON even after many trials. Thus, we had to optimize the tailored synthetic conditions including solvent, building blocks (4-iodo-bromobezene did not work well for this purpose), and catalytic systems for H-MON. In a 100 mL flame dried Schlenk flask, $Pd(PPh_3)_2Cl_2$ (8.4 mg, 0.012 mmol), $PPh_3$(6.3 mg, 0.025 mmol), and CuI (4.6 mg, 0.024 mmol) were added under argon. Triethylamine (20 mL) and toluene (30 mL) were added to the reaction mixture. The reaction mixture was sonicated for 1 h and stirred for 1 h at room temperature. Tris(4-ethynylphenyl)amine (76 mg, 0.24 mmol) and 1,4-diiodobezene (0.12 g, 0.36 mmol) in toluene (10 mL) were added to the reaction mixture and stirred at 100 $^oC$ for 48 h. After the solution was cooled to room temperature, the precipitate was isolated by centrifugation. After being successively washed with DMSO, methanol, dichloromethane, and acetone two times, respectively, the solid was dried under vacuum. The $SiO_2$@MON (0.75 g) was added to the mixture of HF solution (20 mL, 48% aqueous solution) and methanol (5 mL) in a Falcon tube. *Caution: the HF solution is extremely dangerous to touch and to be inhaled. Thus, it should be handled with the utmost caution and specific gloves in hood. Before using the HF solution, please read thoroughly the MSDS sheets.* The reaction mixture was stirred for 1 h at room temperature. After adding 20 mL methanol, the resultant H-MONs were retrieved by centrifugation, washed with a 1:1 mixture of $H_2O$/methanol, methanol, and acetone, and dried under vacuum.

***Synthetic procedure of model compound (MD-1 and MD-2 in text)***

4-Ethynylphenyldiphenylamine was prepared by the procedure in the literature.[3] For the preparation of MD-1, $Pd(PPh_3)_4$ (58 mg, 0.050 mmol), $PPh_3$ (26 mg, 0.10 mmol), and $ZnCl_2$ (0.41 g, 3.0 mmol) were added to a flame-dried 100 mL Schlenk flask under argon, followed by the addition of DMF (10 mL) and triethylamine (20 mL), and the reaction mixture was stirred at room temperature for 1 h. Then, 4-ethynylphenyldiphenylamine (0.27 g, 1.0 mmol) and 5-bromo-2-iodobenzoic acid (0.16 g, 0.50 mmol) in DMF (10 mL) were added to the reaction mixture and stirred at 100 $^oC$ for 48 h. After the solution was cooled to room temperature, the solvent was removed by vacuum-distillation. The residue was extracted with methylene chloride and brine solution. After drying the methylene chloride solution with $MgSO_4$, the solvent

was removed by rotary evaporator. The product was isolated by silica flash column chromatography using a 2:1 mixture of hexane and methylene chloride as an eluent. The obtained product was 0.18 g (0.27 mmol, 54% isolated yield.) Characterization data for MD-1: $^{1}$H NMR (500 MHz, $CDCl_3$): $\delta$ = 8.41 (s, 1H), 7.76 (dd, J = 8.2 Hz, 1H), 7.72 (d, J = 8.9 Hz, 2H), 7.41 (d, J = 8.2 Hz, 1H), 7.38 (d, J = 8.8 Hz, 2H), 7.31 (d, J = 8.6 Hz, 4H), 7.28 (d, J = 8.7 Hz, 4H), 7.11 (m, 14H), 7.01 (d, J = 8.8 Hz, 2H), 6.81 (s, 1H) ppm. $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 161.75, 154.18, 149.67, 148.31, 147.11, 146.96, 137.16, 137.05, 132.69, 132.50, 129.55, 129.49, 126.30, 125.78, 125.38, 125.18, 124.50, 124.04, 123.77, 123.11, 122.06, 121.78, 120.14, 115.36, 99.91, 91.96, 87.73 ppm. FT-IR: 1735, 1589, 1510, 1490, 1326, 1284, 1193, 1178, 1066, 1031, 837 $cm^{-1}$. Elemental Analysis for $C_{47}H_{32}N_2O_2$, calc: C, 85.95; H, 4.91; N, 4.27; O, 4.87. obs: C, 85.89; H, 4.92; N, 4.21; O, 4.95. HRMS (FAB mode) for $C_{47}H_{32}N_2O_2$, calc. [M+1]: 657.2542, obs. 657.2543. MD-2 was prepared by the synthetic procedure in the literature.[4]

**Experimental procedure of fluorescence quenching tests**

Phenol (2,4,6-trinitrophenol, picric acid; PA, 4-nitrophenol; 4-NP, 2,4-dinitrophenol; 2,4-DNP, 2-nitrophenol; 2-NP, 4-chlorophenol, phenol, and 4-methylphenol) solution with various concentrations (1.0 mM, 0.50 mM, 0.25 mM, 0.125 mM, 0.10 mM, 0.080 mM, 0.060 mM, 0.040 mM, 0.020 mM, 0.010 mM, and 0.0050 mM) was prepared in a 2:1 mixture of $H_2O$/THF. The H-IC-MONs (3.0 mg) were added to the THF solution (200 mL). After sonication for 30 min, water (40 mL) was added to the H-IC-MON suspension (20 mL). The suspension of H-IC-MON (2 mL) in a 2:1 mixture of $H_2O$/THF was added to the phenol solution (2 mL). The mixture was sonicated for 20 s. The emission intensity of H-IC-MON (440 nm excitation) was investigated using a JASCO FP-6200 spectrofluorometer at 298K. The *K*sv values were obtained by Stern-Volmer plot ($I_o/I = K_{sv}[M] + 1$, $I_o$: the intensity of original emission, I: the intensity of emission in the presence of nitrophenols, M: the concentration of nitrophenols in a 2:1 mixture of $H_2O$/THF. $R^2 > 0.99$ for linear regression) The H-IC-MON materials showed increasing sensing activities toward nitrophenols in the order of 2NP, 4NP, DNP, and PA with the $K_{sv}$ values of $6.3\times10^3$, $7.9 \times 10^3$, $1.1\times10^4$, and $1.5\times10^4$ $M^{-1}$ at 298K, respectively. 4-Chlorophenol, phenol, and 4-methylphenol solutions did not quench the emission of H-IC-MON. For the recovery tests in text, we increased the scale of solution to 4 L total volume. PA (1.0 mM in a 2:1 mixture of $H_2O$/THF, 2 L) was added to a suspension of H-IC-MON (5.0 μg/mL in a 2:1 mixture of $H_2O$/THF, 2 L, total 10 mg of H-IC-MONs). The emission intensity of H-IC-MON in the mixture was investigated. The H-IC-MONs were retrieved by filtration (membrane filter, Merck isopore, pore size 0.2 μm), washed with $H_2O$ (250 mL) and acetone (500 mL), and dried under vacuum. We have screened the recovery methods including centrifugation. Unexpectedly, the filtration described above was the most efficient method and resulted in the nearly complete recovery of H-IC-MONs. The recovered H-IC-MONs were dispersed in a PA solution (0.50 mM in a 2:1 mixture of $H_2O$/THF, 4 L). The emission intensity of H-IC-MONs in solution was investigated. This process was repeated three times and the recovered H-IC-MONs were analyzed by $N_2$ sorption isotherm curves and SEM.

**Computational simulation**

To shed light on the reason for the sensing mechanism of H-IC-MON, we carried out the density functional theory (DFT) calculations. The geometrical optimization for MD-1, MD-2, H-IC-MON-MD-1–4, H-MON-MD, PA, DNP, 2NP, 4NP, 4-chlorophenol, phenol, and 4-methylphenol were performed within B3LYP/6-31+G(d) level. Firstly, the HOMO/LUMO energy levels and HOMO-LUMO gaps were estimated for all of molecular systems. The time-dependent DFT (TDDFT) calculations were performed to obtain the maximum peak positions ($\lambda_{max}$) in an absorption spectrum. In the simulated UV-vis absorption spectrums, the UV-vis peak half-width at half height was taken to be equal to 2658.83 $cm^{-1}$. Then, our calculated results were compared with the experimental findings regarding absorption properties and quenching behaviors. All calculations were performed using a suite of Gaussian 09 programs. [M. J. Frisch, *et al., Gaussian 09, Revision B.01*, Gaussian, Inc., Wallingford CT, 2009]

**References**


1. W, Stöber, A. Fink and E. Bohn, *J. Colloid Inter. Sci.* 1968, **26**, 62-69.
2. M. Mba, M. D'Acunzo, P. Salice, T. Carofiglio, M. Maggini, S. Caramori, A. Campana, A. Aliprandi, R. Argazzi, S. Carli and C. A. Bignozzi, *J. Phys. Chem. C* 2013, **117**, 19885-19896.
3. H. Gao, Y. Li, L. Wang, C. Ji, Y. Wang, W. Tian, X. Yang and L. Yin, *Chem. Commun.*, 2014, **50**, 10251-10254.
4. M. Grigoras, L. Vacareanu, T. Ivan and A. M. Catargiu, *Dyes Pigments* 2013, **98**, 71-81.

**Fig. S1** Powder XRD patterns of H-IC-MON (red) and control materials: IC-MON (brown, nonhollow MON with isocoumarin moieties), and H-MON (black, hollow MON without isocoumarin moieties).

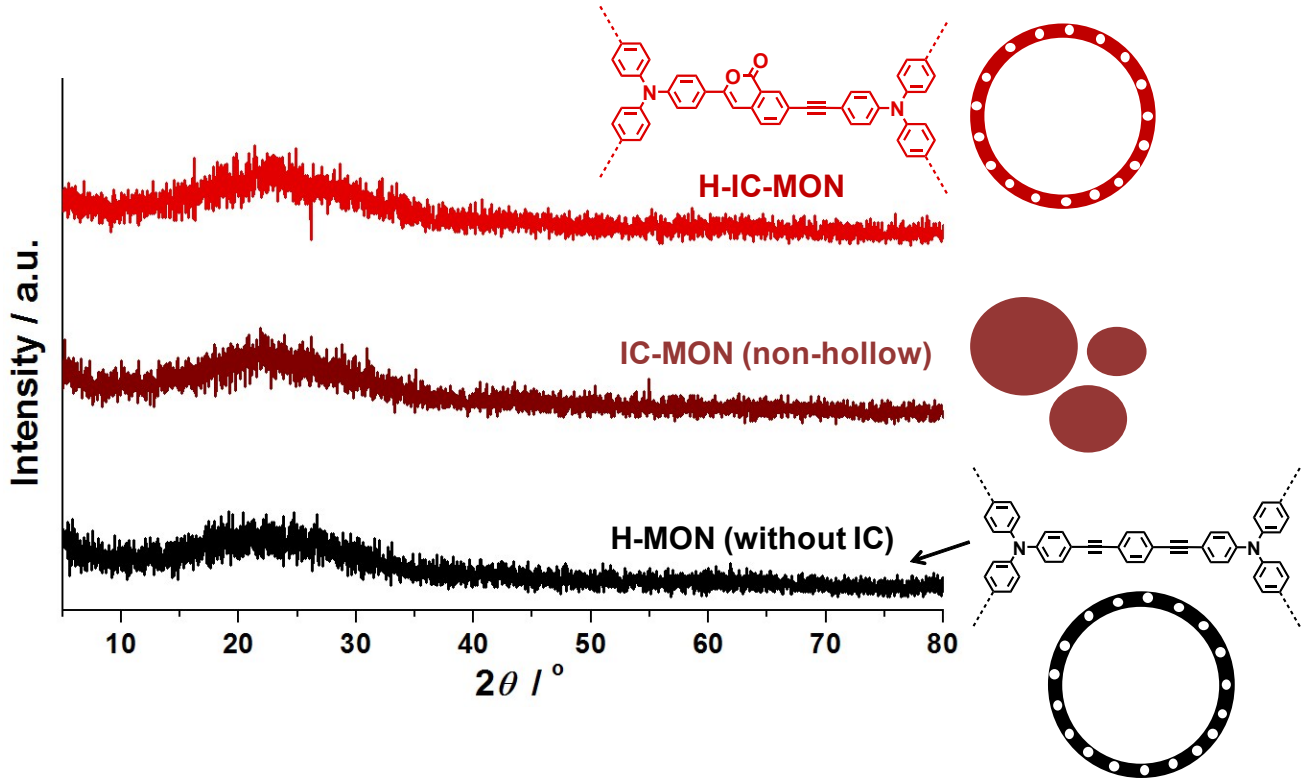


**Fig. S2** Thermogravimetric analysis of H-IC-MON.

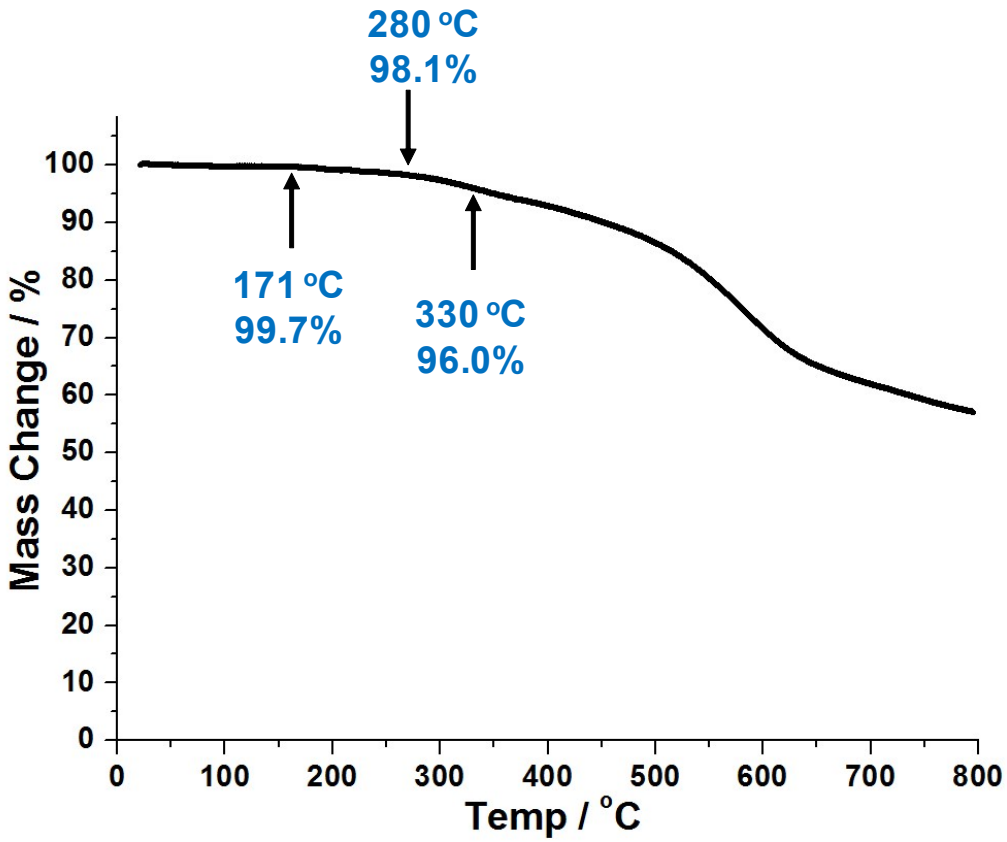


**Fig. S3** (a) Emission properties and (b) decay curves of H-IC-MON in 2:1 $H_2O$/THF and solid (Excitation wavenlength: 440 nm).

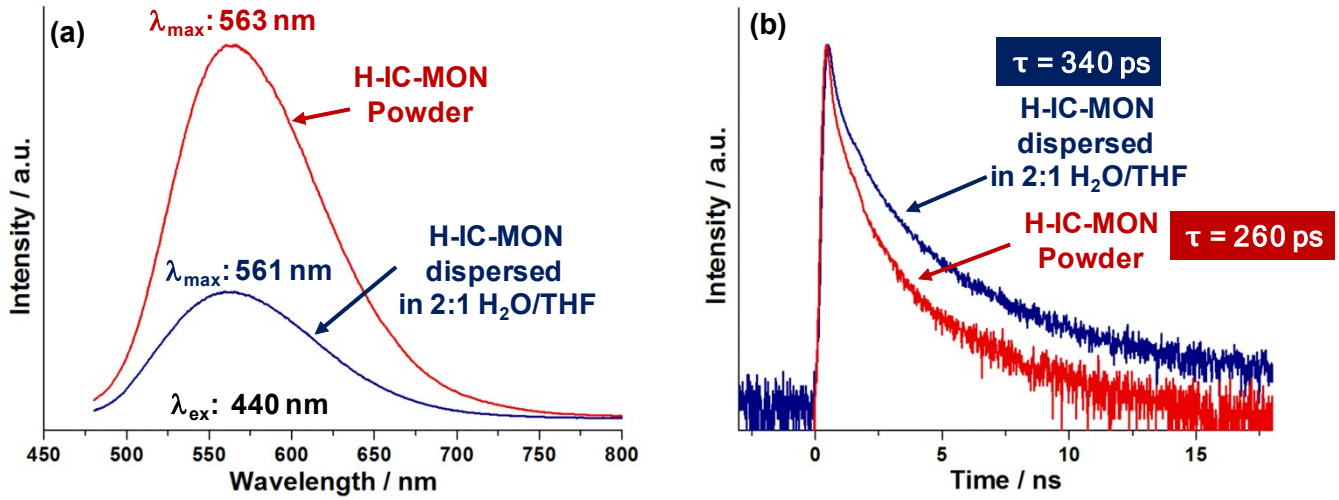


**Fig. S4** SEM, TEM, $N_2$ adsorption-desorption isotherm curves, and pore size distribution diagrams of control materials, IC-MON (brown) and H-MON (black).

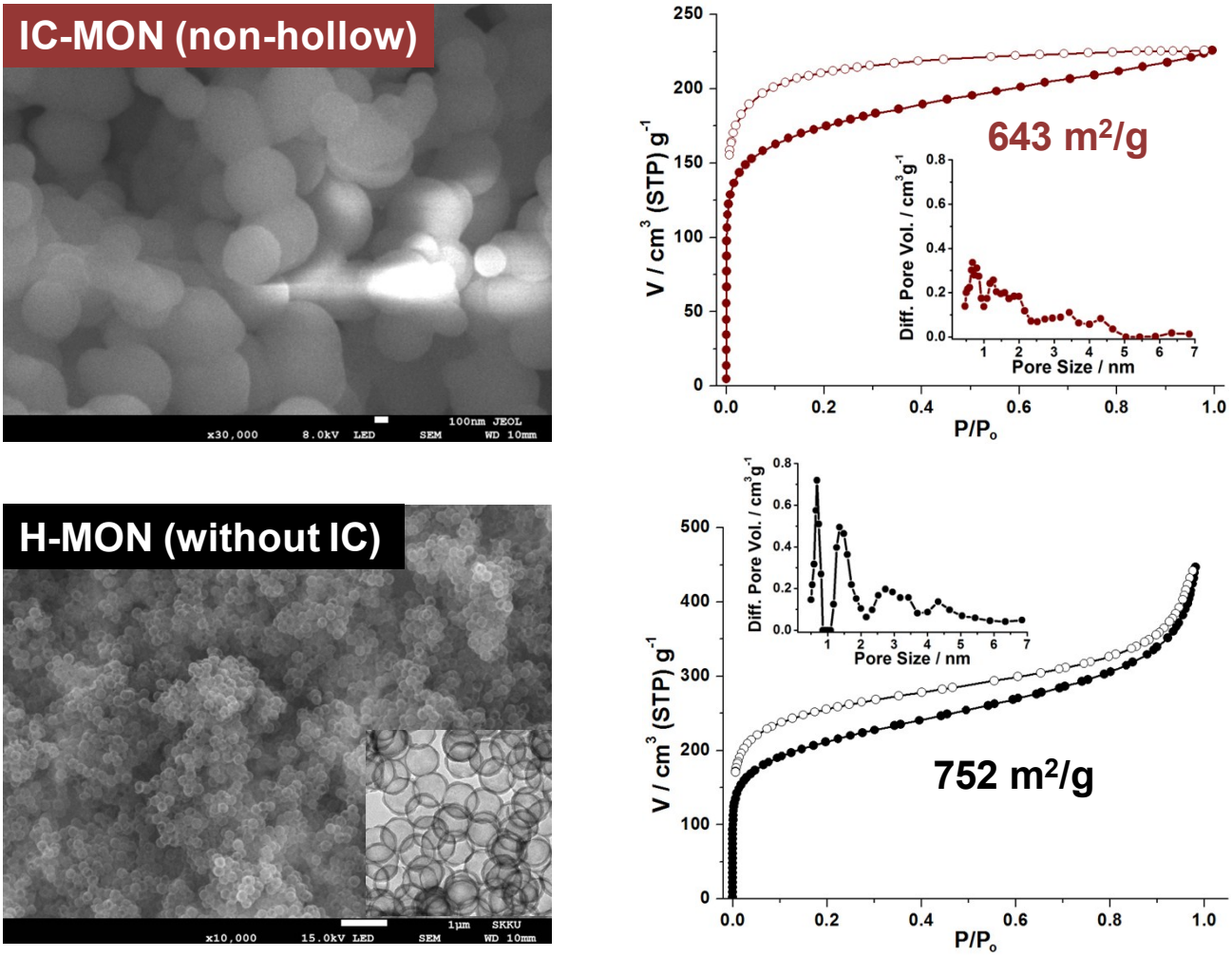


**Fig. S5** UV/vis absorption (solid lines) and emission spectra (dotted lines) of control materials, IC-MON (brown) and H-MON (black). The normalized absorption spectra were obtained through conversion of reflectance spectra of powder samples. The un-normalized emission spectra were obtained with the dispersed solution (2.5 μg/mL) of IC-MON and H-MON in a 2:1 mixture of $H_2O$/THF.

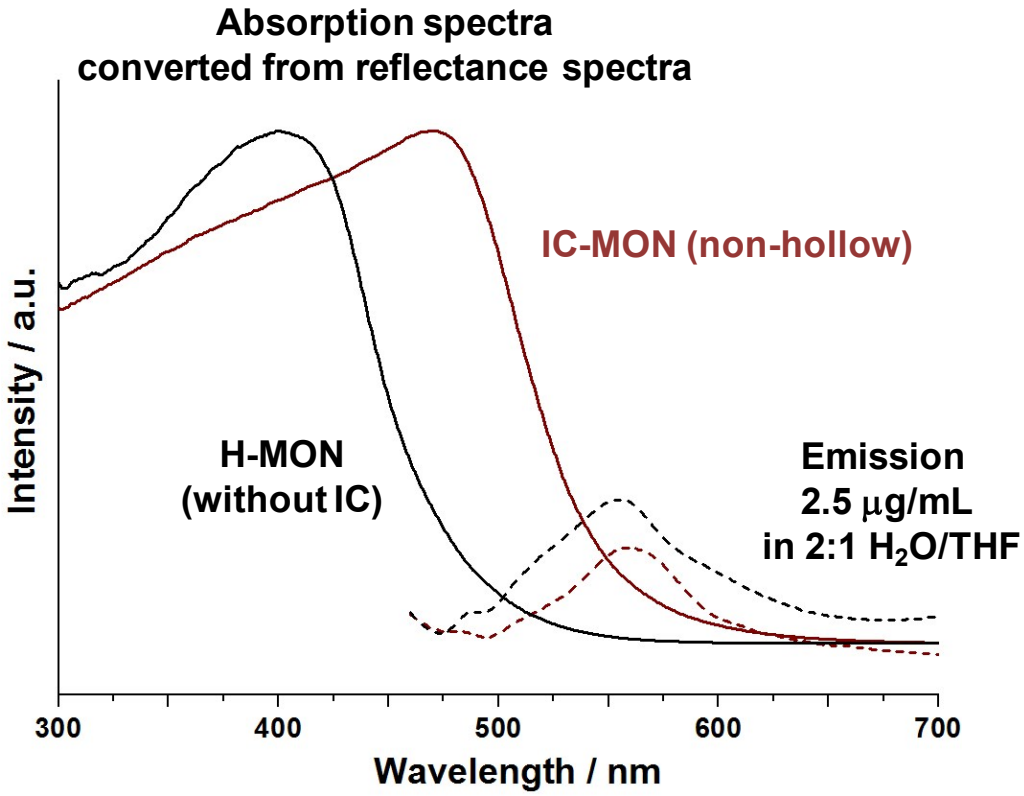


**Fig. S6** Reaction time dependent (a) solid phase $^{13}C$ NMR and (b) IR absorption spectra of H-IC-MON. For comparison, the spectra of MD-1 and IC-MON were added.

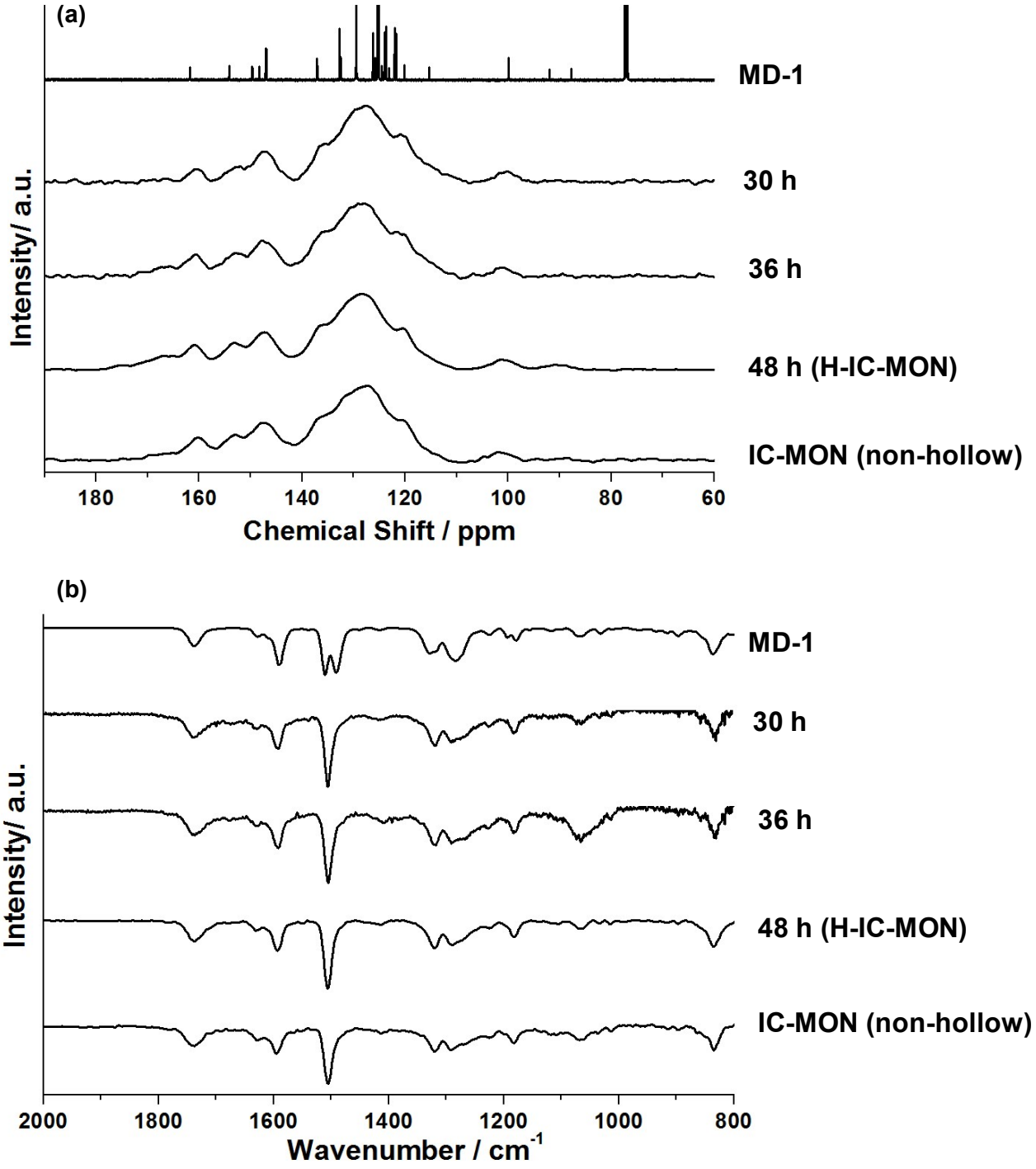


**Fig. S7** Emission ( $\lambda_{max}$: 561 nm, 440 nm excitation) quenching of H-IC-MON (2.5 μg/mL in a 2:1 mixture of $H_2O$/THF) by PA(2,4,6-trinitrophenol), DNP(2,6-dinitrophenol), 4NP(4-nitrophenol), 2NP(2-nitrophenol), 4-chlorophenol, phenol, and 4-methylphenol.

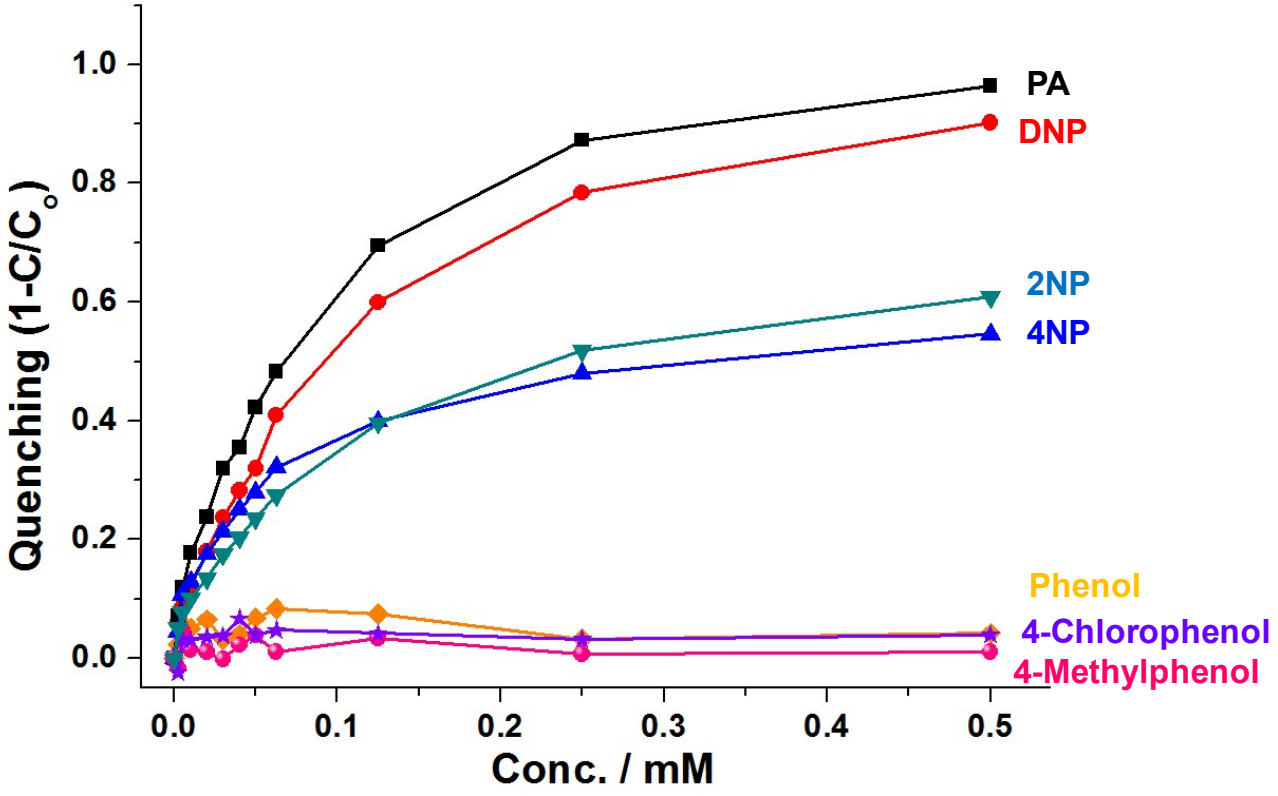
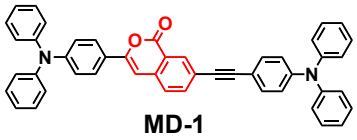
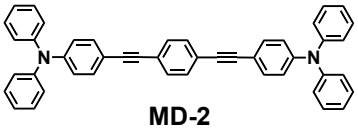


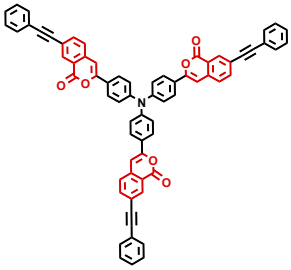
**Fig. S8** Model compounds for computational simulation (Figs. S7-10). In order to understand the optical properties and sensing behavior of H-IC-MON, the density functional theory (DFT) calculations were performed for the model compounds which can represent the local region of the electronic structure for H-IC-MON and H-MON.



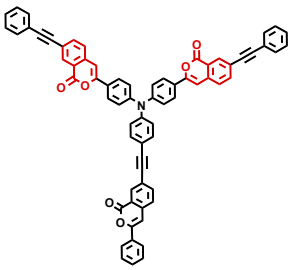
MD-1



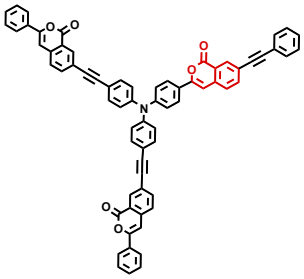
MD-2



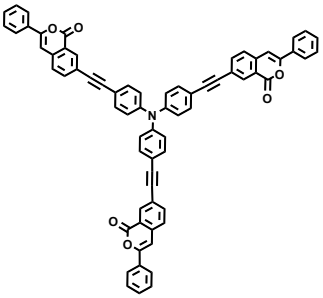
H-IC-MON
-MD-1



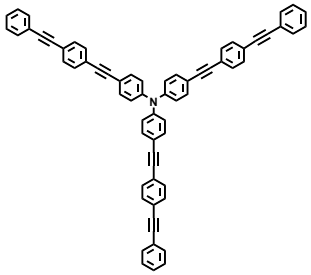
H-IC-MON
-MD-2



H-IC-MON
-MD-3

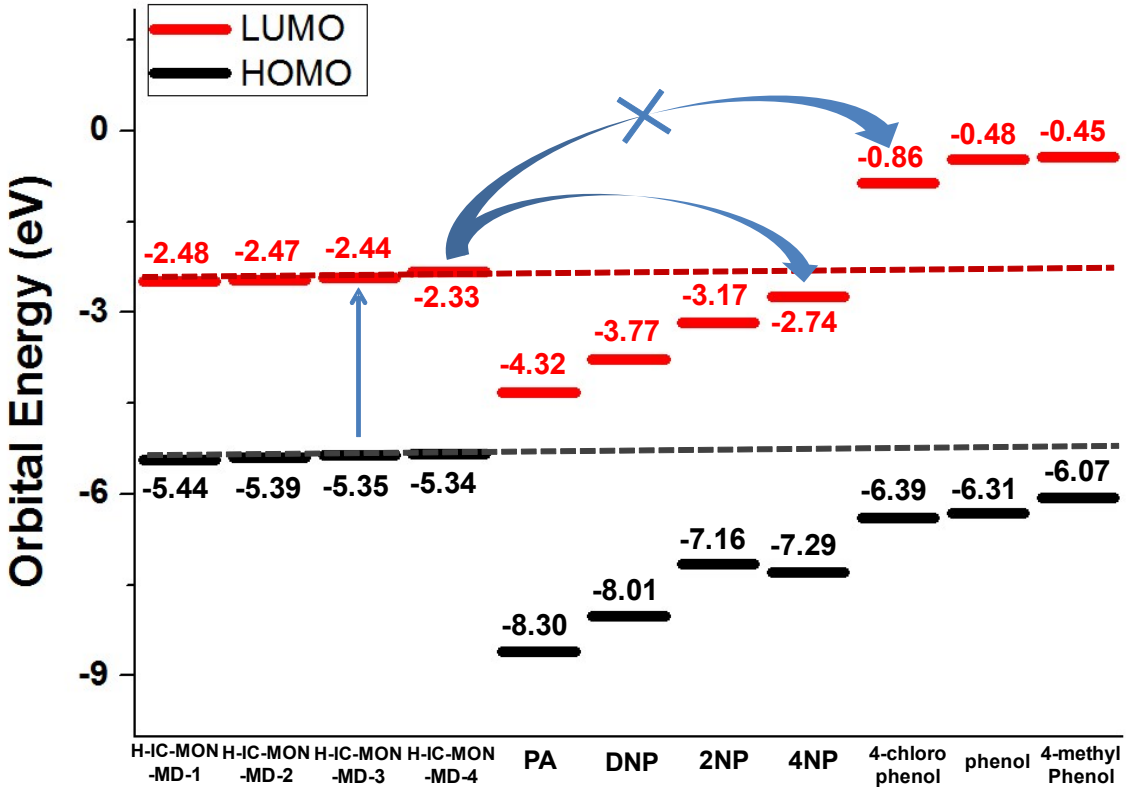


H-IC-MON
-MD-4



H-MON
-MD-1

**Fig. S9** The DFT (the B3LYP/6-31+G(d)) simulated HOMO and LUMO energy levels of the H-IC-MON model species (H-IC-MON-MD-1 ~ 4), PA, DNP, 2NP, 4NP, 4-chlorophenol, phenol, and 4-methylphenol.



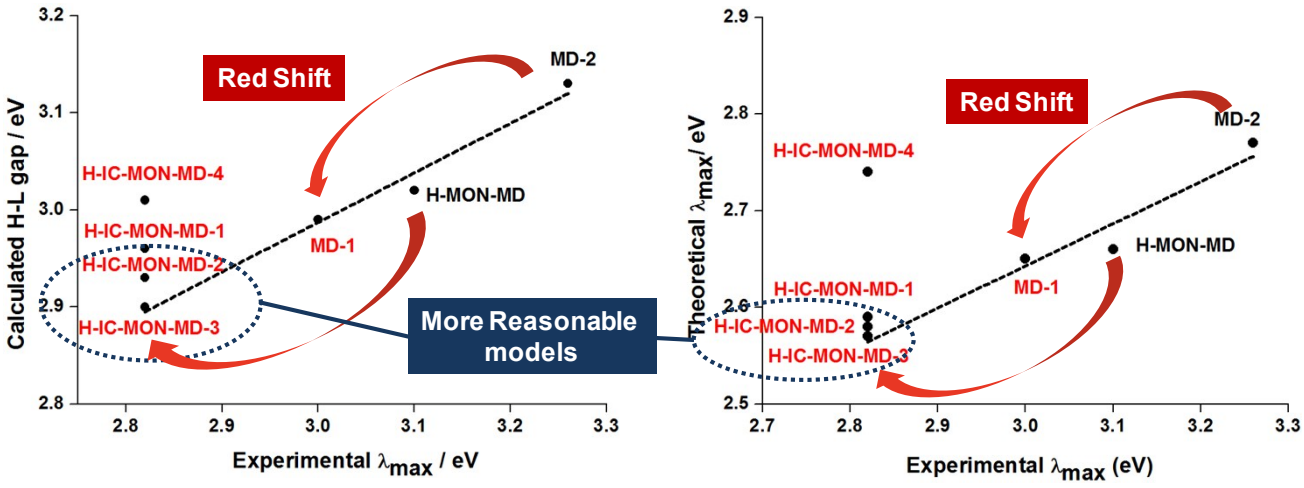

The HOMO and LUMO energy levels for H-IC-MON were estimated as -5.44 ~ -5.34 eV and -2.33 ~ -2.48 eV, respectively, from the calculated results for **H-IC-MON-MD-1-4**. Considering the calculated LUMO energy levels for nitrophenols (PA, DNP, 2NP and 4NP), 4-chlorophenol, phenol, and 4-methylphenol, it is expected that the emission of H-IC-MON can be quenched by the electron transfer from the excited LUMO level of model H-IC-MON species to the LUMO levels of nitophenols (-4.32 ~ -2.74 eV). In comparison, the electron transfer from the excited LUMO level of model H-IC-MON species to LUMO levels for 4-chlorophenol, phenol, and 4-methylphenol (-0.86 ~ -0.45 eV) was unfavorable.

**Fig. S10** (a) The calculated and experimental maximum peak positions ($\lambda_{max}$) of an absorption spectrum for MD-1, MD-2, H-IC-MON-MD-1–4 and H-MON-MD-1. Comparison of experimental maximum peak positions ($\lambda_{max}$) with the calculated HOMO-LUMO gap values (b) as well as theoretical $\lambda_{max}$ values (c).

**(a)**

| Model compounds | HOMO (eV) | LUMO (eV) | H-L Gap (eV) | Theoretical $\lambda_{max}$ (eV) | Experimental $\lambda_{max}$ (eV) |
|---|---|---|---|---|---|
| **MD-1** | -5.14 | -2.14 | 2.99 | 2.65 | 3.00 |
| **MD-2** | -5.06 | -1.92 | 3.13 | 2.77 | 3.26 |
| **H-IC-MON-MD-1** | -5.44 | -2.48 | 2.96 | 2.59 | 2.82 |
| **H-IC-MON-MD-2** | -5.39 | -2.47 | 2.93 | 2.58 | |
| **H-IC-MON-MD-3** | -5.35 | -2.44 | 2.90 | 2.57 | |
| **H-IC-MON-MD-4** | -5.34 | -2.33 | 3.01 | 2.74 | |
| **H-MON-MD-1** | -5.20 | -2.18 | 3.02 | 2.66 | 3.10 |

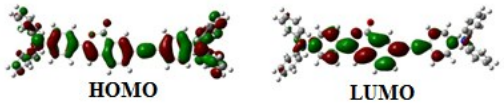
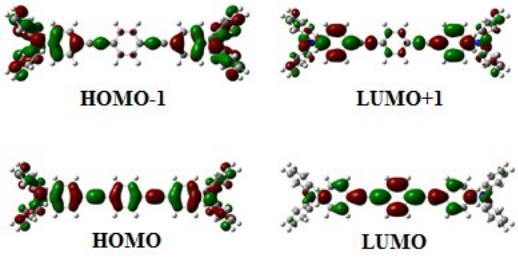
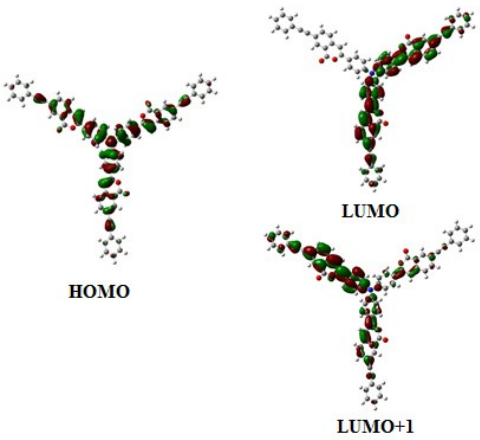
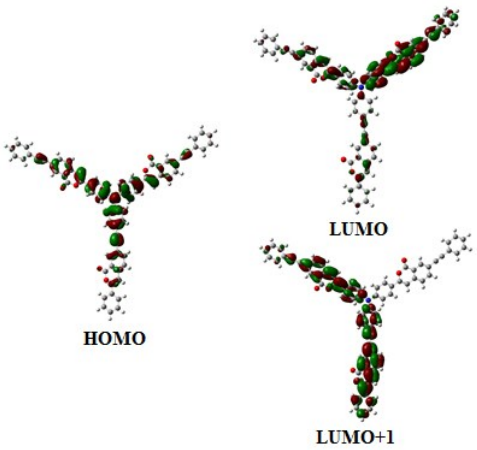
**(b)** **(c)**

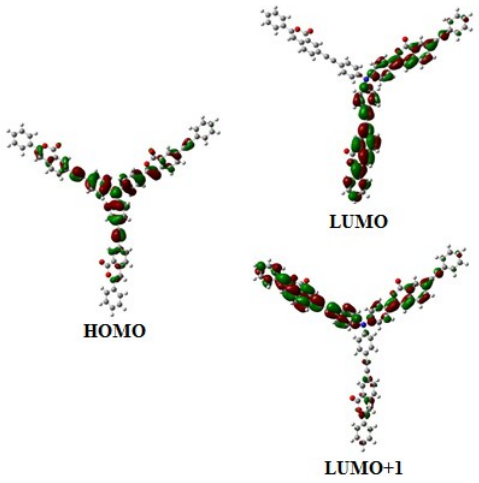
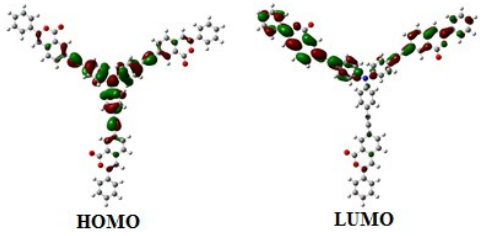
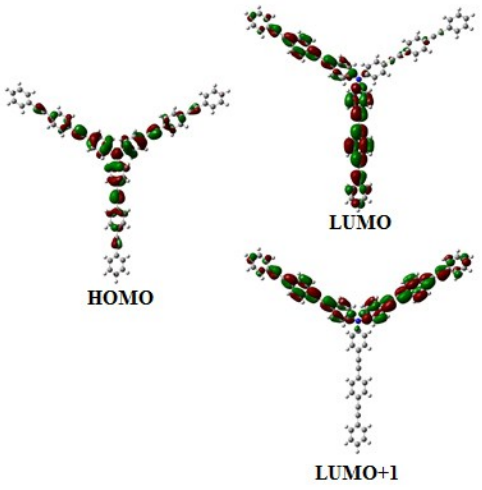



Firstly, to confirm the reliability of designed model systems (H-IC-MON-MD-1–4 and H-MON-MD-1), we tried to compare the calculated HOMO-LUMO gaps and the simulated $\lambda_{max}$ values through time-dependent DFT (TD-DFT) calculations with experimental results. As shown in Figs. S8b-c, the trend of calculated HOMO-LUMO gaps and simulated $\lambda_{max}$ values are in good agreement with experimental $\lambda_{max}$ values. Our calculated results also are in line with the red-shifted $\lambda_{max}$ of MD-1 on the basis of $\lambda_{max}$ value of MD-2. For H-IC-MON-MD-1–4, the trends in Figs. S8b-c indicate that H-IC-MON-MD-2 and H-IC-MON-MD-3 might be more reasonable models of actual H-IC-MON system. By considering the synthetic process making organic networks (Fig.1 in text), the H-IC-MON-MD-2-3 would have higher possibility of existence in actual H-IC-MON systems than H-IC-MON-MD-1 and H-IC-MON-MD-4. Interestingly, H-

IC-MON-MD-2-3 are also expected to be good model systems for actual H-IC-MON from DFT calculations.

**Fig. S11** TD-DFT results: Calculated frontier molecular orbitals and contributions of orbital transitions for the 1st excited state of MD-1, MD-2, H-IC-MON-MD-1–4 and H-MON-MD-1 with B3LYP/6-31+G(d) level of theory.

| | Molecular orbitals | Contributions of orbital transitions |
|---|---|---|
| **MD-1** |   | Excited state 1 : 2.65 eV<br>Oscillator strength : 2.05<br>HOMO → LUMO : 100 % |
| **MD-2** |   | Excited state 1 : 2.77 eV<br>Oscillator strength : 2.41<br>HOMO-1 → LUMO+1 : 2.4 %<br>HOMO → LUMO: 97.6 % |
| **H-IC-MON-MD-1** |   | Excitation energy : 2.59 eV<br>Oscillator strength : 1.72<br>HOMO → LUMO : 31.0 %<br>HOMO → LUMO+1 : 69.0 % |
| **H-IC-MON-MD-2** |   | Excitation energy : 2.56 eV<br>Oscillator strength : 1.74<br>HOMO → LUMO: 94.3 %<br>HOMO → LUMO+1 : 5.7 % |

| | | |
|---|---|---|
| **H-IC-MON-MD-3** |  | Excitation energy : 2.55 eV<br>Oscillator strength : 1.72<br>HOMO → LUMO: 84.8 %<br>HOMO → LUMO+1 : 15.2 % |
| **H-IC-MON-MD-4** |  | Excitation energy : 2.67 eV<br>Oscillator strength : 1.33<br>HOMO → LUMO: 100 % |
| **H-MON-MD-1** |  | Excitation energy : 2.66 eV<br>Oscillator strength : 1.85<br>HOMO → LUMO: 83.1 %<br>HOMO → LUMO+1 : 16.9 % |

The calculated maximum peak position ($\lambda_{max}$) of an absorption spectrum is highly related with the 1st excited state with large oscillator strength. Fig. S9 shows that the details of orbital contribution for the 1st excited state. The main contribution results from the HOMO, LUMO and their symmetrical related orbitals (e g. HOMO-1 or LUMO+1 state).

**Fig. S12** The cartesian coordinates (in Å) of optimized geometry for MD-1, MD-2, H-IC-MON-MD-1–4 and H-MON-MD-1 at the B3LYP/6-31+G(d).

**MD-1**

| | | | |
|---|---|---|---|
| C | 7.24917300 | -1.21859100 | 0.08514000 |
| C | 5.86276800 | -1.26906000 | 0.05633500 |
| C | 5.08597700 | -0.09648500 | -0.03171300 |
| C | 5.76887000 | 1.13410800 | -0.08494300 |
| C | 7.15794800 | 1.19043900 | -0.06652400 |
| C | 7.92731500 | 0.01568700 | 0.02007200 |
| H | 7.81787800 | -2.13891300 | 0.17110200 |
| H | 5.38281500 | -2.24010100 | 0.13309400 |
| H | 5.20119000 | 2.05510500 | -0.15754600 |
| H | 7.65413200 | 2.15397000 | -0.12367800 |
| C | 10.11100800 | -0.95751600 | -0.56906400 |
| C | 9.79005300 | -1.41356900 | -1.85792500 |
| C | 11.21168500 | -1.51606100 | 0.10013200 |
| C | 10.55045000 | -2.41831100 | -2.45762100 |
| H | 8.94633700 | -0.97723900 | -2.38457100 |
| C | 11.97690200 | -2.50946300 | -0.51260300 |
| H | 11.46358300 | -1.16692200 | 1.09716900 |
| C | 11.64911200 | -2.97042000 | -1.79135200 |
| H | 10.28996100 | -2.76004600 | -3.45628400 |
| H | 12.82607100 | -2.93209100 | 0.01862200 |
| H | 12.24314600 | -3.74817900 | -2.26349300 |
| C | 10.00821300 | 1.14611100 | 0.69948300 |
| C | 11.09335800 | 1.78249900 | 0.07635800 |
| C | 9.60068600 | 1.57622200 | 1.97251100 |
| C | 11.75908400 | 2.82687800 | 0.71979200 |
| H | 11.41140300 | 1.45497900 | -0.90908200 |
| C | 10.26087000 | 2.63206400 | 2.60226300 |
| H | 8.76690400 | 1.08217000 | 2.46271900 |
| C | 11.34505400 | 3.26141400 | 1.98254000 |
| H | 12.59726700 | 3.31048200 | 0.22433500 |
| H | 9.93274900 | 2.95447400 | 3.58724400 |
| H | 11.86089300 | 4.07960000 | 2.47767600 |
| N | 9.33727800 | 0.06781900 | 0.04976700 |
| C | 3.62066500 | -0.14537000 | -0.06553700 |
| C | 2.83405700 | -1.24910400 | -0.18296400 |
| O | 3.05097400 | 1.10099800 | 0.03264800 |
| C | 1.40454500 | -1.13054300 | -0.18521100 |
| H | 3.28467100 | -2.22926300 | -0.28318600 |
| C | 1.68250000 | 1.33953700 | 0.02294000 |
| C | 0.81986500 | 0.15551100 | -0.08118100 |
| C | 0.54161800 | -2.24504400 | -0.28884000 |
| O | 1.31731700 | 2.49160200 | 0.10366500 |
| C | -0.56929600 | 0.32016300 | -0.07622800 |
| H | 0.96843300 | -3.24160500 | -0.37209500 |
| C | -0.83172300 | -2.08153500 | -0.28200700 |
| C | -1.41868700 | -0.79202800 | -0.17372500 |
| H | -0.97941800 | 1.32102400 | 0.00589300 |
| H | -1.48271900 | -2.94753500 | -0.35973300 |
| C | -2.83295400 | -0.63989500 | -0.16144800 |
| C | -4.04573800 | -0.51695500 | -0.14543600 |
| C | -5.46023500 | -0.36730300 | -0.11746500 |
| C | -6.31160900 | -1.49297900 | -0.12054200 |
| C | -6.05578000 | 0.91178600 | -0.07925300 |
| C | -7.69280800 | -1.34714200 | -0.08817900 |
| H | -5.87654400 | -2.48746700 | -0.16068000 |
| C | -7.43678600 | 1.05834800 | -0.03560600 |
| H | -5.42025400 | 1.79254700 | -0.06760100 |
| C | -8.28064200 | -0.06866200 | -0.03954400 |
| H | -8.32768300 | -2.22764700 | -0.10091700 |
| H | -7.87102100 | 2.05235900 | 0.00706900 |
| N | -9.68721600 | 0.07805200 | 0.00719000 |
| C | -10.47579100 | -0.82362300 | 0.77833500 |
| C | -10.32350200 | 1.13848300 | -0.70004800 |
| C | -10.07123100 | -1.20040600 | 2.06971900 |
| C | -11.67342700 | -1.34271100 | 0.25970400 |
| C | -11.34265600 | 1.88848700 | -0.09071500 |
| C | -9.94602500 | 1.44348500 | -2.01827200 |
| C | -10.84618100 | -2.08588900 | 2.81973000 |
| H | -9.15055900 | -0.79711600 | 2.48107000 |
| C | -12.45145300 | -2.21436900 | 1.02292200 |
| H | -11.99061000 | -1.05874800 | -0.73942800 |
| C | -11.97406400 | 2.91711800 | -0.79130900 |
| H | -11.63752700 | 1.66023100 | 0.92919400 |
| C | -10.57093200 | 2.48452700 | -2.70609700 |
| H | -9.16378100 | 0.86293500 | -2.49844900 |
| C | -12.04210200 | -2.59555600 | 2.30445800 |
| H | -10.51864900 | -2.36632800 | 3.81778200 |
| H | -13.37613100 | -2.60635900 | 0.60654600 |
| C | -11.59054300 | 3.22521600 | -2.10011800 |
| H | -12.76132400 | 3.48787400 | -0.30501800 |
| H | -10.26687400 | 2.70728600 | -3.72585700 |
| H | -12.64701200 | -3.27920900 | 2.89386800 |
| H | -12.07975800 | 4.03086600 | -2.64075600 |

**MD-2**

| | | | |
|---|---|---|---|
| C | 4.06068200 | 0.00002800 | -0.00025700 |
| C | 2.84129800 | -0.00002100 | -0.00025800 |
| C | 5.48340500 | 0.00003500 | -0.00019700 |
| C | 6.21218600 | -1.20848200 | 0.02373600 |
| C | 6.21217400 | 1.20856100 | -0.02407600 |
| C | 7.60162000 | -1.20904900 | 0.03051800 |
| H | 5.67406300 | -2.15160600 | 0.05239400 |
| C | 7.60160800 | 1.20914300 | -0.03075400 |
| H | 5.67404300 | 2.15167900 | -0.05277700 |
| C | 8.32233400 | 0.00005100 | -0.00009000 |
| H | 8.13894800 | -2.15176500 | 0.06185000 |
| H | 8.13892800 | 2.15186500 | -0.06204800 |
| N | 9.73733100 | 0.00006000 | -0.00003700 |
| C | 10.45635700 | -0.99976100 | -0.71633100 |
| C | 10.45628900 | 0.99988800 | 0.71631600 |
| C | 10.07256700 | -1.36018400 | -2.01859500 |
| C | 11.56423500 | -1.63383400 | -0.13063300 |
| C | 11.56419800 | 1.63398300 | 0.13070100 |
| C | 10.07240000 | 1.36029600 | 2.01855500 |
| C | 10.77818700 | -2.34340000 | -2.71329500 |
| H | 9.22177600 | -0.86805200 | -2.48065000 |
| C | 12.27457700 | -2.60462600 | -0.83820400 |
| H | 11.86445300 | -1.36166500 | 0.87697500 |
| C | 12.27447300 | 2.60478300 | 0.83832900 |
| H | 11.86449400 | 1.36182600 | -0.87688700 |
| C | 10.77795400 | 2.34351800 | 2.71331100 |
| H | 9.22158400 | 0.86814600 | 2.48054500 |
| C | 11.88459000 | -2.96939900 | -2.13047000 |
| H | 10.46814100 | -2.61038800 | -3.72057300 |
| H | 13.12948700 | -3.08635400 | -0.37010600 |
| C | 11.88438800 | 2.96954000 | 2.13057000 |
| H | 13.12940900 | 3.08652800 | 0.37029600 |
| H | 10.46783100 | 2.61049500 | 3.72056900 |
| H | 12.43577900 | -3.73024800 | -2.67639500 |
| H | 12.43552400 | 3.73039600 | 2.67653900 |
| C | 1.41877600 | -0.00012600 | -0.00018500 |
| C | 0.69413900 | 1.21236000 | -0.00024000 |
| C | 0.69431600 | -1.21271700 | -0.00006300 |
| C | -0.69431600 | 1.21225900 | -0.00000400 |
| H | 1.23681600 | 2.15313800 | -0.00030900 |
| C | -0.69413900 | -1.21281900 | -0.00017400 |
| H | 1.23713000 | -2.15341600 | -0.00004600 |
| C | -1.41877600 | -0.00033300 | -0.00005600 |
| H | -1.23712900 | 2.15295800 | 0.00006000 |
| H | -1.23681600 | -2.15359700 | -0.00019100 |
| C | -2.84129800 | -0.00043700 | 0.00000600 |
| C | -4.06068200 | -0.00048500 | 0.00005500 |
| C | -5.48340500 | -0.00035000 | 0.00006800 |
| C | -6.21206600 | 1.20824000 | 0.02397900 |
| C | -6.21229300 | -1.20880400 | -0.02383200 |
| C | -7.60150100 | 1.20894500 | 0.03072000 |
| H | -5.67385200 | 2.15131100 | 0.05265300 |
| C | -7.60172700 | -1.20924800 | -0.03055000 |
| H | -5.67425400 | -2.15197500 | -0.05251600 |
| C | -8.32233400 | -0.00008400 | 0.00009000 |
| H | -8.13873600 | 2.15171400 | 0.06203600 |
| H | -8.13913900 | -2.15191700 | -0.06186000 |
| N | -9.73733100 | 0.00005000 | 0.00009700 |
| C | -10.45622900 | 0.99994200 | -0.71622600 |
| C | -10.45641600 | -0.99970800 | 0.71641900 |
| C | -10.07236200 | 1.36031500 | -2.01848100 |
| C | -11.56405700 | 1.63413800 | -0.13056500 |
| C | -11.56437500 | -1.63368100 | 0.13076500 |
| C | -10.07260600 | -1.36016800 | 2.01866700 |
| C | -10.77785500 | 2.34360000 | -2.71320900 |
| H | -9.22160900 | 0.86808800 | -2.48050600 |
| C | -12.27427400 | 2.60500100 | -0.83816500 |
| H | -11.86433400 | 1.36200800 | 0.87703600 |
| C | -12.27477600 | -2.60441000 | 0.83836300 |
| H | -11.86461100 | -1.36148300 | -0.87683000 |
| C | -10.77828600 | -2.34332100 | 2.71339400 |
| H | -9.22175300 | -0.86811300 | 2.48068800 |
| C | -11.88420900 | 2.96972200 | -2.13042200 |
| H | -10.46775100 | 2.61054800 | -3.72048000 |
| H | -13.12914700 | 3.08682300 | -0.37009600 |
| C | -11.88476900 | -2.96922000 | 2.13061300 |
| H | -13.12974900 | -3.08606000 | 0.37029900 |
| H | -10.46822400 | -2.61033800 | 3.72065900 |
| H | -12.43530000 | 3.73062700 | -2.67636800 |
| H | -12.43600500 | -3.73002000 | 2.67655900 |

**H-IC-MON-MD-1**

| | | | |
|---|---|---|---|
| C | 0.92876600 | 2.12875800 | -0.84577900 |
| C | 0.93884000 | 3.51724200 | -0.84520000 |
| C | 0.03167200 | 4.25469100 | -0.05891600 |
| C | -0.89252500 | 3.53753300 | 0.72450100 |
| C | -0.89803100 | 2.14637400 | 0.73616700 |
| C | 0.01103700 | 1.41936200 | -0.04933800 |
| H | 1.62738300 | 1.58476700 | -1.47389700 |
| H | 1.64549300 | 4.02846400 | -1.49176700 |
| H | -1.60053600 | 4.07899800 | 1.34194000 |
| H | -1.60950300 | 1.61736200 | 1.36270100 |
| C | 1.22368500 | -0.71924000 | -0.04933800 |
| C | 2.30783000 | -0.29546900 | 0.73616700 |
| C | 1.37917500 | -1.86871400 | -0.84577900 |
| C | 3.50985600 | -0.99581700 | 0.72450100 |
| H | 2.20542800 | 0.58518900 | 1.36270100 |
| C | 2.57660100 | -2.57168100 | -0.84520000 |
| H | 0.55875700 | -2.20173900 | -1.47389700 |
| C | 3.66883500 | -2.15477400 | -0.05891600 |
| H | 4.33278400 | -0.65339400 | 1.34194000 |
| H | 2.66600600 | -3.43927100 | -1.49176700 |
| C | -1.23472300 | -0.70012200 | -0.04933800 |
| C | -1.40979900 | -1.85090500 | 0.73616700 |
| C | -2.30794200 | -0.26004400 | -0.84577900 |
| C | -2.61733000 | -2.54171600 | 0.72450100 |
| H | -0.59592500 | -2.20255100 | 1.36270100 |
| C | -3.51544100 | -0.94556200 | -0.84520000 |
| H | -2.18614000 | 0.61697200 | -1.47389700 |
| C | -3.70050700 | -2.09991700 | -0.05891600 |
| H | -2.73224800 | -3.42560400 | 1.34194000 |
| H | -4.31149900 | -0.58919400 | -1.49176700 |
| N | 0.00000000 | 0.00000000 | -0.04967700 |
| C | 0.04136300 | 5.72293600 | -0.04921300 |
| C | 0.99757800 | 6.54159800 | -0.56202200 |
| O | -1.06422400 | 6.25019200 | 0.57142700 |
| C | 0.85792300 | 7.96788900 | -0.47935900 |
| H | 1.88171100 | 6.12099700 | -1.02605400 |
| C | -1.29859000 | 7.61204100 | 0.72499500 |
| C | -0.28395200 | 8.51075000 | 0.15860800 |
| C | 1.81555200 | 8.86378500 | -1.00455000 |
| O | -2.30993300 | 7.94112800 | 1.30311600 |
| C | -0.46333900 | 9.89411300 | 0.26333300 |
| H | 2.70103300 | 8.46818800 | -1.49584200 |
| C | 1.63699300 | 10.23177100 | -0.90126700 |
| C | 0.49038400 | 10.77662500 | -0.26454200 |
| H | -1.35038200 | 10.27360700 | 0.75913800 |
| H | 2.38039500 | 10.90965500 | -1.31036100 |
| C | 0.31832600 | 12.18605300 | -0.16627400 |
| C | 0.17487700 | 13.39305900 | -0.08584600 |
| C | 0.00000000 | 14.80464500 | 0.01239500 |
| C | 0.96138500 | 15.68623600 | -0.52503400 |
| C | -1.13822300 | 15.34274500 | 0.64911600 |
| C | 0.78543800 | 17.06528900 | -0.42640400 |

| | | | |
|---|---|---|---|
| H | 1.83969900 | 15.27761500 | -1.01622800 |
| C | -1.30558200 | 16.72321900 | 0.74302100 |
| H | -1.88142500 | 14.66859400 | 1.06463500 |
| H | 1.53386700 | 17.73358300 | -0.84444500 |
| H | -2.18700900 | 17.12466600 | 1.23633900 |
| C | -0.34661500 | 17.58916500 | 0.20682800 |
| H | -0.48043500 | 18.66509200 | 0.28208500 |
| C | -4.97689000 | -2.82564700 | -0.04921300 |
| C | -6.16397900 | -2.40687100 | -0.56202200 |
| O | -4.88071300 | -4.04674000 | 0.57142700 |
| C | -7.32935600 | -3.24096100 | -0.47935900 |
| H | -6.24179400 | -1.43088900 | -1.02605400 |
| C | -5.94292600 | -4.93063300 | 0.72499500 |
| C | -7.22855000 | -4.50128500 | 0.15860800 |
| C | -8.58403900 | -2.85957800 | -1.00455000 |
| O | -5.72225300 | -5.97102400 | 1.30311600 |
| C | -8.33688400 | -5.34832000 | 0.26333300 |
| H | -8.68418300 | -1.89493100 | -1.49584200 |
| C | -9.67947000 | -3.69820800 | -0.90126700 |
| C | -9.57802300 | -4.96362700 | -0.26454200 |
| H | -8.22201300 | -6.30626900 | 0.75913800 |
| H | -10.63823600 | -3.39334500 | -1.31036100 |
| C | 4.93552700 | -2.89728900 | -0.04921300 |
| C | 5.16640100 | -4.13472700 | -0.56202200 |
| O | 5.94493600 | -2.20345100 | 0.57142700 |
| C | 6.47143200 | -4.72692800 | -0.47935900 |
| H | 4.36008300 | -4.69010800 | -1.02605400 |
| C | 7.24151600 | -2.68140800 | 0.72499500 |
| C | 7.51250200 | -4.00946500 | 0.15860800 |
| C | 6.76848700 | -6.00420700 | -1.00455000 |
| O | 8.03218500 | -1.97010400 | 1.30311600 |
| C | 8.80022300 | -4.54579300 | 0.26333300 |
| H | 5.98315000 | -6.57325700 | -1.49584200 |
| C | 8.04247700 | -6.53356300 | -0.90126700 |
| C | 9.08763800 | -5.81299800 | -0.26454200 |
| H | 9.57239500 | -3.96733800 | 0.75913800 |
| H | 8.25784100 | -7.51631000 | -1.31036100 |
| C | -10.71259400 | -5.81734800 | -0.16627400 |
| C | -11.68616800 | -6.54508200 | -0.08584600 |
| C | -12.82119900 | -7.40232200 | 0.01239500 |
| C | -14.06537200 | -7.01053400 | -0.52503400 |
| C | -12.71809600 | -8.65710300 | 0.64911600 |
| C | -15.17169300 | -7.85243500 | -0.42640400 |
| H | -14.15065300 | -6.04558100 | -1.01622800 |
| C | -13.82994200 | -9.49227700 | 0.74302100 |
| H | -11.76266200 | -8.96365900 | 1.06463500 |
| C | -15.05935600 | -9.09476000 | 0.20682800 |
| H | -16.12466700 | -7.53842300 | -0.84444500 |
| H | -13.73689200 | -10.45633800 | 1.23633900 |
| H | -15.92422700 | -9.74861500 | 0.28208500 |
| C | 10.39426800 | -6.36870500 | -0.16627400 |
| C | 11.51129100 | -6.84797800 | -0.08584600 |
| C | 12.82119900 | -7.40232200 | 0.01239500 |
| C | 13.10398700 | -8.67570200 | -0.52503400 |
| C | 13.85631900 | -6.68564300 | 0.64911600 |
| C | 14.38625500 | -9.21285400 | -0.42640400 |
| H | 12.31095300 | -9.23203400 | -1.01622800 |
| C | 15.13552400 | -7.23094200 | 0.74302100 |
| H | 13.64408800 | -5.70493500 | 1.06463500 |
| C | 15.40597200 | -8.49440500 | 0.20682800 |
| H | 14.59079900 | -10.19515900 | -0.84444500 |
| H | 15.92390100 | -6.66832800 | 1.23633900 |
| H | 16.40466100 | -8.91647800 | 0.28208500 |

## H-IC-MON-MD-2

| | | | |
|---|---|---|---|
| C | 1.18611200 | 2.05420100 | -0.73869200 |
| C | 1.17908300 | 3.44215900 | -0.77119500 |
| C | 0.30692700 | 4.18890600 | 0.04561600 |
| C | -0.56438500 | 3.48007600 | 0.89477600 |
| C | -0.55310100 | 2.08945100 | 0.93820100 |
| C | 0.32114100 | 1.35373400 | 0.12204500 |
| H | 1.85670000 | 1.50338600 | -1.39092100 |
| H | 1.84568500 | 3.94413100 | -1.46570100 |
| H | -1.24525900 | 4.02748700 | 1.53687400 |
| H | -1.22563600 | 1.56784500 | 1.61224700 |
| C | 1.55092100 | -0.77541400 | 0.10692700 |
| C | 2.67624600 | -0.31937900 | 0.81357000 |
| C | 1.66956400 | -1.95284300 | -0.65522200 |
| C | 3.87972000 | -1.01476200 | 0.75906600 |
| H | 2.60432900 | 0.58271500 | 1.41329100 |
| C | 2.86972800 | -2.64931600 | -0.69812400 |
| H | 0.81746800 | -2.31253500 | -1.22342800 |
| C | 4.00255500 | -2.20059000 | 0.00966000 |
| H | 4.73313500 | -0.64671700 | 1.31739800 |
| H | 2.92605000 | -3.54029600 | -1.31597700 |
| C | -0.90448500 | -0.77546100 | 0.22349400 |
| C | -1.03851300 | -1.89017400 | 1.06958200 |
| C | -2.00665400 | -0.37651900 | -0.55262800 |
| C | -2.23723100 | -2.59103100 | 1.13088600 |
| H | -0.19806200 | -2.20272200 | 1.68196100 |
| C | -3.20946300 | -1.06929200 | -0.48197100 |
| H | -1.91515800 | 0.48002500 | -1.21349300 |
| H | -2.32789300 | -3.44762000 | 1.79240400 |
| H | -4.05134900 | -0.75206600 | -1.09013100 |
| N | 0.32507900 | -0.06526300 | 0.15335800 |
| C | 0.29809100 | 5.65710600 | 0.01926400 |
| C | 1.18803500 | 6.47414900 | -0.60396900 |
| O | -0.74959400 | 6.18754500 | 0.73079100 |
| C | 1.03687900 | 7.90024400 | -0.54242900 |
| H | 2.02720500 | 6.05337400 | -1.14476100 |
| C | -0.98730400 | 7.54968900 | 0.87411000 |
| C | -0.04510500 | 8.44573200 | 0.19048100 |
| C | 1.92556900 | 8.79400500 | -1.18060500 |
| O | -1.94199100 | 7.88142500 | 1.54026000 |
| C | -0.23323100 | 9.82894000 | 0.27880100 |
| H | 2.76447800 | 8.39680500 | -1.74664800 |
| C | 1.73823500 | 10.16189800 | -1.09358200 |
| C | 0.65163600 | 10.70912900 | -0.36096100 |
| H | -1.07350800 | 10.20998600 | 0.84923300 |
| H | 2.42804000 | 10.83783300 | -1.59038200 |
| C | 0.46940400 | 12.11837200 | -0.28083300 |
| C | 0.31715200 | 13.32529300 | -0.21693200 |
| C | 0.12952300 | 14.73632600 | -0.13553400 |
| C | 1.01774700 | 15.61838900 | -0.78613000 |
| C | -0.94931900 | 15.27348800 | 0.59815200 |
| C | 0.82875400 | 16.99672000 | -0.70284500 |
| H | 1.85017800 | 15.21067400 | -1.35225600 |
| C | -1.13024200 | 16.65324400 | 0.67582100 |
| H | -1.63615200 | 14.59913000 | 1.10115200 |
| H | 1.52051100 | 17.66519200 | -1.20893700 |
| H | -1.96559900 | 17.05374900 | 1.24437000 |
| C | -0.24394100 | 17.51964000 | 0.02708300 |
| H | -0.38835100 | 18.59499700 | 0.08981300 |
| C | 5.27145900 | -2.93823000 | -0.02233000 |
| C | 5.49187200 | -4.17525000 | -0.54172400 |
| O | 6.29814100 | -2.24064400 | 0.56515900 |
| C | 6.79969900 | -4.76448900 | -0.49458700 |
| H | 4.67547100 | -4.73273200 | -0.98494700 |
| C | 7.59990400 | -2.71448100 | 0.68130100 |
| C | 7.85697100 | -4.04433800 | 0.11307200 |
| C | 7.08439900 | -6.04276000 | -1.02461600 |
| O | 8.40578900 | -1.99882600 | 1.23257500 |
| C | 9.14714800 | -4.57992700 | 0.18665800 |
| H | 6.28721400 | -6.61339400 | -1.49453900 |
| C | 8.36073500 | -6.57142300 | -0.95208300 |
| C | 9.42138800 | -5.84914100 | -0.34336300 |
| H | 9.93152900 | -3.99933800 | 0.66034000 |
| H | 8.56605200 | -7.55521000 | -1.36388200 |
| C | 10.72954300 | -6.40558400 | -0.27376000 |
| C | 11.84758800 | -6.88575200 | -0.21571800 |
| C | 13.15917600 | -7.43995100 | -0.14214500 |
| C | 13.42995600 | -8.71728100 | -0.67646700 |
| C | 14.20809900 | -6.71920700 | 0.46680200 |
| C | 14.71388600 | -9.25439700 | -0.60147600 |
| H | 12.62638000 | -9.27671700 | -1.14654500 |
| C | 15.48878100 | -7.26445200 | 0.53714700 |
| H | 14.00528800 | -5.73527900 | 0.87941400 |
| C | 15.74722400 | -8.53193200 | 0.00456000 |
| H | 14.90908900 | -10.23977200 | -1.01677300 |
| H | 16.28782600 | -6.69853900 | 1.00904300 |
| H | 16.74718200 | -8.95388700 | 0.06128000 |
| C | -3.34971000 | -2.19485500 | 0.35814000 |
| C | -4.57865100 | -2.90943100 | 0.42184200 |
| C | -5.63431700 | -3.51653200 | 0.46819200 |
| C | -6.86590600 | -4.22684500 | 0.52350400 |
| C | -7.96039500 | -3.83541600 | -0.26181100 |
| C | -7.01430400 | -5.35064100 | 1.37928800 |
| C | -9.16609100 | -4.54148500 | -0.19917900 |
| H | -7.88513200 | -2.98053600 | -0.92532700 |
| C | -8.20708800 | -6.04878400 | 1.44179300 |
| H | -6.17139500 | -5.65832500 | 1.99121700 |
| C | -9.31323500 | -5.66263700 | 0.65278400 |
| C | -10.29614700 | -4.10467600 | -1.03062300 |
| H | -8.29947800 | -6.90597700 | 2.10406600 |
| C | -10.57219000 | -6.35262400 | 0.68380300 |
| O | -11.45972100 | -4.85675400 | -0.92477000 |
| O | -10.30685300 | -3.16371400 | -1.79201300 |
| C | -11.60327600 | -5.94474900 | -0.10059000 |
| H | -10.69755800 | -7.19722800 | 1.35039800 |
| C | -12.94681000 | -6.54241500 | -0.18525300 |
| C | -13.98137600 | -5.86970200 | -0.86181900 |
| C | -13.22755100 | -7.79050000 | 0.40394200 |
| C | -15.25952800 | -6.42480100 | -0.93333700 |
| H | -13.77862900 | -4.91175100 | -1.32711100 |
| C | -14.50504100 | -8.34035100 | 0.32931000 |
| H | -12.44479600 | -8.34629300 | 0.91105700 |
| C | -15.52902500 | -7.65935100 | -0.33817700 |
| H | -16.04618900 | -5.88839800 | -1.45734800 |
| H | -14.70015200 | -9.30666600 | 0.78697600 |
| H | -16.52466100 | -8.09106500 | -0.39674000 |

## H-IC-MON-MD-3

| | | | |
|---|---|---|---|
| C | -1.64222300 | 1.22769800 | 0.41228400 |
| C | -2.22436900 | 2.48910000 | 0.37192400 |
| C | -0.64747900 | 3.16148800 | -1.33786400 |
| C | -0.07368100 | 1.89592800 | -1.30625900 |
| C | -0.56027200 | 0.91190700 | -0.42806700 |
| H | -2.02338200 | 0.47915800 | 1.10026300 |
| H | -3.05666900 | 2.72059200 | 1.02990700 |
| H | -0.26327000 | 3.91074000 | -2.02376100 |
| H | 0.75731200 | 1.66295300 | -1.96525000 |
| C | -0.77854600 | -1.53544600 | -0.31410900 |
| C | -1.97529000 | -1.62303900 | -1.04441100 |
| C | -0.40972700 | -2.62241200 | 0.50091700 |
| C | -2.77784900 | -2.75605600 | -0.96116100 |
| H | -2.27594700 | -0.79851000 | -1.68334500 |
| C | -1.20918400 | -3.75499300 | 0.57349100 |
| H | 0.50300100 | -2.56903200 | 1.08620200 |
| C | -2.41137300 | -3.85143300 | -0.15555000 |
| H | -3.69449800 | -2.80224500 | -1.53819700 |
| H | -0.89822900 | -4.56186900 | 1.22994100 |
| C | 1.45031500 | -0.50141000 | -0.42124800 |
| C | 2.06523800 | -1.49330900 | -1.20593500 |
| C | 2.26155500 | 0.36976300 | 0.32736700 |
| C | 3.44956000 | -1.61474700 | -1.23558300 |
| H | 1.45111400 | -2.16612900 | -1.79679800 |
| C | 3.64590000 | 0.25578400 | 0.28878200 |
| H | 1.79973900 | 1.13616400 | 0.94237200 |
| H | 3.91024400 | -2.38208300 | -1.85086600 |
| H | 4.25956800 | 0.93252400 | 0.87596100 |
| N | 0.03593000 | -0.37803500 | -0.38784800 |
| C | -3.26146900 | -5.04628100 | -0.08404800 |
| C | -2.98537000 | -6.21857500 | 0.54723500 |
| O | -4.44771700 | -4.88571700 | -0.75684800 |
| C | -3.93232800 | -7.29684800 | 0.53220100 |
| H | -2.04221400 | -6.35023900 | 1.06361600 |
| C | -5.43273800 | -5.86157700 | -0.85122300 |
| C | -5.15590500 | -7.12815300 | -0.16080200 |
| C | -3.70013700 | -8.53084600 | 1.18002400 |
| O | -6.42717200 | -5.58976400 | -1.48577700 |
| C | -6.10952700 | -8.15055300 | -0.20271600 |
| H | -2.76721900 | -8.68223800 | 1.71740900 |
| C | -4.64412800 | -9.54123800 | 1.13876200 |
| C | -5.87191000 | -9.37153500 | 0.44518100 |
| H | -7.03488700 | -7.98437700 | -0.74376100 |
| H | -4.45333100 | -10.48445200 | 1.64230300 |
| C | -6.83495200 | -10.41898000 | 0.41084400 |
| C | -7.65685200 | -11.31776800 | 0.38520800 |
| C | -8.62649600 | -12.36244700 | 0.35000800 |
| C | -8.38639400 | -13.58844200 | 1.00549000 |
| C | -9.84404900 | -12.18574500 | -0.34073900 |
| C | -9.33913700 | -14.60505600 | 0.96915000 |
| H | -7.45099700 | -13.73032700 | 1.53895500 |
| C | -10.79080900 | -13.20805500 | -0.37159000 |
| H | -10.03426400 | -11.24400800 | -0.84713400 |
| C | -10.54352100 | -14.41997600 | 0.28195800 |
| H | -9.14161600 | -15.54469500 | 1.47867900 |
| H | -11.72470200 | -13.05856700 | -0.90725600 |
| H | -11.28427200 | -15.21482600 | 0.25584600 |
| C | 4.27073200 | -0.74115500 | -0.49122100 |
| C | 5.68860200 | -0.85659900 | -0.52350500 |
| C | 6.90431800 | -0.94071400 | -0.53938000 |

| | | | |
|---|---|---|---|
| C | 8.32391700 | -1.03417600 | -0.55335600 |
| C | 9.10666700 | -0.20596400 | 0.26484000 |
| C | 8.98200000 | -1.96798600 | -1.39713300 |
| C | 10.50149200 | -0.30460200 | 0.24581500 |
| H | 8.63990700 | 0.51996700 | 0.92193100 |
| C | 10.36206300 | -2.06472700 | -1.41701700 |
| H | 8.38259500 | -2.61177500 | -2.03420700 |
| C | 11.15738600 | -1.23598500 | -0.59469500 |
| C | 11.29384500 | 0.57826300 | 1.11274200 |
| H | 10.84527400 | -2.78603300 | -2.07141700 |
| C | 12.59205000 | -1.29729300 | -0.57992600 |
| O | 12.67259200 | 0.41936600 | 1.05015000 |
| O | 10.86236600 | 1.41946500 | 1.86879200 |
| C | 13.31054900 | -0.48294200 | 0.23604000 |
| H | 13.09838900 | -1.99562200 | -1.23527200 |
| C | 14.77623000 | -0.42413100 | 0.37090100 |
| C | 15.37851800 | 0.60021500 | 1.12514300 |
| C | 15.60510300 | -1.38188800 | -0.24520500 |
| C | 16.76683100 | 0.66763500 | 1.24810400 |
| H | 14.75427700 | 1.34131800 | 1.61120000 |
| C | 16.99024100 | -1.31017700 | -0.11917700 |
| H | 15.17164400 | -2.19676300 | -0.81681900 |
| C | 17.57938500 | -0.28354300 | 0.62717300 |
| H | 17.21265600 | 1.46804400 | 1.83272500 |
| H | 17.61146900 | -2.06128700 | -0.59999800 |
| H | 18.66039200 | -0.23020100 | 0.72540900 |
| C | -1.73693900 | 3.48511200 | -0.50136600 |
| C | -2.32664800 | 4.77973000 | -0.53400900 |
| C | -2.83488300 | 5.88716500 | -0.55414500 |
| C | -3.42378200 | 7.18205400 | -0.58108000 |
| C | -4.48765500 | 7.50964800 | 0.27245500 |
| C | -2.94490100 | 8.17433800 | -1.47738100 |
| C | -5.05707000 | 8.78669700 | 0.23716600 |
| H | -4.88140600 | 6.77720200 | 0.96897900 |
| C | -3.50869600 | 9.43716900 | -1.51329300 |
| H | -2.12197900 | 7.92705800 | -2.14162000 |
| C | -4.57845000 | 9.77603200 | -0.65545300 |
| C | -6.17286100 | 9.09897500 | 1.14074100 |
| H | -3.12714500 | 10.18180500 | -2.20748900 |
| C | -5.19751100 | 11.07181300 | -0.65539300 |
| O | -6.68296100 | 10.38895500 | 1.05915000 |
| O | -6.68162000 | 8.34713100 | 1.94143600 |
| C | -6.21868400 | 11.34969100 | 0.19595700 |
| H | -4.84920200 | 11.82553500 | -1.35116800 |
| C | -6.95094000 | 12.62151300 | 0.32214900 |
| C | -8.13102400 | 12.68819200 | 1.08600800 |
| C | -6.49200400 | 13.79255200 | -0.31165000 |
| C | -8.83447300 | 13.88788400 | 1.19982800 |
| H | -8.49274800 | 11.79695100 | 1.58613400 |
| C | -7.19773400 | 14.98756800 | -0.19463700 |
| H | -5.57170700 | 13.77956700 | -0.88747000 |
| C | -8.37437800 | 15.04144600 | 0.56065200 |
| H | -9.74542000 | 13.91872400 | 1.79180300 |
| H | -6.82425600 | 15.88105700 | -0.68806100 |
| H | -8.92253600 | 15.97534100 | 0.65270200 |

## H-IC-MON-MD-4

| | | | |
|---|---|---|---|
| C | 2.20197400 | -0.74457300 | 0.60874800 |
| C | 3.24171000 | -1.66726600 | 0.61395200 |
| C | 2.00307400 | -3.07098000 | -0.91826400 |
| C | 0.97091100 | -2.14027000 | -0.93776400 |
| C | 1.05145600 | -0.96502500 | -0.16956400 |
| H | 2.27634800 | 0.15376700 | 1.21359700 |
| H | 4.12150300 | -1.48444000 | 1.22380000 |
| H | 1.92690400 | -3.97192600 | -1.51973600 |
| H | 0.09439600 | -2.32008300 | -1.55252200 |
| C | 0.28334200 | 1.37186100 | -0.19248800 |
| C | 1.31912600 | 1.88037900 | -0.99594300 |
| C | -0.45841200 | 2.26558200 | 0.60014700 |
| C | 1.61436000 | 3.23873600 | -0.99450300 |
| H | 1.89285900 | 1.20434700 | -1.62239900 |
| C | -0.17558800 | 3.62665700 | 0.58700500 |
| H | -1.25643300 | 1.88672900 | 1.23118800 |
| H | 2.41611100 | 3.61656800 | -1.62207000 |
| H | -0.75338000 | 4.30341100 | 1.20955900 |
| C | -1.35742300 | -0.46011300 | -0.17789000 |
| C | -2.32064800 | 0.17911100 | -0.97809600 |
| C | -1.75775700 | -1.54105000 | 0.62771700 |
| C | -3.64535500 | -0.24186400 | -0.96411600 |
| H | -2.02520800 | 1.00842100 | -1.61333600 |
| C | -3.07892600 | -1.97368000 | 0.62751500 |
| H | -1.02769300 | -2.03907800 | 1.25827800 |
| H | -4.37660600 | 0.26018600 | -1.59066800 |
| H | -3.37347300 | -2.80628200 | 1.25947700 |
| N | -0.00721700 | -0.01884000 | -0.18141200 |
| C | -4.05331400 | -1.32925200 | -0.16337800 |
| C | -5.41230000 | -1.75765500 | -0.14891500 |
| C | -6.57680500 | -2.11581600 | -0.13466500 |
| C | -7.94490600 | -2.51355000 | -0.11031000 |
| C | -8.30732600 | -3.86378600 | 0.00033900 |
| C | -8.97574100 | -1.54049600 | -0.19820000 |
| C | -9.65623400 | -4.23534900 | 0.02774200 |
| H | -7.54745800 | -4.63580800 | 0.06157700 |
| C | -10.30967200 | -1.90673200 | -0.16753500 |
| H | -8.70099500 | -0.49321700 | -0.28571500 |
| C | -10.68324200 | -3.26368500 | -0.04945400 |
| C | -10.00498000 | -5.66005600 | 0.12665500 |
| H | -11.08318800 | -1.14518000 | -0.23175100 |
| C | -12.05295100 | -3.69491200 | -0.01078900 |
| O | -11.36255100 | -5.95679600 | 0.16683500 |
| O | -9.22878400 | -6.58791600 | 0.17654000 |
| C | -12.35754800 | -5.01294600 | 0.10679500 |
| H | -12.84641700 | -2.96148300 | -0.09567700 |
| C | -13.70465100 | -5.60518400 | 0.16229600 |
| C | -13.89547900 | -6.96914800 | -0.12850600 |
| C | -14.82503700 | -4.82217900 | 0.50119900 |
| C | -15.17519500 | -7.52481500 | -0.10300600 |
| H | -13.03882400 | -7.58621100 | -0.37838100 |
| C | -16.10054900 | -5.38247300 | 0.52708200 |
| H | -14.69866000 | -3.77689000 | 0.76884900 |
| C | -16.28253900 | -6.73593300 | 0.22096100 |
| H | -15.30594800 | -8.57844300 | -0.33754600 |
| H | -16.95279500 | -4.76412500 | 0.79784600 |
| H | -17.27793300 | -7.17184200 | 0.24333500 |
| C | 3.16290200 | -2.85367700 | -0.14495800 |
| C | 4.22021700 | -3.80867800 | -0.12704600 |
| C | 5.12088200 | -4.62909800 | -0.10880400 |
| C | 6.15826600 | -5.60524900 | -0.08118800 |
| C | 7.50691100 | -5.23064100 | 0.00376800 |
| C | 5.84203500 | -6.98841400 | -0.13866300 |
| C | 8.51230900 | -6.20371000 | 0.03527300 |
| H | 7.78691700 | -4.18324900 | 0.04180200 |
| C | 6.83508800 | -7.95122100 | -0.10376500 |
| H | 4.79924100 | -7.28460000 | -0.20623600 |
| C | 8.19520700 | -7.58275900 | -0.01181900 |
| C | 9.91804300 | -5.78012800 | 0.10730800 |
| H | 6.57071500 | -9.00503600 | -0.14491300 |
| C | 9.26224900 | -8.54364300 | 0.02800500 |
| O | 10.86354900 | -6.79899300 | 0.14957400 |
| O | 10.32502500 | -4.64014000 | 0.13423600 |
| C | 10.55411400 | -8.13583800 | 0.11761800 |
| H | 9.03162100 | -9.60053700 | -0.03533000 |
| C | 11.74791300 | -8.99626300 | 0.16774300 |
| C | 13.01411300 | -8.47785000 | -0.16087400 |
| C | 11.64668700 | -10.35081800 | 0.53824700 |
| C | 14.14131700 | -9.30006000 | -0.14040400 |
| H | 13.10710000 | -7.43274700 | -0.43589600 |
| C | 12.77564400 | -11.16708500 | 0.55894600 |
| H | 10.68711700 | -10.76427600 | 0.83493100 |
| C | 14.02825500 | -10.64667400 | 0.21543100 |
| H | 15.11094100 | -8.88557700 | -0.40428100 |
| H | 12.67941300 | -12.20865900 | 0.85461300 |
| H | 14.90825000 | -11.28433600 | 0.23338300 |
| C | 0.87225700 | 4.14208500 | -0.20469700 |
| C | 1.17872100 | 5.53358700 | -0.19998300 |
| C | 1.44696200 | 6.72206200 | -0.18773200 |
| C | 1.78246100 | 8.10625300 | -0.16411800 |
| C | 0.79576700 | 9.09020100 | -0.00584200 |
| C | 3.13502700 | 8.51829700 | -0.29692200 |
| C | 1.14442000 | 10.44508200 | 0.02606600 |
| H | -0.24880900 | 8.81331600 | 0.09051400 |
| C | 3.48118000 | 9.85738400 | -0.26256000 |
| H | 3.90360300 | 7.76096300 | -0.42134900 |
| C | 2.49465800 | 10.85409300 | -0.09551600 |
| C | 0.08589400 | 11.45436600 | 0.17746600 |
| H | 4.52344600 | 10.15112400 | -0.36139100 |
| C | 2.80262800 | 12.25646600 | -0.05020200 |
| O | 0.50453900 | 12.77946000 | 0.21954100 |
| O | -1.10227000 | 11.24124100 | 0.27029500 |
| C | 1.81544900 | 13.17421600 | 0.11578300 |
| H | 3.82973300 | 12.58176100 | -0.16913600 |
| C | 1.97407500 | 14.63658700 | 0.18405900 |
| C | 0.87689100 | 15.48404300 | -0.05878600 |
| C | 3.22120600 | 15.21476300 | 0.48781900 |
| C | 1.03185900 | 16.87035500 | -0.01997900 |
| H | -0.09198800 | 15.05037400 | -0.28083400 |
| C | 3.37012800 | 16.59959800 | 0.52733000 |
| H | 4.07368900 | 14.58197700 | 0.71834700 |
| C | 2.27684200 | 17.43457500 | 0.26924400 |
| H | 0.17560500 | 17.51088000 | -0.21707600 |
| H | 4.33880800 | 17.02804500 | 0.77077300 |
| H | 2.39424000 | 18.51472700 | 0.30200400 |

## H-MON-MD-1

| | | | |
|---|---|---|---|
| C | 0.93189500 | -2.11571000 | 0.46386400 |
| C | 0.94507800 | -3.50527600 | 0.48419900 |
| C | 0.03629000 | -4.25281100 | -0.29525400 |
| C | -0.87814600 | -3.54666800 | -1.10631400 |
| C | -0.88290300 | -2.15712300 | -1.13660800 |
| C | 0.01784300 | -1.41981700 | -0.34736000 |
| H | 1.62951100 | -1.56034900 | 1.08335500 |
| H | 1.65214200 | -4.02794900 | 1.12170700 |
| H | -1.57898800 | -4.10172400 | -1.72295500 |
| H | -1.58860100 | -1.63306900 | -1.77410300 |
| C | 1.22067600 | 0.72536100 | -0.34736000 |
| C | 2.30957400 | 0.31394500 | -1.13660800 |
| C | 1.36631200 | 1.86490000 | 0.46386400 |
| C | 3.51057800 | 1.01283800 | -1.10631400 |
| H | 2.20858000 | -0.55923400 | -1.77410300 |
| C | 2.56311900 | 2.57110000 | 0.48419900 |
| H | 0.53654600 | 2.19137200 | 1.08335500 |
| C | 3.66489700 | 2.15783300 | -0.29525400 |
| H | 4.34169100 | 0.68341800 | -1.72295500 |
| H | 2.66223500 | 3.44477100 | 1.12170700 |
| C | -1.23851900 | 0.69445600 | -0.34736000 |
| C | -1.42667200 | 1.84317700 | -1.13660800 |
| C | -2.29820600 | 0.25081100 | 0.46386400 |
| C | -2.63243200 | 2.53383100 | -1.10631400 |
| H | -0.61997900 | 2.19230400 | -1.77410300 |
| C | -3.50819700 | 0.93417700 | 0.48419900 |
| H | -2.16605700 | -0.63102400 | 1.08335500 |
| C | -3.70118700 | 2.09497700 | -0.29525400 |
| H | -2.76270300 | 3.41830500 | -1.72295500 |
| H | -4.31437700 | 0.58317800 | 1.12170700 |
| N | 0.00000000 | 0.00000000 | -0.36643400 |
| C | 4.89618600 | 2.86964900 | -0.25533300 |
| C | 5.95255900 | 3.47660900 | -0.20677700 |
| C | 0.03709600 | -5.67504600 | -0.25533300 |
| C | 0.03455200 | -6.89337200 | -0.20677700 |
| C | -4.93328200 | 2.80539700 | -0.25533300 |
| C | -5.98711100 | 3.41676300 | -0.20677700 |
| C | 0.02766100 | -8.31430400 | -0.13664100 |
| C | -0.91454000 | -9.07170000 | -0.86682900 |
| C | 0.95906600 | -9.00141400 | 0.67267100 |
| C | -0.92823700 | -10.45792100 | -0.78659400 |
| H | -1.63618100 | -8.55679000 | -1.49414300 |
| C | 0.94548200 | -10.38754200 | 0.75229900 |
| H | 1.69026500 | -8.43200700 | 1.23884200 |
| C | 0.00000000 | -11.14455500 | 0.02637700 |
| H | -1.66021000 | -11.02737700 | -1.35171800 |
| H | 1.66640600 | -10.90250700 | 1.38036200 |
| C | -7.21422900 | 4.13319700 | -0.13664100 |
| C | -8.27498600 | 3.67013200 | 0.67267100 |
| C | -7.39905300 | 5.32786500 | -0.86682900 |
| C | -9.46861700 | 4.37495900 | 0.75229900 |
| H | -8.14746500 | 2.75219100 | 1.23884200 |
| C | -8.59270700 | 6.03283700 | -0.78659400 |
| H | -6.59230600 | 5.69537000 | -1.49414300 |
| C | -9.65146700 | 5.57227700 | 0.02637700 |
| H | -10.27505100 | 4.00810400 | 1.38036200 |
| H | -8.71988400 | 6.95147300 | -1.35171800 |
| C | 7.18656800 | 4.18110700 | -0.13664100 |
| C | 8.31359200 | 3.74383500 | -0.86682900 |
| C | 7.31592100 | 5.33128300 | 0.67267100 |
| C | 9.52094300 | 4.42508400 | -0.78659400 |
| H | 8.22848800 | 2.86142000 | -1.49414300 |
| C | 8.52313400 | 6.01258300 | 0.75229900 |
| H | 6.45719900 | 5.67981600 | 1.23884200 |
| C | 9.65146700 | 5.57227700 | 0.02637700 |
| H | 10.38009400 | 4.07590400 | -1.35171800 |
| H | 8.60864500 | 6.89440400 | 1.38036200 |
| C | -0.01990800 | -12.56491500 | 0.11679000 |

| | | | |
|---|---|---|---|
| C | -0.04011200 | -13.78050600 | 0.20028200 |
| C | 10.89149000 | 6.26521700 | 0.11679000 |
| C | 11.95432400 | 6.85551500 | 0.20028200 |
| C | -10.87158200 | 6.29969800 | 0.11679000 |
| C | -11.91421200 | 6.92499100 | 0.20028200 |
| C | -0.06536900 | -15.20233700 | 0.30291800 |
| C | 0.87977300 | -15.88136600 | 1.10088000 |
| C | -1.03773900 | -15.95543600 | -0.38888400 |
| C | 0.84935200 | -17.27116700 | 1.20142500 |
| H | 1.63098000 | -15.30769900 | 1.63607100 |
| C | -1.06076200 | -17.34495300 | -0.28224900 |
| H | -1.76839500 | -15.43889000 | -1.00457400 |
| C | -0.11942000 | -18.00837100 | 0.51201600 |
| H | 1.58366300 | -17.78100200 | 1.82003600 |
| H | -1.81607500 | -17.91218300 | -0.82034200 |
| H | -0.14054900 | -19.09198300 | 0.59321000 |
| C | -13.13292600 | 7.65778000 | 0.30291800 |
| C | -13.29894300 | 8.87642600 | -0.38888400 |
| C | -14.19355300 | 7.17877700 | 1.10088000 |
| C | -14.49078900 | 9.59112300 | -0.28224900 |
| H | -12.48627400 | 9.25092000 | -1.00457400 |
| C | -15.38194500 | 7.90002300 | 1.20142500 |
| H | -14.07234600 | 6.24137900 | 1.63607100 |
| C | -15.53599600 | 9.10760600 | 0.51201600 |
| H | -14.60436800 | 10.52885900 | -0.82034200 |
| H | -16.19063100 | 7.51900800 | 1.82003600 |
| H | -16.46386800 | 9.66771100 | 0.59321000 |
| C | 13.19829500 | 7.54455800 | 0.30291800 |
| C | 13.31378000 | 8.70258900 | 1.10088000 |
| C | 14.33668200 | 7.07901000 | -0.38888400 |
| C | 14.53259300 | 9.37114300 | 1.20142500 |
| H | 12.44136600 | 9.06632000 | 1.63607100 |
| C | 15.55155100 | 7.75383000 | -0.28224900 |
| H | 14.25466900 | 6.18797000 | -1.00457400 |
| C | 15.65541700 | 8.90076400 | 0.51201600 |
| H | 14.60696800 | 10.26199300 | 1.82003600 |
| H | 16.42044300 | 7.38332500 | -0.82034200 |
| H | 16.60441700 | 9.42427300 | 0.59321000 |

**Fig. S13** SEM, TEM, and $N_2$ adsorption-desorption isotherm curves of recovered H-IC-MON after five sensing cycles. (Refer to the experimental section in the ESI for detail recovery process)