Supporting Information

Stimuli-Response in Organic Cocrystals with Different Donor-Acceptors

Darya Khan Hassand[1*], Nawrooz Ali zahedi[1], Abdul Samad Hamid[1] and Mohammad Sharif Stanikzai[2]

[1]*Department of Chemistry, Education Faculty, Ghazni University, Ghazni 2301, Afghanistan.*

[2]*Department of Petrochemical and Gas industrial Engineering, Faulty of Chemical Industrial Engineering, Kabul Polytechnic University, Kabul 100, Afghanistan.*

*Corresponding authors:

dk.hassand@gmail.com (A. Prof. Darya khan Hassand)

Crystal growth and preparation of cocrystals

Acenaphthylene (AE), dithieno[3,2-b:2',3'-d]thiophene (DTT), and 3-aminopyridine (3-AP) were used as different donor molecules, while tetracyanobenzene (TCNB) served as the common acceptor, to prepare organic cocrystals in various solvents. Additionally, a mixture of AE (4.5 mg, 0.03 mmol), DTT (5.88 mg, 0.03 mmol), and 3-AP (2.82 mg, 0.03 mmol) was combined with TCNB (5.34 mg, 0.03 mmol) and gradually dissolved in 5 mL of tetrahydrofuran (THF), ethyl acetate (EA), or dichloromethane (DCM). The cocrystals were then prepared in a 1:1 stoichiometric ratio of donor to acceptor using the solvent evaporation method. Specifically, the solvent evaporation method usually dissolves a certain proportion of the reaction mixture solution in a bottle and then stores it in a dark environment and at room temperature. The solute gradually reaches a saturated state in the solution, and forms cocrystal nuclei driven by intermolecular interactions and gradually precipitates out after a few days. This method usually requires donor and acceptor molecules to have similar solubility in the same solvent and it is highly dependent on factors such as solvent, concentration, temperature, and other external conditions.

However, for the crystal structure analyses and more characterization, we used powder X-ray diffraction (PXRD) and optical microscope (OM). For the studies and determination of photophysical chemical properties, we used solid-state samples of the AETC, DTTC and 3-ATC cocrystals with different instrument measurements such as UV-vis, photoluminescence (PL), thermal gravimetric analysis (TGA), differential scanning calorimetry (DSC) and Fourier-transform infrared (FTIR).

Table S1 The single-crystal data of AETC, DTTC and 3-ATC cocrystals.

Chemical formula	**$C_{22}H_{10}N_4$**	**$C_{18}H_6N_4S_3$**	**$C_{15}H_8N_6$**

CCDC	2287450	2287435	2347457
Formation weight	330.34	374.45	272.27
Temperature /K	160/K	160/K	160 K
Wavelength	1.54184	1.54184	1.54184
Space group	P-1	P-1	C2/c
Crystal system	triclinic	triclinic	monoclinic
a/Å	6.7303(3)	7.2203(2)	7.2422(1)
b/Å	8.0525(3)	9.1337((2)	15.4771(1)
c/Å	15.2393(5)	12.6626(3)	11.6557(1)
α/°	94.320(3)	92.056(2)	90
β/°	99.821(3)	94.846(2)	92.677(1)
γ/°	97.783(3)	95.128(2)	90
Volume/ Å3	802.20 (5)	827.97(5)	1305.04(2)
Z	2	2	4
ρ_{calc}g/cm^3	1.368	1.502	1.386
μ /mm−1	0.667	4.161	0.733
F(000)	340.0	380.0	560.0
R_{int}	0.0677	0.0462	0.0291
Goof	1.072	1.061	1.115
Final R indexes [I>=2σ (I)]	wR_1 = 0.0677, wR_2 = 0.2146	wR_1 = 0.0462, wR_2 = 0.1390	wR1 = 0.0291, wR2 = 0.0824

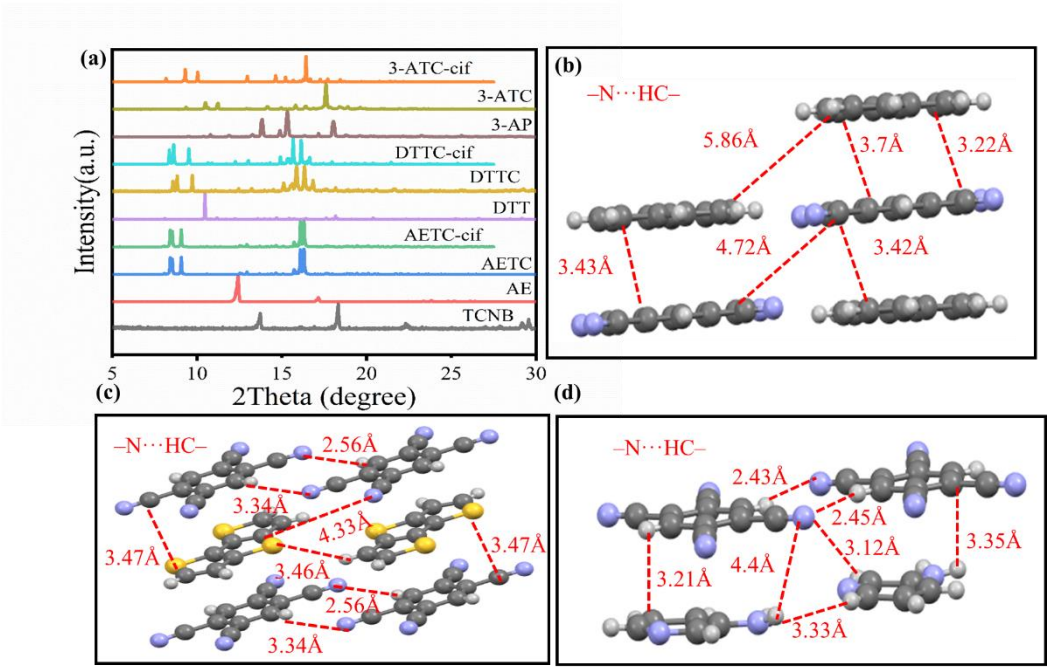

Fig. S1, a) PXRD, and b-d the distance in the π-π direction of AETC, DTTC and 3-ATC organic cocrystal.

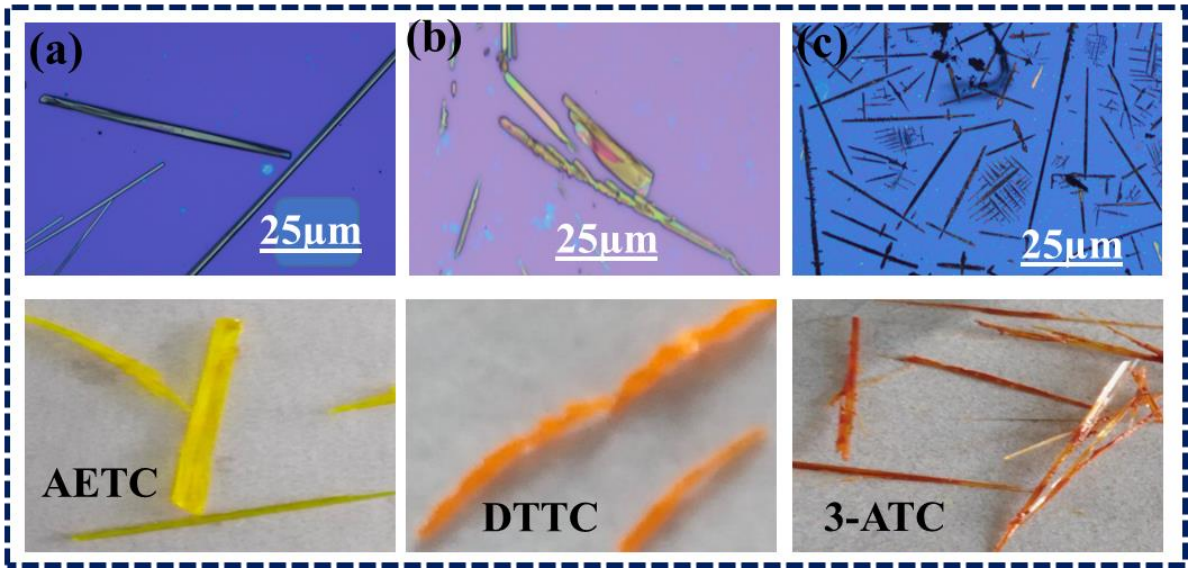

Fig. S2, a-c) The OM, images of AETC, DTTC and 3-ATC organic cocrystal shown 2D for AETC, 1D DTTC and 3-ATC organic cocrystal.

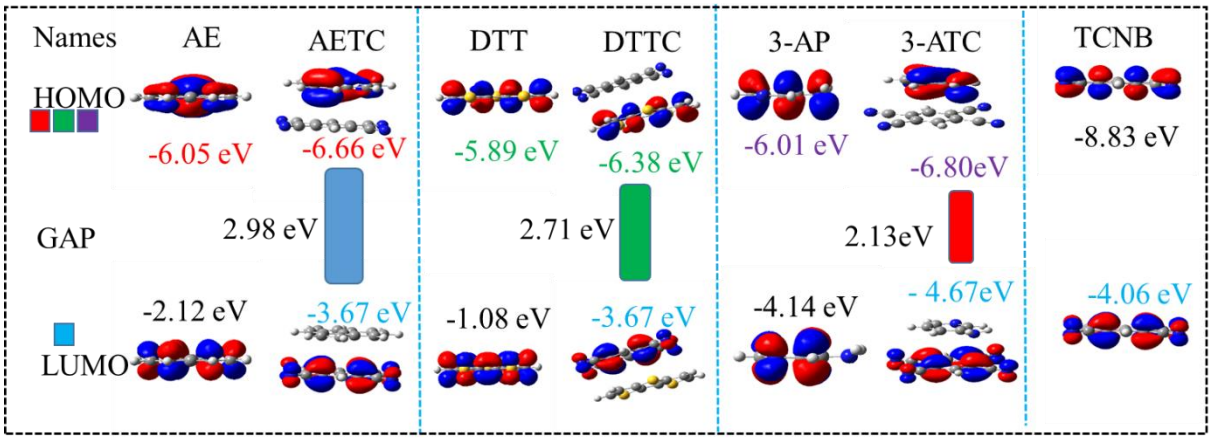

Fig. S3), the band gap of AETC, DTTC and 3-ATC organic cocrystals and host materials AE,DTT and 3-AP.

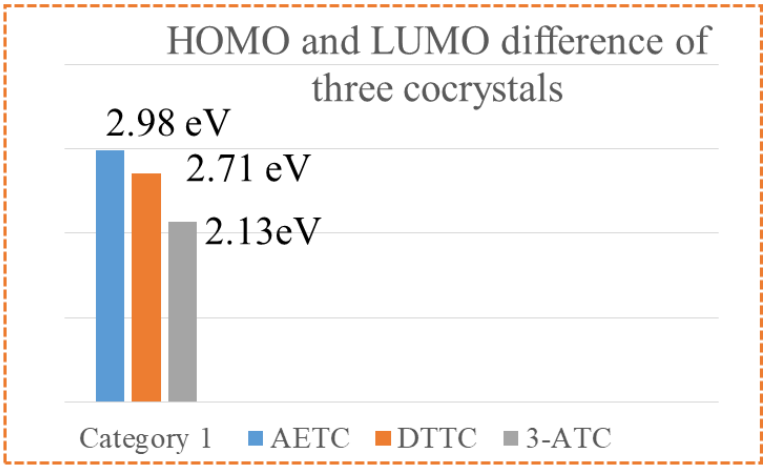

Fig. S4), the band gap of AETC, DTTC and 3-ATC organic cocrystals.

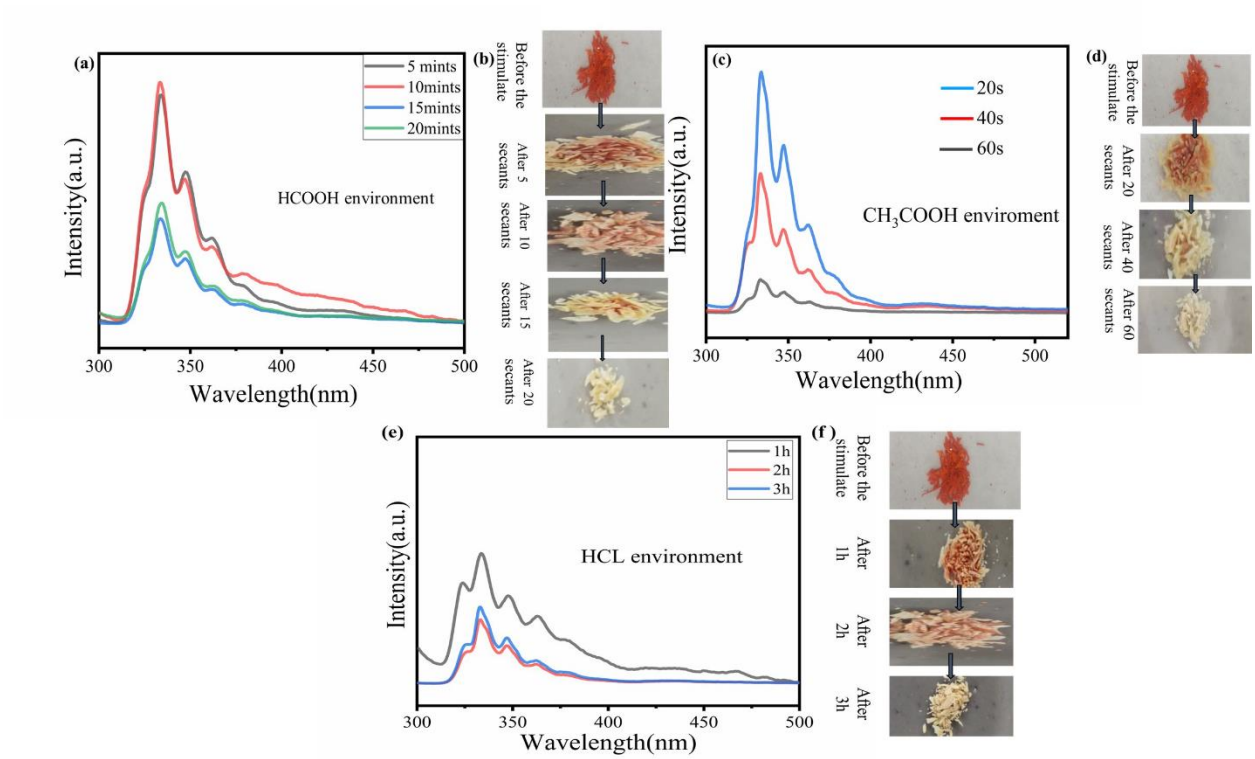

Fig. S5. a-b) Intensities of fluorescence and color change in formic acid environment,c-d) in acetic acid environment, e-f) and in hydrochloric acid environment.

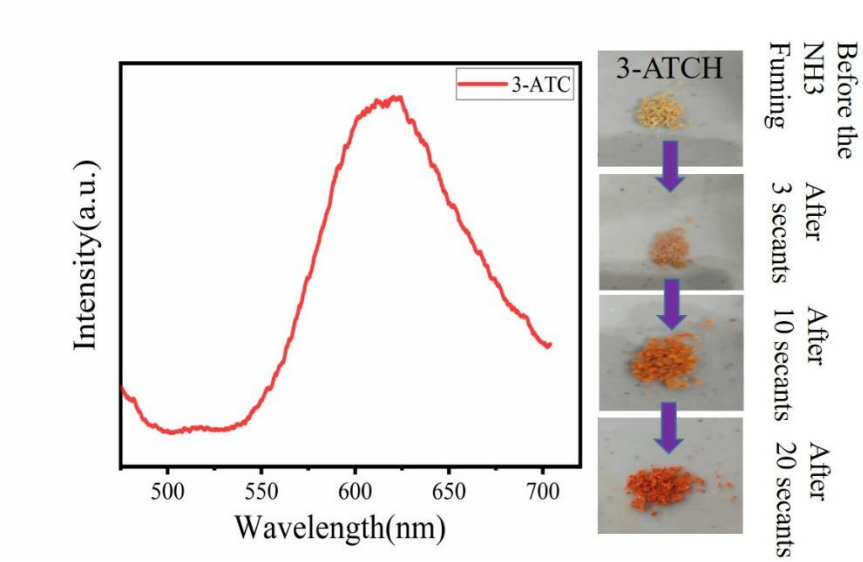

Fig. S6. Intensities of fluorescence and color recycal in NH_3 environment.