Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Inorganic-organic hybrid sorbent for aromatic desulfurization of hydrocarbons: Regenerative adsorption based on charge-transfer complex

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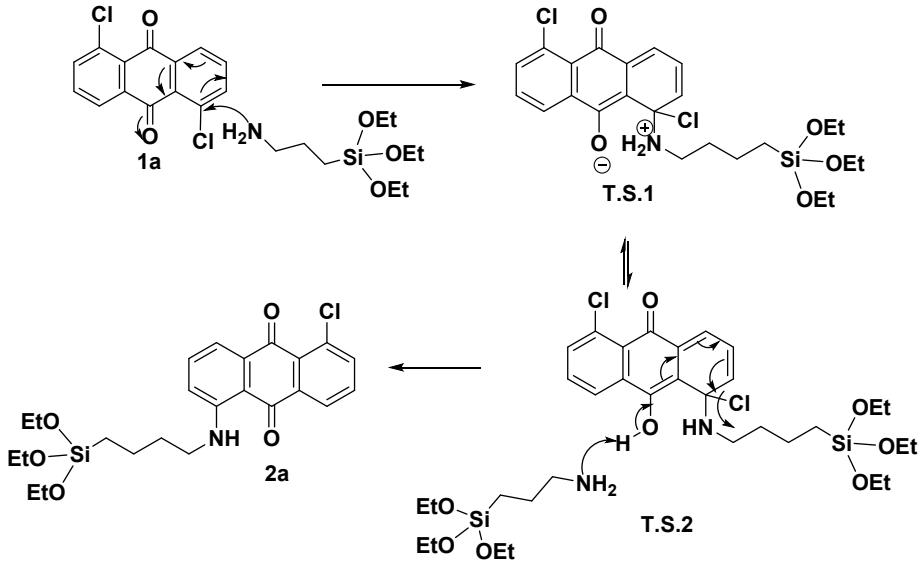
Table S1. X-ray crystallographic data for **2d**

Parameter	**2d**
Empirical formula	$C_{20}H_{22}ClNO_5Si$
Formula weight	419.93
Crystal size (mm)	0.30 × 0.20 × 0.01
Crystal color	Red/Plate
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal system	monoclinic
Space group	*P* $2_1/c$
a (Å)	7.145(5)
b(Å)	35.461(16)
c (Å)	10.506(7)
α (°)	90.00
β (°)	133.00(11)
γ (°)	90.00
v(Å^3)	1947(2)
Z	4
Absorption coefficient (mm^{-1})	0.290
Calculated density (mg/m^3)	1.433
F(000)	880
θ Range for data	2.89–25.00
Reflections collected	16740
Unique reflections [R(int)]	0.1717
Data/restrains/parameters	3434/126/254
Goodness–of–fit on F2	1.111
Final R indices [I>2σ(I)]	R1 = 0.1825 wR2 = 0.4127



Scheme S1. The possible mechanism for functionalization of 1-chloro-5-((3-(triethoxysilyl)propyl)amino)anthracene-9,10-dione (**2a**, AQ-Cl).

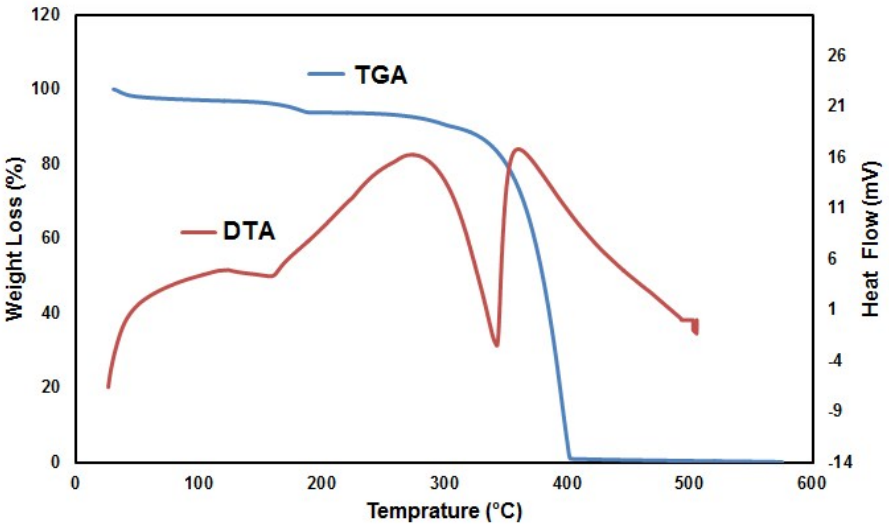


Figure S1. TGA and DTA curves of 1,5-dichloro-4,8-dinitroanthraquinone (**1c**).

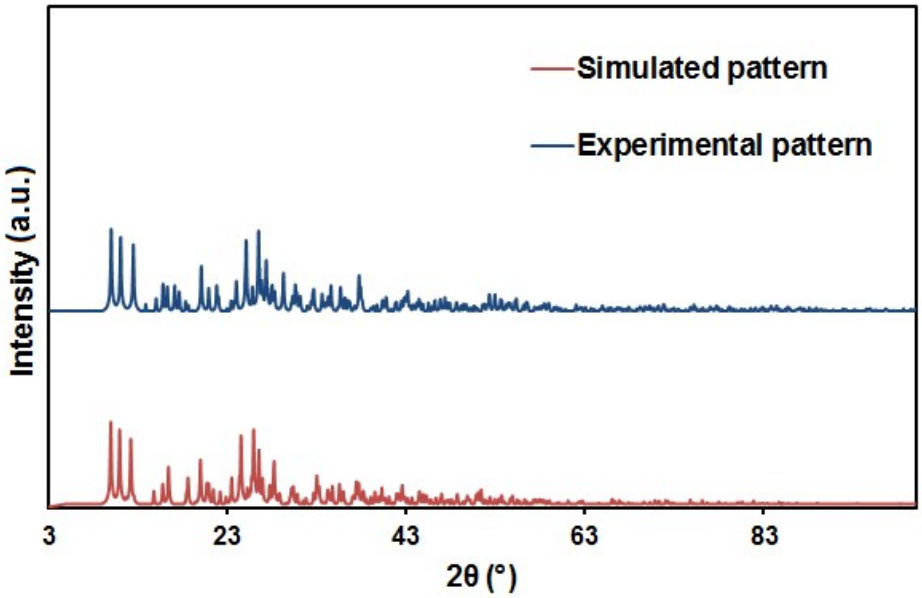


Figure S2. Experimental (blue) and simulated (red) powder X-ray diffraction pattern (PXRD) for the charge-transfer complex.

Table S2. X-ray Crystallographic data for CTC

Parameter	**CTC**
Empirical formula	$C_{28}H_{16}C_{l2}N_2O_6S$
Formula weight	579.40
Crystal size (mm)	0.35× 0.20 × 0.10
Crystal color	Orange/needle
Temperature (K)	298(2)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	*P cnb*
a (Å)	10.6317(8)
b(Å)	14.5110(10)
c (Å)	16.1526(9)
α (˚)	90.00
β (˚)	90.00
γ (˚)	90.00
v($Å^3$)	2492.0(3)
Z	4
Absorption coefficient (mm^{-1})	0.394
Calculated density (mg/m^3)	1.544
F(000)	1184
θ Range for data	2.29 –29.19
Reflections collected	11048
Unique reflections [R(int)]	0.0569
Data/restrains/parameters	3355/0/177
Goodness–of–fit on F2	0.979
Final R indices [I>2σ(I)]	R1 = 0.0610 wR2 = 0.1423

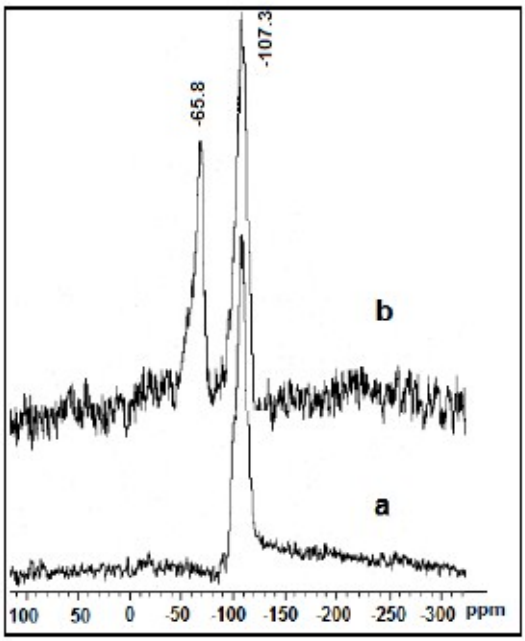


Figure S3. ^{29}Si CP/MAS NMR spectra of a) Si-MCM-41, and, b) AQ-NO_2@Si-MCM-41.

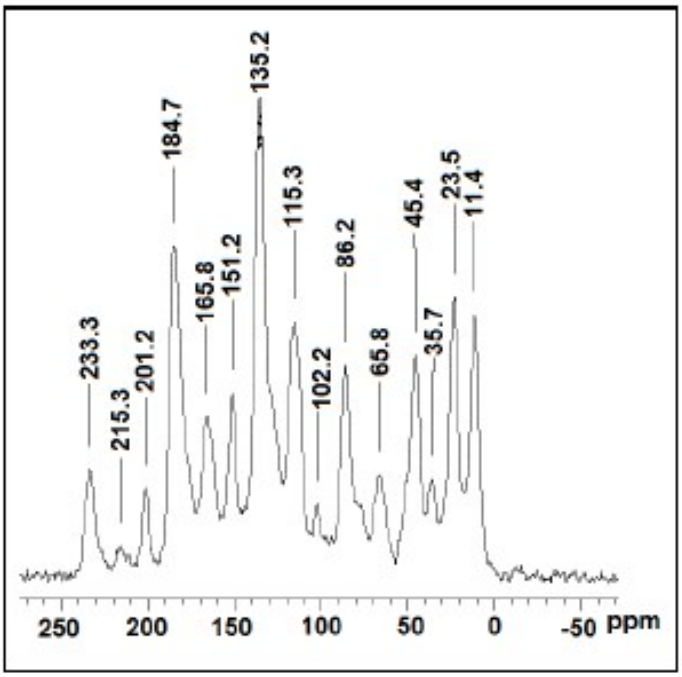


Figure S4. ^{13}C CP/MAS NMR spectrum of AQ-NO_2@Si-MCM-41.

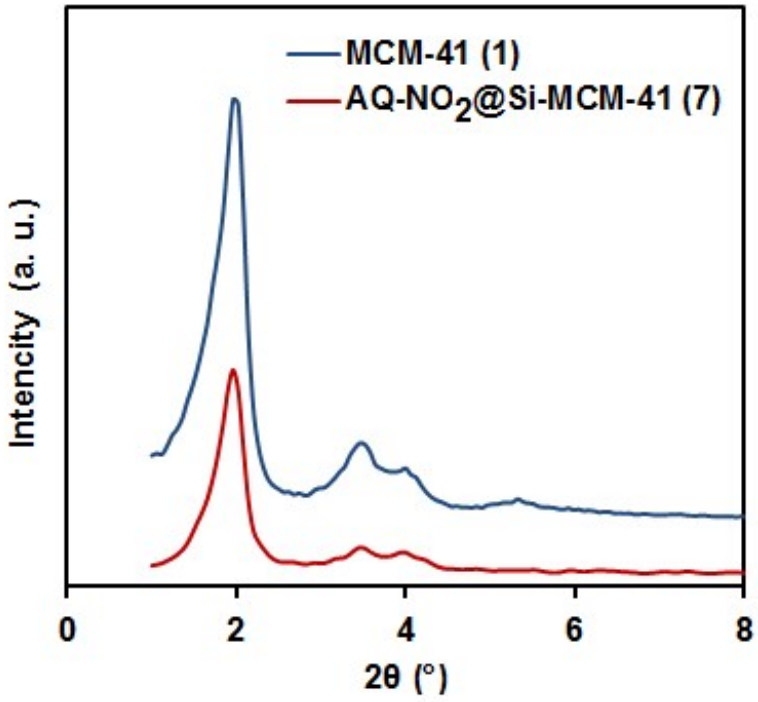


Figure S5. X-ray diffraction patterns of Si-MCM-41 and AQ-NO_2@Si-MCM-41.

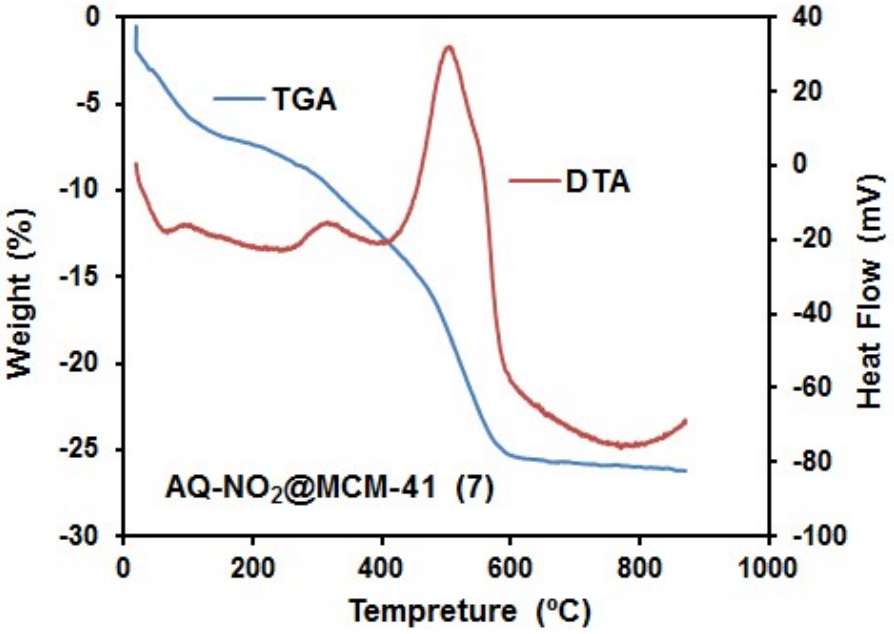


Figure S6. TGA-DTA curves of AQ-NO_2@Si-MCM-41.

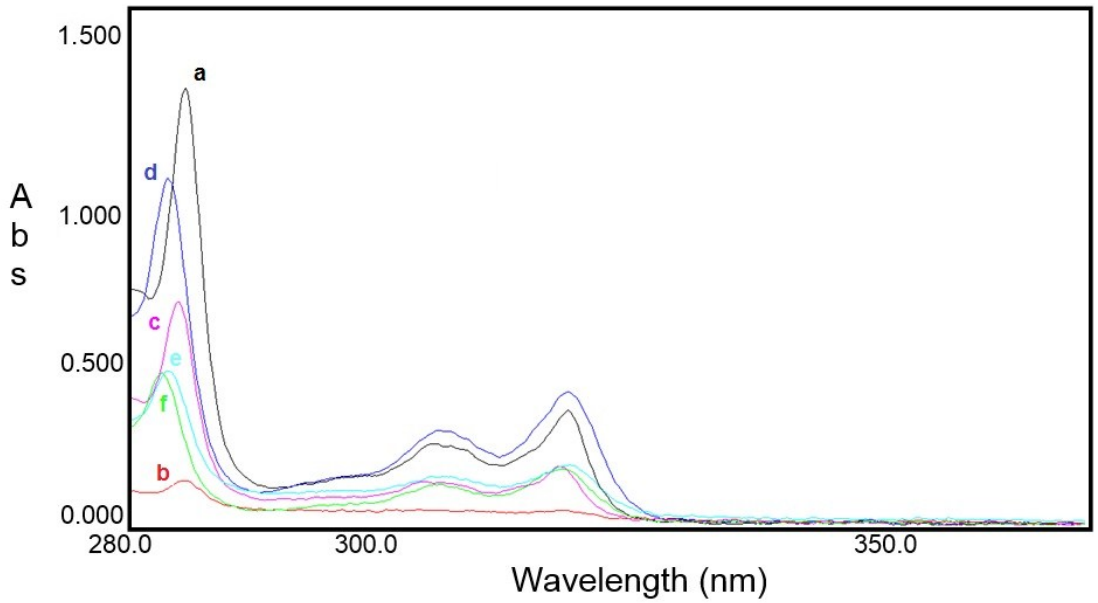


Figure S7. UV-Vis spectrum of DBT before adsorption (a), after adsorption on AQ-NO_2@Si-MCM-41 (9, 7) (b) (c), DBT before adsorption (d), and after adsorption on AQ-NO_2@Si-MCM-41 (10, 8) (e) (f).

Figure S7 shows the UV-Vis absorption spectrum of a DBT and 4,6-DMDBT solution with an initial concentration of 20 mg/L (0.10 mM) before and after contact with the AQ-NO_2@Si-MCM-48 at different conditions. The intensities of the distinct peak of DBT and 4,6-DMDBT at 286 and at 284 nm respectively dropped significantly in the UV-Vis spectrum of the 4,6-DMDBT solution after contact with sorbent.

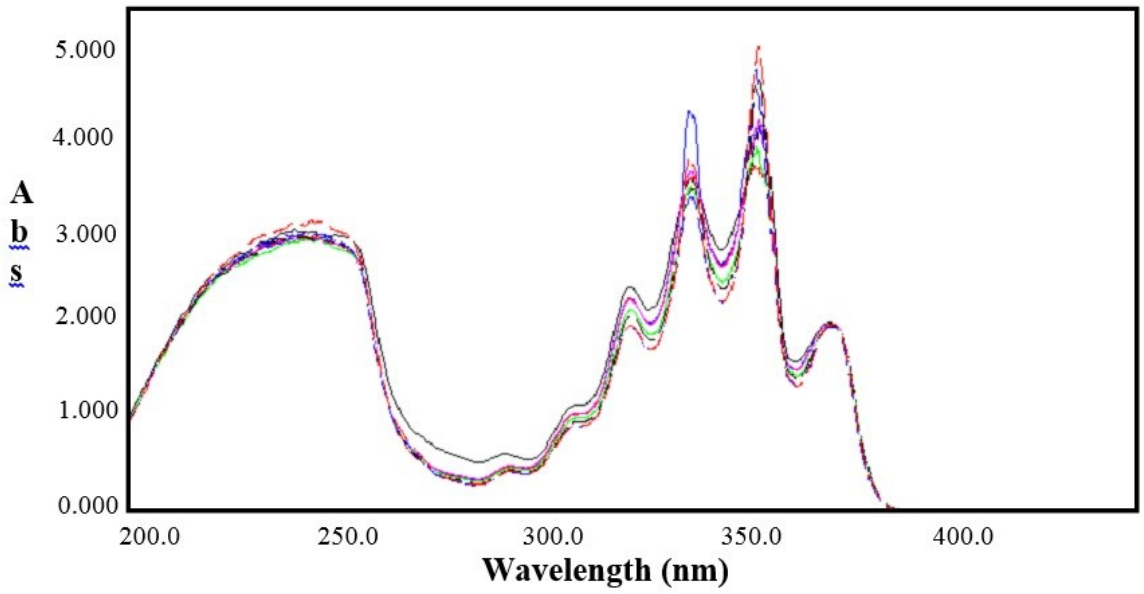


Figure S8. UV-Vis spectrum of anthracene before and after contact with AQ-NO_2@Si-MCM-41 for two days at room temperature.

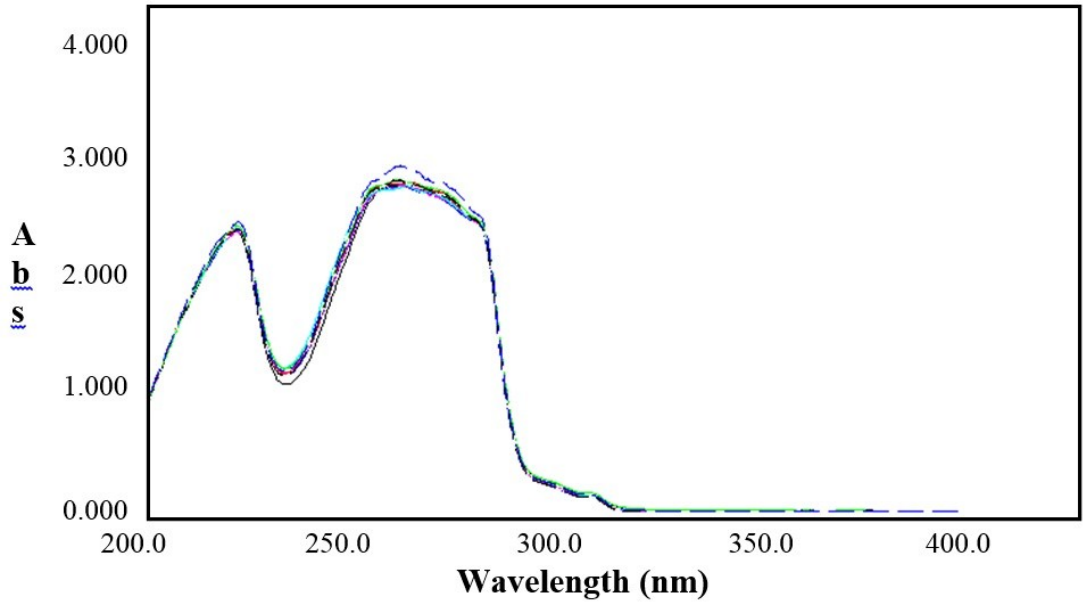


Figure S9. UV-Vis spectrum of naphthalene before and after contact with AQ-NO_2@Si-MCM-41.

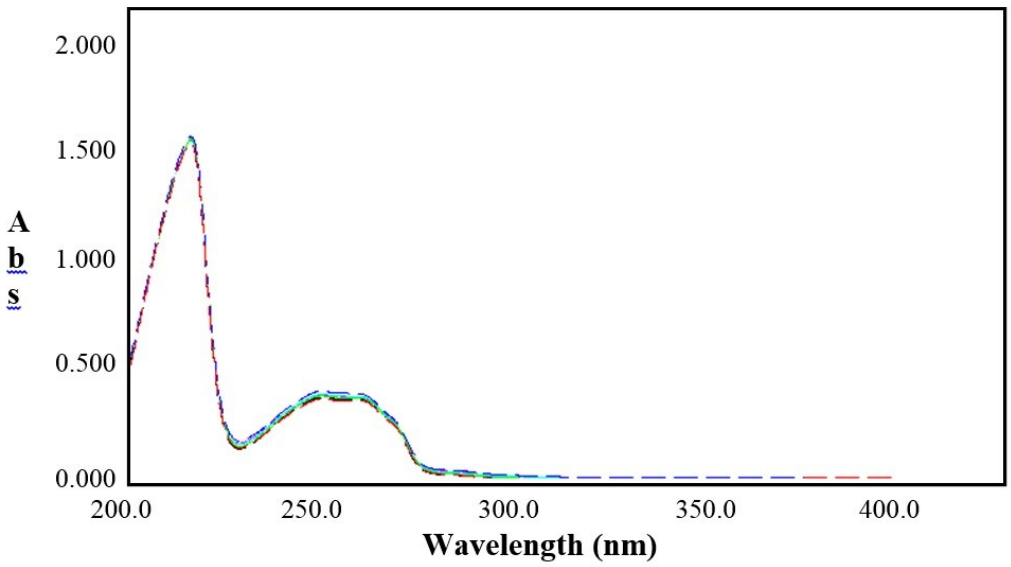


Figure S10. UV-Vis spectrum of xylene before and after contact with AQ-NO_2@Si-MCM-41.

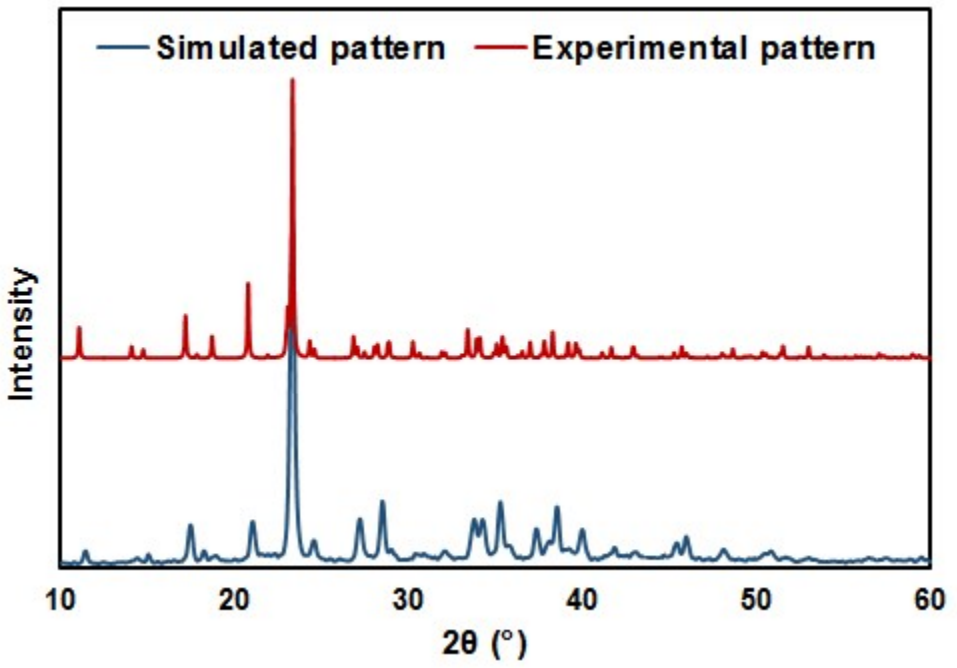


Figure S11. Simulated (red) and experimental (blue) powder X-ray diffraction pattern (PXRD) of 1,5-dichloro-4,8-dinitroanthraquinone (**1c**) generated after heating CTC to 200 °C under reduced pressure.