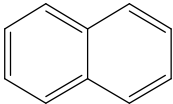
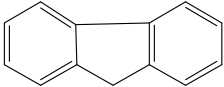
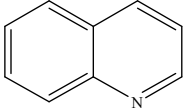
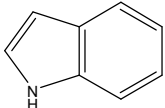
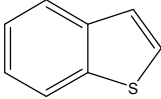
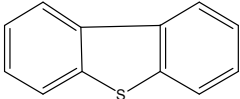


Adsorption of Heterocyclic Sulfur and Nitrogen Compounds in Liquid Hydrocarbons on Activated Carbons Modified by Oxidation: Capacity, Selectivity and Mechanism

Dong Qu^a, Xiao Feng^a, Na Li^{a*}, Xiaoliang Ma^{b*}, Chao Shang^a, Xiao Dong Chen^a

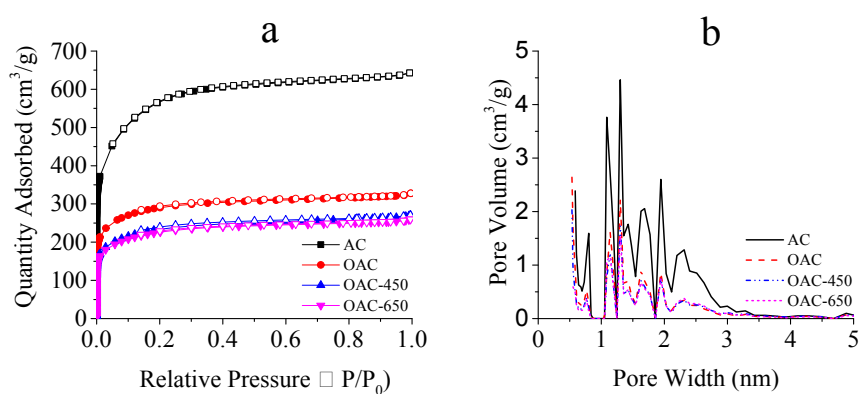
Table S1. Some properties of adsorbates.

Adsorbate	Chemical structure	Molar mass (g/mol)	Charge on S/N (a.u.)	Number of C (sp ²) atoms	Dipole magnitude (D)	Diameter (Å)
Na		128	-	10	0.000	7.2
Fl		166	-	12	0.370	7.5
Qu		129	-0.059	9	1.844	7.1
In		117	+0.288	10	2.004	7.2
BT		134	+0.261	9	1.090	6.9
DBT		184	+0.242	13	1.362	8.0

^acritical diameter is defined as “the smallest diameter of a cylinder through which the molecule can pass without distortion”. Na: naphthalene; Fl: fluorene; Qu: quinoline; In: indole; BT: benzothiophene; DBT: dibenzothiophene.

Table S2. Composition of model fuel with different compounds.

Chemicals	Purity	Molar concentration	Concentration	
	(wt %)	($\mu\text{mol/g}$)	(wt %)	S or N (ppmw)
Na	99	10	0.128	-
Fl	98	10	0.166	-
Qu	98	10	0.129	140
In	99	10	0.117	140
BT	98	10	0.134	320
DBT	99	10	0.184	320
Heptane	97	-	99.142	-
Total	-	-	100	-

**Figure S1.** a) Nitrogen adsorption-desorption isotherms and b) pore size distribution of the original and modified activated carbons.

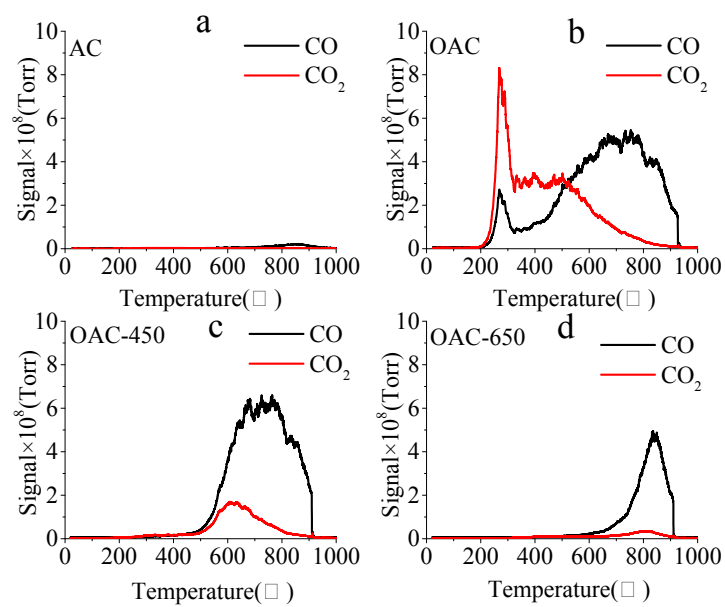


Figure S2. TPD-CO and TPD-CO₂ profiles of different activated carbons.