## Electronic supplementary information (ESI)

## Research on the reaction mechanistic and molecular stacking of acid

## catalyzed naphthalene to prepare mesophase pitch

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Carbon atom number	12	13	14	15	16	17	18
Carbon charge	-0.046	-0.038	-0.057	-0.049	-0.044	-0.045	-0.061
Protonation energy barrier (kJ/mol)	65.37	73.50	48.38	68.12	70.03	70.85	59.54
reaction heat(kJ/mol)	58.85	46.94	38.11	42.80	51.75	65.47	27.09
Carbon cation number	G1	G2	G3	G4	G5	G6	G7
Carbocation structure	H H H	H H H	H H H	H H	H H H	H H H	H H H
Type of electrophilic addition reaction	Intermolecular	Intermolecular	Intermolecular	Intermolecular	Intermolecular	Intramolecular	Intermolecular
Carbon cation number	H1	H2	H3	H4	H5	Ι	H6
Electrophilic addition product	H H H		H H H H			H H H H	H H H H H H H H

Table S1 Protonation of D molecules and electrophilic addition reactions of different carbocations





Reaction coordinate

Fig. S1 (a) Detailed generation reaction process of molecule  $C_{50}H_{40}$ . (b)Relative energy of substances in the generation reaction process of molecule  $C_{50}H_{40}$ .





## **Reaction coordinate**

Fig. S2 (a) Detailed reaction pathway of molecule  $C_{50}H_{28}$ . (b)Relative energy of substances in the generation reaction process of molecule  $C_{50}H_{28}$ .