Electronic Supplementary Material

Regulation of radicals by hydrogen donor solvent in direct coal liquefaction

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Supporting information:

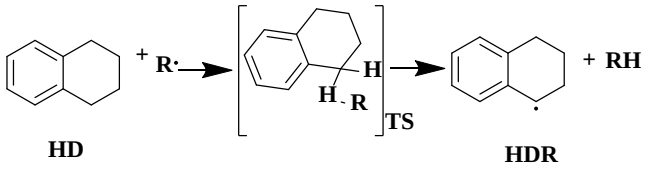

Figure S1 H extracted by radicals from hydrogen donor solvent (·, radicals; TS, transition state) [7]

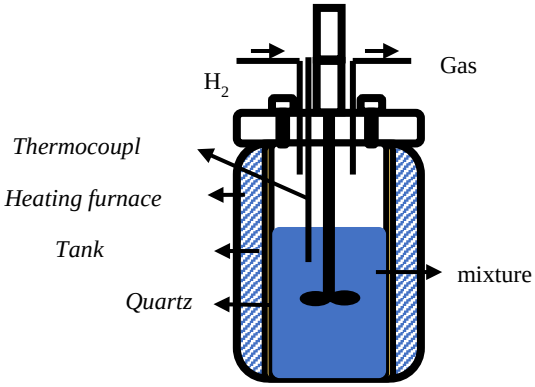

Figure S2 A diagram of reaction device

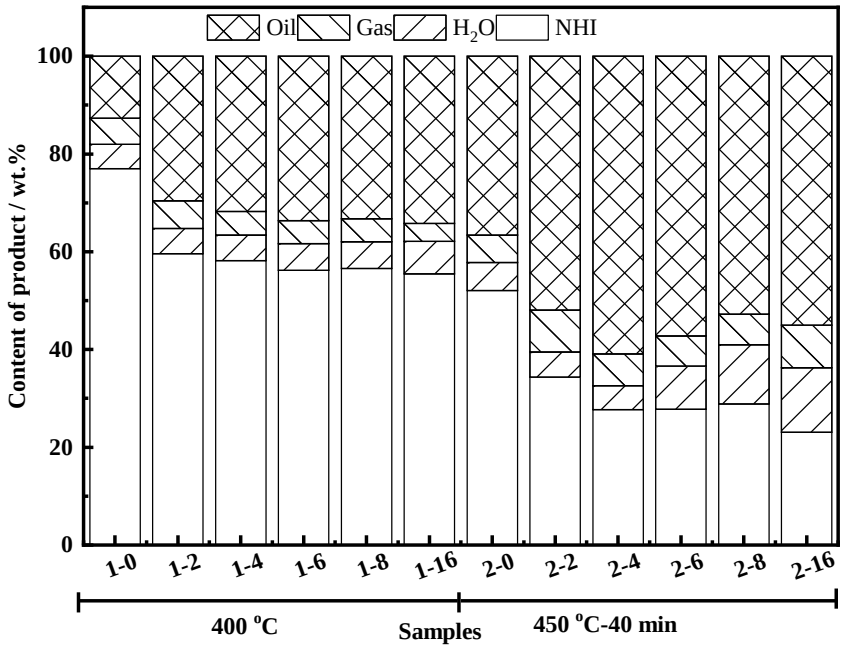

Figure S3. Product distribution of direct coal liquefaction with different ratios of tetralin to coal (T = 400 ºC /450 ºC-40 min; P = 6 MPa H_2; s-n: series number-m_{THN}/m_{coal}).

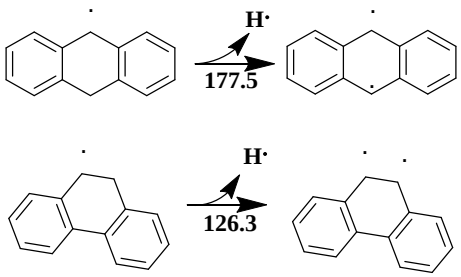

Figure S4 Dehydrogenation of 9,10-dihydroanthracene and 9,10-dihydrophenanthrene scheme **(**·, radicals; **BDE**, kJ/mol; TS, transition state, T=450 °C**)**

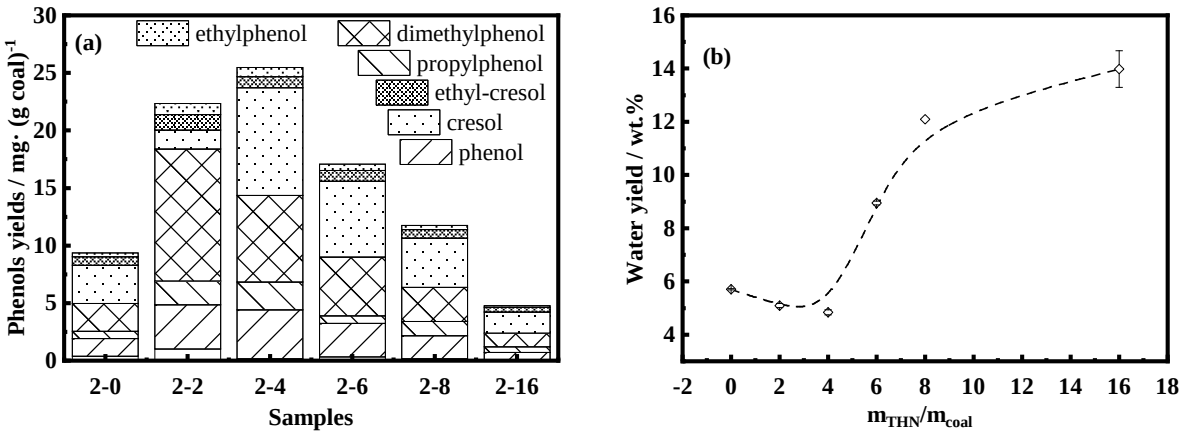

Figure S5. Phenolic compounds and water yield with different ratios of tetralin to coal (Reaction condition: T = 450 °C, lasting for 40 min; a: phenols in oil; b: water yield)

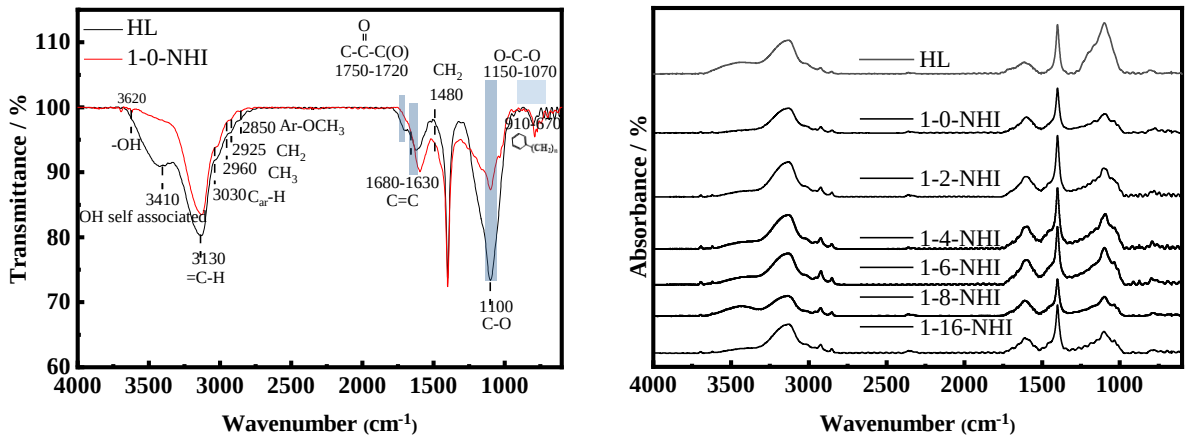

Figure S6. FT-IR spectra of **NHI** with different ratios of tetralin to coal at 400 °C

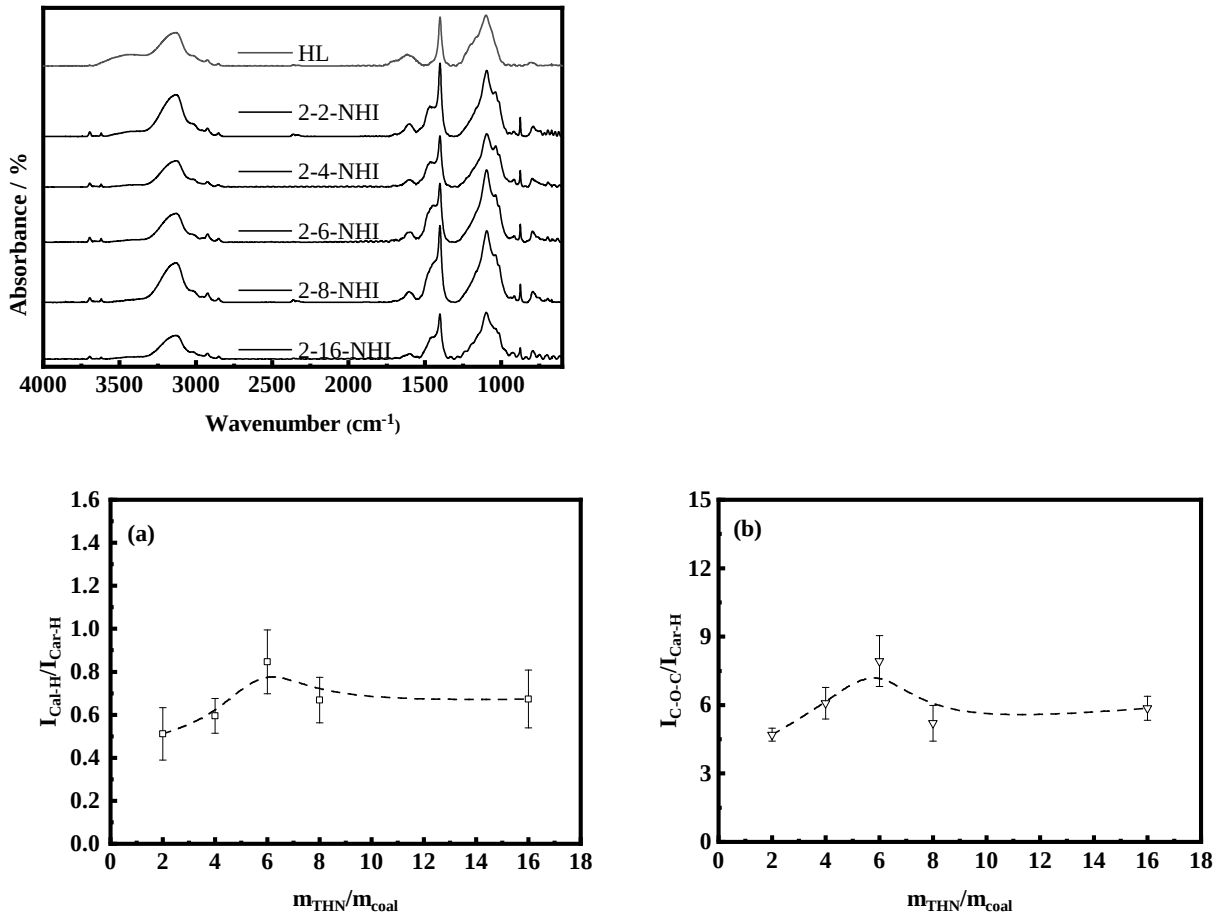

Figure S7. FT-IR spectra of **NHI** with different ratios of tetralin to coal at 450 °C lasting for 40 min

Table S1a. Materials balance at 400 ºC

	Reactant / g				Product /g			Balance /*wt*%
400	lignite	THN	MN	H_2	mixture	gas [a)]	other [b)]	
0	4.28	0.00	17.61	0.16	20.09	0.20	0.66	95.04
2	4.43	8.75	8.76	0.15	20.34	0.24	0.78	96.69
4	4.56	18.00	0.00	0.15	20.76	0.19	0.82	95.79
6	3.09	18.04	0.00	0.15	19.07	0.13	0.72	93.68
8	2.29	18.54	0.00	0.15	18.76	0.10	0.89	94.14
16	1.24	19.51	0.00	0.16	19.59	0.02	0.67	96.96

Table S1b. Materials balance at 450 ºC lasting for 40 min.

	Reactant / g				Product / g			Balance / *wt*%
450-40	lignite	THN	MN	H_2	mixture	gas [a)]	other [b)]	
0	4.00	0.00	16.04	0.15	18.46	0.21	0.47	94.77
2	4.06	8.00	8.03	0.15	17.68	0.35	0.66	92.30
4	3.99	16.11	0.00	0.15	18.27	0.26	0.47	93.79
6	2.54	15.03	0.00	0.15	16.37	0.16	0.39	95.47
8	1.92	15.02	0.00	0.16	15.48	0.12	0.59	94.71
16	1.29	20.00	0.00	0.15	20.53	0.11	0.55	98.83

Notes: a) including H_2, CH_4, CO and CO_2 detected by GC; b) indicates that the product sticks to the reactor wall and is wiped with absorbent cotton.