

Table of peak positions of functional groups

Functional group	Peak /cm ⁻¹	Peak position attribution	Proportion of peak area before nFeS-lignite reaction	Proportion of peak area after nFeS-lignite reaction	Proportion of peak area before lignite reaction	Proportion of peak area after lignite reaction
Aromatic hydrocarbon	900	Benzene ring disubstitution	72.16	61.64	72.26	54.66
	~	Benzene ring trisubstitution	17.26	13.97	23.52	40.7
	700	Benzene ring tetra substitution	10.58	24.62	4.22	4.65
Oxygenated functional group		Alkyl ethers	6.15	1.59	2.81	2.76
		C-O phenols, ethers	28.81	21.51	21.41	22.39
	1800	C-O in aryl ethers	6.51	8.41	8.73	8.75
	~	Aymmetric Ar-CH ₃	8.86	11.76	11.9	11.95
	1000	Asymmetric -CH ₃ , -CH ₂	8.22	9.91	9.25	9.7
Aliphatic hydrocarbon		Aromatic C=C	34.43	39.02	38.82	36.34
		-COOH	7.02	7.79	7.09	8.10
	3000	Symmetric R ₂ CH ₂	19.09	34.23	23.81	28.72
	~	R ₃ CH	35.45	22.6	18.21	19.24
	2800	Asymmetric R ₂ CH ₂	31.66	29.86	42.41	36.88
Hydroxyl		Asymmetric RCH ₃	13.81	13.32	15.58	15.16
	3600	OH-N	6.89	6.18	9.8	14.14
	~	Ring hydroxyl	16.13	24.86	19.8	25.57
	3000	Phenol OH	48.73	35.94	46.83	34.1
		OH-π	28.26	33.02	23.57	26.2