Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The involvement of carbon-centered radicals in the aging process of coals under atmospheric conditions: An EPR study

Tze'ela Taub[1], Sharon Ruthstein[2, #], and Haim Cohen[1, 3, #]

[1]Dept. of Chemical Sciences, Ariel University, Ariel, Israel

[2]Chemistry Dept., Faculty of Exact Science, Bar Ilan University, Ramat Gan, Israel

[3]Chemistry Dept., Ben-Gurion University, Be'er Sheva, Israel

[#]Corresponding authors

Supportive Information

Table S1: g-values of stable radicals in BA coal. The effect of aging and gas atmosphere.

Coal oxidation time	g_1*				g_2**			
	air	vacuum	CO_2	He	air	vacuum	CO_2	He
fresh	2.0032	2.0030	2.0032	2.0031	2.0029	2.0029	2.0027	2.0027
2w	2.0032	2.0033	2.0032	2.0031	2.0029	2.0028	2.0029	2.0027
5w	2.0032	2.0031	2.0034	2.0032	2.0029	2.0028	2.0027	2.0029
10w	2.0032	2.0033	2.0032	2.0031	2.0029	2.0028	2.0028	2.0027
22w	2.0032	2.0033	2.0033	2.0031	2.0029	2.0029	2.0030	2.0027

*g_1 for the carbon-centered radical, **g_2 for the aliphatic carbon-centered radical
Evaluation error: ±0.0001

Table S2: g-values of stable radicals in HA coal. The effect of aging and gas atmosphere.

Coal oxidation time	g_1*				g_2**			
	air	vacuum	CO_2	He	air	vacuum	CO_2	He
fresh	2.0042	2.0043	2.0039	2.0041	2.0028	2.0028	2.0029	2.0029
2w	2.0039	2.0039	2.0039	2.0039	2.0029	2.0027	2.0029	2.0030
5w	2.0039	2.0040	2.0039	2.0040	2.0029	2.0029	2.0030	2.0031
10w	2.0039	2.0037	2.0037	2.0038	2.0029	2.0030	2.0028	2.0029
22w	2.0036	2.0037	2.0036	2.0037	2.0027	2.0029	2.0029	2.0030

*Carbon centered with an adjacent oxygen atom, **g_2 for the aliphatic carbon-centered radical
Evaluation error: ±0.0001

The extent of each species is derived from the simulations taking into account the line width. The linewidth depends on the amount of radicals and the proximity between them as well as mobility of the electron spins. Since each sample is different, the linewidth is varied. Figure S1 shows a fitting of each specie alone: species 1 and species 2 and its fitting.

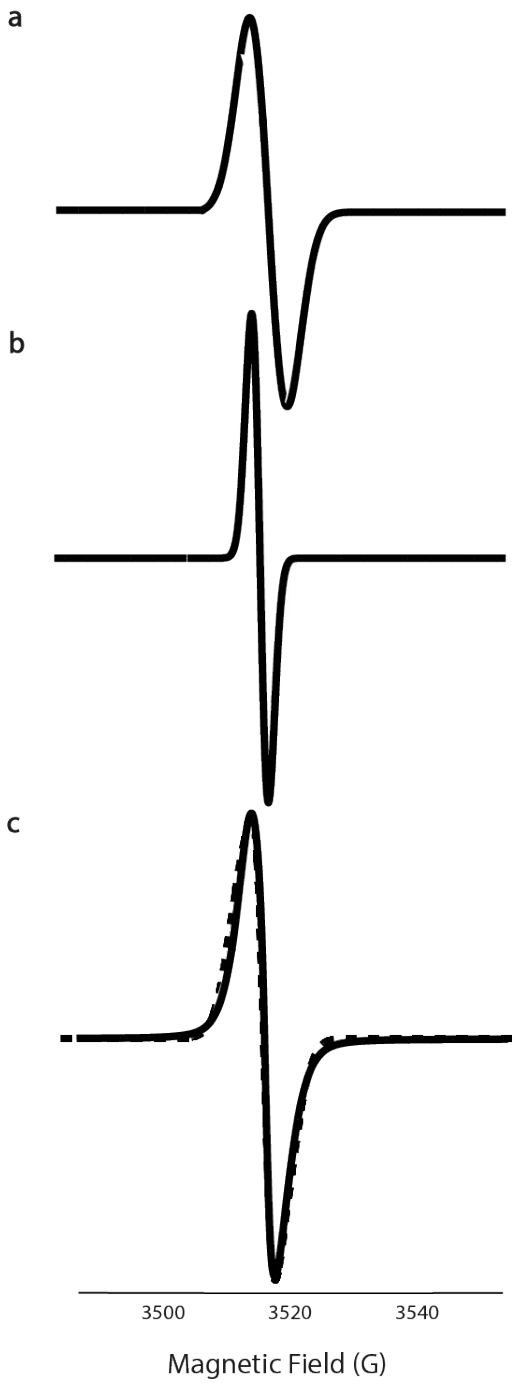

Figure S1: An example of EPR spectra (lorentzian line) of (a) spec 1 as 100% (b) spec 2 as 100% (c) a fitting of two lorentzian lines (dashed) to the experimental spectra (solid), where the distribution is: spec 1 – 90%, spec 2 – 10%.