Supporting Information for the Manuscript:

Quantitative Analysis of Lewis Acid Centers of γ-Alumina by Using EPR of the Adsorbed Anthraquinone as a Probe Molecule: Comparison with the Pyridine, Carbon Monoxide IR and TPD of Ammonia

Marat R. Gafurov[a†], Ildar N. Mukhambetov[b], Boris V. Yavkin[a], Georgy V. Mamin[a], Alexander A. Lamberov[b], Sergei B. Orlinskii[a]

[a] Kazan Federal University, Institute of Physics, 420008 Kazan

[b] Kazan Federal University, A. Butlerov Institute of Chemistry, 420008 Kazan

[†]to whom correspondence should be addressed

e-mail: marat.gafurov@kpfu.ru

1. Continuous-wave (CW) EPR experiments and deconvolution of CW-EPR spectra

For the correct quantitative analysis of the whole concentration range of AQ-alumina samples a proper choice of the registration parameters (first of all of incident microwave power) is in need. Figure S1 demonstrates the changes of the parameters of EPR curves with the microwave (MW) power. As it can be seen, at high values of MW power the EPR spectra broaden and lose their resolved structure. To avoid saturation effects we have applied microwave power P = 20 μW in our measurements. Table S1 presents the results of the CW EPR spectra deconvolutions.

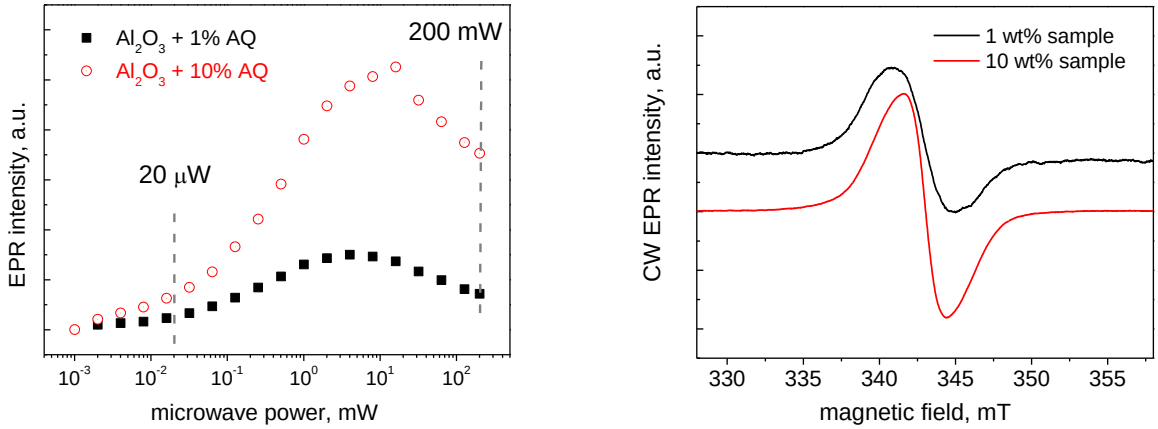

Figure S1. *Left panel*: power dependencies (saturation curves) of the CW EPR intensities for 1 wt% AQ (squares) and 10 wt% AQ (circles) samples registered at room temperature. *Right panel:* EPR spectra for 1 wt% AQ (upper curve) and 10 wt% AQ (lower curve) samples registered at high microwave power of P = 200 mW at room temperature (RT).

Table S1. Concentration dependence of linewidth, number of spins and value of the hyperfine interaction for all of the three paramagnetic centres as followed from the decomposition of corresponding CW spectra taken at RT.

$AQ:Al_2O_3$, mg (AQ wt%)	Al pair centre			S1 centre		S2 centre	
	hyperfine, mT	linewidth, mT	abs. spins, $*10^{17}$	linewidth, mT	abs. spins, $*10^{17}$	linewidth, mT	abs. spins, $*10^{17}$
0.05:10 (0.5%)	0.7	0.6	0.34	3.5	0.56	-	-
0.1:10 (1%)	0.7	0.6	0.67	3.5	1.13	-	-
0.3:10 (3%)	0.7	0.6	0.83	3.3	1.45	0.9	0.02
0.5:10 (5%)	0.7	0.6	0.73	3.2	1.90	1.0	0.17
1.0:10 (10%)	0.7	0.6	0.25	3.0	1.95	1.0	0.3
2.0:10 (20%)	0.7	0.6	0.04	2.7	3.40	1.0	0.9

2. Pulsed EPR experiments.

The main text of manuscript is dealing with the CW EPR spectra. Although ESE detected EPR spectra (Figure S2) and ESE decays (Figure S3) were recorded. As it was pointed out in the main text of the manuscript, because of the complex behavior of the ESE detected spectra of AQ-alumina system expressed in the sophisticated character of T_2 curves correct numerical computations from the ESE spectra are problematic.

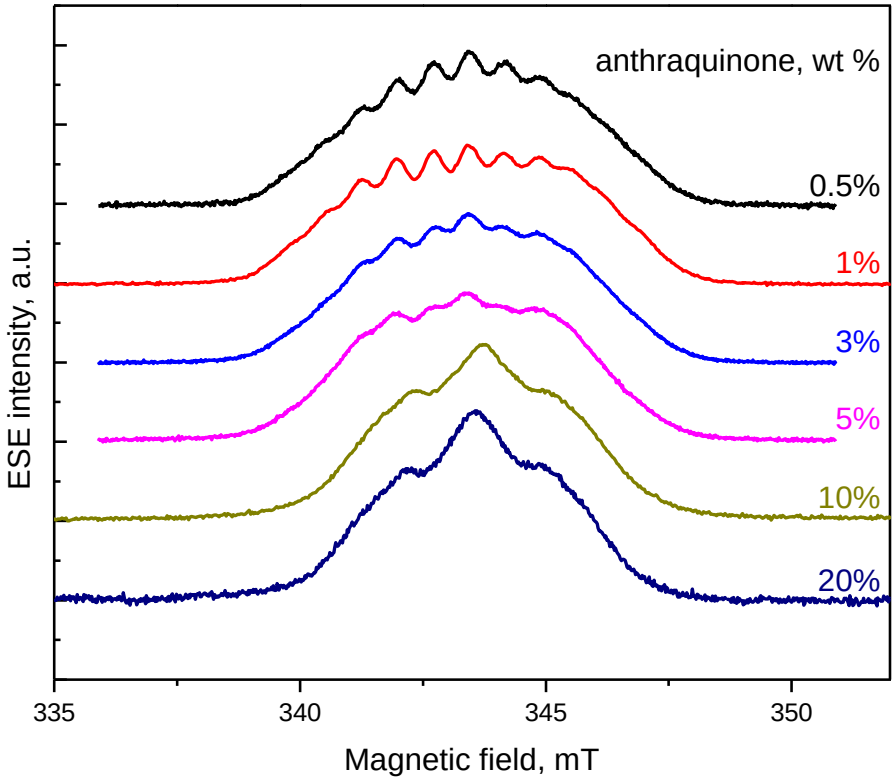

Figure S2. Room temperature ESE EPR spectra of six synthesized anthraquinone-alumina samples at τ = 240 ns

The ESE decays measurements were done in the magnetic field, corresponding to the centre of each ESE detected spectrum. The relaxation curves (Figure S3) were fitted by mono-exponential decays. The extracted T_2 parameters are presented in Table S2. FFT of decays' modulation signal are presented in the inset.

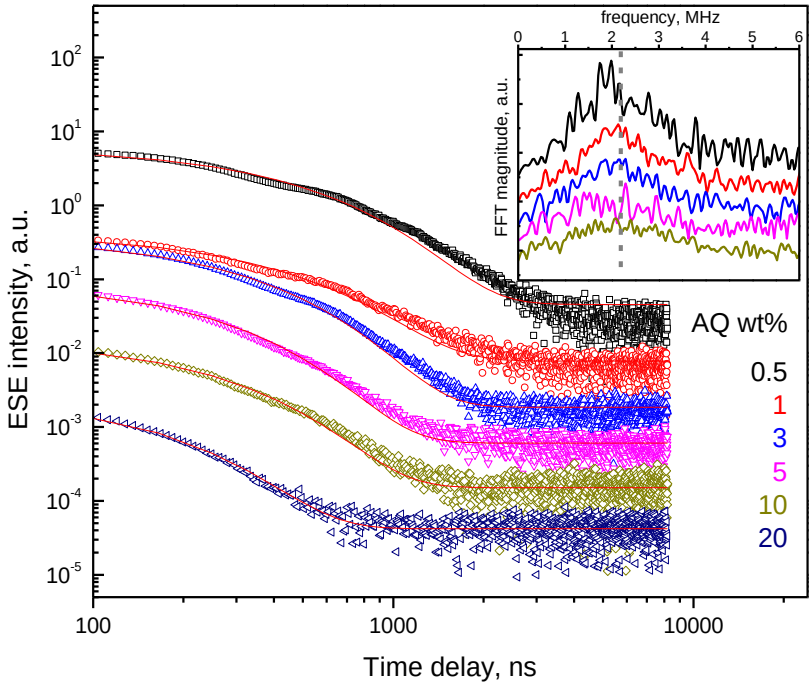

Figure S3. Experimental T_2 curves of six synthesized anthraquinone-alumina samples at RT and their exponential fittings. Inset shows Fourier-transformed modulation pattern of the relaxation curves for five AQ concentrations. Modulation frequency of 2MHz corresponds to the weak hyperfine interaction with the remote ^{27}Al nuclei.

Table S2. The room temperature spin relaxation time T_2 as a function of AQ amount.

AQ weight, %	*T_2, ns*
0.5	380
1	330
3	245
5	196
10	200
20	124