Supporting information

# Effect of the surface properties of the resorcinol-formaldehyde resin/carbon nanocomposites and their carbonization products on the solid-phase extraction of explosives

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### 1. Raman spectroscopy



**Fig. ESI 1.** Raman spectra of the fillers CNT (thick line) and EG (thin line) on the left graph. Deconvolution of the Raman spectrum of CNT (thick line) on the right, line with open circles presents the total sum of Lorentz components.

#### 2. SPE – statistical analysis

**Table ESI 1.** The results of the analysis of variance (F-Snedecor's test) for the adsorption and desorption rates. The critical value of  $F_{0.05,1,4}$  (tabulated elsewhere) is 7.71. The marked grey values are for F <  $F_{0.05,1,4}$ .

	Adsorption rate									
Variables (composites)	Calculated statistic F for the experiments for:									
	нмх	TEX	ROX	CI-20	NG	DNTG	PETN	TNT	DNT	
RFR-43, RFR-44	2.1	2.1	1.8	1.5	12.7	9.1	16.8	1.5	1.5	
RFC-43, RFC-44	208.8	239.3	156.2	29.8	376.1	108.5	43.3	19.7	22.9	
	Desorption rate									
RFR-43, RFR-44	2.6	5.0	3.8	2.3	27.2	15.9	12.7	1.1	1.3	
RFC-43, RFC-44	33.9	11.9	30.6	13.9	18.7	12.7	13.0	28.1	21.1	

## 3. XPS analysis

Surface composition of RFC-43 and RFC-44 sample was determined by XPS. High-resolution (HR) XPS measurements were performed using a PHI 5000 VersaProbe<sup>TM</sup> (ULVAC-PHI) spectrometer with microfocused and monochromatic AI K  $\alpha$  radiation. The spectrometer was equipped with a spherical capacitor energy analyzer with multi-channel detection with a 100  $\mu$ m × 100  $\mu$ m area for XPS analysis. The X-ray beam was incident on the sample surface at an angle of 45° with respect to the surface normal, and the analyzer axis was located at 45° with respect to the surface. HR XPS spectra were recorded with the energy step of 0.1 eV at the analyzer pass energy of 23.5 eV. All XPS spectra were recorded on the as-delivered composites, pre-sputtered by 2 keV argon ions (at angle of incidence of 35° with respect to the surface normal, rastered over a 2 mm × 2 mm surface area; a maximal ion current of 1.1  $\mu$ A) for 5 min. The Ar<sup>+</sup> sputtering rate was 7 nm/min, as measured using a SiO<sub>2</sub>/Si reference sample.

ULVAC-PHI MultiPak software (ver. 9.6.0.15) was used to evaluate the XPS data. Deconvolution of XPS spectra were performed using a Shirley background and a Gaussian peak shape with 30% Lorentzian character. The binding energies (BE) of all detected spectra were calibrated with respect to the BE of C 1s at 285.0 eV. Atomic concentration (AC) of oxygen at the samples surface was quantified using the multiline software [A. Jablonski, Determination of surface composition by X-ray photoelectron spectroscopy taking into account elastic photoelectron collisions, Anal. Sci. 26(2010) 155–164].

**Table 2 ESI** C (1s) peak fitting results obtained for RFR-43 and RFR-44 samples, for oxygen functionalities on carbon surfaces. In parentheses are shown binding energies.

Sample		C=0 %	С-О-С %	
Sample	C-017C-0 /8 (EV)	(eV)	(eV)	
RFR-43	3.3 (285,9)	-	1.0 (286,8)	
RFR-44	3.4 (286,3)	1.4 (287.6)	-	

Using results of XPS measurements the surface concentration of the major oxygen containing functionalities were quantified. The results demonstrate similar surface concentration of C-OH/C-O groups and higher surface concentration of the polar group i.e. carbonyl on RFR-44 composite, in comparison to RFR-43 one. This can explain the higher SPE adsorption rate of aliphatic nitrate esters on RFR-44 composite.

## 4. SPE equipment

The SPE experiments were carried out using SPE 12-G system (Baker). It consist of 12 port vacuum manifold (glass vacuum container, cover with Luer fittings, individual flow control valves and PTFE lids), collection rack for graduated flask, and vacuum gauge/controller. The reduced pressure was obtained using vacuum pump.



Fig. ESI 2. SPE 12-G system used in experiments.