

# Intercalation Compounds of Oxidized Carbon Black

Mario Maggio, Maria Rosaria Acocella, Gaetano Guerra\*

*Department of Chemistry and Biology and INSTM Research Unit, Università di Salerno, via  
Giovanni Paolo II 132, 84084 Fisciano (SA), Italy*

## Supporting Information

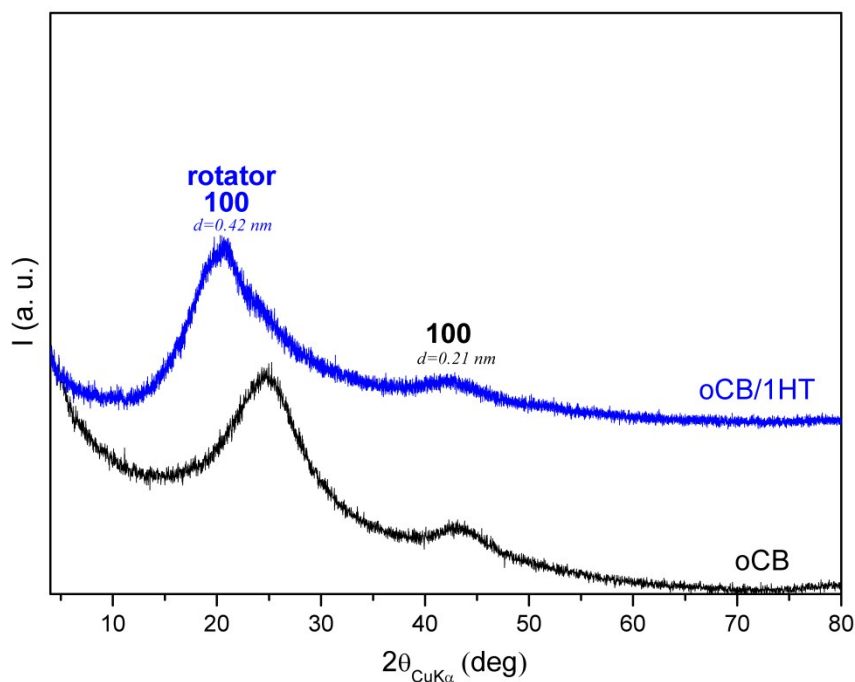
### **oCB/1HT adducts**

oCB/1HT adducts have been prepared with the oCB samples described in Figure 4.

X-ray diffraction patterns of the obtained adducts show the presence of the diffraction peak of the rotator order and the absence of the low  $2\theta$  peaks of the intercalate order. This is shown, for instance, by the WAXD pattern ( $\text{CuK}\alpha$ ) of the oCB/1HT adduct as prepared with the oCB sample with O/C wt ratio equal to 0.83 (Figure S1, upper curve), which roughly contains 30 wt % of 1HT. A comparison with the WAXD pattern of the starting oCB sample (Figure S1, lower curve), clearly show that the typical amorphous halo of oCB remains only as a shoulder in the pattern of the adduct (Figure S1a) while a broad 100 rotator peak appears at  $d = 0.42$  nm.

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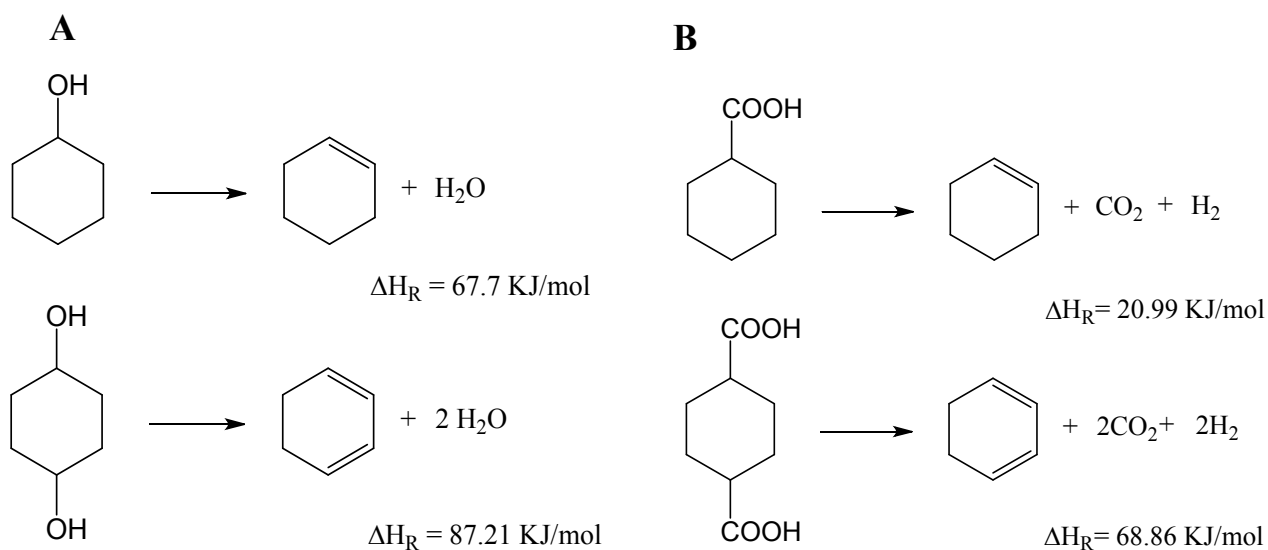
\* Corresponding author. Fax: +39 089 969603. E-mail: [gguerra@unisa.it](mailto:gguerra@unisa.it) (G. Guerra)



**Figure S1.** X-ray diffraction patterns ( $\text{CuK}\alpha$ ) of: (a) the prepared oCB sample with C/O wt ratio equal to 1.2; b) of the corresponding oCB/1HT adducts.

### Thermodynamic considerations on enthalpy of deoxygenation reactions

We add here some simple thermodynamic considerations, relative to dehydration and decarboxylation reactions, leading to double bond formations. These reactions, when lead to isolated or even conjugated double bonds, are generally endothermic. This is shown, for instance, for reactions of low molecular mass compounds (Figure S2) analogous to reactions occurring by heating on oCB.



**Figure S2.** Dehydration and decarboxylation reactions leading to isolated or conjugated double bonds, as model reactions for those occurring by heating of oCB. The reaction enthalpy changes ( $\Delta H_R$ ) have been evaluated by considering the enthalpy of formation of reactant and products (Hess law).<sup>S1</sup>

Enthalpy changes of these reactions ( $\Delta H_R$ ) have been evaluated from enthalpies of formation of reactants and products (Hess law).<sup>S1</sup>

**Single Dehydration:**

$$\Delta H_R = H_f - H_i = (H_{\text{Cyclohexene(l)}} + H_{\text{water(g)}}) - (H_{\text{Cyclohexanol}}) = (-38.5 \text{ KJ/mol} - 241.82 \text{ KJ/mol}) - (-348 \text{ KJ/mol}) = 67.7 \text{ KJ/mol}$$

**Double dehydration:**

$$\Delta H_R = H_f - H_i = (H_{\text{Cyclohexadiene(l)}} + 2 H_{\text{water(g)}}) - (H_{\text{Cyclohexandiol}}) = (71.41 \text{ KJ/mol} - 2 \times 241.82 \text{ KJ/mol}) - (-500.28 \text{ KJ/mol}) = 87.86 \text{ KJ/mol}$$

**Single decarboxylation:**

$$\Delta H_R = H_f - H_i = (H_{\text{Cyclohexene(l)}} + H_{\text{CO}_2(\text{g})}) - (H_{\text{cyclohexanecarboxylic acid (l)}}) = (-38.5 \text{ KJ/mol} - 393.51 \text{ KJ/mol}) - (-453.0 \text{ KJ/mol}) = 20.99 \text{ KJ/mol}$$

**Double decarboxylation:**

$$\Delta H_R = H_f - H_i = (H_{\text{Cyclohexadiene(l)}} + 2 H_{\text{CO}_2(\text{g})}) - (H_{\text{cyclohexane-1,4-dicarboxylic acid(l)}}) = (71.41 \text{ KJ/mol} - 2 \times 393.51 \text{ KJ/mol}) - (-784.46 \text{ KJ/mol}) = 68.86 \text{ KJ/mol}$$

It is worth adding that the occurrence in DSC scans of GO and eGO of exothermal (rather than endothermal) peaks is due to prevalence of analogous deoxygenation (dehydration and decarboxylation) reactions leading to aromatization. In fact, aromatization implies large exothermal contributions (typically of the order of 150 KJ/mol per 6-membered aromatic rings).<sup>S2</sup>

**References**

S1 David. R. Lide " Chemistry and Physics" 87<sup>th</sup> Edition 2006-2007, CRC Press Taylor and Francis.

S2 McMurry, J. (2012). Organic Chemistry, 8th edition. Cengage Learning.