

# ADDITIONS AND CORRECTIONS

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**J. Oscar C. Jiménez-Halla, Juvencio Robles, and Miquel Solà\*:** Coordination and Haptotropic Migration of  $\text{Cr}(\text{CO})_3$  in Polycyclic Aromatic Hydrocarbons: The Effect of the Size and the Curvature of the Substrate

Page 1203. Equation 1 has an error when including the BSSE correction to the total energy. It should read

$$\Delta E = \Delta E_{\text{el}} + \text{ZPE}(\text{AB}) - \text{ZPE}(\text{A}) - \text{ZPE}(\text{B}) + \delta^{\text{BSSE}} \quad (1)$$

Page 1208. This error affects the results presented at Table 1 and the references to these numbers in the text, but it does not change the trends observed and the conclusions of the work remain the same. Thus, Table 1 should read

**TABLE 1: Binding Energies ( $\Delta E$ ), Activation Barriers ( $\Delta E^\ddagger$ ), and Relative Energy of the Intermediate 2 ( $\Delta E_2$ ) with Respect to the  $(\eta^6\text{-PAH})\text{Cr}(\text{CO})_3$  Reactant for the Two Reaction Routes Found at Level B3LYP/(Wachters' basis, 6-31G(d,p))<sup>a</sup>**

route A	$\Delta E$	$\Delta E_2$	$\Delta E^\ddagger_{(1 \rightarrow \text{TS}_2)}$
$\text{C}_{16}\text{H}_{10}$	−27.05	17.76	18.24
$\text{C}_{28}\text{H}_{14}$	−10.74	4.01	4.40
route B	$\Delta E$	$\Delta E_2$	$\Delta E^\ddagger_{(1 \rightarrow \text{TS}_1)}$
$\text{C}_{10}\text{H}_8$	−39.26		23.40
$\text{C}_{26}\text{H}_{12}$	−18.58		10.44

<sup>a</sup> For the notation of the calculated structures see Figure 8. All energies (in  $\text{kcal}\cdot\text{mol}^{-1}$ ) are corrected by BSSE.

Values that should be corrected in the text are the following:

Page 1205, column 1, line 12: 39.3 instead of 50.2  
 Page 1206, column 1, line 12: 10.3 instead of 11.8  
 Page 1206, column 1, line 20: 23.4 instead of 25.7  
 Page 1206, column 1, line 42: 27.0 instead of 40.6  
 Page 1206, column 2, line 6: 18.2 instead of 19.8  
 Page 1206, column 2, line 29: 10.7 instead of 22.9  
 Page 1206, column 2, line 37: 4.4 instead of 6.2  
 Page 1206, column 2, line 49: 18.6 instead of 30.2 and 7.8 instead of 7.3

Page 1207, column 1, line 7: 10.4 instead of 13.3

Page 1211, column 2, line 9: it should read “derivative than for  $(\eta^6\text{-C}_{28}\text{H}_{14})\text{Cr}(\text{CO})_3$  species (Table 3).”

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