ADDITIONS AND CORRECTIONS

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J. Oscar C. Jiménez-Halla, Juvencio Robles, and Miquel Solà*: Coordination and Haptotropic Migration of $Cr(CO)_3$ 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

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

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 1should read

TABLE 1: Binding Energies (ΔE), Activation Barriers ($\Delta E^{\ddagger}$), and Relative Energy of the Intermediate 2 (ΔE_2) with Respect to the (η^6-PAH)$Cr(CO)_3$ Reactant for the Two Reaction Routes Found at Level B3LYP/(Wachters' basis, 6-31G(d,p))[a]

route A	ΔE	ΔE_2	$\Delta E^{\ddagger}_{(1\rightarrow TS2)}$
$C_{16}H_{10}$	−27.05	17.76	18.24
$C_{28}H_{14}$	−10.74	4.01	4.40
route B	ΔE	ΔE_2	$\Delta E^{\ddagger}_{(1\rightarrow TS1)}$
$C_{10}H_8$	−39.26		23.40
$C_{26}H_{12}$	−18.58		10.44

[a] For the notation of the calculated structures see Figure 8. All energies (in kcal·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 (η^6-$C_{28}H_{14}$)$Cr(CO)_3$ species (Table 3)."

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