J|A|C|S
ADDITIONS AND CORRECTIONS

Kinetics and Thermodynamics of H• Transfer from (η^5-C_5R_5)$Cr(CO)_3H$ (R = Ph, Me, H) to Methyl Methacrylate and Styrene

[*J. Am. Chem. Soc.* **2003**, *125*, 10093−10102]. Lihao Tang, Elizabeth T. Papish, Graham P. Abramo, Jack R. Norton,* Mu-Hyun Baik, Richard A. Friesner, and Anthony Rappé

The redox potential *in CH_3CN* of $C_5Ph_5Cr(CO)_3$•/$C_5Ph_5Cr(CO)_3^-$ vs Fc/Fc^+ was transcribed incorrectly from the publication cited as ref 3. Substitution of the correct redox potential in CH_3CN (−0.50 V) changes the Cr−H bond strength for $C_5Ph_5Cr(CO)_3H$ from 59.6(3) kcal/mol to *64.0(3)* kcal/mol in CH_3CN, the C−H bond strength in a methyl isobutyryl radical from 45.6 kcal/mol to *50.0* kcal/mol in toluene, and the C−H bond strength in an α-methylbenzyl radical from 47.9 kcal/mol to *52.4* kcal/mol in toluene. The methyl isobutyryl C−H bond strength now agrees with that (50 kcal/mol) reported by Woska, Xie, Gridnev, Ittel, Fryd, and Wayland (*J. Am. Chem. Soc.* **1996**, *118*, 9102−9109) for the cyanoisopropyl radical and is very close to the value (49.5 kcal/mol) obtained by the present authors from DFT calculations. The α-methylbenzyl C−H bond strength is now slightly higher than the value (49.9 kcal/mol) obtained by the present authors from DFT calculations. The authors are grateful to Jongwook Choi for pointing out the error in transcription.

JA069969Z

10.1021/ja069969z
Published on Web 08/03/2006