2006, Volume 110A

Aimee Clements and Michael Lewis*: Arene—Cation Interactions of Positive Quadrupole Moment Aromatics and Arene—Anion Interactions of Negative Quadrupole Moment Aromatics

Page 12705. Additional calculations requested upon review changed the F^- binding of C_6H_6 and $C_6H_2I_4$ reported in the abstract. The BSSE corrected MP2(full)/6-311++G** F^- -C₆H₆ ΔH_{298} value should be -0.14 kcal/mol, as is correctly reported in Tables 2 and 5. The reported value of -5.51 kcal/mol is the non-BSSE corrected MP2(full)/6-311G** ΔH_{298} value. The rest of the manuscript contains the correct F^- -C₆H₆ ΔH_{298} value. The reported F^- -C₆H₂I₄ ΔH_{298} value of -20.13 kcal/mol was also calculated at the MP2(full)/6-311G** level of theory without BSSE correction. The BSSE corrected MP2(full)/6-311G** ΔH_{298} value is -2.26 kcal/mol. Due to challenges optimizing the F^- -C₆H₂I₄ complex at the MP2(full)/6-311++G** level of theory in a timely manner it was ultimately dropped from the manuscript, but unfortunately not from the abstract.

All other binding enthalpy values in the abstract and the manuscript are correct and all of the findings of the paper remain unchanged. We gratefully thank Professor Steven Wheeler for alerting us to the error. We apologize for not recognizing the mistake earlier.

10.1021/jp106292u Published on Web 07/23/2010