JCTC Journal of Chemical Theory and Computation

Improving the QM/MM Description of Chemical Processes: A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. [*J. Chem. Theory Comput. 1*, 1008−1016 (2005)]. By Sergio Martí, Vicente Moliner, and Iñaki Tuñón. Departament de Ciències Experimentals, Universitat Jaume I, Box 224, 12080 Castellón, Spain and Departament de Química Física/IcMol, Universidad de Valencia, 46100 Burjasot, Valencia, Spain

Pages 1013 and 1014. In the last example discussed in the paper we used a combination of B3LYP/6-31+G* and PM3 methods combined with molecular mechanics (MM) named as B3LYP:PM3/MM. At the end of the section (p 1014) we erroneously named it twice as B3LYP:AM1/MM, instead of B3LYP:PM3/MM. This typographical correction has no bearing with any of our results or conclusions.

CT058001A

10.1021/ct058001a
Published on Web 12/02/2005