

ADDITIONS AND CORRECTIONS

2009, Volume 113A

**Pankaj Kulshrestha, N. Sukumar, Jane S. Murray,*
Rossman F. Giese, and Troy D. Wood:** Computational
Prediction of Antibody Binding Sites on Tetracycline Antibiot-
ics: Electrostatic Potentials and Average Local Ionization
Energies on Molecular Surfaces

Page 756. Reference 47 is in error. The correct reference
should be: Aga, D. S.; Goldfish, R.; Kulshrestha, P. *Analyst*
2003, 128, 658.

In addition, the binding isotherm data presented in Figure 1
were measured in Dr. Diana Aga's laboratory under NSF
sponsorship (NSF Career Grant CHE-0233700) and should have
been cited in the acknowledgments.

10.1021/jp903095g

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2006, Volume 110A

Edward F. C. Byrd* and Betsy M. Rice: Improved Prediction
of Heats of Formation of Energetic Materials Using Quantum
Mechanical Calculations

Pages 1005–1013. The names of the group equivalents in
Table 3 were mislabeled. The results as published in the paper
are consistent with the new, properly labeled, group equivalents
shown in the corrected Table 3.

TABLE 3: Atom or Group Equivalent Energies and Parameters for Equations 3 and 4 using B3LYP/6-31G* Geometries, B3LYP/6-311++G(2df, 2p) Energies, and Electrostatic Surface Potential Mappings

atom or group equivalent	ϵ (hartree)	eq 3		eq 4	
C	−38.123748	a (kcal/mol-Å ^{−1})	2.130167	a (kcal/mol-Å ^{−4})	0.000267
H	−0.597580	b (kcal/mol)	0.930065	b (kcal/mol)	1.650087
N	−54.785466	c (kcal/mol)	−17.843973	c (kcal/mol)	2.966078
O	−75.187087				
C'	−38.129456				
N'	−54.788487				
O'	−75.186033				
C−NO ₂	−205.160396				
N−NO ₂	−205.163484				
O−NO ₂	−205.166631				
C−N ₃	−164.364907				
X−NO	−129.976691				

We apologize for any inconvenience this might have caused to the readers. We would like to thank Dr. Didier Mathieu for bringing these typographical errors to our attention.

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