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Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. [Erratum to document cited in CA103(2):11627f]

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Additions and Corrections

AM1: A New General Purpose Quantum Mechanical Molecular Model [*J. Am. Chem. Soc.* **1985**, 107, 3902–3909].

MICHAEL J. S. DEWAR,* EVE G. ZOEBISCH, EAMONN F. HEALY, AND JAMES J. P. STEWART

In eq 1, in the expression for $F(A)$ and $F(B)$, a factor was omitted. Each summation should have been multiplied by $(1/\gamma_{ss}R_{AB})$. The correct version was used in the calculations reported in the paper and presumably also in all other published AM1 calculations, given that the algorithms used in all versions of the MOPAC and AMPAC computer programs have been correct. We appreciate M. Banerjee and A. K. Chandra calling attention to the fact that a correction had not been printed in the journal.

Photoinduced Electron Transfer in Covalently Linked Ruthenium Tris(bipyridyl)–Viologen Molecules: Observation of Back Electron Transfer in the Marcus Inverted Region [*J. Am. Chem. Soc.* **1992**, 114, 8081–8087].

EDWARD H. YONEMOTO, RICHARD L. RILEY, YEONG IL KIM, STEPHEN J. ATHERTON, RUSSELL H. SCHMEHL,* AND THOMAS E. MALLOUK*

Due to a programming error, incorrect values of the square of the electronic coupling matrix element, $|V(r)|^2$, were reported in the caption for Figure 4 and in the text on p 8086. The other parameters (S , λ , λ_s , $h\nu$) and fits to the data shown in the figure represent the correct $|V(r)|^2$ values, which are as follows:

		$ V(r) ^2$, eV ²
forward reaction:	$n = 1$	8.00×10^{-6}
	$n = 2$	8.82×10^{-6}
back reaction:	$n = 1$	1.79×10^{-5}
	$n = 2$	6.97×10^{-6}

The assertion made on p 8086 that electronic coupling for the forward reactions, which occur through a shorter spacer, is significantly stronger than it is for the back reactions should be disregarded in light of the corrected $|V(r)|^2$ values.

Structures of Sweet and Bitter Peptide Diastereomers by NMR, Computer Simulations, and X-ray Crystallography [*J. Am. Chem. Soc.* **1993**, 115, 428–432].

MURRAY GOODMAN,* TOSHIMASA YAMAZAKI, YUN-FEI ZHU, ETTORRE BENEDETTI, AND RAJ K. CHADHA

Page 428: In Table I, the cutoff for “unique reflections used” should be $895[F_o > 3.0\sigma(F_o)]$ and $868[F_o > 4.0\sigma(F_o)]$.

Page 429: In Table II, the values given in the column “Asp(*R*)-Chg-OCH₃” should be (in descending order of entry) the following: 167.1, 176.5, –77.9, 173.6, 88.1, –131.8, 178.2, and 69.0/–169.0.

Page 429, second column: In line 4, the torsion values for the L-*R*-isomer should be (167.1°, –77.9°); in line 6, the torsion values for aspartame should be (149.0°, –71.7°); in line 8, the torsion values for Asp(*S*)gAlaTMCP should be (166.2°, –75.4°).

In references 13 and 17a,b,c, the correct spelling of the author’s name is Lelj, F.

These changes do not alter the findings of the paper.