Erratum: “Ab initio computed diabatic potential energy surfaces of OH–HCl”

Paul E. Wormer, Jacek A. Kłos, Gerrit C. Groenenboom, and Ad van der Avoird

Citation: J. Chem. Phys. 126, 079902 (2007); doi: 10.1063/1.2472333
View online: http://dx.doi.org/10.1063/1.2472333
View Table of Contents: http://jcp.aip.org/resource/1/JCPSA6/v126/i7
Published by the American Institute of Physics.

Additional information on J. Chem. Phys.
Journal Homepage: http://jcp.aip.org/
Journal Information: http://jcp.aip.org/about/about_the_journal
Top downloads: http://jcp.aip.org/features/most_downloaded
Information for Authors: http://jcp.aip.org/authors

Paul E. S. Wormer, Jacek A. Kłos,a) Gerrit C. Groenenboom, and Ad van der Avoirdb)

Theoretical Chemistry, IMM, Radboud University Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

(Received 9 January 2007; accepted 10 January 2007; published online 20 February 2007)

[DOI: 10.1063/1.2472333]

Equation (47) of the article has a small typographical error. In the second binomial coefficient $\alpha$ must be replaced by $\beta$. The correct equation for the $d$ functions is

$$d_{m'm}^{l}(\theta) = (-1)^{l} \binom{2j - k}{k + \alpha} \binom{k + \beta}{\beta}^{-1/2} \left( \sin \frac{\theta}{2} \right)^{\alpha} \left( \cos \frac{\theta}{2} \right)^{\beta} P_{l}^{(\alpha, \beta)}(\cos \theta).$$

---

a)Present address: Department of Chemistry & Biochemistry, University of Maryland, College Park, Maryland 20742-4454.

b)Electronic mail: A.vanderAvoird@theochem.ru.nl