Theor Chem Acc (2011) 130:725–726
DOI 10.1007/s00214-011-1064-z

ERRATUM

Erratum to: (Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers

Masayoshi Nakano · Hitoshi Fukui · Takuya Minami · Kyohei Yoneda · Yasuteru Shigeta · Ryohei Kishi · Benoît Champagne · Edith Botek · Takashi Kubo · Koji Ohta · Kenji Kamada

Published online: 2 November 2011

Erratum to: Theor Chem Acc
DOI 10.1007/s00214-010-0871-y

Due to publisher's error that occurred at the typesetting stage and which was not corrected at the proof stage, reference 81 was inadvertently deleted with the result that references 81–104 should be 82–105, with reference 81 being

Bulat FA, Toro-Labbe A, Champagne B, Kirtman B, Yang W (2005) J Chem Phys 123:014319

The only reference in the text that then needs to be changed is reference 104 (above Sect. 5 Concluding remarks) which should then be reference 105. The corrected line is given below:

These properties will be reintroduced well by the complete active space (CAS)-DFT method [94–105].

The amended list of references 81–105 are as follows:

81. Bulat FA, Toro-Labbé A, Champagne B, Kirtman B, Yang W (2005) J Chem Phys 123:014319
82. Mori-Sanchez P, Wu Q, Yang W (2003) J Chem Phys 119:11031
83. Sekino H, Maeda Y, Kamiya M, Hirao K (2007) J Chem Phys 126:014107
84. Kirtman B, Bonness S, Ramirez-Solis A, Champagne B, Matsumoto H, Sekino H (2008) J Chem Phys 128:114108
85. Bonness S, Fukui H, Yoneda K, Kishi R, Champagne B, Botek E, Nakano M (2010) Chem Phys Lett 493:195
86. Nakano M, Takebe A, Kishi R, Ohta S, Nate M, Kubo T, Kamada K, Ohta K, Champagne B, Botek E, Takahashi H, Furukawa S, Morita S, Nakasuji K (2006) Chem Phys Lett 432:473
87. Song J-W, Hirosawa T, Tsuneda T, Hirao K (2007) J Chem Phys 126:154105
88. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA Jr, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R,

The online version of the original article can be found under doi:10.1007/s00214-010-0871-y.

M. Nakano (✉) · H. Fukui · T. Minami · K. Yoneda · Y. Shigeta · R. Kishi
Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan
e-mail: mnaka@cheng.es.osaka-u.ac.jp

B. Champagne · E. Botek
Laboratoire de Chimie Théorique, Facultés Universitaires Notre-Dame de la Paix (FUNDP), rue de Bruxelles, 61, 5000 Namur, Belgium
e-mail: benoit.champagne@fundp.ac.be

T. Kubo
Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan
e-mail: kubo@chem.sci.osaka-u.ac.jp

K. Ohta · K. Kamada
Research Institute for Ubiquitous Energy Devices, National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan
e-mail: k.ohta@aist.go.jp

K. Kamada
e-mail: k.kamada@aist.go.jp

Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam NJ, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas Ö, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2009) Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT

89. Filatov M, Cremer D (2005) J Chem Phys 123:124101
90. Nakano M, Yamada S, Shigemoto I, Yamaguchi K (1996) Chem Phys Lett 250:247
91. Nakano M, Yamaguchi K (1994) Phys Rev A 50:2989
92. Nakano M, Yamaguchi K, Matsuzaki Y, Tanaka K, Yamabe T (1995) J Chem Phys 102:2986
93. Yanai T, Tew DP, Handy NC (2004) Chem Phys Lett 393:51
94. Savin A, Flad HJ (1995) Int J Quantum Chem 56:327
95. Gori-Giorgi P, Savin A (2006) Phys Rev A 73:3250
96. Fromager E, Toulouse J, Jensen HJA (2007) J Chem Phys 126:074111
97. Kusakabe K (2001) J Phys Soc Jpn 70:2038
98. Yamanaka S, Nakata K, Takada T, Kusakabe K, Ugalde JM, Yamaguchi K (2006) Chem Lett 35:242
99. Yamanaka S, Nakata K, Ukai T, Takada T, Yamaguchi K (2006) Int J Quantum Chem 16:3312
100. Miehlich B, Stoll H, Savin A (1997) Mol Phys 91:527
101. Gräfenstein J, Cremer D (2000) Chem Phys Lett 316:569
102. Gusarov S, Malmqvist PÅ, Lindh R, Roos BO (2004) Theor Chem Acc 112:84
103. Pérez-Jiménez, AJ, Pérez-Jord JM (2007) Phys Rev A 75:012503
104. Takeda R, Yamanaka S, Yamaguchi K (2002) Chem Phys Lett 366:321
105. Takeda R, Yamanaka S, Yamaguchi K (2004) Int J Quantum Chem 96:463