NJC

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *New J. Chem.*, 2020, **44**, 15299

Correction: Understanding the reactivity of carbene-analogous phosphane complexes with group 13 elements as a central atom: a theoretical investigation

Zheng-Feng Zhang,[a] Tsung-Lung Li*[b] and Ming-Der Su*[ac]

DOI: 10.1039/d0nj90117b

rsc.li/njc

Correction for 'Understanding the reactivity of carbene-analogous phosphane complexes with group 13 elements as a central atom: a theoretical investigation' by Zheng-Feng Zhang *et al.*, *New J. Chem.*, 2020, **44**, 12815–12826, DOI: 10.1039/D0NJ01708F.

The authors regret that eqn (6) and (7) shown on page 12817 were incorrect in the original article. The correct equations are as shown below:

$$\mathbf{0M} + CH_4 \rightarrow \mathbf{TS1M} \rightarrow \mathbf{1M} \quad (6)$$

$$\mathbf{0M} + C_2H_4 \rightarrow \mathbf{TS2M} \rightarrow \mathbf{2M} \quad (7)$$

The authors also regret that the following details were omitted from the last paragraph of II. Theoretical methods on page 12817:

The bonding energies and characteristics of a single complex may be affected by the choice of the density functionals[1] as well as the inclusion of the solvent models[2] in the computations. However, for the chemical energetics and bonding interactions along the reaction profiles, all characteristics of the complexes in their transition and product states are relative to those of the reactants. The effects due to the choice of density functionals and the inclusion of solvent models are largely canceled.[3] Therefore, the density functional BP86 without solvent effects is employed throughout this DFT work.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

1 E. J. Baerends and V. G. Oleg, A quantum chemical view of density functional theory, *J. Phys. Chem. A*, 1997, **101**, 5383–5403.
2 D. M. Chipman, Comparison of solvent reaction field representations, *Theor. Chem. Acc.*, 2002, **107**, 80–89.
3 D. Young, *Computational chemistry: a practical guide for applying techniques to real world problems*, Wiley-VCH, John Wiley and Sons, Inc., New York, 2001.

[a] *Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan. E-mail: midesu@mail.ncyu.edu.tw*
[b] *Department of Electrophysics, National Chia-Yi University, Chiayi 60004, Taiwan. E-mail: quantum@mail.ncyu.edu.tw*
[c] *Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 80708, Taiwan*