## **PCCP**



## CORRECTION

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## Correction: The stability of biradicaloid versus closed-shell $[E(\mu-XR)]_2$ (E = P, As; X = N, P, As) rings. Does aromaticity play a role?†

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Correction for The stability of biradicaloid versus closed-shell  $[E(\mu-XR)]_2$  (E = P, As; X = N, P, As) rings. Does aromaticity play a role?' by Rafael Grande-Aztatzi et al., Phys. Chem. Chem. Phys., 2016, 18, 11879-11884.

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We would like to inform the reader of a correction that needs to be made to our previous publication. The energy differences  $(\Delta E)$ between the planar and butterfly isomers of the  $[P(\mu-PH)]_2$ ,  $[P(\mu-AsH)]_2$ , and  $[As(\mu-AsH)]_2$  compounds are incorrectly reported to be -98.9, -176.3 and -180.7 kcal  $\text{mol}^{-1}$ , respectively, on page 11882 and in Table 1. The correct values are -47.3, -46.4, and -44.1 kcal mol<sup>-1</sup>, respectively, which appeared in the Table S1 of the supporting information.†

Thus the correct sentence should read "However, when N is substituted by heavier atoms, like P or As, the butterfly isomer turns out to be the most stable isomer, by  $47.3 \text{ kcal mol}^{-1}$  for  $[P(\mu\text{-PH})]_2$  and  $46.4 \text{ kcal mol}^{-1}$  for  $[P(\mu\text{-AsH})]_2$ , and by  $27.7 \text{ kcal mol}^{-1}$ for  $[As(\mu-PH)]_2$  and 44.1 kcal mol<sup>-1</sup> for  $[As(\mu-AsH)]_2$ ".

The corrected version of Table 1 is given below.

Table 1 Relative energies at the MCQDPT level, and the lowest frequency and geometry parameters of the MCSCF(2,2)/aug-cc-pVTZ optimizations.  $\Delta E$  in kcal mol<sup>-1</sup>,  $\nu_{min}$  in cm<sup>-1</sup>, bond lengths in Å, bond angles and dihedral angles in degrees

|                     | $[P(\mu$ -AsH)] <sub>2</sub> |       |       | $[As(\mu-PH)]_2$ |       |       |
|---------------------|------------------------------|-------|-------|------------------|-------|-------|
|                     | N                            | P     | As    | N                | P     | As    |
| Planar              |                              |       |       |                  |       |       |
| $\Delta E$          | 0.0                          | 0.0   | 0.0   | 0.0              | 0.0   | 0.0   |
| $ u_{\mathrm{min}}$ | 338.6                        | 175.8 | 39.3  | 238.6            | 102.3 | -19.8 |
| E-X                 | 1.684                        | 2.055 | 2.333 | 1.814            | 2.268 | 2.453 |
| E-E                 | 2.580                        | 3.308 | 3.393 | 2.814            | 3.494 | 3.531 |
| X-H                 | 0.990                        | 1.396 | 1.508 | 0.992            | 1.400 | 1.510 |
| E-X-E               | 100.0                        | 107.2 | 93.3  | 101.8            | 100.5 | 92.1  |
| X-E-X               | 80.0                         | 77.9  | 86.7  | 78.2             | 100.8 | 87.6  |
| X-E-E-X             | 180.0                        | 176.5 | 179.9 | 180.0            | 180.0 | 167.8 |
| Butterfly           |                              |       |       |                  |       |       |
| $\Delta E$          | 21.5                         | -47.3 | -46.4 | 17.2             | -27.7 | -44.1 |
| $ u_{\mathrm{min}}$ | 468.4                        | 234.5 | 148.4 | 280.9            | 192.1 | 127.0 |
| E-X                 | 1.760                        | 2.212 | 2.333 | 1.893            | 2.339 | 2.450 |
| E-E                 | 2.084                        | 2.206 | 2.170 | 2.337            | 2.445 | 2.463 |
| X-H                 | 1.004                        | 1.410 | 1.516 | 1.004            | 1.409 | 1.515 |
| E-X-E               | 72.6                         | 58.8  | 55.4  | 76.2             | 63.0  | 60.3  |
| X-E-X               | 80.1                         | 82.1  | 84.3  | 78.1             | 80.4  | 81.6  |
| X-E-E-X             | 106.0                        | 98.6  | 97.5  | 106.4            | 98.4  | 98.1  |
|                     |                              |       |       |                  |       |       |

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

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