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ADDITION/CORRECTION

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Correction to "Binding of CO, NO, and O_2 to Heme by Density Functional and Multireference ab Initio Calculations"

[*The Journal of Physical Chemistry A* **2008**, *112*, 11824–11832. DOI: 10.1021/jp806075b]. Mariusz Radoń,* and Kristine Pierloot

An incorrect configuration was given in the discussion of the quintet state ($S = 2$) for the free hemes (the right column on p 11827). The correct quintet configuration for $Fe^{II}P$ reads

$$(d_{x^2-y^2})^1(d_{xz})^1(d_{yz})^1(d_{z^2})^2(d_{xy})^1$$

(pointing to the $^5A_{1g}$ state). The correct quintet configuration for $Fe^{II}P(Im)$ reads

$$(d_{x^2-y^2})^1(d_{xz})^2(d_{yz})^1(d_{z^2})^1(d_{xy})^1$$

(pointing to the $^5A'$ state). (P = porphyrin, Im = imidazole, as defined in the article.)

The error was limited to specifying a wrong configuration in the discussion only. Because the correct configurations have been used everywhere else in this work, in particular to calculate the spin splittings in Table 3 (the top of p 11827), the present correction does not affect any of the results reported or any of the conclusions drawn.

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