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Coordination Chemistry Reviews 249 (2005) 1133
COORDINATION CHEMISTRY REVIEWS
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Erratum

# Erratum to "Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site" [Coord. Chem. Rev. 238/239 (2003) 255–266]

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Available online 9 March 2005

The senior computational author (MBH) regrets that an undetected coding error resulted in errors for the overall exothermicity of the reactions reported in this paper. This error is purely numerical and does not affect the qualitative aspects or the chemistry reported and discussed in this paper. The following corrections should be noted.

1. In Fig. 5 the final relative energy of species **5a-Na** should be $-5.65\,\text{kcal mol}^{-1}$.
2. In Fig. 6 the final relative energy of species **10** should be $6.57\,\text{kcal mol}^{-1}$.
3. On page 265, column 1, line 10. The sentence should read "Compared with intermediate **3**, the monosubstituted complex **5a-Na** is $8.10\,\text{kcal mol}^{-1}$ more stable".

DOI of original article:10.1016/S0010-8545(02)00326-0
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doi:10.1016/j.ccr.2005.02.006