

Accepted Manuscript

Modeling the hydrogen sulfide binding to heme

B.D. Ostojić, P. Schwerdtfeger, D.S. Đorđević



PII: S0162-0134(17)30805-X
DOI: doi:[10.1016/j.jinorgbio.2018.04.012](https://doi.org/10.1016/j.jinorgbio.2018.04.012)
Reference: JIB 10479
To appear in: *Journal of Inorganic Biochemistry*
Received date: 18 November 2017
Revised date: 14 April 2018
Accepted date: 17 April 2018

Please cite this article as: B.D. Ostojić, P. Schwerdtfeger, D.S. Đorđević , Modeling the hydrogen sulfide binding to heme. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Jib(2017), doi:[10.1016/j.jinorgbio.2018.04.012](https://doi.org/10.1016/j.jinorgbio.2018.04.012)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Modeling the Hydrogen Sulfide Binding to Heme

B. D. Ostojic^{a,*} P. Schwerdtfeger^b and D. S. Dorđević^a

^a Center of Excellence in Environmental Chemistry and Engineering, Institute for Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, Belgrade 11000, Serbia

^b Centre for Theoretical Chemistry and Physics (CTCP), The New Zealand Institute for Advanced Study (NZIAS), Massey University Auckland, Private Bag 102904, North Shore City, 0745 Auckland, New Zealand

Abstract

The binding of hydrogen sulfide to a model heme compound is investigated by coupled-cluster singles-doubles augmented by a perturbative triple excitations, CCSD(T), and density functional theory, DFT. The minimum energy path for the H₂S addition to an isolated heme center of the heme protein is evaluated by adopting as a model the heme compound FeP(Im) (P=porphyrin; Im=imidazole). The FeP(Im)-H₂S adduct is bound by 13.7 kcal/mol at the CCSD(T) level of theory. Relaxed potential energy curves for the lowest lying spin states of the H₂S to FeP(Im) binding using DFT reveal that the binding process is associated with a "double spin-crossover" reaction with the existence of long-distance van der Waals minima only 5-7 kcal/mol above the FeP(Im)-H₂S ground state. The fact that the energy of the singlet ground state of FeP(Im)-H₂S is so close in energy to the dissociation products FeP(Im)+H₂S points towards the reversibility of the H₂S adsorption/desorption process in biochemical reactions.

Keywords: heme; imidazole; H₂S binding; electronic states; density functional theory; coupled cluster theory.

* Corresponding author. E-mail: bostojic@chem.bg.ac.rs (B. D. Ostojic).

Phone: +381 113336893; fax: +381 112636061

Download English Version:

<https://daneshyari.com/en/article/7753803>

Download Persian Version:

<https://daneshyari.com/article/7753803>

[Daneshyari.com](https://daneshyari.com)