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COMPUTATIONAL AND EMPIRIC CONSIDERATIONS REGARDING THE ELECTRO CATALYTIC REDUCTION OF CO2 BY WATER SOLUBLE COBALT PORPHYRINS

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The electrochemical reduction of CO_2 offers one of the possible solutions to current energy and sustainability issues since it can sequester carbon from the atmosphere and can be used to produce fuels and useful chemicals. In this respect, some metalloporphyrins have been reported to catalyse the electro reduction of CO_2. However, key issues still remain in regard to the elucidation of the effect of the porphyrin structure on the reaction mechanism and catalyst activity. An essential and necessary stage in the proposed mechanism for the catalytic reduction of CO_2 by the Co(II)/Co(I) porphyrin redox couple is the formation of an intermediate Co(II)porphyrin-CO_2- complex. In an attempt to examine the effect of positively and negatively charged porphyrin substituents on the catalytic activity, we report here on a combined density functional theory (DFT) and empirical study regarding the electrochemical reduction of CO in the presence of the Cobalt(II) 5,10,15,20-(tetra-N-methyl-4-pyridyl) porphyrin - Co(II)TMPyP and Cobalt(II) 5,10,15,20-(tetra-4-sulfonatophenyl) porphyrin – *Co(II)TPPS* complexes, with charges of +4 and -4, respectively. The lower catalytic activity of the CoTPPS complex as compared to that of CoTMPyP, both dissolved in aqueous alkaline solutions, as demonstrated by cyclic voltammetry experiments, are in agreement with the DFT study. Columbic interactions seem to dictate the cobalt-carbon bond length and strength in the porphyrin-CO_2 intermediate, and consequently have an impact on its stability and on the overall catalytic activity towards CO_2 reduction

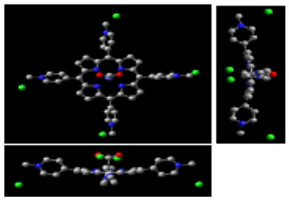

Figure 1: Calculated CoTMPyP-CO2 complex, top and side views

Biography

Yeshayahu Ben Eliyahu has received all his degrees in Chemistry from the Hebrew University of Jerusalem. His MSc and PhD theses were done under the supervision of the late Prof Yehuda Haas from the Physical Chemistry Department. He is working in the NRCN, Department of Chemistry since 1995. He has served as the Head of Department of Chemistry in NRCN from 2010-2013 and as the Head of Nuclear Engineering Department in the IAEC from 2013-2018. Now he is on Sabbatical in the Department of Chemical Engineering in Ben-Gurion University of the Negev in Israel.

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