CATALASE ACTIVITY OF MANGANESE(III) COMPLEXES

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The study of oxidative stress and the close relationship this has with ageing means there is much interest in the effects of antioxidant complexes, which often contain manganese. Although experimental data in biological studies have shown very positive effects in prolonging the lifespan of mice, [1] there is much uncertainly about what is the origin of these effects and how they could be improved. Interestingly, very few chemical investigations have been performed on this subject, [2,3] and even less using computational chemistry. Therefore, we studied the mechanism of a catalase reaction of manganese-salen complex that proved beneficial at the biological level, using advanced methods of computational chemistry. [4] The catalase mechanism contains two phases, a first one in which a Mn^{III}-salen complex captures an oxyigen from a hydrogen-peroxide into water and oxygen:

(i) Mn^{III}-salen + HOOH => Mn^{V}=O-salen + H_2O
(ii) Mn^{V}=O-salen + HOOH => Mn^{III}-salen + H_2O + O_2

Besides a detailed description of all the different reaction pathways present in the mechanism and the important role of the spin state, [5] we have found new results and concept that open the possibility of improving the efficiency and feasibility of the antioxidant complex. This is especially relevant for the initial part of the mechanism. Where the manganese complex gas to capture the hydrogen-peroxide in order to activate it. Two important aspects for the description of the reaction mechanism is the ability of the computational methods to correctly describe the spin-state and the weak interactions, for which S12g performs excellently. [4]

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