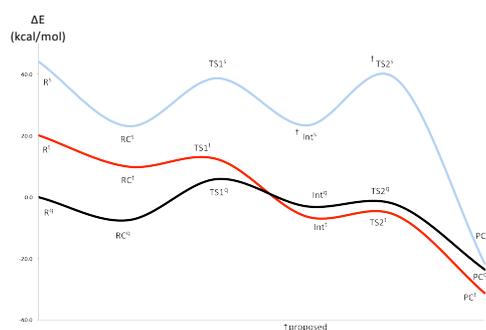
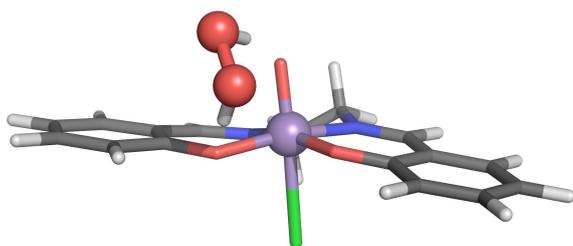


MECHANISM OF ACTION OF SALEN-MANGANESE ANTIOXIDANT COMPLEXES: THE CATALASE REACTION TO NEUTRALIZE OXYGEN SPECIES

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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 uncertainty 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 a salen-manganese complex that proved beneficial at the biological level, using advanced methods of computational chemistry.^[4] Besides a detailed description of all the different reaction pathways present in the mechanism, we have found new results and concepts 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 has 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 method to correctly describe the spin-state and the weak interactions, for which S12g performs excellently.^[4]

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