MOLECULAR MECHANICS MODELLING OF A MANGANESE(II) TRICYCLIC CHELATE OF N,N'-PENTAMETHYLENEBIS(SALICYLIDENEIMINE)

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Manganese plays an important role in the oxygen metabolism, and therefore numerous synthetic high-oxidation state manganese complexes with Schiff base ligands and their Mn(II) precursors enjoy considerable interest as possible biomimetic models. One representative of such complexes is the tricyclic chelate of Mn(II) with N,N'-pentamethylenebis(salicylideneimine). In the present study we performed a conformational analysis of this complex on the basis of molecular mechanics (MMX) calculations. As initial approximations to the geometry of the eight-membered chelate ring, three of the lowest in energy minimum-energy conformations (MECs) of the cyclooctane molecule were chosen: boat-chair (bc), twist-chair-chair (tcc) and crown, with energies of 81, 85 and 86 kJ mol⁻¹, respectively. Starting from the bc-based structures, five MECs of the complex were obtained, corresponding to the five different positions which Mn- and the two N-atoms can occupy on the bc-shaped ring. Three of them have very similar energies (148-152 kJ mol⁻¹), one of them possesses the highest energy (175 kJ mol⁻¹), and the remaining one has the lowest energy (145 kJ mol⁻¹) with respect to all of the MECs obtained. The geometry of this conformation is depicted below.

In a similar way, from the corresponding tcc-structures, two MECs of the complex were produced, and from the crown-structure, one MEC was obtained. Their energies are 148, 152 and 148 kJ mol⁻¹, respectively.

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