عنوان مقاله:

DFT study of the Jahn-Teller Effect in six coordinate copper(II) complexes

محل انتشار:

سومین همایش ملی تحقیقات نوین در شیمی و مهندسی شیمی (سال: 1390)

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خلاصه مقاله:

Molecular distortion due to an electronically degenerate ground state is named as Jahn Teller effect. In this study the structure of copper (II) complexes with different ligands which have different ligand field, were optimized by the B3LYP method and the LANL2DZ basis set. The optimized structures of these complexes don't show any difference between lengths of ligands to Cu ion. Calculation of the molecular orbital of complexes with the B3LYP method and 6-311++G** basis set shows that the M.O. of them is different. The results show that the HOMO in 2 directions vary from others and may be the reason of difference seen in bond length. The results of this research may be the beginning of the interpretation of Jahn Teller effect.

کلمات کلیدی:

Jahn-Teller , DFT , B3LYP , LANL2DZ ،Orbital

لینک ثابت مقاله در پایگاه سیویلیکا: