Molecular structures of iridium(III) complexes containing protonated (enH^+) and non-protonated (en*) monodentately bound 1,2-ethanediamine: *mer*-$[Ir(en)(enH)Cl_3]^+$ and *mer*-$[Ir(en)(en^*)Cl_3]$. Comparative DFT and ab initio theoretical study.

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Streszczenie

Extensive density functional theory (DFT) and correlated ab initio calculations are performed to study geometrical structures of the title Ir complexes. All the structures are fully optimized and the associated charge distribution is computed with the natural population analysis (NPA). For the cation mer-[Ir(en)(enH)Cl3]+ (1), two nearly degenerate geometrical isomers denoted (1a) and (1b) and differing by the conformation of the bidentately attached 1,2-ethanediamine (en) ligand have been found. The calculated conformation of en in mer-[Ir(en)(enH)Cl3]+ (1a) and in the non-protonated complex mer-[Ir(en)(en*)Cl3] (2) are in a close agreement with the X-ray diffraction values by Galsbøl et al. The conformation of the monodentate enH+ ligand in the isolated cation is found to be stabilized via intramolecular N–H···Cl hydrogen bonds. For the complex (2), the theoretical predictions of the bond distances and bond angles involving the unique non-chelate 1,2-ethanediamine (en*) are expected to be more reliable than the X-ray results. A good agreement between the DFT B3LYP and ab initio MP2 results is observed.

Słowa kluczowe

Iridium(III) complexes, Ab initio, Density functional study

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