

عنوان مقاله:

The effect of Mg atom on proton affinities of CH₃CONHO Ligand; A theoretical study

محل انتشار:

بیست و یکمین سمینار شیمی معدنی انجمن شیمی ایران (سال: 1398)

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خلاصه مقاله:

A theoretical study on protonation of CH₃CONHO Ligand in the presence of Mg atom has been reported. The gas-phase protonation energies (PA1) were computed using density functional theory (DFT) calculation. The proton affinity of a monobasic neutral ligand (related to the acidity) at 0 K is defined as the negative of the electronic energy difference between HL⁺ and L together with a correction for the difference in zero point energies. Two species CH₃CO (H⁺)NOH and CH₃CON(H⁺)OH can be considered in protonation of the above ligand. In order to understand the effect of Mg atom on protonation of CH₃CONHO Ligand which connect to OH group of this ligand (Fig. 1), the values of PA1 for two species before and after connection of Mg atom were calculated. The connection of Mg atom to OH group of this ligand has a decreasing effect on PA1 of two species.

کلمات کلیدی:

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