

Metal-Ligand Bond Vibrations In Alkaline Earth Metal Acetylacetonates

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The infrared and Raman spectra of alkaline earth metal acetylacetonates were recorded. The absorption bands below 900 cm⁻¹ were assigned in terms of the calculated fundamentals. Density functional theory (DFT) calculations were carried out at the B3LYP/LANL2DZ level to optimize the structures and obtain the vibrational spectra of these compounds. These calculations were also repeated for Be, Mg, and Ca acetylacetonates at the B3LYP and BLYP levels using 6-311++G**, 6-311G*, and 6-31G* basis sets. Analysis of the vibrational spectra indicates that there are several bands related to the metal-oxygen vibration. To investigate the effect of the central metal ion on the bond order, the charge distributions, electron delocalization, and bond energies in alkaline earth metal acetylacetonates were also studied by the natural bond orbital (NBO) analysis [1,2] and the atoms in molecules (AIM) theory [3]. The results of NBO analysis indicate that the resonance effects have an important role in stabilization of these complexes. A good correlation was obtained between stability constant and the symmetric M-O stretching of these complexes.

References

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