

Abstract

This thesis compares the results of four theoretical methods to calculate the molecular orbitals against the experimental data. The calculations were carried out in five basis sets, differing mainly in size, upon the set of reference molecules – diatomic hydrides of transition metals. The values, compared to the experiment, include interatomic distance, dissociation energy, anharmonicity and selected vibrational data.

Calculations ignoring the theory of relativity provided unusable results. Coupled cluster method was confirmed as the most accurate one and the accuracy of the basis sets was corresponding with their sizes.

Results of one of the smaller-sized basis sets were significantly improved with the addition of several polarizing orbitals. Keeping the calculation times significantly shorter, its accuracy was similar to the largest of the used basis sets.