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Potential energy surface, quartic force fields and vibrational levels of chlorine dioxide anion

A Shayesteh, E Falatooni, and M Sadat Motallebipour

School of Chemistry, College of Science, University of Tehran, Tehran, Iran

E-mail: ashayesteh@ut.ac.ir

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Abstract

Potential energy surface was calculated for the ground electronic state of the triatomic ion ClO_2^- using the coupled-cluster method CCSD(T). Calculations were carried out for 1200 points on the potential energy surface, and the calculated points were fitted to the potential energy expression in terms of the internal coordinates, from which the quadratic, cubic and quartic force fields were determined. Using the second-order rovibrational perturbation theory, harmonic vibrational frequencies, anharmonicity constants and several other spectroscopic parameters were calculated, and accurate fundamental vibrational frequencies were obtained. Also, the energies of 30 lowest vibrational levels were calculated using the anharmonicity constants.

Keywords: potential energy surface, coupled cluster method, quartic force fields, vibrational anharmonicity

For full article, refer to the Persian section