THEORETICAL COMPARISON OF THE EXCITED ELECTRONIC STATES OF THE URANYL AND URANATE IONS

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Understanding the nature of the uranium oxide compounds at fundamental levels of theory, especially the electronic structure of uranium oxides, is essential to monitoring chemical changes of uranium oxides with time and environment using electronic spectroscopy. The work performed involved calculating theoretical electronic states of uranium (VI) oxides using a new relativistic effective core potential for uranium. Theoretical electronic states of the linear uranyl (UO_2^{2+}) ion were calculated. Particular focus was paid to those electronic transitions occurring at optical frequencies. Excited electronic states of a uranate ion (UO_4^{2-}) are also calculated, in order to examine the effect of oxygen coordination on the electronic spectra of uranium oxides. Both results are compared with experimental results. The uranyl ion results were excellent agreement with experimental measurements of the fluorescent series.