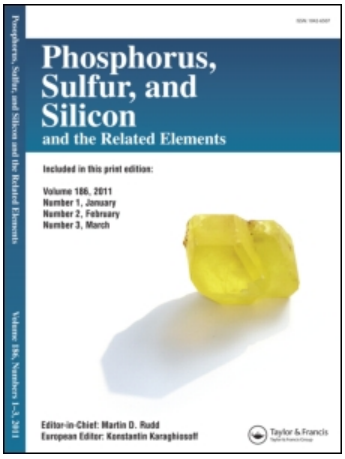

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SEMIEMPIRICAL CALCULATION OF THE INNER SHELL BINDING ENERGY SHIFTS IN MOLECULES INVOLVING SULPHUR ATOM

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The inner core binding energy shifts of sulphur atom in various chemical environments were studied by the semiempirical self-consistent charge molecular orbital method,. The relaxation energy was taken into account by using two distinct approaches: (a) reorganization potential method and (b) transition potential method. The changes in ESCA chemical shifts of sulphur are satisfactorily accounted for by the latter method, the standard deviation from the experimental data being 0.2 eV. It appears that the reorganization energy plays an important role in rationalizing inner core binding energy shifts of sulphur.