

Sulfur K-Edge X-Ray Absorption Spectra of SF₆, H₂S and SO₂

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Abstract

Sulfur K-edge x-ray absorption spectra of gaseous compounds SF₆, H₂S and SO₂ were measured using a synchrotron radiation source at Ritsumeikan University. Two kinds of method for x-ray absorption measurements, a transmission mode and a total electron yield mode, were applied to this study, and the spectra obtained experimentally were compared with those calculated non-empirically by means of the DV-X α molecular orbital method. Orbitals related to the resonant absorption observed at 2484 eV in the SF₆ spectrum were found to be 7t_{1u}, 8t_{1u} and 9t_{1u}, while those observed at 2470 eV in the H₂S spectrum were 3b₂ and 6a₁. The spectrum for SO₂ is quite similar to that for H₂S, except that the absorption band positions for SO₂ shift slightly to the high energies compared to those for H₂S. Spectra obtained by the DV-X α molecular orbital calculation based on the transition state of the electronic excitation agreed excellently with the experimental results.

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