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تقنيات حسابية في أطياف الجزيئات ثنائية الذرة

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Abstract : In diatomic spectroscopy, computational techniques are required in a number of problems. The oxygen molecule is very important to us and life would not be possible without it. The oxygen and ozone molecules protect life on Earth from harmful solar UV radiation. Therefore, we have developed an ideal model to study the atmospheric absorption spectrum due to pure molecules in the UV region (175 - 300 nm). These include the Herzberg I bands ( ), the Herzberg II bands ( ), the Schumann – Runge bands ( ) and the Herzberg continuum. The BOUND computer program of Telle and Telle (1982) is used for constructing the Rydberg - Klein - Rees potential energy curves of the , , and as well as in calculating the Franck - Condon factors of the three systems involved. We have simulated the absorption spectrum of the ( ) system for ?- progression (,) using the TRISING program which is developed in this work. We have also simulated the absorption spectrum due to the ( ) system for (,) and to the ( ) system for ?- progression (,) using the TRIPLET program which is also developed in this work. The simulated spectra are then compared with the experimental spectra. Using the simulated spectra we could also determine the ratios of band oscillator strength

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