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: Comparative study of five-parameter potential energy function of diatomic

molecule

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**Abstract** 

: There are different methods by which the potential energy curve for a molecule can be obtained. One of the methods is the Rydberg – Klein – Rees (RKR) method. Another method is based on the empirical functions where the parameters in the expressions are evaluated from the known spectroscopic constants. We have used the later method in the potential curve calculation of stable diatomic molecules. we have proposed four proposed function of five – parameters to perform the potential curve calculation of 15 molecular states of different diatomic molecules . In order to perform a comparative study, calculation of potential curves have been done using the three-parameter Morse function (1929), the five-parameter Hulburt-Hirschfelder function (1941) and the five-parameter Al-Senany functions (1999) for the 15 molecular states. All these values are compared with the RKR values. We have studied different methods which are used for describing the asymptotic part of the potential curve; we also used these methods and others to obtain the dissociation energy. This part is described by the long-range potential function. We have found the dissociation energy and the long-range constants using both the near-dissociation theory and the extended near-dissociation theory for the XOg+ state of I2. The Birge-Sponer and the atomic products method are another way for determining the dissociation energy, which is also included in this work

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