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Abstract

: The electronic spectra of diatomic molecules comprise of the vibrational and rotational structure in the UV and visible region mostly. If sufficient spectroscopic data is available, potential energy curves are built from the experimentally determined vibration-rotation energy levels by well known Rydberg-Klein-Rees method. An alternative procedure of proposing empirical potential functions is adopted when the data is insufficient. In order to devise our own methods of analyzing the spectroscopic data, the experimental data of Rafi et al (1993c, 1991) of the G-X system of Bi2 and F-X system of Na2 have been used for vibrational analysis in these studies. For rotational analysis we chose the data of F -X sys- tem of hydrides and deuterides of Ca, Sr and Ba of Edvinsson et al (1963). We analyzed these bands: CaH O-O CaD 0-0, 1-0 SrH 0-0,1-0~ SrD 0-0, 1-0~ BaH 0-0, 1-0. With our computer methods of analysis, we obtained the results which are in agreement with the earlier work. On the availability of large amount of data on the photo absorption spectra of LiH, NaH and KH Al E+ -Xl E+ systems we have extended this work to construct the Rydberg-Klein-Rees potential curves of Al E+ states in the new regions. Computer program of Professor Le Roy has been used in these calculations of RKR curves. We have also proposed a new five-parameter empirical potential function. Potential curve calculations on fifteen molecular states have been made using this function and these are compared with Rydberg-Klein-

Rees method calculations

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