

# Response to the comment on: “Universal relation between spectroscopic constants”

SARVPREET KAUR and C G MAHAJAN

Department of Physics, Panjab University, Chandigarh 160 014, India

E-mail: cgm@pu.ac.in

- (1) The author, S Chandra, has used his own definition of Sutherland parameter,  $\Delta = \omega_e r_e^2 / 2D_e$  at variance with the correct relation  $\Delta = k_e r_e^2 / 2D_e$  where  $k_e = \mu \omega_e^2$  (see *J. Chem. Phys.* **8**, 161 (1940) and also [1443] in *Spectra of diatomic molecules*, G Herzberg, vol. I, 2nd ed., p. 459, paragraph 2). His wrong definition has resulted in highly erroneous values of  $r_e$ .
- (2) With our equation  $\ln G = 1.91578 + 0.9711 \ln \Delta$  (omitting the standard deviations) the value of  $r_e$  for  $\text{Li}_2 X^1\Sigma_g^+$  comes out to be 2.52 Å against the experimental value of 2.6729 Å.

Furthermore, the author has approximated the above equation to  $\ln G = 2 + \ln \Delta$ . This has further introduced the error in determining the value of  $r_e$ . Even with this approximated equation and using the correct definition of Sutherland parameter the value of  $r_e$  turns out to be 2.359 Å instead of the alarmingly high 14.27 Å given in table 1. We have checked only one molecular state, i.e.,  $\text{Li}_2$ ; we are however sure this will be the situation for the rest of the molecular states.

- (3) The author has used eq. (6) of his paper to calculate  $D_e$ . This relation leads to a large deviation from the correct value depending upon the extent to which experimental values are known. Guided by this fact, in our work, we used experimentally observed  $D_e$  values to derive the relation between spectroscopic constants. We may further mention that the relation  $\Delta = 2.2r_e$  is based on the experimental values (values taken from literature) of  $\mu, \omega_e, r_e$  and  $D_e$  of alkali diatomic molecules. Nowhere in our work we attempted to derive an analytical relation and had simply observed the factual experimental facts as shown in table 3 of our paper.

Incidentally we may mention that the author has again committed a mistake in putting that the column 4 of table 2 (author's paper) gives the value of Kaur and Mahajan. In fact these are experimental values taken from the literature.