

Rejoinder

Authors' reply to the comments* made by Suresh Chandra on their paper† entitled "Dissociation energy of diatomic molecules"

SARVAPREET KAUR and C G MAHAJAN

1. Suresh Chandra has started his comments on the presumption that we have used experimental data on D_e to evaluate it. This seems to be constructed on the basis of our inclusion of D_e experimental data in table 1 of our paper. We have not used experimental values of D_e as input for computations. As mentioned on page 399 of our paper, we have only approximated D_e by $\omega_e^2/4\omega_e x_e$ to initiate the iteration. In fact, this is same as $(Y_{10})^2/(-4Y_{20})$ employed by him to obtain the value of D_e .
2. He writes that the Klein integral f is given analytically by eq. (6) of his paper which, for limited Dunham's coefficients, yields

$$\text{Dissociation energy, } U = (Y_{10})^2/(-4Y_{20}) \quad (1)$$

or in terms of spectroscopic notations

$$U = \omega_e^2/4\omega_e x_e. \quad (1a)$$

Equation (1a) is the one we have used to have the approximate values. Relations (1) are applicable when the quadratic equation, $\omega_0 v - \omega_0 x_0 v^2$ represents all the vibrational levels correctly. That means, ΔG is a linear function of v . Usually, this is not the case with most of the molecules as ΔG vs v curve deviates significantly at large v and particularly near the dissociation point. On the other hand, unlike the consideration of only two parameters $\omega_e(Y_{10})$ and $\omega_e x_e(-Y_{20})$ as is done by him, in the empirical relation (eq. (3) in our paper) C represents the commutative effects of rotational, vibrational, rotation-vibration constants and also possibly the finer interaction constants. In other words, we have taken into consideration a large number of Dunham's coefficients that yield, as very rightly pointed out by him, results very close to the experimental values. Even in the analytical relation for C (eq. (5) of our paper) where the relation is limited to five parameters only, the rotation-vibration interaction, α_e and rotational constant, B_e play significant role in the accurate determination of C (also refer our other paper, *Pramana - J. Phys.* **52**, 409-420, April 1999).

I sincerely hope that our response will clarify the situation/misunderstanding. We beg to say that in our views, the comments/communication of the author has no meaningful substance in it. The relation Suresh Chandra has arrived at does not lead to even close approximate values (see, G Herzberg, *Molecular spectra and molecular structure*, 2nd edition, vol. 1, p. 100, eq. III-97, Van Nostrand Reinhold Company, New York).

* Appeared in *Pramana - J. Phys.*, **56**, (4), April 2001, pp. C585-C587.

† *Pramana - J. Phys.* **50**(5), May 1998, 397-403