ON THE DETERMINATION OF THE AVERAGE IMPACT PARAMETER IN THE RATCF MODEL

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A procedure for deriving the average impact parameter $b_{av}(i, f)$ using a refined version of the Anderson–Tsao–Curnutte–Frost model is reported. It is shown that this way of determinating $b_{av}(i, f)$ has no appreciable effect on the accuracy of calculation of the line half–widths and lineshifts of molecules.

In our construction of a refined version of the Anderson—Tsao—Curnutte—Frost model (RATCF)[1] for absorption at the frequency $\omega_{fi} = E_f - E_i$ we used the average impact parameter $b_{av}(i, f)$. Let us examine its derivation. This parameter appears when integrating the real and imaginary parts of the differential collision cross section (S_2 and $\tilde{S}_2$) over the impact parameter in problems of the lineshift and line broadening. In order that the results of integration of the functions S_2 and $\tilde{S}_2$ over the impact parameter be independent of the method used (the Anderson–Tsao–Curnutte–Frost model[2,3] or the Srivastava approach[1,4]), the following equality must be satisfied:

$$S_{2t}(b(i,f), \upsilon(i,f), F_{Nt}(b(i,f))) = \frac{2S_{2t}(b(i,f),\upsilon(i,f),f_{Nt}(b_{av}(i,f)))}{h_t - 2}, \quad (1)$$

which transforms into

$$f_{Nt}(b_{av}(i, f)) = \frac{(h_t - 2)}{2} F_{Nt}(b(i, f)),$$

$$\tilde{f}_{Nt}(b_{av}(i, f)) = \frac{(h_t - 2)}{2} \tilde{F}_{Nt}(b(i, f)), \quad (2)$$

where $\upsilon(i, f)$ is the average relative velocity of motion of the interacting molecules associated with the states i and f of the absorbing molecules, f_N is the nonadiabatic function derived before integrating the differential collision cross section over the impact parameter, F_N is the nonadiabatic function derived after integrating S_2 and $\tilde{S}_2$ over the impact parameter, and h_t is the power of the impact parameter which enters into the functions:

$$S_2 = \sum_t S_{2t} = \sum \lambda_t / b^{h_t} \text{ and } \tilde{S}_2 = \sum_t \tilde{S}_{2t} = \sum \lambda_t / b^{h_t}$$

where $1/b^{h_t}$ determines the explicit part of the impact parameter.

If in the definition of the parameters $k = \frac{b(i, f)}{t(i, f)} \Delta\omega$ we use the values $k' = k + 0.7$ and we take the increment Δb to be equal to $\frac{0.7 \cdot \upsilon(i, f)}{\Delta\omega}$, then

$$b_{av}(i, f) = b(i, f) + \Delta b \quad (3)$$

and Eqs. (1) and (2) are accurate to within 1–5% for each t–type of the interaction (see Figs. 1 and 2).

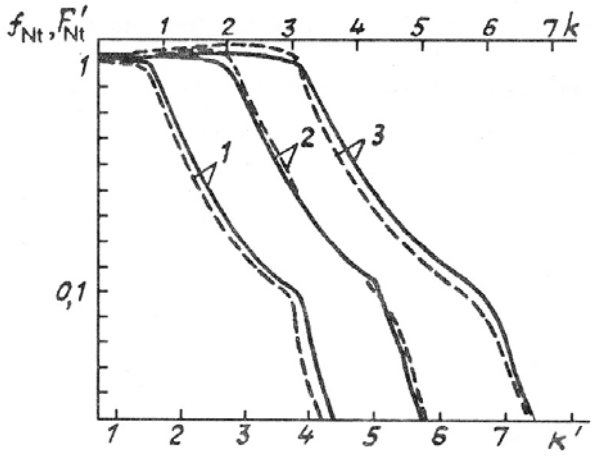

FIG. 1. The nonadiabatic functions f_t and F'_t for the three main interaction types: dipole–dipole (curve 1, $t = 1$), dipole–quadrupole (curve 2, $t = 2$), and quadrupole–quadrupole (curve 3, $t = 3$). The solid lines stand for $f_{Nt}(k')$, the broken lines for $F'_{Nt}(k) = \frac{h_t - 2}{2} F_{Nt}(k)$.

According to the RATCF approach the half–width parameter $\gamma(b(i, f), F_{Nt}(b(i, f)))$ is then replaced by $\gamma\left(b(i, f), \frac{2f_{Nt}(b_{av}(i, f))}{h_t - 2}\right)$ with an error of not more than 1% (Fig. 1). In the calculations of the line center shift

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$\delta(b(i, f), F_{Nt}(b(i, f))$ is then replaced by $\delta\left(b(i, f), \frac{2\tilde{f}_{Nt}(b_{av}(i, f))}{h_t - 2}\right)$, which results in a slight increase in the computational error (up to ~ 2–5%). However, the calculation of the lineshift in terms of the average shift $b_{av}(i, f)$ makes it possible to estimate the contributions of the third– and the fourth–order interaction to the line center shift, which may significantly exceed (by a few tens of percent) the computational error in the parameter δ.

Thus, the calculations of the relaxation parameter by the following formulas:

$$\gamma\left(b(i, f), \frac{2f_{Nt}(b_{av}(i, f))}{h_t - 2}\right) \text{ and } \delta\left(b(i, f), \frac{2\tilde{f}_{Nt}(b_{av}(i, f))}{h_t - 2}\right)$$

makes it possible to increase the information content without any appreciable effect on the computational accuracy.

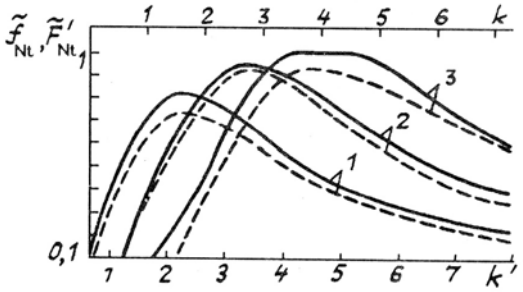

FIG. 2. The nonadiabatic functions $\tilde{f}_t$ and $\tilde{F}'_t$. The notation is the same as in Fig. 1.

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