$$\begin{aligned}
S_1(\omega) = & \cos^2 \phi \{ Y_1 \delta(\omega) + \frac{1}{2} (I/2\pi T)^{1/2} (1+c)^{1/2} \int_{-1}^1 dx (1-x^2) \omega^{*2} \exp[-(1+cx^2)(\frac{1}{2}\omega^{*2})] \\
& + \sin^2 \phi \frac{1}{4} (I/2\pi T)^{1/2} (1+c)^{1/2} \{ \int_{-1}^1 dx [(1-x^2)/|cx|^3] \omega^{*2} \exp\{-\frac{1}{2} [(1+cx^2)/(cx)^2] \omega^{*2}\} \\
& + \int_{-1}^1 dx [(1+x)^2/(1+cx)^3] \omega^{*2} \exp(-\frac{1}{2} [(1+cx^2)/(cx)^2] \omega^{*2}) \}, \quad (29)
\end{aligned}$$

with $\omega^* = (I/T)^{1/2} \omega$. The higher-order spectral density functions can be obtained by substituting the corresponding expression for the rotational correlation function in Eq. (28). While the first- and second-order spectral density functions have been shown to be related to the appropriately normalized infrared and Raman band shapes,⁸ the physical interpretation of the higher-order functions is not available.

We have applied Eq. (9) to the analysis of neutron-scattering measurements on gaseous ammonia and water vapor. The calculation is based on a Gaussian representation of χ_r , and the procedure has been discussed in some detail in Ref. 1. In the case of NH_3 , the time-of-flight distributions of neutrons scattered at 20° and 90° are shown in Fig. 2 along with the experimental points⁹ and the earlier calculation [Eq. (14)]. In addition, exact quantum-mechanical results are available at 20° .¹⁰ In the case of H_2O , the moments of inertia of the asymmetric molecule are $I_x = 1.0243$, $I_y = 1.9207$, and $I_z = 2.9470 \times 10^{-40} \text{ g cm}^2$, and the H-O-H angle is $104^\circ 27'$.¹¹ Since rotational correlation functions for an asymmetric rotor have not yet been derived, we assume that H_2O can be treated as a symmetric

molecule with moments of inertia $I'_x = I'_y = \frac{1}{2}(I_x + I_y)$, $I'_z = I_z$, and ϕ as half of the H-O-H angle. The comparison of absolute scattering intensities with experimental data¹² is shown in Fig. 3.¹³ For the 21° scattering angle, we also include the spectrum computed using the Krieger-Nelkin model (effective mass 1.81).¹⁴ The discrepancy in the vicinity of $400 \mu\text{sec/m}$ could possibly arise from experimental effects, such as multiple scattering or small amounts of moisture in the sample.

In summary, we note that the two methods of deriving classical rotational correlation functions, the use of quantum-mechanical results for the intermediate scattering function,⁶ and the use of classical conditional distribution functions,² give identical results for freely rotating molecules. Model calculations which incorporate intermolecular torque effects are of interest, and for this purpose the approach of St. Pierre and Steele seems to be more appropriate.

ACKNOWLEDGMENT

We are grateful to W. Glaser for sending us his data on water vapor.

*Work performed under the auspices of the U.S. Atomic Energy Commission.

[†]Work supported by the National Science Foundation.

¹A. K. Agrawal and S. Yip, Phys. Rev. **171**, 263 (1968).

²A. G. St. Pierre and W. A. Steele, Phys. Rev. **184**, 172 (1969).

³A. Rahman, J. Nucl. Energy **13**, 128 (1961).

⁴In all subsequent equations, we use $\hbar = k_B = 1$.

⁵M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

⁶V. F. Sears, Can. J. Phys. **45**, 237 (1967).

⁷Handbook of Mathematical Functions, edited by M. Abramowitz and I. A. Stegun (Dover Publications, Inc.,

New York, 1965).

⁸R. G. Gordon, J. Chem. Phys. **43**, 1307 (1965).

⁹F. J. Webb, Proc. Phys. Soc. (London) **92**, 912 (1967).

¹⁰G. Venkataraman, K. R. Rao, B. A. Dasannacharya, and P. K. Dayanidhi, Proc. Phys. Soc. (London) **89**, 379 (1966).

¹¹G. Herzberg, *Molecular Spectra and Molecular Structure, Spectra of Diatomic Molecules* (D. Van Nostrand Co., Inc., New York, 1950).

¹²W. Glaser (private communication).

¹³A. K. Agrawal, Trans. Am. Nucl. Soc. **12**, 194 (1969).

¹⁴T. J. Kreiger and M. S. Nelkin, Phys. Rev. **106**, 290 (1957).

ERRATUM

Pressure Effects of Foreign Gases on the Absorption Lines of Cesium, S. Y. Ch'en and Robert O. Garrett [Phys. Rev. 144, 59 (1966); 144 66 (1966); 155, 38 (1967)]. An error has recently been discovered which necessitates our making certain corrections in the values of relative densities of foreign gases reported in the first four papers in our series. Papers V and VI are not in error. The original calculation made the incorrect assumption that the relative density (r.d.) of foreign gas is identical to the pressure in atmospheres that the gas in question would have if the temperature were reduced to 0°C. Our recalculation of r.d. assumes, instead, that it is the ratio of the molar volume of the foreign gas at 1 atm and 0°C to that of the foreign gas under the experimental conditions. Figure 1 gives a correction curve to enable one to redraw any figure in the four papers. Corrections are negligibly small for r.d.'s less than 10, for all graphs in the four papers. Since higher r.d. points are the most severely affected, some of the slopes reported in the text of the four papers also need revision. Those slopes needing correction are included in Table I.

TABLE I. Revised slopes of linear portions of certain graphs in papers I-IV.

Spectral line	Shift ($\Delta\nu_m/\text{r.d.}$) (in $\text{cm}^{-1}/\text{r.d.}$)		Half-width ($\Delta\nu_{1/2}/\text{r.d.}$) (in $\text{cm}^{-1}/\text{r.d.}$)	
	Former	Revised	Former	Revised
Cs(1)/He $^2P_{1/2}$	0.60 ± 0.01	0.68 ± 0.01	0.77 ± 0.02	0.78 ± 0.02
$^2P_{3/2}$	0.72 ± 0.02	0.86 ± 0.02	0.70 ± 0.02	0.71 ± 0.02
Cs(2)/Ne $^2P_{1/2}$	1.19 ± 0.02	1.24 ± 0.02	No slope reported	
$^2P_{3/2}$	1.31 ± 0.02	1.38 ± 0.02	No slope reported	
Cs(1)/Ar $^2P_{1/2}$	-0.51 ± 0.01	-0.46 ± 0.01	0.53 ± 0.03	0.49 ± 0.03
$^2P_{3/2}$	-0.94 ± 0.01	-0.88 ± 0.01	0.84 ± 0.02	0.77 ± 0.02
Cs(2)/Ar $^2P_{1/2}$	-2.75 ± 0.02	-2.71 ± 0.02	1.86 ± 0.02	1.82 ± 0.02
$^2P_{3/2}$	-2.83 ± 0.02	-2.79 ± 0.02	2.00 ± 0.05	1.96 ± 0.05
Cs(1)/Kr $^2P_{1/2}$	-1.32 ± 0.01	-1.24 ± 0.01	0.86 ± 0.03	0.78 ± 0.03
$^2P_{3/2}$	-2.09 ± 0.01	-1.87 ± 0.01	1.92 ± 0.05	1.78 ± 0.05

FIG. 1. Correction curves for relative density values in papers I-IV.