direct comparison between these two pulse-height distributions were obtained. Figure 1 shows a superposition of the two spectra measured simultaneously. It can be seen that the difference in the end-point values of the two distributions is less than 5 percent of the α-particle energy.

Since this surface effect is so small, it cannot be responsible for nonlinearity of response of (chemically cleaned) NaI crystals to α-particles. An incidental result is that trace amounts of polonium in a NaI(Tl) crystal do not affect its characteristic performance as a scintillation crystal.

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The Scattering of Slow Neutrons by O_2 Molecules*

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The scattering of slow neutrons by O_2 is due to nuclear interaction as well as magnetic forces arising from two magnetically active electrons. The molecular (nuclear) scattering is subdivided into elastic (coherent and incoherent) transitions and inelastic (mostly hyperelastic) transitions. The magnetic scattering is purely incoherent and essentially elastic. Numerical values are obtained for the integral cross sections of these various scattering processes in dependence upon the wavelength. The case of very long neutron wavelength is of greatest physical interest, since only then can a sizable magnetic effect be expected. The analysis requires careful consideration of the thermal motion of the O_2 molecules, which sometimes influences the order of magnitude of the result. More accurate experiments can be expected to lead to an independent measurement of the distribution of the magnetically active shell of valence electrons.

1. INTRODUCTION

THE present paper contains a detailed theoretical analysis of the scattering of very slow neutrons by O_2 molecules. One of us (O.H.) has announced some time ago, in very brief form, some theoretical estimates.[1] We present here a full quantitative discussion of this problem which will justify previous expectations that more refined experiments may lead to an analysis of the distribution of valence electrons in O_2.

The interaction between a neutron and the O_2 molecule is essentially twofold. There exists first the customary nuclear interaction caused by the two nuclei. In addition to it, the paramagnetic O_2 gives rise to a magnetic type of neutron scattering caused by the interaction between the magnetic moment of the neutron and the molecule.

This magnetic interaction, which has previously been analyzed in great detail,[2] has so far been studied experimentally mostly through observation on the salts of elements of the iron group in polycrystalline form. While very recent experiments[3] seem to lead to a satisfactory agreement between experiment and even finer points of the theory, it must be kept in mind that scattering experiments with solid targets are often accompanied by some disturbing features. The paramagnetic scattering of a neutron by O_2 can be expected to be essentially undisturbed; one can therefore hope to draw conclusions from a comparison of calculation and experiment which will lead to information concerning the distribution of the magnetically active shell.

It is, of course, necessary for this purpose clearly to isolate the magnetic scattering from the purely nuclear scattering. As shown before,[2] the magnetic scattering does not interfere with the nuclear scattering so that the latter may be calculated quite independently and the resulting total cross section can be subtracted from the observed cross section to obtain a value for the paramagnetic cross section.

Since, on the other hand, the earlier theory[2] of paramagnetic scattering leads us to expect that only neutrons of very long wavelength will have sufficiently large a form factor so that a sizable magnetic scattering can be expected, the analysis must be carried out for a range of wavelengths which make the calculations of inelastic transitions somewhat complicated. It will turn out that the change in the neutron energy accompanying inelastic (mostly hyperelastic) transitions will be, in general, large compared with the orignial neutron energy. This fact requires an individual study of all the matrix elements of significance, which are very numerous, since O_2 at room temperature occupies rotational states with quantum numbers 1 to 23 with appreciable frequency. Customary simplifications in the theory of neutron scattering by molecules are, therefore, no longer applicable.

It will also turn out that the thermal velocity of O_2 is comparable with the neutron velocity. The thermal motion of O_2 needs to be taken into account rather accurately in the study of the various contributions.

* Supported in part by the U. S. Office of Naval Research.
[1] O. Halpern, Phys. Rev. **72**, 746 (1947).
[2] O. Halpern and M. H. Johnson, Phys. Rev. **55**, 898 (1939).
[3] Smith, Taylor, and Havens, Phys. Rev. **88**, 163 (1952).

The experimental side of the question will be discussed in Sec. 7 of this paper.

2. THE NUCLEAR INTERACTION

The neutron is characterized by its wave vectors $\mathbf{k}$ and $\mathbf{k}'$, referring to the momentum before and after the collision in the mass center system of neutron and molecule. To describe the nuclear interaction we introduce, as is customary,[4] the simplified Fermi potential for use in Born approximation:

$$-(2\pi\hbar^2/m)a[\delta(\mathbf{r}-\mathbf{r}_1)+\delta(\mathbf{r}-\mathbf{r}_2), \quad (1)$$

in which m=neutron mass, $\mathbf{r}$=position vector of neutron, and $\mathbf{r}_1$, $\mathbf{r}_2$=position vectors of nuclei. The single atom potential gives for scattering by an atom of infinite mass the cross section $4\pi a^2$. Experimentally, it has been found by Melkonian[5] that the cross section of a free oxygen atom amounts to 3.73 barns. This means that $4\pi a^2$ for the case of oxygen must be put equal to $3.73(17/16)^2$ to account for the reduction in cross section due to the reduced mass of the system of neutron and oxygen atom. The molecule is characterized by its rotational and magnetic quantum numbers l and m. The vibrational eigenfunction is treated as a delta-function, which introduces the equilibrium nuclear separation of the ground state, denoted by d. This assumption is modified later when a correction to d due to vibrational motion is discussed.

The matrix element leading, for the neutron, from the state $\mathbf{k}$ to the state $\mathbf{k}'$ and, for the molecule, from the state l, m to the state l', m' is then proportional to the quantity

$$(\mathbf{k}, l, m|M|\mathbf{k}', l', m') = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta Y_{l,m}^*(\theta,\phi) \times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)Y_{l',m'}(\theta,\phi), \quad (2)$$

in which $Y_{l,m}(\theta,\phi)$ are normalized spherical harmonics and in which $(\mathbf{k}-\mathbf{k}')$ has been chosen as the Z axis of the internal coordinates of the molecule, as is permitted by the principle of spectroscopic stability. The electronic eigenfunction of O_2 is antisymmetric in the nuclear coordinates; this limits l to odd integers in order that the total eigenfunction be symmetric in the nuclear coordinates. For calculation of the total cross section (i.e., both coherent and incoherent), we must sum the squares of the matrix elements over the final, and average over the initial degeneracies in the magnetic quantum number to obtain for the differential cross section (via the Born formula), in the center-of-mass system of neutron and molecule, the expression:

$$d\sigma_{\mathbf{k},l;\mathbf{k}',l'} = 4a^2\left(\frac{\mu}{m}\right)^2\frac{k'}{k} \times\frac{1}{2l+1}\sum_{m,m'}|(\mathbf{k},l,m|M|\mathbf{k}',l',m')|^2 d\Omega, \quad (3)$$

in which μ is the reduced mass of neutron and oxygen molecule and $d\Omega=\sin\Theta d\Theta d\Phi$ is the element of solid angle of the sphere of scattering. Because of the orthogonality of the $Y_{l,m}$ in ϕ and the ϕ-independence of our operator, the sum over m' of the squares of expression (2) reduces to

$$\sum_{m'}|(\mathbf{k},l,m|M|\mathbf{k}',l',m')|^2 = \left|\int_0^{\pi}\sin\theta d\theta P_{l,m}(\cos\theta) \times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)P_{l',m}(\cos\theta)\right|^2, \quad (4)$$

in which $P_{l,m}(\cos\theta)$ are the normalized θ-dependent parts of $Y_{l,m}(\theta,\phi)$. The total cross section for the transition k, l to k', l' becomes

$$\sigma(p,l)_{k,l;k',l'} = 4\cdot 4\pi a^2\left(\frac{\mu}{m}\right)^2\int\frac{d\Omega}{4\pi} \times\left\{\frac{1}{2l+1}\sum_m\frac{k'}{k}\left|\int_0^{\pi}\sin\theta d\theta P_{l,m}P_{l',m} \times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)\right|^2\right\}, \quad (5)$$

in which $k'/k=(p^2+2\mu\Delta E)^{\frac{1}{2}}/p$ and $p=k\hbar$ denotes the initial neutron momentum, and ΔE is the energy change of the neutron which is positive for hyperelastic and negative for inelastic transitions. The strength factor $4\cdot 4\pi a^2(\mu/m)^2$ has the value of 15.84 barns.

Since the number of neutrons removed from the beam per unit time is invariant with respect to Galilei transformations, we have, for our case of a gas target in which the neutron has initial laboratory velocity $\mathbf{v}$ and the molecule initial laboratory velocity $\mathbf{u}$, the following expression for the cross section at a given gas temperature for the above transition:

$$\sigma(v,l)_{k,l;k',l'} = \int|\mathbf{v}-\mathbf{u}|/vN(\mathbf{u})\sigma(p,l)_{k,l;k',l'}d\mathbf{u}, \quad (6)$$

in which $p=\mu|\mathbf{v}-\mathbf{u}|$ and $N(\mathbf{u})$ is the normalized Maxwell velocity distribution in $\mathbf{u}$. This Doppler correction is an average, with multiplication by the factor $|\mathbf{v}-\mathbf{u}|/v$, over all p's. For a given laboratory neutron wavelength $\lambda=h/mv$, the cross section at a given gas temperature will be an average over l of expression (6).

[4] J. Schwinger and E. Teller, Phys. Rev. **52**, 286 (1937).
[5] E. Melkonian *et al.*, Phys. Rev. **76**, 1750 (1949).

3. ELASTIC TRANSITIONS

Our procedure is to calculate $\sigma(p, l)$ of expression (5) for the various types of transitions as a function of $p=\mu|\mathbf{v}-\mathbf{u}|$ and then to perform the Maxwell averaging as indicated in (6). We obtain the elastic cross section by setting $l=l'$ and $k=k'$. It should be emphasized that all of the result will not be coherent. Only transitions involving no change in the magnetic quantum number m are in this category. We will see, however, that the coherent part of the elastic scattering is large compared with the incoherent. Our calculation proceeds by expanding $\cos(\frac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)$ to the fourth power in $\cos\theta$. The validity of this expansion is justified by the long wavelengths considered. It should be remarked that the fourth-power contributions are significant in the range 5 to 10A only because of an effective wavelength shortening due to the thermal motion of the molecules. Our calculation of expression (5) for the total elastic cross section (averaged over the thermal distribution in l) leads to

$$\sigma(p, l)_{k;k}=15.84[1-\tfrac{1}{6}(kd)^2+0.01682(kd)^4 -9.00\times10^{-4}(kd)^6+2.08\times10^{-5}(kd)^8]. \quad (7)$$

The above formula is derived in the Appendix where also the Maxwell averaging is discussed. We have tabulated the total and coherent values for the elastic cross section at a gas temperature of 300°K in Table I. The distinction between coherent and incoherent elastic scattering, with formulas for the former, is presented in the Appendix.

4. INELASTIC TRANSITIONS

It will turn out that among the inelastic transitions only the hyperelastic are of quantitative significance in the wavelength range studied. If we again use the simplifications introduced in Sec. 3 of replacing the cosine operator by its power expansion, then obviously the first term gives no contribution on account of the orthogonality of the rotational eigenfunctions referring to l. The second term which is proportional to $\cos^2\theta$ permits only transitions between rotational states l and $l\pm2$. The third term, proportional to $\cos^4\theta$, has matrix elements for $|\Delta l|=2$ and 4. We shall here only discuss transitions $l\rightarrow l-2$; the Appendix shows that, for all wavelengths, the quantitative contribution coming from transitions $l\rightarrow l-4$ is small. Expression (5) for the case $l\rightarrow l-2$ is

$$\sigma(p, l)_{k,l;k',l-2}=15.84\int\frac{d\Omega}{4\pi}\left[\frac{1}{2l+1}\sum_m\frac{(p^2+2\mu\Delta E)^{\frac{1}{2}}}{p} \times\left|\int_0^\pi\sin\theta d\theta P_{l,m}(\cos\theta) \times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)P_{l-2,m}(\cos\theta)\right|^2\right]. \quad (8)$$

The essential difference occurring in (8) as compared with the elastic is the appearance of the factor $(p^2+2\mu\Delta E)^{\frac{1}{2}}/p$. It arises from the energy increase of the scattered neutron, which carries away some of the rotational energy of the O_2 molecules. This factor must not be confused with the factor $|\mathbf{v}-\mathbf{u}|/v$ of expression (6), which is exclusively caused by the translational thermal motion of the O_2 molecules.

TABLE I. Total elastic and coherent cross sections in barns at a gas temperature of 300°K.

λ	5.1A	7.5A	10.0A
Total elastic cross section	11.01	14.59	17.95
Coherent cross section	10.89	14.46	17.84

The method of evaluation of (8) and its averaging over the various states of the O_2 molecules is shown in the Appendix. One sees from the results given in Table II that the hyperelastic transitions make a very substantial contribution to the total nuclear cross section. It is perhaps surprising at first to notice that the hyperelastic cross section increases slightly if the wavelength of the incident neutron increases from 5 to 10A. One would have expected, from the expansion of the cosine operator in (8), that hyperelastic transitions become less significant with longer wavelengths. The reason for the opposite behavior is to be found in the energy acquired by the neutron in a hyperelastic collision which is usually much larger than the original energy of the incident neutron. The $|\mathbf{k}-\mathbf{k}'|$ factors in (8), therefore, are not very much influenced by the fact that p decreases strongly if λ increases from 5 to 10A. It is kept almost constant by the large value of p' while the factors k'/k and $|\mathbf{v}-\mathbf{u}|/v$ of formula (6) in front of the cross section increase with decreasing neutron velocity. This explains qualitatively the quantitatively obtained increase of the hyperelastic cross section.

5. DISCUSSION OF SOME CORRECTIONS

The treatment given so far is incomplete, since inelastic transitions accompanied by an energy loss of the neutron have not yet been included. We shall here refrain from presenting in detail the quantitative justification for the omission. They can obviously be calculated in perfect analogy with the hyperelastic collisions which were treated in detail, but one sees almost by inspection that their contribution to the cross section will be small.

One finds easily that, for the wavelength range studied, inelastic transitions can only occur as far as $l=5$. These first rotational states are not very strongly occupied. Furthermore, the factor k'/k in front of any inelastic

TABLE II. Total hyperelastic cross section in barns at a gas temperature of 300°K.

λ	5.1A	7.5A	10.0A
σ	1.11	1.22	1.38

cross section is considerably smaller than 1. One can so readily believe the result of a closer calculation which makes the inelastic cross section less than 1 percent of the total.

We should here also mention the justification of our treatment of vibrational eigenfunctions. At room temperature, most O_2 molecules will be in the lowest vibrational state and transitions to a higher state are energetically impossible. Taking the vibrational motion into account means eventually an increase of the square of the interatomic distance, as it occurs in the matrix elements, by about one percent. The small diminution of the elastic scattering thereby occasioned is about balanced by the equally small addition of the inelastic transitions. This was observed to be the case for 5.1A. At longer wavelengths the percentage influence of both these effects is still less.

6. MAGNETIC TRANSITIONS

Having thus determined the total nuclear cross section (see Table III), we now have to add the contribution due to the magnetic interaction. No calculations are required for this, since the result is contained in a general form in reference 2. We only have to comment on the transfer of the expression 5.41 of that paper, which was derived under the assumption of a free

TABLE III. Total nuclear cross section in barns at a gas temperature of 300°K.

λ	5.1A	7.5A	10.0A
σ	12.12	15.81	19.33

magnetic moment, to the case of O_2, where the electronic spin is coupled to the rotational momentum of the molecule. This procedure can be justified by referring to investigations by Van Vleck[6] and Kramers,[7] who first determined the coupling energy for the present case. It turns out that this coupling energy is small compared to the energy of the slowest neutron ($\frac{1}{8}$ of the average neutron energy at 10.0A and 300°K); it therefore seems correct to use the results of reference 2 as if the electron spin would be completely free. We must correct for our case of a free target the result 5.41 calculated for a rigidly bound target. We give below the corrected form for the differential magnetic cross section.

$$d\sigma(\text{magnetic}) = (\mu/m)^2(2/3)\int S(S+1)[e^2\gamma/m_eC^2]^2 F d\Omega, \quad (9)$$

in which S is the total spin of the molecule; e, m_e, c are electronic charge and mass, and light speed in absolute units; and γ is the magnetic moment of the neutron in nuclear magnetons. The differential form factor F is

$$\left|\int \exp(i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r})\rho(\mathbf{r})d\mathbf{r}\right|^2,$$

in which $\rho(\mathbf{r})$ is the distribution function of the magnetically active electrons which is so normalized as to give unit form factor in the limit of long wavelengths.

The only remaining problem then is given by the expression of the form factor; i.e., the distribution of the magnetically active shell which leads us back to the starting point of the whole investigation. It will, of course, be necessary to establish experimentally the dependence of the total magnetic cross section on the wavelength of the incident neutron. One can then empirically obtain an expression for the form factor due to the distribution of the magnetic moment.

To assist such future evaluations, we are here presenting form factors as functions of the incident wavelength under the undoubtedly arbitrary assumption that the magnetic shell is very thin and thus essentially characterized by its radius. If the description on this basis should, as we expect, not be quite satisfactory one can always obtain a better one by the superposition of a number of such shells.

It is shown in the Appendix that the integral form factor (in the mass center system) for a shell of radius $d'/2$ can be given rigorously by the expression

$$\int F d\Omega/4\pi = (kd')^{-2}[\log_e(2kd') - \mathrm{Ci}(2kd') + 0.5772], \quad (10)$$

in which

$$\mathrm{Ci}(x) = -\int_x^\infty (\cos t/t)dt.$$

For our wavelength range ($\lambda > 5.1$A), the laboratory form factor can be expressed with sufficient accuracy by the formula given in Table VI of the Appendix.

7. GENERAL DISCUSSION

There exist two groups of observations on the scattering of slow neutrons by O_2. In the experiments of Fermi and Marshall,[8] the scattering cross section of O_2 was found to be in excess of 16 barns; the wavelength was not sharply determined but was stated to be closely centered near 5.1A.

Later experiments by Melkonian[5] extend over a large wavelength range up to about 5.3A. The points of longest wavelength should undoubtedly fall within the range of our theory. Melkonian's value is about 2 barns smaller than that of Fermi and Marshall. No explanation is given for this experimental disagreement. Since, according to our formulas (see Table III), the total nuclear cross section at 5.1A amounts to 12.12

[6] Van Vleck, *Electric and Magnetic Susceptibilities* (Oxford University Press, London, 1932).

[7] H. A. Kramers, Z. Physik **53**, 422 (1927).

[8] E. Fermi and L. Marshall, Phys. Rev. **71**, 666 (1947).

barns, the experiments give widely different values for the residue, which is interpreted by us as the magnetic cross section. It seems clear that no successful determination of the size of the magnetic shell can be attempted under these circumstances. We would be somewhat inclined to think that the effective wavelength in the experiment of Fermi and Marshall has been underrated. If their value should be correct the magnetic form factor would be about 80 to 90 percent, which would mean that the magnetic shell is essentially contained within the sphere described by the molecular radius. This result seems to us somewhat unlikely, but we prefer to refrain from any quantitative discussion until future experiments have established more accurate values for the total scattering cross section.

It should be mentioned that the method here used can be equally applied to the treatment of paramagnetic NO. In this case, the calculation will be more complicated. In computing the contributions coming from inelastic transitions, one will have to remember that all rotational states will be present in NO. Furthermore, the active magnetic moment as shown by Van Vleck[6] is due to a complicated super position of quantum states. It does not seem doubtful, on the other hand, that a similar analysis will lead to interesting information concerning the active magnetic shell in NO.

It will equally be possible to extend the line of reasoning here presented to an analysis of the magnetic scattering by solid O_2.

APPENDIX

The following discusses our procedure of evaluation of the various integral form factors. For the nuclear scattering, we require

$$\int\frac{d\Omega}{4\pi}\left\{\frac{1}{2l+1}\sum_m\left|\int_0^\pi \sin\theta d\theta P_{l,m}\times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)P_{l,m}\right|^2\right\}$$

from formula (5) for the elastic scattering,

$$\int\frac{d\Omega}{4\pi}\left\{\frac{1}{2l+1}\sum_m\frac{(p^2+2\mu\Delta E)^{\frac{1}{2}}}{p}\left|\int_0^\pi \sin\theta d\theta P_{l,m}\times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)P_{l-2,m}\right|^2\right\} \quad (12)$$

from formula (8) for $l\to l-2$, and a similar factor for $l\to l-4$. The magnetic form factor, under our assumption of a thin shell distribution, is

$$\int(d\Omega/4\pi)\left|\int d\mathbf{r}\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\delta(r-\tfrac{1}{2}d')/4\pi\right|^2, \quad (13)$$

where $\delta(r-\frac{1}{2}d')/4\pi$ is the appropriately normalized $\rho(\mathbf{r})$. We first calculate the total elastic form factor (11), then average over the molecular velocity according to (16). In the second part, the coherent elastic and the magnetic form factors are shown to be equal except for differences in the shell diameter, and the magnetic form factor (as a function of d' and λ) is obtained from the coherent expression. Finally, the hyperelastic form factors are calculated.

(a) Elastic Form Factors

In formula (11) we set $|\mathbf{k}-\mathbf{k}'|=2k\sin(\Theta/2)$ and expand the cosine to the fourth power in its argument to obtain

$$\int\frac{d\Omega}{4\pi}\left\{\frac{1}{2l+1}\sum_m\left|\int_0^\pi \sin\theta d\theta(P_{l,m})^2\left[1-\frac{1}{2}\left(kd\sin\frac{\Theta}{2}\right)^2\times\cos^2\theta+\frac{1}{24}\left(kd\sin\frac{\Theta}{2}\right)^4\cos^4\theta\right]\right|^2\right\}. \quad (14)$$

Representing

$$\int_0^\pi \sin\theta d\theta(P_{l,m})^2\cos^2\theta \quad \text{by} \quad (l,m|\cos^2\theta|l,m),$$

and so forth, we have

$$\int\frac{d\Omega}{4\pi}\left\{\frac{1}{2l+1}\sum_m\left[1-\left(kd\sin\frac{\Theta}{2}\right)^2(l,m|\cos^2\theta|l,m)+\frac{1}{4}\left(kd\sin\frac{\Theta}{2}\right)^4(l,m|\cos^2\theta|l,m)^2+\frac{1}{12}\left(kd\sin\frac{\Theta}{2}\right)^4(l,m|\cos^4\theta|l,m)-\frac{1}{24}\left(kd\sin\frac{\Theta}{2}\right)^6(l,m|\cos^2\theta|l,m)(l,m|\cos^4\theta|l,m)+\left(\frac{1}{24}\right)^2\left(kd\sin\frac{\Theta}{2}\right)^8(l,m|\cos^4\theta|l,m)^2\right]\right\}. \quad (15)$$

The averages over the sphere of scattering are given by

$$\int\frac{d\Omega}{4\pi}\sin^{2n}\frac{\Theta}{2}=\frac{1}{n+1},$$

so that our formula becomes

$$\begin{aligned}&1-\tfrac{1}{2}(kd)^2\langle(l,m|\cos^2\theta|l,m)\rangle_m\\&+(1/12)(kd)^4\langle(l,m|\cos^2\theta|l,m)^2\rangle_m\\&+(1/36)(kd)^4\langle(l,m|\cos^4\theta|l,m)\rangle_m\\&-(1/96)(kd)^6\langle(l,m|\cos^2\theta|l,m)(l,m|\cos^4\theta|l,m)\rangle_m\\&+(1/5)(1/24)^2(kd)^8\langle(l,m|\cos^4\theta|l,m)^2\rangle_m, \quad (16)\end{aligned}$$

in which $\langle\ \rangle_m$ denotes the m average, $[1/(2l+1)]\sum_m$. The terms $\langle(l,m|\cos^2\theta|l,m)\rangle_m$ and $\langle(l,m|\cos^4\theta|l,m)\rangle_m$ are $\frac{1}{3}$ and $\frac{1}{5}$, respectively. The other terms require the

TABLE IV. Cosine matrix element factors for elastic and hyperelastic form factors. Except where noted, the arguments for the functions A, B, and C are l and m. The numerical values in the elastic case are averages over the thermal distribution in l for a temperature of 300°K. The hyperelastic values are for $l=15$.

Elastic transitions		
$\langle(l, m\|\cos^2\theta\|l, m)^2\rangle_m$	$\frac{1}{2l+1}\sum_m B^2$	0.1352
$\langle(l, m\|\cos^2\theta\|l, m)(l, m\|\cos^4\theta\|l, m)\rangle_m$	$\frac{1}{2l+1}\sum_m [A^2B+B^2+C^2B]$	0.0864
$\langle(l, m\|\cos^4\theta\|l, m)^2\rangle_m$	$\frac{1}{2l+1}\sum_m [A^2+B^2+C^2]^2$	0.063
Hyperelastic transitions		
$\langle(l, m\|\cos^2\theta\|l-2, m)^2\rangle_m$	$\frac{2}{15}\frac{l(l-1)}{4l^2-1}$	
$\langle(l, m\|\cos^2\theta\|l-2, m)(l, m\|\cos^4\theta\|l-2, m)\rangle_m$	$\frac{1}{2l+1}\sum_m [C^2B+C^2B(l-2, m)]$	0.027
$\langle(l, m\|\cos^4\theta\|l-2, m)^2\rangle_m$	$\frac{1}{2l+1}\sum_m [CB+CB(l-2, m)]^2$	0.025
$\langle(l, m\|\cos^4\theta\|l-4, m)^2\rangle_m$	$\frac{1}{2l+1}\sum_m [C(l-2, m)C(l, m)]^2$	0.002

following evaluation procedure. By successive application of the expansion formula,

$$\cos^2\theta P_{l,m}(\cos\theta)=A(l, m)P_{l+2,m}(\cos\theta)+B(l, m)P_{l,m}(\cos\theta)+C(l, m)P_{l-2,m}(\cos\theta), \quad (17)$$

in which

$$A(l, m)=\left\{\frac{[(l+1)^2-m^2][(l+2)^2-m^2]}{(2l+1)(2l+3)^2(2l+5)}\right\}^{\frac{1}{2}},$$

$$B(l, m)=\frac{2l^2+2l-1-2m^2}{(2l+3)(2l-1)} \quad (18)$$

$$C(l, m)=\left\{\frac{[l^2-m^2][(l-1)^2-m^2]}{(2l+1)(2l-1)^2(2l-3)}\right\}^{\frac{1}{2}},$$

one obtains algebraic expressions in l. For example,

$$(l, m|\cos^2\theta|l, m)^2=[B(l, m)]^2.$$

Hence, $\langle(l, m|\cos^2\theta|l, m)^2\rangle_m=[1/(2l+1)]\sum_m B^2$. All such expressions are reduced to algebraic functions of l by means of the formulas for the sums of even powers of the integers in terms of the upper limit.

The cosine matrix element factors are given as functions of A, B, and C in Table IV. Terms appearing in the hyperelastic form factor are included. The numbers for the elastic terms are averages over the thermal distribution in l for a gas temperature of 300°K. The first two elastic factors are exact, but the third is in error by about 20 percent. Since this latter appears in the eighth power term of the form factor expansion, it introduces negligible error into the cross section. The form factor now appears as a power series in (kd), formula (7) of the text:

$$1-\tfrac{1}{6}(kd)^2+0.01682(kd)^4-9.00\times10^{-4}(kd)^6+2.08\times10^{-5}(kd)^8.$$

We transform (kd) to laboratory quantities. Since $\lambda=h/mv$, k may be expressed as $k=(1/\hbar)\mu|\mathbf{v}-\mathbf{u}|(h/mv\lambda)$ which gives $kd=(2\pi d\mu/m\lambda)(|\mathbf{v}-\mathbf{u}|/v)$. This form facilitates the Maxwell averaging procedure and the numerical evaluation. We define $A(\lambda)=(2\pi d\mu/m\lambda)$ and $f_n=|\mathbf{v}-\mathbf{u}|^n/v^n$. Formula (11) now appears in abbreviated notation as

$$1-\tfrac{1}{6}A^2f_2+0.01682A^4f_4-9.00\times10^{-4}A^6f_6+2.08\times10^{-5}A^8f_8.$$

If we denote by $\bar{f}_n$ the Maxwell average over $\mathbf{u}$ of $|\mathbf{v}-\mathbf{u}|^n/v^n$, then the effective form factor of expression (6) reads

$$\bar{f}_1-\tfrac{1}{6}A^2\bar{f}_3+0.01682A^4\bar{f}_5-9.00\times10^{-4}A^6\bar{f}_7+2.08\times10^{-5}A^8\bar{f}_9, \quad (19)$$

in which, of course, the average over l has already been performed.

We now develop formulas for the $\bar{f}_n$ expressions for odd n, in terms of the dimensionless variable α defined by $\alpha^2=Mv^2/2kT$, in which M is the mass of O_2 and T is the gas temperature. One has the integral $\int d\mathbf{u}N(\mathbf{u})|\mathbf{v}-\mathbf{u}|^n/v^n$, in which $N(\mathbf{u})$ is normalized by the condition $\int d\mathbf{u}N(\mathbf{u})=1$ to be $(M/2\pi kT)^{\frac{3}{2}}\times\exp(-Mu^2/2kT)$. Our integral under the transformation[9] $\mathbf{u}=\mathbf{v}+\mathbf{w}$ becomes

$$\left(\frac{M}{2\pi kT}\right)^{\frac{3}{2}}\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta d\theta\int_0^{\infty}w^2dw\times\left[\exp\left(\frac{-M|\mathbf{v}+\mathbf{w}|^2}{2kT}\right)w^n/v^n\right]. \quad (20)$$

[9] These integrals can be done in $\mathbf{u}$ space without this transformation, but then one must reduce by partial integrations integrals of the form $\int_0^1\exp(-\alpha^2x^2)x^m dx$ and $\int_1^{\infty}\exp(-\alpha^2x^2)x^p dx$ for higher powers of x than are required by the method described.

Choosing the Z axis along $\mathbf{v}$ and using the transformation $x=-\cos\theta$, one gets

$$2\pi\left(\frac{M}{2\pi kT}\right)^{\frac{3}{2}}\int_0^\infty w^2dw\left[\left(\frac{w^n}{v^n}\right)\exp\left(-\frac{Mv^2}{2kT}-\frac{Mw^2}{2kT}\right)\times\int_{-1}^{1}\exp\left(\frac{2Mvwx}{2kT}\right)dx\right], \quad (21)$$

which equals

$$2\pi\left(\frac{M}{2\pi kT}\right)^{\frac{3}{2}}\left(\frac{kT}{M}\right)\int_0^\infty\left(\frac{1}{vw}\right)w^2dw\frac{w^n}{v^n}\times\exp\left(-\frac{Mv^2}{2kT}-\frac{Mw^2}{2kT}\right)\left[2\sinh\left(\frac{2Mvw}{2kT}\right)\right]. \quad (22)$$

Introducing α^2 defined above and the new variable $y=w/v$, we reduce the integral to

$$(\alpha/\sqrt{\pi})2\int_0^\infty\exp[-\alpha^2(y^2+1)]\sinh(2y\alpha^2)y^{n+1}dy, \quad (23)$$

or

$$(\alpha/\sqrt{\pi})\int_0^\infty\{\exp[-\alpha^2(y-1)^2]-\exp[-\alpha^2(y+1)^2]\}y^{n+1}dy.$$

Separation of the integral and the transformations, $x=y-1$ and $x=y+1$, applied to the respective parts give

$$(\alpha/\sqrt{\pi})\left\{\int_{-1}^{\infty}[\exp(-\alpha^2x^2)](x+1)^{n+1}dx-\int_1^\infty[\exp(-\alpha^2x^2)](x-1)^{n+1}dx\right\}. \quad (24)$$

In the interval $[-1, 1]$ for the first integral, only the even powers in x contribute, so that one gets, for the even powers, terms of the form

$$(2\alpha/\sqrt{\pi})\int_0^1\exp(-\alpha^2x^2)\binom{p}{n+1}x^pdx,$$

in which $(p, n+1)$ is the appropriate binomial coefficient. In the interval $[1, \infty]$ for both integrals, the even power terms are canceled, and one gets, for odd m, terms of the form

$$(2\alpha/\sqrt{\pi})\int_1^\infty\exp(-\alpha^2x^2)\binom{m}{n+1}x^mdx.$$

Our notation is m for odd powers and p for even powers. We define

$$E(p)=2\int_0^1\exp(-\alpha^2x^2)x^pdx, \quad (25)$$

and

$$G(m)=2\int_1^\infty\exp(-\alpha^2x^2)x^mdx. \quad (26)$$

The latter are quite easily evaluated. In the p terms, the transformation $u=\alpha x$ and partial integration give the recurrence relation

$$E(p)=-[\exp(-\alpha^2)]/\alpha+[(p-1)/2\alpha^2]E(p-2), \quad (27)$$

and for $p=0$,

$$E(0)=(2/\alpha)\int_0^\alpha\exp(-u^2)du=(\sqrt{\pi}/\alpha)\,\mathrm{erf}(\alpha), \quad (28)$$

in which $\mathrm{erf}(\alpha)$ is the error function of α defined as

$$(2/\sqrt{\pi})\int_0^\alpha\exp(-u^2)du.$$

With tables of E and G for $m=1$ through 9 and $p=0$ through 10, we have obtained formulas for $\bar{f}_n$ for $n=1$ through 9 by substitution in the appropriate $(n+1)$

TABLE V. Formulas for $\bar{f}_n$, the average over Maxwellian distribution in $\mathbf{u}$, at the temperature T, of the quantity $|\mathbf{v}-\mathbf{u}|^n/v^n$ as a function of $\alpha^2=Mv^2/2kT$, in which M is the molecular mass. The numerical values are for a gas temperature of 300°K.

n	$\bar{f}_n$	$\bar{f}_n$ $\lambda=5.1$A	$\lambda=7.5$A	$\lambda=10.0$A
1	$\left[\frac{1}{\sqrt{\pi}}\frac{\exp(-\alpha^2)}{\alpha}\right]+[\mathrm{erf}(\alpha)]\left(1+\frac{0.5}{\alpha^2}\right)$	1.1295	1.2758	1.4702
3	$\left[\frac{1}{\sqrt{\pi}}\frac{\exp(-\alpha^2)}{\alpha}\right]\left(1+\frac{2.5}{\alpha^2}\right)+[\mathrm{erf}(\alpha)]\left(1+\frac{3}{\alpha^2}+\frac{0.75}{\alpha^4}\right)$	1.8283	2.9165	4.7154
5	$\left[\frac{1}{\sqrt{\pi}}\frac{\exp(-\alpha^2)}{\alpha}\right]\left(1+\frac{7}{\alpha^2}+\frac{8.25}{\alpha^4}\right)+[\mathrm{erf}(\alpha)]\left(1+\frac{7.5}{\alpha^2}+\frac{11.25}{\alpha^4}+\frac{1.88}{\alpha^6}\right)$	3.7338	9.0725	21.486
7	$\left[\frac{1}{\sqrt{\pi}}\frac{\exp(-\alpha^2)}{\alpha}\right]\left(1+\frac{13.5}{\alpha^2}+\frac{46.25}{\alpha^4}+\frac{34.88}{\alpha^6}\right)+[\mathrm{erf}(\alpha)]\left(1+\frac{14}{\alpha^2}+\frac{52.5}{\alpha^4}+\frac{52.5}{\alpha^6}+\frac{6.56}{\alpha^8}\right)$	9.0998	35.263	125.56
9	$\left[\frac{1}{\sqrt{\pi}}\frac{\exp(-\alpha^2)}{\alpha}\right]\left(1+\frac{22}{\alpha^2}+\frac{147}{\alpha^4}+\frac{330}{\alpha^6}+\frac{180.9}{\alpha^8}\right)+[\mathrm{erf}(\alpha)]\left(1+\frac{22.5}{\alpha^2}+\frac{157.5}{\alpha^4}+\frac{393.8}{\alpha^6}+\frac{295.4}{\alpha^8}+\frac{295.4}{\alpha^{10}}\right)$	25.66	163.4	890.1
2	$1+1.5/\alpha^2$	1.389	1.841	2.495

binomial formula. For example,

$$\bar{f}_3=(\alpha/\sqrt{\pi})[E(4)+4G(3)+6E(2)+4G(1)+E(0)]. \quad (29)$$

The $\bar{f}_n$ formulas are given in Table V. We have included $\bar{f}_2$, which appears in our treatment of the hyperelastic form factor.

(b) Coherence and Incoherence

The distinction between coherent and incoherent parts of the elastic form factor appears in the treatment of the matrix element in the Born formula. For the total elastic cross section, the square of the matrix element given in formula (2), in which the $Y_{l,m}(\theta,\phi)$ are the eigenfunctions, was summed over m' and averaged over m, since, in this case, we did not specify the transitions between the degenerate states. Proceeding more generally, let us represent an internal l state of our rigid rotator by the linear combination of eigenfunctions, $\sum_m(C_{l,m}Y_{l,m})$, with the normalization condition, $\sum_m(C_{l,m}{}^*C_{l,m})=1$.

The matrix element for a transition from this state to some other is proportional to

$$\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta d\theta[(\sum_m C_{lm}{}^*Y_{lm}{}^*)\times\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)(\sum_{m'}C_{l',m'}{}'Y_{l',m'})], \quad (30)$$

where $\sum_m(C_{l',m}{}'Y_{l',m})$ is the eigenfunction of the final state with the same normalization condition. For coherence, we examine a diagonal matrix element ($C_{l,m}{}'=C_{l,m}$ in above). The square of this matrix element enters the Born formula for the coherent transition from state C to state C. The orthogonality of the $Y_{l,m}$ in ϕ and our ϕ-independent Hamiltonian reduce this matrix element to

$$\int_0^{\pi}\sin\theta d\theta\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta)(\sum_m C_{lm}{}^*C_{lm}P_{lm}{}^*P_{lm}).$$

Equal *a priori* probability for the m's demands that the $C_{lm}{}^*C_{lm}$ be the same for all m so that the matrix element is now proportional to

$$\tfrac{1}{2}\int_0^{\pi}\sin\theta d\theta\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta),$$

since

$$\sum_m(P_{l,m}{}^*P_{l,m})=(2l+1)/2 \quad \text{and} \quad C_{lm}{}^*C_{lm}=1/(2l+1).$$

The integral coherent form factor then is the expression

$$\int(d\Omega/4\pi)\left|\tfrac{1}{2}\int_0^{\pi}\sin\theta d\theta\cos(\tfrac{1}{2}d|\mathbf{k}-\mathbf{k}'|\cos\theta\right|^2. \quad (31)$$

Let us now consider the magnetic form factor of formula (13).

$$\int(d\Omega/4\pi)\left|\int d\mathbf{r}[\delta(r-\tfrac{1}{2}d')/4\pi]\times[\cos(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}+i\sin(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\right|^2. \quad (32)$$

With Z axis along $(\mathbf{k}-\mathbf{k}')$, we see that the sin factor gives zero in the θ-integration over $\mathbf{r}$ space. Thus, the magnetic form factor is

$$\int(d\Omega/4\pi)\left|\tfrac{1}{2}\int_0^{\pi}\sin\theta d\theta\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|d'\cos\theta)\right|^2, \quad (33)$$

which is the same as the coherent nuclear factor except for the shell diameter. Aside from this trivial difference these factors become

$$\int\frac{d\Omega}{4\pi}\left[\frac{\sin(|\mathbf{k}-\mathbf{k}'|d/2)}{|\mathbf{k}-\mathbf{k}'|d/2}\right]^2,$$

which can be evaluated to give formula (10) of the text:

$$(1/kd)^2[\log_e(2kd)-\mathrm{Ci}(2kd)+0.5772]. \quad (34)$$

The procedure is as follows. Since the collisions are elastic, $|\mathbf{k}-\mathbf{k}'|$ is equal to $2k\sin(\Theta/2)$. In terms of the variable $y=2kd\sin(\Theta/2)$ our integral form factor becomes

$$(kd)^{-2}\int_0^{2kd}(1-\cos y)/y dy.$$

This integral is expressed in terms of Euler's constant and the cosine integral as given above.

Since the exact form factor of expression (34) does not permit an easy Maxwellian averaging, we have evaluated (31) by expansion of $\cos(\frac{1}{2}|\mathbf{k}-\mathbf{k}'|d\cos\theta)$. For the proper choices of shell diameter, the resulting expression gives both the coherent and magnetic form factors.

Formula (31) becomes in our approximation:

$$\int\frac{d\Omega}{4\pi}\left[1-\frac{1}{2}\left(kd\sin\frac{\Theta}{2}\right)^2\frac{1}{3}+\frac{1}{24}\left(kd\sin\frac{\Theta}{2}\right)^4\frac{1}{5}\right]. \quad (35)$$

One gets upon squaring, in a way similar to that used in the total elastic case, the following power series in (kd) for the coherent nuclear form factor:

$$1-\tfrac{1}{6}A^2f_2+0.01481A^4f_4-6.944\times10^{-4}A^6f_6+1.389\times10^{-5}A^8f_8. \quad (36)$$

The effective coherent form factor is obtained in the same way as for the total elastic case.

In Table VI we give the form factor formulas and strength factors for the total elastic, coherent, and magnetic cross sections at a gas temperature of 300°K.

TABLE VI. Strength factors (in barns) and form factor formulas for the various cross sections, for a gas temperature of 300°K.

Type of scattering	Strength factor (barns)	Form factor formula
Total elastic	15.84	$\tilde{f}_1-0.1667A^2\tilde{f}_3+0.01682A^4\tilde{f}_5-9.00\times10^{-4}A^6\tilde{f}_7+(2.08)\times10^{-5}A^8\tilde{f}_9$
Coherent	15.84	$\tilde{f}_1-0.1667A^2\tilde{f}_3+0.01481A^4\tilde{f}_5-6.944\times10^{-4}A^6\tilde{f}_7+1.389\times10^{-5}A^8\tilde{f}_9$
Magnetic	4.53	$\tilde{f}_1-0.1667A^2\tilde{f}_3(d'/d)^2+0.01481A^4\tilde{f}_5(d'/d)^4-6.944\times10^{-4}A^6\tilde{f}_7(d'/d)^6+1.389\times10^{-5}A^8f_9(d'/d)^8$

(c) Hyperelastic Form Factors

The hyperelastic formulas require evaluation of

$$\left(\frac{1}{2l+1}\right)\sum_m\left\{\frac{k'}{k}\left|\int_0^\pi \sin\theta d\theta P_{l-2,m}P_{l,m}\times\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|d\cos\theta)\right|^2\right\}, \quad (37)$$

and a similar term for $l\to l-4$. Upon expansion of the cosine to the fourth power in its argument we obtain with the aid of the selection principles implicit in the expansion formulas of the Legendre functions (see paragraph 4):

$$\left(\frac{1}{2l+1}\right)\sum_m\left\{\frac{k'}{k}\left[-\frac{1}{2}\left(|\mathbf{k}-\mathbf{k}'|\frac{d}{2}\right)^2(l,m|\cos^2\theta|l-2,m)+\frac{1}{24}\left(|\mathbf{k}-\mathbf{k}'|\frac{d}{2}\right)^4(l,m|\cos^4\theta|l-2,m)\right]^2\right\} \quad (38)$$

for the $l\to l-2$ transition, and

$$\left(\frac{1}{2l+1}\right)\sum_m\left\{\frac{k'}{k}\left[\frac{1}{24}\left(|\mathbf{k}-\mathbf{k}'|\frac{d}{2}\right)^4\times(l,m|\cos^4\theta|l-4,m)\right]^2\right\} \quad (39)$$

for the $l\to l-4$ transition. Upon squaring we have

$$\left(\frac{1}{2l+1}\right)\sum_m\left\{\frac{k'}{k}\left[\frac{1}{4}\left(\frac{d}{2}\right)^4|\mathbf{k}-\mathbf{k}'|^4(l,m|\cos^2\theta|l-2,m)^2-\frac{1}{24}\left(\frac{d}{2}\right)^6|\mathbf{k}-\mathbf{k}'|^6(l,m|\cos^2\theta|l-2,m)\times(l,m|\cos^4\theta|l-2,m)+\left(\frac{1}{24}\right)^2\left(\frac{d}{2}\right)^8\times|\mathbf{k}-\mathbf{k}'|^8(l,m|\cos^4\theta|l-2,m)^2\right]\right\}, \quad (40)$$

and

$$\left(\frac{1}{2l+1}\right)\sum_m\left\{\frac{k'}{k}\left[\left(\frac{1}{24}\right)^2\left(\frac{d}{2}\right)^8|\mathbf{k}-\mathbf{k}'|^8\times(l,m|\cos^4\theta|l-4,m)^2\right]\right\}, \quad (41)$$

which must be averaged over the sphere of scattering. The angular dependence is contained only in the $|\mathbf{k}-\mathbf{k}'|$ factors. We require $\int(d\Omega/4\pi)|\mathbf{k}-\mathbf{k}'|^n$ for $n=4$, 6, 8, which are represented as

$$(1/\hbar)^n\tfrac{1}{2}\int_0^\pi \sin\Theta d\Theta|\mathbf{p}-\mathbf{p}'|^n,$$

in which $p'^2=p^2+2\mu\Delta E$ and Θ is the angle between $\mathbf{p}$ and $\mathbf{p}'$. Let us denote $2\mu\Delta E$ by β^2. We need β^2 for transitions $l\to l-2$ and $l\to l-4$. One expands $|\mathbf{p}-\mathbf{p}'|^n$ as even powers of the squared magnitude $(p^2-2pp'\cos\Theta+p'^2)$ and then substitutes for p' as above. One then has to average the even powers of $\cos\Theta$ and to discard the odd powers in the final expression. For example,

$$|\mathbf{p}-\mathbf{p}'|^4=p^4+4p^2p'^2\cos^2\Theta+p'^4-4p^3p'\cos\Theta-4pp'^3\cos\Theta+2p^2p'^2.$$

In the average over Θ, $\cos^2\Theta$ becomes $\frac{1}{3}$ and the terms linear in $\cos\Theta$ vanish, to give

$$\int(d\Omega/4\pi)|\mathbf{p}-\mathbf{p}'|^4=p^4+(10/3)p^2p'^2+p'^4=p^4+(10/3)p^2(p^2+2\mu\Delta E)+(p^2+2\mu\Delta E)^2.$$

In briefer notation the result is

$$\int(d\Omega/4\pi)|\mathbf{k}-\mathbf{k}'|^4=(1/\hbar)^4[(16/3)p^4+(16/3)p^2\beta^2+\beta^4], \quad (42a)$$

and for the sixth and eighth powers

$$\int(d\Omega/4\pi)|\mathbf{k}-\mathbf{k}'|^6=(1/\hbar)^6(16p^6+24p^4\beta^2+10p^2\beta^4+\beta^6), \quad (42b)$$

$$\int(d\Omega/4\pi)|\mathbf{k}-\mathbf{k}'|^8=(1/\hbar)^8(41p^8+81p^6\beta^2+57p^4\beta^4+16p^2\beta^6+\beta^8]. \quad (42c)$$

The powers of $|\mathbf{k}-\mathbf{k}'|$ will be used to specify the respective terms—fourth, sixth, and eighth order. We take the dominant (fourth-order) term to illustrate our calculation procedure:

$$[(p^2+\beta^2)^{\frac{1}{2}}/p]\langle(l,m|\cos^2\theta|l-2,m)^2\rangle_m(1/4)(d/2)^4\times(1/\hbar)^4[(16/3)p^4+(16/3)p^2\beta^2+\beta^4]. \quad (43)$$

In the elastic case the form factor was expressed in

TABLE VII. Effective hyperelastic form factor formulas, in our notation, for the $l \to l-2$ transition. The $l \to l-4$ term is identical with the 8th-order term except for a different cosine factor and that the a^2 factor refers to a larger energy change.

4th order	$\frac{1}{4}\left(\frac{A}{2}\right)^4 \langle (l, m\|\cos^2\theta\|l-2, m)^2\rangle_m \left[\frac{16}{3}F_4(l)+\frac{16}{3}F_2(l)a^2(l)+F_0(l)a^4(l)\right]$
6th order	$-\frac{1}{24}\left(\frac{A}{2}\right)^6 \langle (l, m\|\cos^2\theta\|l-2, m)(l, m\|\cos^4\theta\|l-2, m)\rangle_m [16F_6(l)+24F_4(l)a^2(l)+10F_2(l)a^4(l)+a^6(l)F_0(l)]$
8th order	$+\left(\frac{1}{24}\right)^2\left(\frac{A}{2}\right)^8 \langle (l, m\|\cos^4\|l-2, m)^2\rangle_m [41F_8(l)+81F_6(l)a^2(l)+57F_4(l)a^4(l)+16F_2(l)a^6(l)+F_0(l)a^8(l)]$

terms of $A(\lambda)$ and $|\mathbf{v}-\mathbf{u}|/v$ to facilitate the averaging over $\mathbf{u}$ and the numerical evaluation. To achieve a similar expression here, we substitute $\mu|\mathbf{v}-\mathbf{u}|$ for p and multiply by unity in the form $(\mu v/\mu v)^4$ to obtain

$$\frac{(\mu^2|\mathbf{v}-\mathbf{u}|^2+\beta^2)^{\frac{1}{2}}}{\mu|\mathbf{v}-\mathbf{u}|}\frac{1}{4}\left(\frac{1}{2}\right)^4\left(\frac{d\mu v}{\hbar}\right)^4\langle (l, m|\cos^2\theta|l-2, m)^2\rangle_m \times\left[\frac{16}{3}\frac{\mu^4|\mathbf{v}-\mathbf{u}|^4}{\mu^4v^4}+\frac{16}{3}\frac{\mu^2|\mathbf{v}-\mathbf{u}|^2\beta^2}{\mu^2v^2\mu^2v^2}+\frac{\beta^4}{\mu^4v^4}\right].$$

The notation introduced in the elastic case is supplemented by the characteristic hyperelastic parameter, $a^2(\lambda, l)=\beta^2(l)/(\mu v)^2$. These parameters are given as functions of l in Table IX. Formula (43) now reads:

$$\frac{(\mu^2|\mathbf{v}-\mathbf{u}|^2+\beta^2)^{\frac{1}{2}}}{\mu|\mathbf{v}-\mathbf{u}|}\langle (l, m|\cos^2\theta|l-2, m)^2\rangle_m\frac{1}{4}\left(\frac{A}{2}\right)^4 \times\left[\frac{16}{3}\frac{|\mathbf{v}-\mathbf{u}|^4}{v^4}+\frac{16}{3}\frac{|\mathbf{v}-\mathbf{u}|^2}{v^2}a^2+a^4\right]. \quad (44)$$

The sixth- and eighth-order terms have a similar expression as a polynomial in even powers of $|\mathbf{v}-\mathbf{u}|/v$ and a, multiplied by the square root factor. These are:

$$-\frac{(\mu^2|\mathbf{v}-\mathbf{u}|^2+\beta^2)^{\frac{1}{2}}}{\mu|\mathbf{v}-\mathbf{u}|} \times\langle (l, m|\cos^2\theta|l-2, m)(l, m|\cos^4\theta|l-2, m)\rangle_m \times\frac{1}{24}\left(\frac{A}{2}\right)^6\left[16\frac{|\mathbf{v}-\mathbf{u}|^6}{v^6}+24\frac{|\mathbf{v}-\mathbf{u}|^4}{v^4}a^2 +10\frac{|\mathbf{v}-\mathbf{u}|^2}{v^2}a^4+a^6\right], \quad (45)$$

and

$$\left(\frac{1}{24}\right)^2\left(\frac{A}{2}\right)^8\langle (l, m|\cos^4\theta|l-2, m)^2\rangle_m \times\left[41\frac{|\mathbf{v}-\mathbf{u}|^8}{v^8}+81\frac{|\mathbf{v}-\mathbf{u}|^6}{v^6}a^2+57\frac{|\mathbf{v}-\mathbf{u}|^4}{v^4}a^4 +16\frac{|\mathbf{v}-\mathbf{u}|^2}{v^2}a^6+a^8\right]. \quad (46)$$

The characteristic term to be averaged over the molecular velocities is

$$\frac{|\mathbf{v}-\mathbf{u}|}{v}\frac{(\mu^2|\mathbf{v}-\mathbf{u}|^2+\beta^2)^{\frac{1}{2}}}{\mu|\mathbf{v}-\mathbf{u}|}\frac{|\mathbf{v}-\mathbf{u}|^m}{v^m}, \quad (47)$$

with m taking on even values 0 through 8. This expression simplifies to $(|\mathbf{v}-\mathbf{u}|^2/v^2+a^2)^{\frac{1}{2}}|\mathbf{v}-\mathbf{u}|^m/v^m$, whose Maxwell average we denote as $F_m(l)$. We can proceed in the same way as in the evaluation of the $\bar{f}_n$ formulas for the elastic form factor in part (a) of the Appendix up to the integration over the magnitude of $\mathbf{w}$. The representation of $F_m(l)$ as a quadrature over the variable $y=w/v$ as defined in the $\bar{f}_n$ evaluation is

$$F_m(l)=(2\alpha/\sqrt{\pi})\int_0^\infty \exp[-\alpha^2(y^2+1)] \times\sinh(2\alpha^2y)(y^2+a^2)^{\frac{1}{2}}y^{m+1}dy. \quad (48)$$

For $a=0$, $F_m(l)$ reduces to $\bar{f}_{m+1}$. [See formula (23).] Table VII contains the form factor formulas in terms of the functions $F_m(l)$ and $a^2(l)$. Both these quantities increase monotonically with λ. These formulas show clearly the quantitative details of the qualitative argument of paragraph 4 regarding the relative independence of wavelength of the hyperelastic cross section. The coefficients $A(\lambda)$ in front decrease with increasing wavelength while $F_m(l)$ and $a^2(l)$ increase, with the effect of maintaining the form factor approximately constant. The slight increase with increasing λ comes about from the competition between the positive fourth-order and the negative sixth-order terms.

The l dependence of $F_m(l)$ and a^2 is a very important factor in the evaluation. Since a^2 varies directly as $(2l-1)$, it can be accounted for exactly in averaging the form factors over the thermal distribution in l. It is necessary to approximate the l- and λ-dependence of the $F_m(l)$ factors for purposes of averaging, because the combination of these with the a^2 quantities which appear in the formulas make impossible the choice of some average l value at which all quantities could be evaluated. Our choice of an approximation was determined by the following factors: (1) the fourth-order term is by far the largest and determines the order of magnitude of the cross section, (2) the sixth-order term is still sufficiently large and very important because of the negative sign. We chose an approximation

TABLE VIII. Results of calculation of the hyperelastic form factors at 300°K, itemized according to the two transitions and the various terms.

Transition	Term	5.1A	7.5A	10.0A
$l\to l-2$	4th	0.175	0.152	0.158
$l\to l-2$	6th	−0.125	−0.087	−0.081
$l\to l-2$	8th	0.015	0.009	0.006
$l\to l-4$	8th	0.005	0.003	0.004
Total		0.070	0.077	0.087

which is very good for F_0 through F_4 and then applied corrections. Our approximation is

$$F_m(l)=[1+a^2(l)/\bar{f}_2]^{\frac{1}{2}}\bar{f}_{m+1}. \quad (49)$$

The motivation for this choice is indicated by formula (47) in the form:

$$(1+\beta^2(l)/\mu^2|\mathbf{v}-\mathbf{u}|^2)^{\frac{1}{2}}(|\mathbf{v}-\mathbf{u}|^{m+1}/v^{m+1}). \quad (50)$$

In our notation the Maxwell average of $|\mathbf{v}-\mathbf{u}|^2$ is $v^2\bar{f}_2$. In treating the square root factor in this way we are using the k'/k factor for the collision in which the squared magnitude of the relative velocity has its mean value and then incorporating the Doppler correction in the p terms of the form factor. In terms of the integral (49) this approximation amounts to approximating that integral as

$$F_m(l)=(2\alpha/\sqrt{\pi})[1+a^2(l)/(y^2)_{\text{Av}}]^{\frac{1}{2}} \times\int_0^\infty \exp[-\alpha^2(y^2+1)]\sinh(2\alpha^2y)y^{m+2}dy. \quad (51)$$

We have taken $(y^2)_{\text{Av}}$ to be $\bar{f}_2$. Formula (51) shows that our approximation expressed in formula (49) is poor for the higher m values since $(y^2)_{\text{Av}}$ should increase with m. For large m the peak of the integrand moves toward higher y values where $y^2>a^2(l)$. The $(y^2+a^2)^{\frac{1}{2}}$ of (48) then is approximately y and $F_m(l)$ is more nearly $\bar{f}_{m+1}$. However, the thermal distribution in l peaks at $l=9$ and, for all terms, the most probable l values occur between $l=9$ and $l=15$ where $a^2(l)$ is sufficiently large to affect the values of $F_m(l)$. Thus the effectiveness of the approximation is better than the above examination of formula (51) would seem to indicate. Numerical integrations of (48) at $l=9$ and $l=15$ established the corrections for the $F_m(l)$. The net effect of these corrections for the various terms of the form factor (each of which involves several of the F_m factors) were negative and of magnitudes: 2 percent for fourth order, 10 percent for sixth order, and 40 to 60 percent for eighth order. The magnitudes of the correction were larger for larger wavelengths.

TABLE IX. Numerical values for parameters defined in the calculation.

Parameter	λ = 5.1A	λ = 7.5A	λ = 10.0A
$A(\lambda)=2\pi d\mu/m\lambda$	1.442	0.9806	0.7354
$\alpha^2(\lambda,T)=Mv^2/2kT$	3.857	1.783	1.003
$a^2(\lambda,l)=2\mu\Delta E/(\mu v)^2$	0.1176(2l−1)	0.2543(2l−1)	0.4522(2l−1)

TABLE X. Rotational distribution in percent at 300°K.

l	Occupation No.	l	Occupation No.
1	4.1	13	10.9
3	8.8	15	8.3
5	12.2	17	6.0
7	14.0	19	4.1
9	14.0	21	2.6
11	12.8	23	1.6

One further approximation was made in treating the l-dependence of the cosine matrix element factors appearing in front of all the terms of Table VII. This factor was treated exactly for the fourth-order term since the l dependence was quite simple. The other terms varied very slowly in the l interval of consequence and were taken to be constant at their values for $l=15$. (See Table IV.)

The accuracy of this calculation is largely determined by the error in the sixth-order terms, as Table VIII shows. We estimate then the error to be about 10 percent of the hyperelastic cross section, which introduces an error of definitely less than 2 percent into the nuclear cross section. Table IX contains numerical values for the parameters introduced, and Table X gives the rotational occupation numbers in percent at 300°K.