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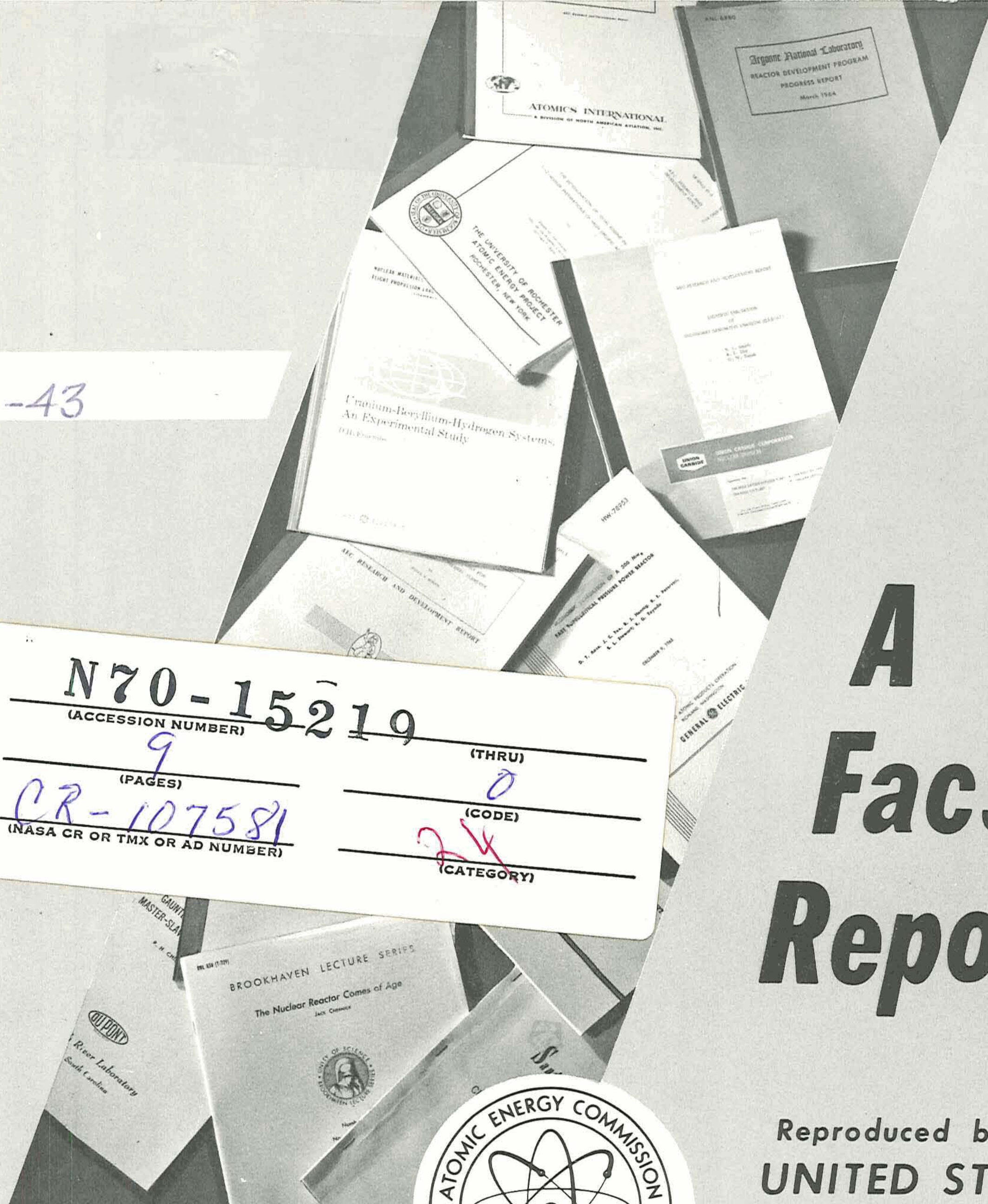

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Determination of Differential Elastic and Vibrational Excitation Cross Sections for e - H_2 Scattering

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ABSTRACT

The elastic scattering of electrons by H_2 has been studied together with the pure vibrational excitation (rotational levels are not resolved). Angular distributions of the elastically and inelastically scattered electrons causing the fundamental and first and second overtone excitations have been measured in the 8° to 80° range. Certain aspects of the experimental procedures and the angular behavior of some of the inelastic to elastic scattering intensity ratios (R) at 7 and 60 eV impact energies are presented here.

The experimental procedure consists of scattering an energy selected electron beam by a static low-pressure H_2 target gas and measuring the scattered signal intensities at fixed electron impact energies (E) and scattering angles (θ) as a function of energy-loss. Due to the weak inelastic signal intensities a long integration time is required to achieve adequate signal-to-noise ratios and the experimental conditions corresponding to measurements at different angles and energies are somewhat different. The quantity that one can extract from these measurements which is least subject to experimental uncertainties is R and its angular dependence at different energies. Figure 1 shows the ratio R_1 of the

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scattered signal intensity at an energy-loss corresponding to the excitation of the fundamental vibration to the signal intensity of the elastic peak at incident energies of 7 and 60 eV. The individual points are experimental values. The curves are calculated in the Born approximation with static and polarization potentials which take account of the non-spherical nature of the molecule and with exchange included in the Ochkur-Rudge approximation. The calculation is discussed in more detail elsewhere. The ratios R_2 for excitation of the second vibrational state have been determined with less accuracy. They are about ten times smaller but have approximately the same angular dependence as the ratios R_1.

The elastic differential scattering cross sections (DCS) have been determined under identical experimental conditions in arbitrary units and at 7 eV normalized to the absolute scale by using the total scattering cross sections of Golden, Bandel and Salerno.[1] The shape of elastic DCS curve agrees very well with the experimental curve of Ehrhardt, et al.[2] From the intensity ratios and from the elastic DCS the inelastic DCS have also been obtained in absolute scale. Extrapolation of the DCS to 0° and to 180° yields an integrated cross section for the fundamental vibrational excitation of 0.61 a_0^2 (± 40%, including an estimate of the extrapolation error) as compared to that of 0.76 a_0^2 of Ehrhardt, et al.. The vibrational excitation DCS at 60 eV has a minimum at 30° and rises to a plateau at 50°-80°.

Measurements carried out at different scattering angles correspond to different $(\ell\, d\Omega)_{eff}$ (explained below) and cannot be directly compared even when other experimental conditions (target density, beam intensity, instrument efficiency, etc.) are the same. The usual expressions relating cross sections and scattered signal intensities contain the path length in an overly simplified way. In a realistic experiment, one has a large number of target particles distributed over the scattering volume and a beam containing many electrons with some kind of energy and spatial distribution. The measured scattered signal is the result of scattering events associated with different path lengths, cross sections and solid angles of detection. One can define only an effective (path length) x (solid angle). This quantity $(\ell \, d\,\Omega)_{eff}$ is a function of the scattering angle and has to be known for absolute DCS determination (or its relative value as a function of scattering angle has to be known to be able to compare DCS measured at different angles).

Previous calculations of $(\ell \, d\,\Omega)_{eff}$ involved simplifications and approximations in scattering geometry, particle distribution and in angular dependence of ℓ and/or σ. The effect of a more rigorous treatment is described here. Circular apertures define the beam cone and similarly apertures A_1 and A_2 define the view cone (see Fig. 2). Scattered signal can be detected from the volume defined by the surfaces of these two intersecting cones. The incoming electron beam density distribution is represented by a Gaussian function having its maximum density along the cone axis. To each volume element within the scattering volume a weighting factor is assigned which is composed of three factors: (a) the electron beam density at that volume element, (b) the solid angle subtended by the detector at that volume element, and (c) the appropriate correction for the change of DCS with angle within the view cone. The

weighted volume elements are then integrated over the scattering volume. (The limits of integration are determined by the equations of the cone surfaces.) This integral is by definition proportional to $(\ell \, d\,\Omega)_{eff}$ and is normalized to unity at 90° for relative DCS determination and error estimation. In the limiting case of very narrow beams and a cross section constant over the whole scattering volume the integral is inversely proportional to sin θ. The energy dependence of the DCS and the energy spread of the electron beam were neglected. The integration was truncated at 2 θ_B in the beam cone. The scattering geometry for the case considered here: $\theta_B = \theta_v = 5°$, $S_B = 3.89$ cm, $S_v = 0.98$ cm, $D_{12} = 0.89$ cm, and $A_1 = A_2 = 0.038$ cm. θ_B is the beam cone angle where the intensity falls to one half of its peak value; A_1 and A_2 are the radii of the exit apertures; for the definition of the other quantities, see Fig. 2. Figure 3 shows the error (%) introduced into the DCS by using sin θ instead of the inverse $(\ell \, d\,\Omega)_{eff}$ correction for the various cases of $\sigma(\theta)$. The error is defined as

$$\text{Error} = \left| \frac{\sin\theta - (\ell \, d\,\Omega)^{-1}_{eff}}{(\ell \, d\,\Omega)^{-1}_{eff}} \right| \times 100\%$$

When DCS are determined from experimental data, the procedure for finding $(\ell \, d\,\Omega)_{eff}$ must be iterative because an <u>approximate</u> form for DCS(θ) has to be assumed to start with. Once an approximate $(\ell \, d\,\Omega)_{eff}$ is known, a better DCS(θ) can be determined, and so on.

Here we do calculations designed to test the error introduced by using an improper scattering length correction. In these calculations a guessed $\sigma_{guess}(\theta)$ is used (in step C above) to compute the $(\ell\, d\,\Omega)^{-1}_{eff}$ correction without iterating, and we determine what error this will cause if the actual DCS is a given different one $\sigma_{actual}(\theta)$. The calculation shows that for this scattering geometry and for a case where $\sigma_{aotual}(\theta) \propto 10^{-0.0322\,\theta}$ (H_2 elastic DCS at 60 eV) one introduces a 40%, 14%, or 10% error in the DCS at 10° by using a sin θ correction, a $(\ell\, d\,\Omega)^{-1}_{eff}$ correction with $\sigma_{guess}(\theta) = 1$, or a $(\ell\, d\,\Omega)^{-1}_{eff}$ correction with $\sigma_{guess}(\theta) \propto 10^{-0.0122\,\theta}$ (H_2 elastic DCS at 10 eV), respectively.

Relatively large (but not unreasonable) cone angles have been considered here to illustrate the importance of the proper path length correction. The errors introduced into the DCS at low scattering angles can be significant even for very slightly diverging beams.

REFERENCES

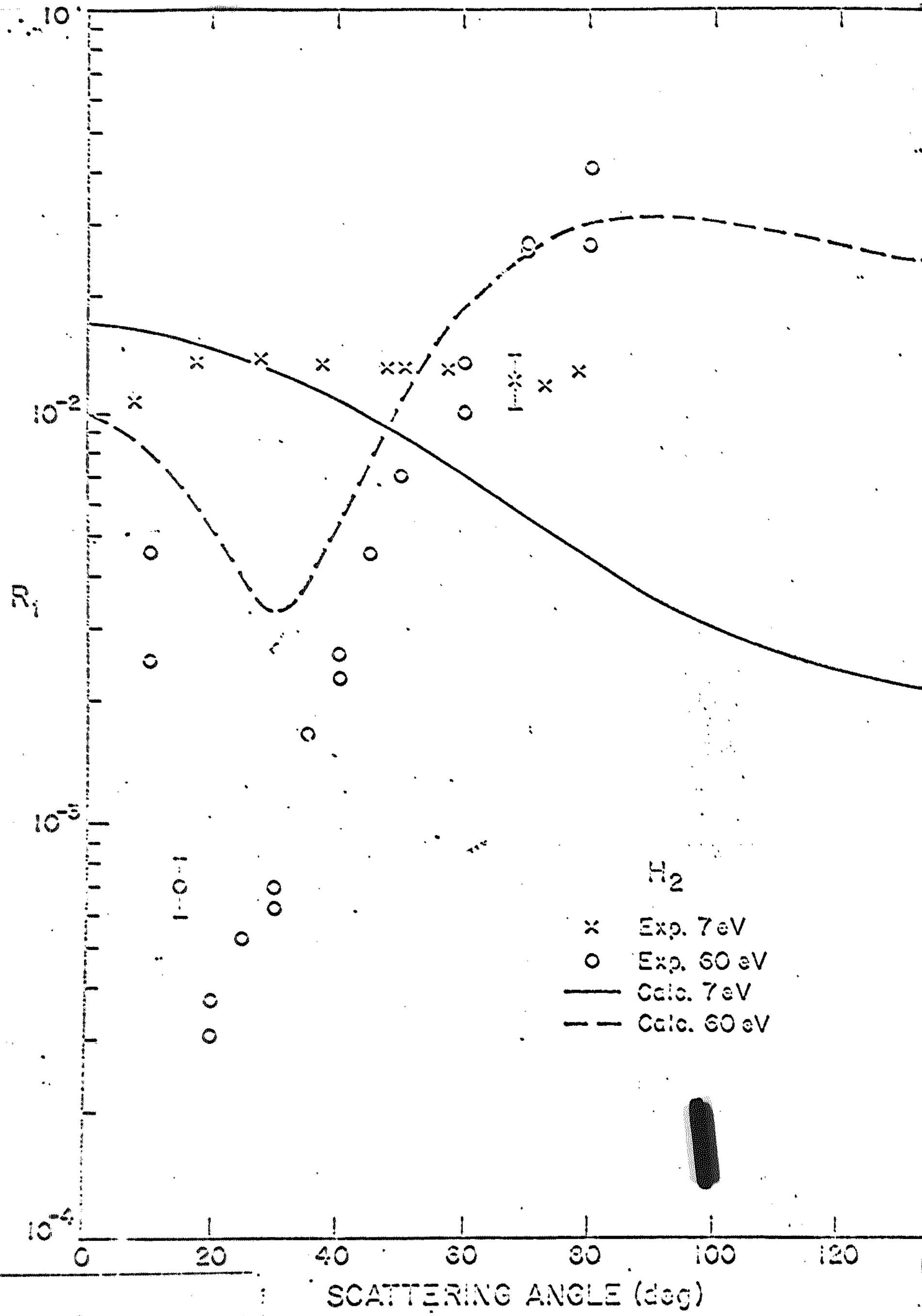
1. D. E. Colden, H. W. Bandel, and J. A. Salerno, Phys. Rev., 146, 40 (1966).
2. H. Ehrhardt, L. Langhans, F. Linder, and H. S. Taylor, Phys. Rev., 173, 222 (1968).

FIGURE CAPTIONS

Figure 1. Vibrational excitation to elastic scattering intensity ratios at 7 and 60 eV impact energies.

Figure 2. Scattering geometry. Dashed lines drawn through the axes of the beam and view cones define the nominal scattering angle θ.

Figure 3. Error (%) introduced into the DCS by using (sin θ) instead of $(\ell\, d\,\Omega)^{-1}_{eff}$ correction for various cases of σ(θ).



10⁻¹
10⁻²
10⁻³
10⁻⁴
R₁
H₂
Exp. 7 eV
Exp. 60 eV
Calc. 7 eV
Calc. 60 eV
0
20
40
60
80
100
120
SCATTERING ANGLE (deg)

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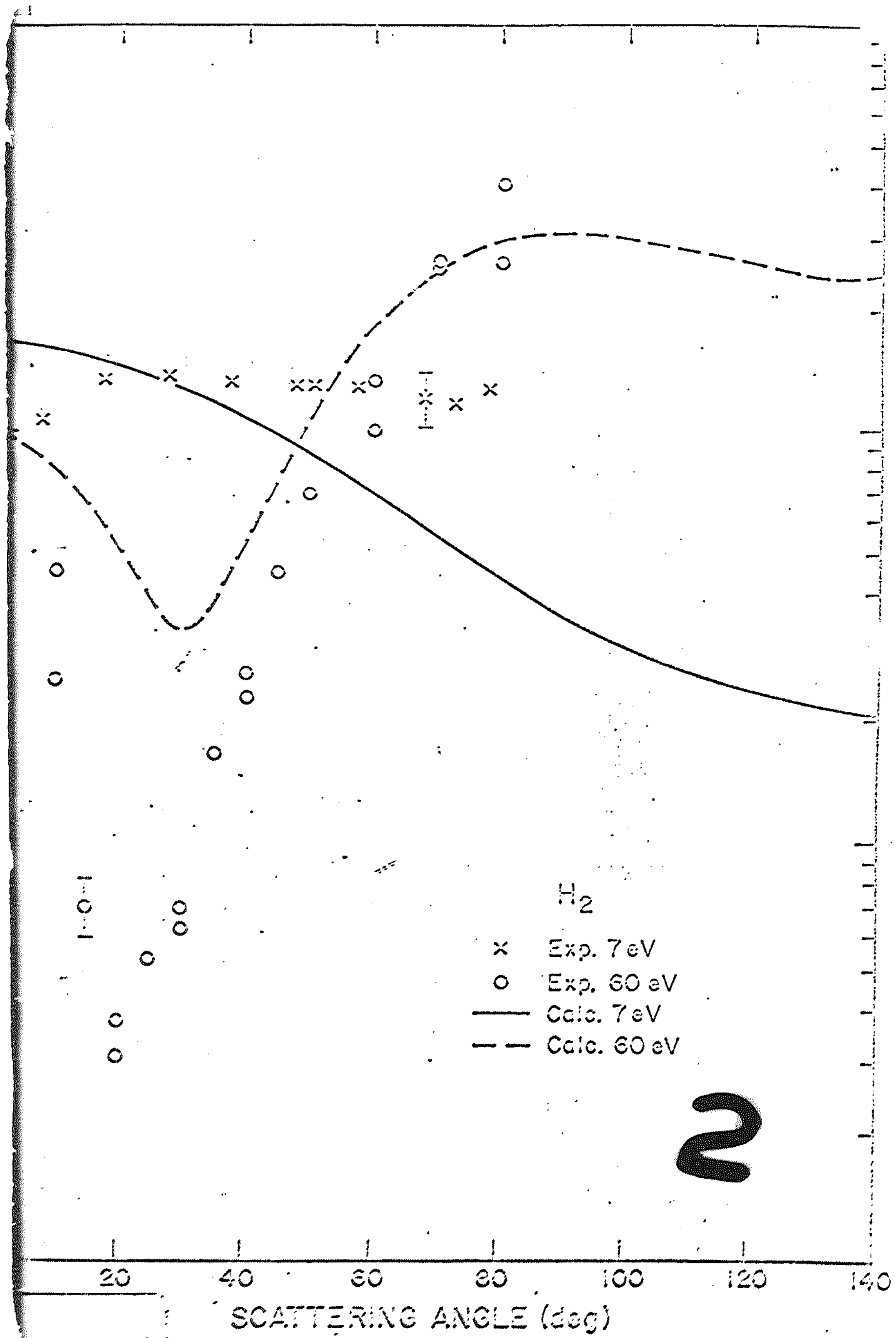
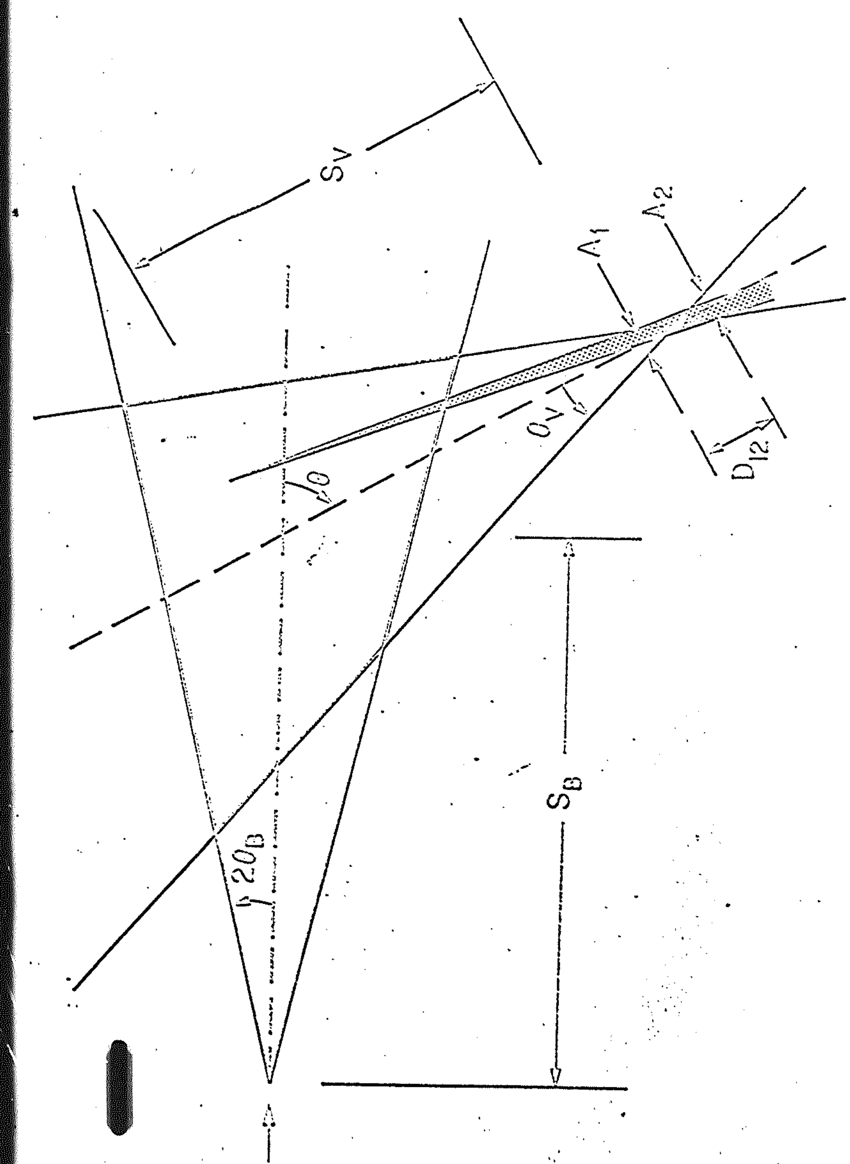


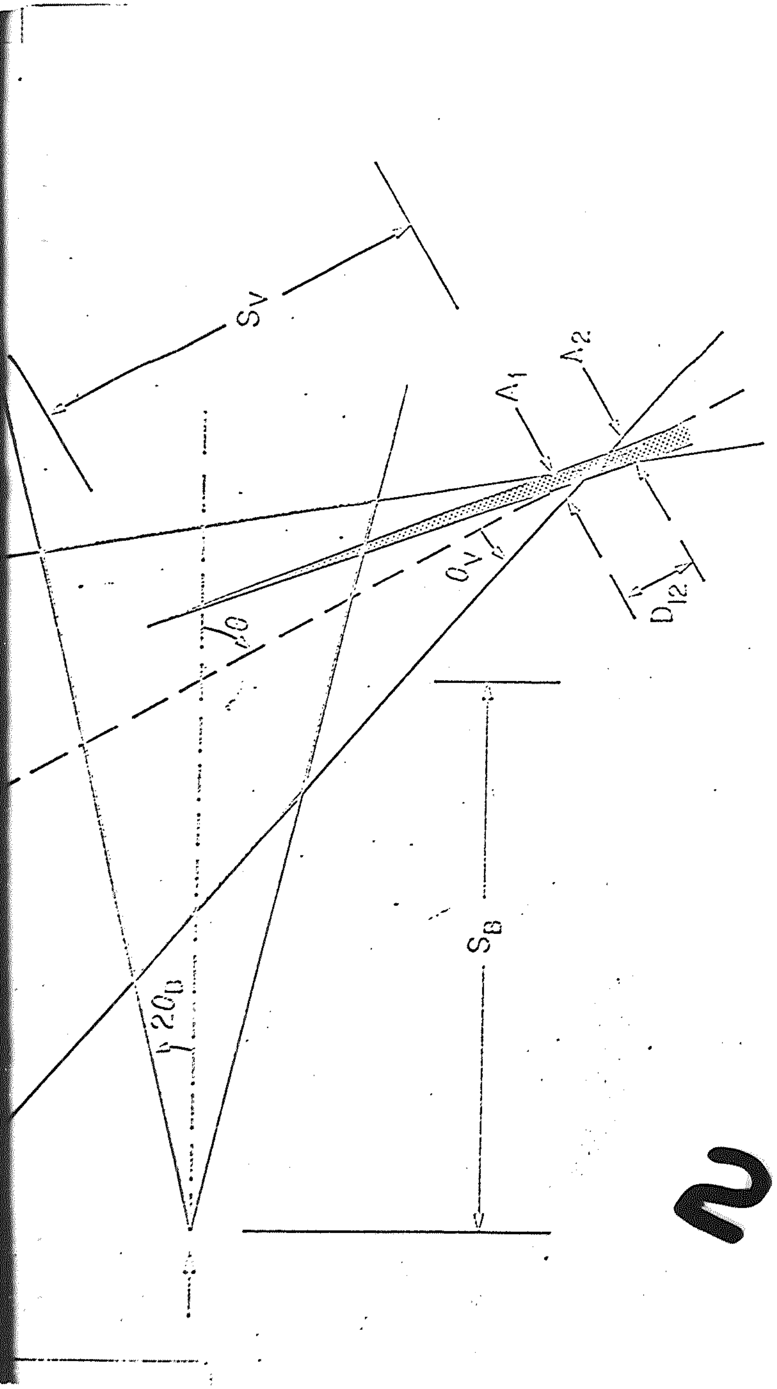
H2
× Exp. 7 eV
○ Exp. 60 eV
Calc. 7 eV
Calc. 60 eV
20
40
60
80
100
120
140
SCATTERING ANGLE (deg)

2



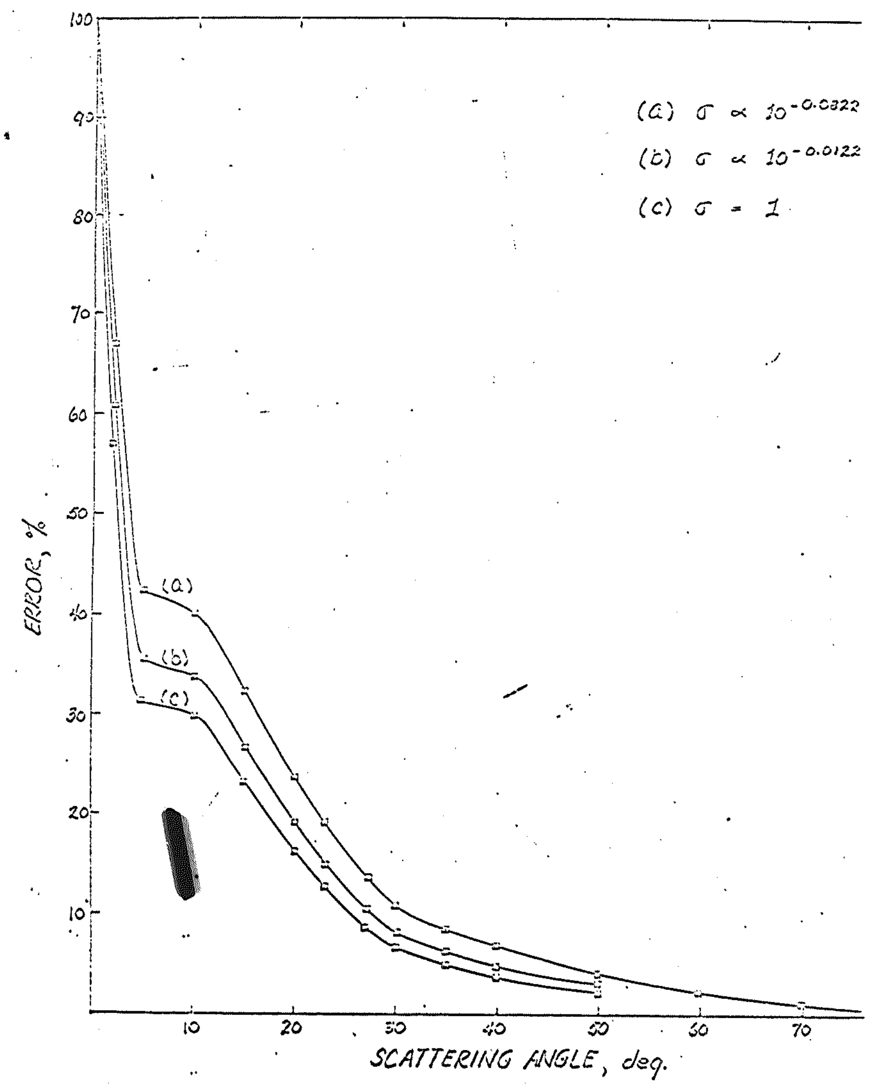
SV
A1
A2
θV
θ
D12
SB
2θB

1



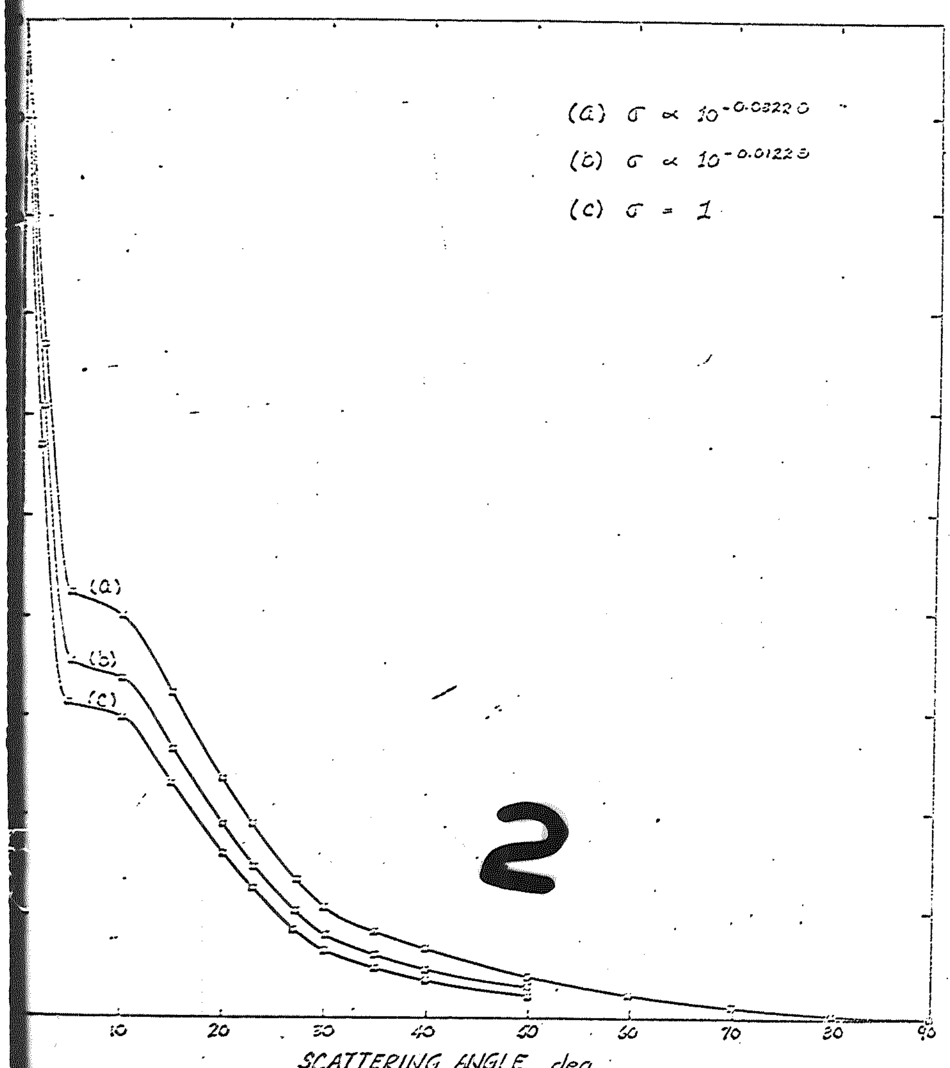
SV
SB
Λ1
Λ2
D12
θ
θV
2θB

2



(a) σ ∝ 10^-0.0322
(b) σ ∝ 10^-0.0122
(c) σ = 1
(a)
(b)
(c)
ERROR, %
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
SCATTERING ANGLE, deg.

Fig.3



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