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Elastic scattering of electrons by benzene

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Abstract. Relative differential cross-sections for the elastic scattering of electrons from benzene have been measured at incident energies 300, 500, 700 and 900 eV and for scattering angles between 30° and 120°. The results are discussed and compared with the independent atom model (IAM) calculations. Two different sets of scattering amplitudes for the constituent atoms of benzene were used in these calculations, one obtained from first Born approximation and the other from partial wave analysis of the Dirac equation. Only the static interaction was taken into account in the calculations. The higher the incident energy, the better is the observed agreement between experiment and theory. This indicates that at higher energies, absorption, exchange and polarization effects are not significant as compared to the static interaction and that the IAM satisfactorily predicts the interference of scattering from the individual atoms of C_6H_6.

Keywords. Elastic scattering of electrons; C_6H_6; energy region 300–900 eV; differential cross sections.

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1. Introduction

While a large number of theoretical and experimental results on elastic differential cross-sections (DCS) for electron scattering have been reported for simple molecules like H_2 and N_2 (Csanak *et al* 1984), data for polyatomic molecules are rather scarce. In fact, there are hardly any data on heavier hydrocarbons in the energy range 200–1000 eV. For C_6H_6, which is the target of the present study, no measurements or calculations of DCS have been reported, though its electronic structure has been extensively investigated by conventional spectroscopic techniques. It is, therefore, worthwhile reviewing the existing theoretical and experimental data for simpler hydrocarbons in the above energy region to find out the range of validity of the different theoretical models in the prediction of DCS.

Fink *et al* (1975) have reported DCS measurements for CH_4, C_2H_2 and C_2H_6 at energies from 100 to 1000 eV and observed good agreement with the independent atom model (IAM) (Bidkar 1990) calculations at scattering angles greater than 40°. Jain (1983) has made calculations for CH_4 in the 25–800 eV energy range using a spherically symmetric analytical static potential along with model dependent local exchange and polarization potentials. His results are in satisfactory agreement with the experimental data at higher energies. Jain and Baluja (1992) have studied a large number of diatomic and polyatomic molecules including CH_4 and C_2H_2 by employing a semiempirical complex optical potential model (SCOP) and reported good agreement

with the measured total (elastic plus inelastic) cross sections in the 100–5000 eV energy range.

It is known that at incident energies much greater than the binding energies of the target electrons, the first Born approximation (FBA) is valid and that the static potential plays an important role. However, FBA underestimates the cross-sections even for the simplest molecule H_2 for scattering angles greater than 100° (Csanak *et al* 1984), though it predicts the shapes of DCS curves quite well in the energy region 200–1000 eV. It would, therefore, be instructive to test the validity of FBA and IAM in this energy region for both simple and complex molecules which have, hitherto, not been investigated.

In the present work, we report DCS measurements on C_6H_6 in the energy region 300–900 eV.

2. Experimental

Measurements of the angular distributions of elastically scattered electrons were carried out using a crossed-beam apparatus. As the details of the apparatus (Bharathi and Srinivasa Rao 1982) and the experimental procedure (Rao and Bharathi 1987) have been described elsewhere, only a brief description of the salient features and necessary modifications relevant to the present measurements will be given here.

Electrons from a commercial electron gun (LEG32, VG, UK) accelerated to the desired energy are allowed to collide orthogonally with the target vapours of interest in a field free region in an aluminium collision chamber of 50·8 cm internal diameter and 61 cm in height. An electron beam current of 2–15 μA is used in the present experiments. The unscattered electron beam is collected in a Faraday cup. A glass manifold connected to an argon gas cylinder serves as the calibration source. The manifold is also coupled to a test tube containing high-pure (GR grade) benzene. Either benzene vapours or argon gas could be leaked into the interaction region through a needle valve and a stainless steel syringe of 0·25 mm inner diameter after passing through a moisture trap assembly.

In order to ensure that high-pure sample gas enters the interaction region, the process of freezing the sample to liquid nitrogen temperature and evacuation of the column above the sample is repeated several times. After attaining a base pressure of about 5×10^{-7} Torr in the collision chamber, the electron beam is made to collide with the target vapours at about 1·5 mm below the tip of the syringe needle. The system is kept on for several hours, before data collection, to ensure stability of experimental conditions. The whole apparatus is maintained at a temperature of 50°C throughout the experiment to avoid deposition of the benzene vapours on the walls of the collision chamber. A cylindrical mirror analyzer (CMA) with energy resolution of 0·4% and acceptance angle of 1·5° was used to record the elastic peaks at different angles of scattering. A parallel plate analyzer (PPA) with energy resolution of 1% was used to monitor the elastically scattered electrons at a fixed angle of 70° to the direction of the incident beam. Philips X919BL channeltrons are used as electron detectors in the analyzers. The details of the data acquisition system employed in the present study have been described in detail in a previous report (Bidkar 1990).

In the present work, no efforts were made to determine absolute differential cross-sections. The following procedure was adopted to obtain the relative differential cross

sections. Both the energy spectra in the CMA and the peak counts in the PPA were recorded simultaneously for the same time interval at the desired impact energy. The area of the CMA spectrum at each angle was normalized to the same number of PPA counts. This procedure ensured that any variations in beam current or target vapour density in the interaction region were taken into account. The area of the CMA spectrum thus obtained is directly proportional to DCS. Several runs were taken to check the reproducibility of the data, particularly at forward angles.

Any possible instrumental anisotropy and the angular calibration of the apparatus were checked by DCS measurements for elastic scattering from argon at 300 eV incident energy. The position of the minimum observed at 110° as well as the values of DCS were found to be in good agreement with those reported earlier (Srinivasa Rao 1985).

Contribution to the error in the relative DCS is mainly due to the reproducibility of the scattering angle and the statistics. The statistical error is maximum (4%) at the minimum of the cross-section curves which occurs at 110°. This is due to the fact that the signal counts at backward angles were not collected for sufficiently long time to get the same statistics as in the data at forward angles. In fact, reproducibility of data could be achieved only when minimum possible time period for data collection was chosen at each angle. This ensured minimum variation of experimental conditions during a single angular distribution run.

Another significant error in the measured DCS arises from the technical impossibility of reproducing the scattering angles to better than 0·25°. However, this error was observed to be much smaller than the statistical error at backward angles. At 500 eV, where the slope of the DCS curve is the steepest at 30°, an extrapolation of the curve to 29° showed a change of cross-section by as much as 24%. Thus an error of 0·25° in the scattering angle at 30° would result in an error of 6%. This error becomes smaller as the angle increases due to the relatively slow variation of cross-section with angle and is negligible as compared to the statistical error at backward angles.

The maximum overall error in the relative DCS is 6%.

3. Results and discussion

Figure 1(a–d) shows the elastic DCS data for C_6H_6 at energies of 300, 500, 700 and 900 eV. The FBA and the partial wave analysis (PWA) (Fink and Yates 1970) calculations obtained by solving the Dirac equation were used to compute the scattering amplitudes for carbon and hydrogen atoms. The IAM (Bidkar 1990) was used to determine the molecular cross-sections for C_6H_6. The theoretical curves shown in figure 1(a–d) are the best fit ones obtained by adjusting the normalization factors at each energy which yield the minimum χ^2.

It is seen that both FBA and PWA calculations fit the DCS data reasonably well at 900 eV. Even at the lowest energy (300 eV), the shape is well-predicted except at backward angles. The diffraction pattern, which is more marked at lower energies, is the result of interference of scattering amplitudes from the different atoms of C_6H_6. Whereas FBA underestimates the cross-sections at lower energies and larger angles, the PWA calculations predict the shapes of the curves satisfactorily except at 300 eV. Surprisingly, at 900 eV, FBA seems to agree better with experiment than does PWA, which is expected to be more accurate than FBA. However, a change in the

normalization factor could shift the theoretical curves below or above the experimental points. Thus in the absence of absolute DCS data, it would not be possible to compare the accuracies of PWA and FBA in predicting the cross-sections, particularly when both the models give DCS values close to the experimental points.

The satisfactory agreement between theory and experiment at higher energies can be understood from the following considerations. The static potential has been proved to be the most important among the interactions in electron-molecule scattering in the 100–1000 eV energy region (Fink *et al* 1975). Polarization and distortion effects become

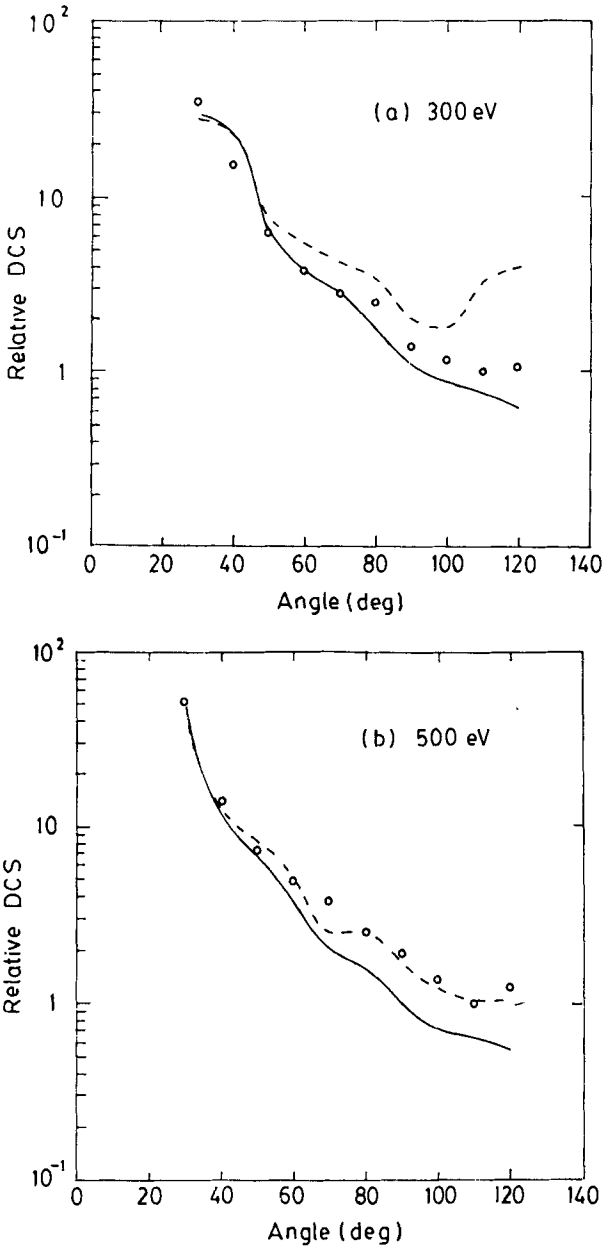

Figure 1(a–b).

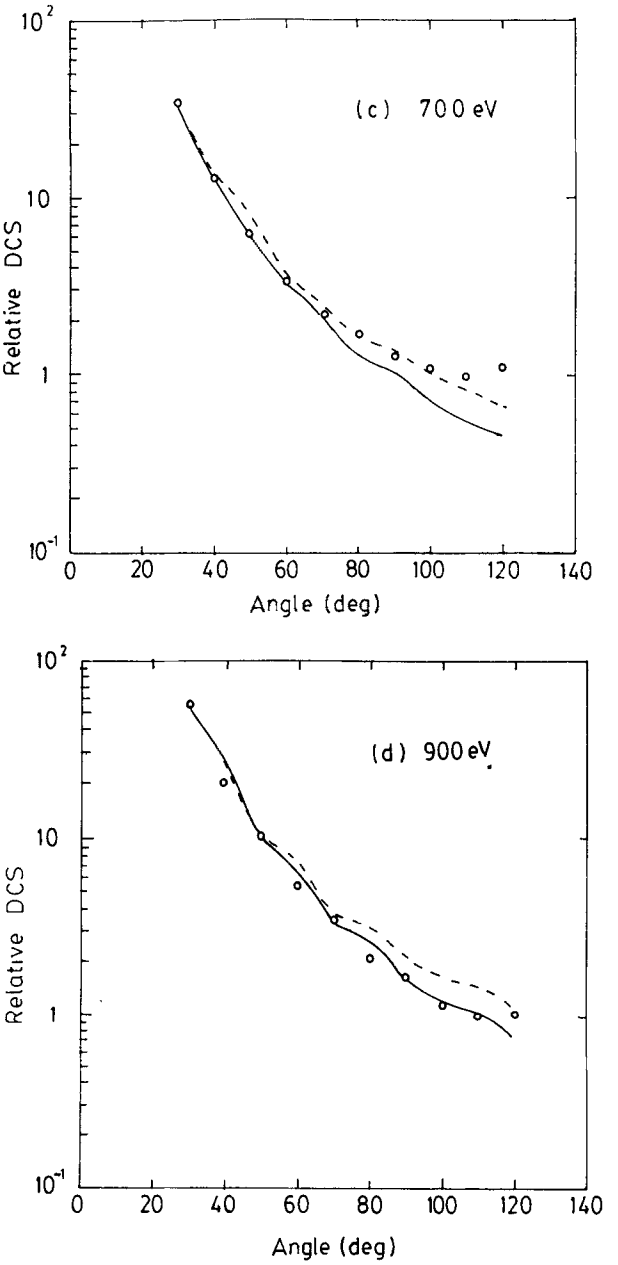

Figure 1(c–d).

Figure 1. Angular distributions for elastic scattering of electrons by benzene molecules at **(a)** 300 eV, **(b)** 500 eV, **(c)** 700 eV, and **(d)** 900 eV. The dashed and solid lines are the PWA-IAM and the FBA-IAM calculations respectively. The open circles are the present experimental data.

more significant at smaller energies. The polarization potential affects the DCS at forward angles less than 30° due to its dependence on the impact parameter (Gupta and Khare 1978). Thus the FBA, which uses only a static potential and a perturbative approach to the solution of Schrödinger equation, is expected to yield reasonably accurate values of the atomic scattering amplitudes. The IAM using the scattering

amplitudes from FBA calculations has been found to be adequate by Fink *et al* (1975) for the simpler hydrocarbons in the energy region of the present study. Thus both FBA- and PWA-IAM should satisfactorily predict the experimental DCS for C_6H_6 at higher energies.

The effect of inclusion of exchange term in the Dirac equation on the DCS at intermediate and high energies has been discussed by Fink and Yates (1970). For all the atoms studied by these authors, it only shifts the cross-section curves as a whole, 2° to 3° toward larger scattering angles.

At 300 eV, where both FBA- and PWA-IAM disagree with experiment, the SCOP model of Jain and Baluja (1992), which takes into account absorption, polarization and exchange along with the static interaction, is expected to fit the experimental data quite well.

4. Conclusions

The present work, carried out at incident electron energies in the region 300–900 eV, shows that the static interaction is the most dominant among the interactions in electron–C_6H_6 scattering. This is consistent with the earlier and theoretical observations in electron scattering from both simple and complex molecules in the intermediate and high energy region. The satisfactory agreement obtained between experiment and IAM calculations is indicative of the fact that the atoms in C_6H_6 scatter the incident electrons independently giving rise to interference pattern in the DCS curves. Since polarization, exchange and absorption potentials are not included in these calculations, it can be concluded that they are less significant as compared to the static interaction at energies above 300 eV. It also appears that FBA–IAM can predict the DCS quite well at energies above 1 keV. At the lowest energy of the present study, 300 eV, only an optical model calculation taking into account static, absorption and exchange potentials would fit the experimental data, as was shown by Jain and Baluja (1992) in polyatomic molecules. The long range polarization potential, which is important at forward angles ($< 30°$), need not be considered in the present work as the angular range covered in the DCS measurements was from 30° to 120°.

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