

## Electron scattering by lithium fluoride

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**Abstract.** Calculations of elastic and rotational excitation cross sections for electron scattering by LiF are presented. A model potential is used and the cross sections computed using the close-coupling and a number of other theoretical methods. The accuracy of the various methods is assessed and a comparison with experimental data shows close agreement at an energy of 5.4 eV.

### 1. Introduction

In an earlier paper (Rudge 1974) it was suggested that the interaction between an electron and a polar molecule could be modelled by a spherically symmetric hard sphere plus a dipole potential. It was shown that if a plane-wave approximation is used then the momentum-transfer cross section may be very different from the point-dipole result, depending upon the value of the hard-sphere radius. In a subsequent paper (Rudge *et al* 1976) the model was improved by making the choice of hard-sphere radius in such a way that the affinity of the molecule was obtained correctly. Furthermore distorted waves, which give exact elastic scattering phase-shifts in the limit of zero dipole moment, were used in place of plane waves.

In the present paper cross sections are computed by using the same model but by solving the close-coupling equations which describe the rotational excitation process. A comparison is then effected between these results and those of a variety of approximate methods which includes the plane-wave and distorted-wave approximations.

The system studied is the collision between an electron and the strongly polar molecule LiF, for which recent experimental data have been obtained (Vuskovic *et al* 1978). Atomic units ( $e = m = \hbar = 1$ ) are used except where otherwise stated.

### 2. Theory

#### 2.1. The scattering equations

The model Hamiltonian is

$$\mathcal{H} = -\frac{\Lambda^2}{2I} - \frac{1}{2}\nabla_r^2 + \sum_{\lambda=0}^1 v_{\lambda}(r)P_{\lambda}(\hat{\mathbf{r}} \cdot \hat{\mathbf{R}}) \quad (1)$$

where  $\Lambda^2$  is an angular momentum operator,  $I$  is the moment of inertia of the molecule and

$$v_0(r) = \begin{cases} \infty & r < R_0 \\ 0 & r > R_0 \end{cases} \quad (2)$$

$$v_1(r) = -\frac{D}{r^2}. \quad (3)$$

Let  $\gamma$  denote collectively the quantum numbers ( $jlJM$ ) and let

$$k_j^2 = 2E - \frac{j(j+1)}{I} \quad (4)$$

where  $E$  is the total energy. Following Arthurs and Dalgarno (1960) a solution of the Schrödinger equation corresponding to entrance channel  $\gamma_0$  can be sought in the form

$$\Psi^{\gamma_0} = r^{-1} \sum_{\gamma} y(\gamma | \hat{\mathbf{R}} \hat{\mathbf{r}}) F_{\gamma}^{\gamma_0}(r) \quad (5)$$

where  $y$  denotes coupled spherical harmonics. It then follows that

$$\left( \frac{d^2}{dr^2} + k_j^2 \right) F_{\gamma}^{\gamma_0} = \sum_{\gamma'} V_{\gamma\gamma'} F_{\gamma'}^{\gamma_0} \quad (6)$$

where

$$r^2 V_{\gamma\gamma'} = -2Df_1(jlj'l'J) + l(l+1)\delta_{\gamma\gamma'} \quad (7)$$

and  $f_1$  denotes an algebraic coefficient defined by Percival and Seaton (1957).

The coupled equations (6) must be solved subject to the boundary conditions

$$F_{\gamma}^{\gamma_0}(R_0) = 0 \quad (8)$$

$$F_{\gamma}^{\gamma_0}(r) \underset{r \rightarrow \infty}{\sim} k_j^{-1/2} [\delta_{\gamma_0\gamma} \sin(k_j r - \frac{1}{2}l'\pi) + R_{\gamma_0\gamma} \cos(k_j r - \frac{1}{2}l'\pi)]. \quad (9)$$

The real symmetric matrix with elements  $V_{\gamma\gamma'}$  may be diagonalised by an orthogonal matrix  $\mathbf{U}$  in the form

$$\mathbf{V} = \mathbf{U}\mathbf{X}\mathbf{\tilde{U}}. \quad (10)$$

Defining a column vector  $\mathbf{F}^{\gamma_0}$ , which has the  $F_{\gamma}^{\gamma_0}$  as elements, and

$$\mathbf{G}^{\gamma_0} = \mathbf{\tilde{U}}\mathbf{F}^{\gamma_0} \quad (11)$$

it follows that the scattering equation (6) can be written

$$(\mathbf{D}^2 + \mathbf{\tilde{U}}\mathbf{K}\mathbf{U})\mathbf{G}^{\gamma_0} = r^{-2}\mathbf{X}\mathbf{G}^{\gamma_0} \quad (12)$$

where

$$\mathbf{D}_{ik}^2 = \delta_{ik} \frac{d^2}{dr^2} \quad (13)$$

and

$$\mathbf{K}_{ik} = k_i^2 \delta_{ik}. \quad (14)$$

The close-coupling equations (6) and (12) have been solved in two ways. In the first method they have been integrated inwards and outwards, using the Runge-Kutta algorithm, and matched to yield the  $\mathbf{R}$  matrix. In the second method the small off-diagonal elements of  $\mathbf{UKU}$  have been set to zero so that the set of equations (12) are then uncoupled. These  $N$  equations can then be more rapidly solved to yield  $N$  phaseshifts. If  $l_k$  denotes the  $l$  value for channel  $k$  then defining matrices with elements

$$\begin{aligned} t_{ik} &= \delta_{ik} \tan \eta_k \\ c_{ik} &= \delta_{ik} \cos \frac{1}{2} l_k \pi \\ s_{ik} &= \delta_{ik} \sin \frac{1}{2} l_k \pi \end{aligned} \quad (15)$$

and

$$\mathbf{R}' = \mathbf{U} \mathbf{t} \mathbf{U} \quad (16)$$

it follows that the  $\mathbf{R}$  matrix is given by

$$\mathbf{R} = (\mathbf{cR}' + \mathbf{s})(\mathbf{c} - \mathbf{sR}')^{-1}. \quad (17)$$

At the energies considered, which are much greater than the rotational spacing, numerical tests show that the second method is accurate and computationally faster than the first method. Results were therefore mainly obtained from the second procedure.

## 2.2. The plane-wave approximation and cross section expressions

The scattering amplitude for rotational excitation may be expressed in the form

$$f_{jm_j j' m_j'}(\mathbf{k}_j, \mathbf{k}_{j'}) = 2\pi i (-1)^{m_{j'}} (k_j k_{j'})^{-1/2} \sum_{ll'LM} C_{m_j - m_{j'}, M}^{j j' L} A_{ll' j j' L} Y(ll' LM | \hat{\mathbf{k}}_j \hat{\mathbf{k}}_{j'}) \quad (18)$$

where

$$A_{ll' j j' L} = \sum_J i^{l-l'} (-1)^{j+l-j'+l'+L-J} W(jl j' l' J L) T_{jl j' l' J} \quad (19)$$

and the  $\mathbf{T}$  matrix is related to the  $\mathbf{R}$  matrix by

$$\mathbf{T} = -2i\mathbf{R}(\mathbf{I} - i\mathbf{R})^{-1}. \quad (20)$$

In these equations  $C$  and  $W$  denote Clebsch-Gordan and Racah coefficients, respectively. The cross sections may be directly evaluated through the  $\mathbf{T}$  matrix elements but due to slow convergence it is better to adopt an alternative procedure. The plane-wave approximation to the scattering amplitude is given by

$$\begin{aligned} f_{jm_j j' m_j'}^{\text{PW}}(\mathbf{k}_j, \mathbf{k}_{j'}) \\ = \frac{(-1)^{m_{j'}}}{3\sqrt{3}} [-16\pi D^2 (2j+1)(2j'+1)]^{1/2} C_{000}^{j j' 1} C_{m_j - m_{j'}, m}^{j j' 1} \frac{\sin qR_0}{q^2 R_0} Y_{1m}(\hat{\mathbf{q}}) \end{aligned} \quad (21)$$

where

$$\mathbf{q} = \mathbf{k}_j - \mathbf{k}_{j'}. \quad (22)$$

The differential cross section (DCS) is given by

$$\frac{dQ_{jj'}}{d\Omega} = \frac{k_{j'}}{(2j+1)k_j} \sum_{m_j m_{j'}} |f_{jm_j j'm_{j'}}(\mathbf{k}_j, \mathbf{k}_{j'})|^2 \quad (23)$$

and if we write

$$f = f^{\text{PW}} + (f - f^{\text{PW}}) \quad (24)$$

then this becomes

$$\frac{dQ_{jj'}}{d\Omega} = \left( \frac{dQ}{d\Omega} \right)_{\text{PW}} + \left( \frac{dQ}{d\Omega} \right)_1 + \left( \frac{dQ}{d\Omega} \right)_2 \quad (25)$$

where

$$\left( \frac{dQ}{d\Omega} \right)_{\text{PW}} = \frac{4D^2 k_{j'}}{3k_j(2j+1)} \left( \frac{\sin qR_0}{q^2 R_0} \right)^2 \max(j, j') \quad (26)$$

$$\left( \frac{dQ}{d\Omega} \right)_1 = \frac{1}{4k_j^2(2j+1)} \sum_{\lambda} \alpha_{\lambda} P_{\lambda}(\hat{\mathbf{k}}_j \cdot \hat{\mathbf{k}}_{j'}) \quad (27)$$

with

$$\alpha_{\lambda} = (2\lambda + 1) \sum_{ll'l_1L} (2L + 1) f_{\lambda}(ll'l_1L) (A_{ll'jj'L} - A_{ll'jj'L}^{\text{PW}}) (A_{l_1l_1jj'L}^* - A_{l_1l_1jj'L}^{\text{PW}}) \quad (28)$$

and

$$\begin{aligned} \left( \frac{dQ}{d\Omega} \right)_2 &= \frac{2Dk_j^{1/2} \sin qR_0}{3R_0 k_j^{3/2} q^3} \left( \frac{2j' + 1}{2j + 1} \right)^{1/2} C_{000}^{jj'1} \sum_{ll'} C_{000}^{l'l'1} [(2l + 1)(2l' + 1)]^{1/2} \\ &\quad \times \text{Re} (A_{ll'jj'1} - A_{ll'jj'1}^{\text{PW}}) [k_j P_l(\hat{\mathbf{k}}_j \cdot \hat{\mathbf{k}}_{j'}) - k_{j'} P_{l'}(\hat{\mathbf{k}}_j \cdot \hat{\mathbf{k}}_{j'})]. \end{aligned} \quad (29)$$

The subtraction method (25) differs from a similar procedure adopted by Itikawa (1969) and Crawford and Dalgarno (1971).

### 2.3. Other theoretical methods

**2.3.1. Distorted-wave method (DW).** The standard distorted-wave scattering amplitude is given by

$$f_{jm_j j'm_{j'}}^{\text{DW}}(\mathbf{k}_j, \mathbf{k}_{j'}) = -(2\pi)^{-1} \int \psi(-\mathbf{k}_{j'}|\mathbf{r}) Y_{j'm_{j'}}^*(\hat{\mathbf{R}}) (\mathcal{H} - E) \psi(\mathbf{k}_j|\mathbf{r}) Y_{jm_j}(\hat{\mathbf{R}}) d\mathbf{r} d\hat{\mathbf{R}} \quad (30)$$

where, if  $j_l(x)$ ,  $n_l(x)$  are spherical Bessel functions,

$$\psi(\mathbf{k}|\mathbf{r}) = \sum_l i^l (2l + 1) e^{im_l} P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) [\cos \eta_l j_l(kr) + \sin \eta_l n_l(kr)] \quad (31)$$

and

$$\tan \eta_l = - \frac{j_l(kR_0)}{n_l(kR_0)}. \quad (32)$$

This approximation was used by Rudge *et al* (1976). The corresponding  $\mathbf{T}$  matrix element is given to a close approximation by

$$T_{\gamma\gamma'}^{\text{DW}} = \frac{1}{2}(e^{2i\eta_l} + e^{2i\eta_{l'}})T_{\gamma\gamma'}^{\text{BPD}} + \delta_{\gamma\gamma'}(1 - e^{2i\eta_l}) \quad (33)$$

where the Born point-dipole (BPD) element is

$$T_{\gamma\gamma'}^{\text{BPD}} = -\frac{2iDf_1(jl'l'J)\sin\frac{1}{2}\pi(l' - l)}{l'(l' + 1) - l(l + 1)}. \quad (34)$$

It may be shown that if  $\hat{\mathbf{k}}_j \cdot \hat{\mathbf{k}}_{j'} = -1$  then the inelastic DW scattering amplitude differs from the BPD amplitude only by a phase factor. Hence, independent of the cut-off radius, the DCS at a scattering angle of  $\pi$  for the  $j' = j \pm 1$  transition in the DW treatment is identical with its BPD value. This is an unsatisfactory feature of the approximation.

**2.3.2. Unitarised approximation.** The unitarity of the  $\mathbf{S}$  matrix, where  $\mathbf{S} = \mathbf{I} - \mathbf{T}$ , is satisfied for the  $N \times N$   $\mathbf{S}$  matrix in the close-coupling approximation where  $N$  is the number of channels. This in some degree is a defect of the method where there are open channels which are omitted in the calculation. However, following Seaton (1961), plane-wave and distorted-wave approximations may be unitarised in which case they may be expected to conform more closely with close-coupling values. There is no unique way of effecting unitarisation but one method is to calculate from an approximate  $\mathbf{T}$  matrix

$$\mathbf{T} = \mathbf{T}_r + i\mathbf{T}_i \quad (35)$$

an  $\mathbf{R}$  matrix given by

$$\mathbf{R} = (-2\mathbf{I} + \mathbf{T}_r)^{-1}\mathbf{T}_i \quad (36)$$

and to then use equation (20). Results using this method have been calculated and are labelled UPW (unitarised plane wave) and UDW (unitarised distorted wave).

**2.3.3. Analytic approximation.** In the second approach described in §2.1 it is unnecessary to evaluate all the phaseshifts numerically. For large values at the angular momentum the phaseshifts may be adequately approximated by the formula

$$\eta_k \simeq -\frac{1}{2}l\pi + \tan^{-1}\left(\frac{\pi[l(l+1) + \beta^2]}{2(2l+1)}\right) \quad (37)$$

where  $\beta^2 = -X_{kk}$  and  $l$  is chosen to be the integer such that  $\beta^2 + l(l+1)$  has its least value. A very simple analytic approximation results if all the phaseshifts are approximated and calculations have been carried out using the formula (37) where the quadratic in  $l$  has real solutions and using the alternative formula

$$\eta_k \simeq -(\beta^2 + k^2R_0^2)^{1/2} - \beta \ln\left(\frac{(\beta^2 + k^2R_0^2)^{1/2} - \beta}{kR_0}\right) \quad (38)$$

otherwise.

### 3. Results

The affinity of LiF has been computed by Jordan *et al* (1976) using a Hartree-Fock approximation and by Rudge (1978) using the model interaction. Taking  $D = 2.4728$

**Table 1.** Reduced differential cross sections (see equation (39)).

Scattering angle	Incident energy (eV)							
	0.5	1.0	2.0	4.0	5.4	8.0	12.0	20.0
5	1.05	1.05	1.04	1.04	1.04	1.04	1.03	1.03
10	1.01	1.01	1.01	1.00	0.99	0.99	0.98	0.97
15	0.93	0.94	0.93	0.92	0.92	0.91	0.89	0.88
20	0.85	0.85	0.85	0.84	0.83	0.81	0.80	0.78
30	0.63	0.64	0.64	0.62	0.61	0.59	0.57	0.55
40	0.45	0.46	0.46	0.45	0.44	0.43	0.41	0.39
50	0.32	0.34	0.35	0.35	0.34	0.32	0.30	0.29
60	0.24	0.27	0.29	0.28	0.27	0.26	0.25	0.25
70	0.19	0.22	0.25	0.25	0.24	0.23	0.23	0.25
80	0.17	0.21	0.24	0.24	0.23	0.22	0.22	0.26
90	0.17	0.22	0.25	0.23	0.22	0.21	0.22	0.27
110	0.28	0.30	0.27	0.23	0.22	0.22	0.24	0.30
130	0.56	0.49	0.34	0.24	0.22	0.22	0.25	0.32
150	0.96	0.73	0.41	0.24	0.23	0.23	0.26	0.34
180	1.32	0.93	0.47	0.25	0.23	0.24	0.27	0.35

(Brumer and Karplus 1973), the value of  $R_0$  was chosen to be 1.15. The equations (6) were solved for an initial value of  $j = 0$  including channels up to a maximum of  $j' = 4$ .

It is convenient to present the angular distribution results as a reduced cross section equal to the ratio of the DCS to its BPD value. Thus for  $\theta \neq 0$  the DCS to an adequate approximation is given in terms of the reduced cross section by

$$\frac{dQ}{d\Omega} = \sum_{j'} \frac{dQ_{jj'}}{d\Omega} = \frac{1}{3} \left( \frac{D}{k_j \sin \theta/2} \right)^2 \left( \frac{dQ}{d\Omega} \right)_R. \quad (39)$$

Table 1 displays the calculated reduced cross sections for a range of energies. It is clear from this table that at angles less than  $10^\circ$  there is little departure from the BPD value and that below  $60^\circ$  the reduced cross sections are almost independent of energy. At large scattering angles there is a marked variation in the reduced cross section with energy.

The shape of the experimental and theoretical curves displayed in figure 1 are in close agreement at 5.4 eV but at 20 eV there is a significant departure. The comparison is complicated by the fact that the experimental data represent an average over initial rotational states and the finite energy spread of the electron beam and include also other unresolved inelastic processes. The model, however, is likely to be less satisfactory at high energies where the short-range forces are more significant.

Table 2 compares the total cross sections calculated by various theoretical methods. The differences are not great due to the dominant forward peak in the scattering which all the methods reproduce.

Table 3 compares the calculated momentum-transfer cross sections. Here the differences are very significant. The only simple procedure which is at all adequate is the analytic approximation. The DW calculations overestimate the cross section due to the fact that the  $j' = j \pm 1$  DCS reduces to the BPD value at  $\theta = \pi$ .

**Table 2.** Total cross sections ( $\pi a_0^2$ ).

Energy (eV)	$Q_{CC}$	$Q_{PW}$	$Q_{UPW}$	$Q_{DW}$	$Q_{UDW}$	$Q_{AA}$	$Q_{CPT}^\dagger$
0.5	3.44,3 $\ddagger$	3.84,3	3.34,3	3.84,3	3.38,3	3.42,3	3.42,3
1.0	1.88,3	2.07,3	1.83,3	2.07,3	1.83,3	1.87,3	1.86,3
2.0	1.10,3	1.11,3	9.89,2	1.11,3	9.90,2	1.01,3	1.01,3
4.0	5.42,2	5.85,2	5.32,2	5.87,2	5.33,2	5.43,2	5.43,2
5.4	4.13,2	4.42,2	4.06,2	4.46,2	4.07,2	4.14,2	4.14,2
8.0	2.89,2	3.06,2	2.84,2	3.10,2	2.85,2	2.90,2	2.90,2
12.0	1.99,2	2.09,2	1.96,2	2.13,2	1.97,2	2.01,2	2.01,2
20.0	1.25,2	1.28,2	1.23,2	1.34,2	1.24,2	1.29,2	1.29,2

$^\dagger$  Dickinson (1977).

$\ddagger$  The figure following the comma denotes the power of ten by which the number should be multiplied.

A more detailed comparison of the various theoretical procedures is shown in figure 2. Figures 2(a), (c) and (e) compare, at three different energies, the reduced DCS as given by the PW, DW, CC and classical perturbation method of Dickinson (1977). Figures 2(b), (d) and (f) similarly compare the UPW, UDW, AA and CC methods. Tables 4 and 5 show the total and momentum-transfer cross sections to individual final rotational states. In table 5 results obtained by Collins and Norcross (1977a,b) using a different model are shown for comparison.

**Table 3.** Momentum-transfer cross sections ( $\pi a_0^2$ ).

Energy (eV)	$Q_{CC}$	$Q_{PW}$	$Q_{UPW}$	$Q_{DW}$	$Q_{UDW}$	$Q_{AA}$	$Q_{CPT}^\dagger$
0.5	1.91,2 $\ddagger$	4.30,2	1.30,2	4.36,2	1.34,2	1.75,2	2.45,2
1.0	9.14,1	2.08,2	6.42,1	2.14,2	6.85,1	9.27,1	1.22,2
2.0	3.99,1	9.75,1	3.15,1	1.04,2	3.59,1	4.25,1	6.12,1
4.0	1.72,1	4.29,1	1.52,1	5.02,1	1.96,1	1.81,1	3.06,1
5.4	1.22,1	2.91,1	1.10,1	3.66,1	1.54,1	1.28,1	2.27,1
8.0	8.01,0	1.67,1	7.01,0	2.44,1	1.16,1	8.62,0	1.53,1
12.0	5.48,0	8.80,0	4.27,0	1.64,1	8.96,0	6.23,0	1.02,1
20.0	3.71,0	3.46,0	2.10,0	1.02,1	6.15,0	4.32,0	9.96,0

$^\dagger$  Dickinson (1977).

$\ddagger$  The figure following the comma denotes the power of ten by which the number should be multiplied.

**Table 4.** Total cross sections for individual final states ( $\pi a_0^2$ ).

Energy (eV)	$j' = 0$	$j' = 1$	$j' = 2$	$j' = 3$	$j' = 4$
0.5	232	3105	82	19	4.6
1.0	119	1703	41	11	2.6
2.0	56	927	23	6.6	1.4
4.0	23	502	12	3.4	0.6
5.4	16	385	9.3	2.4	0.4
8.0	9.4	271	6.4	1.4	0.2

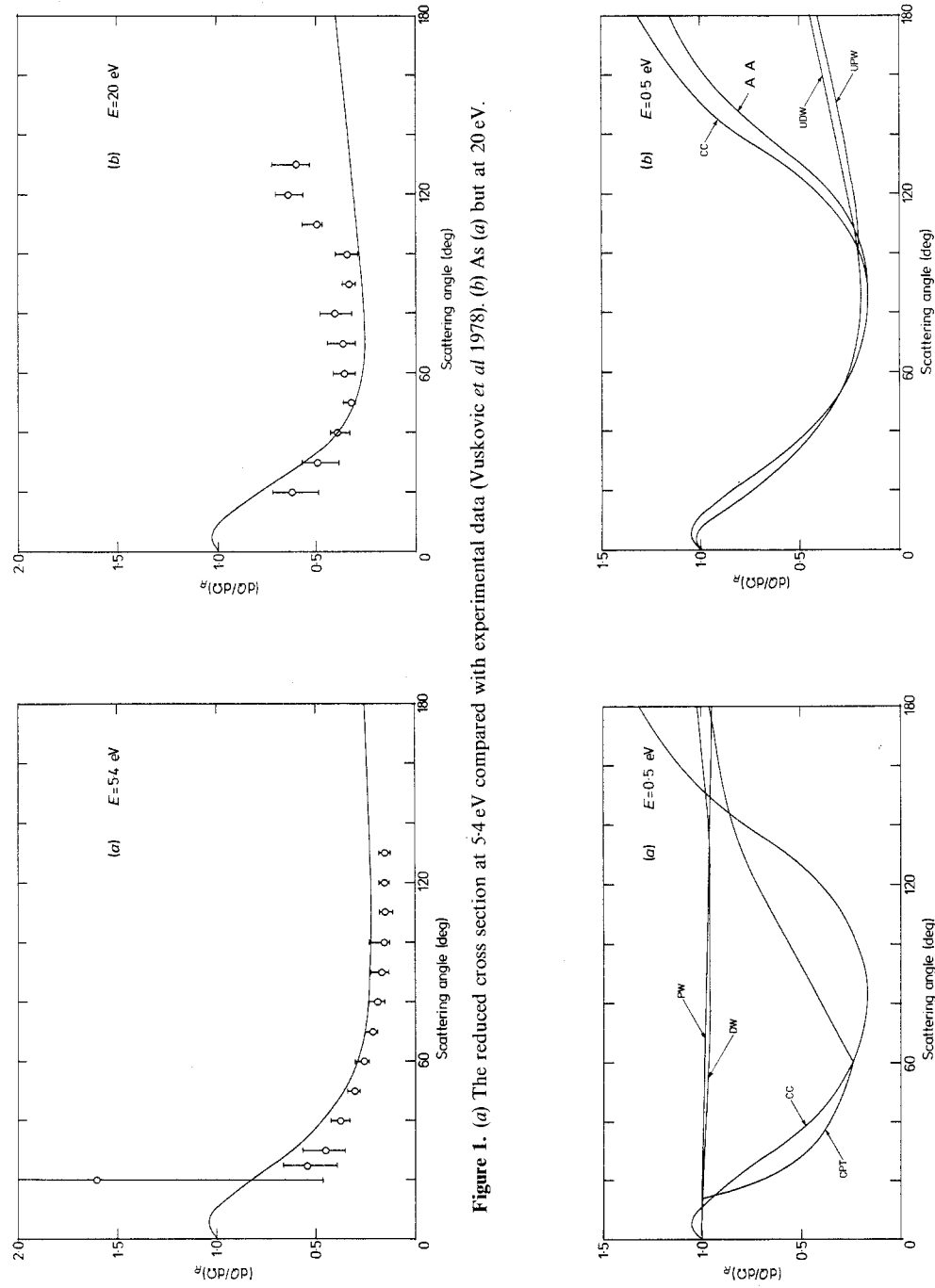
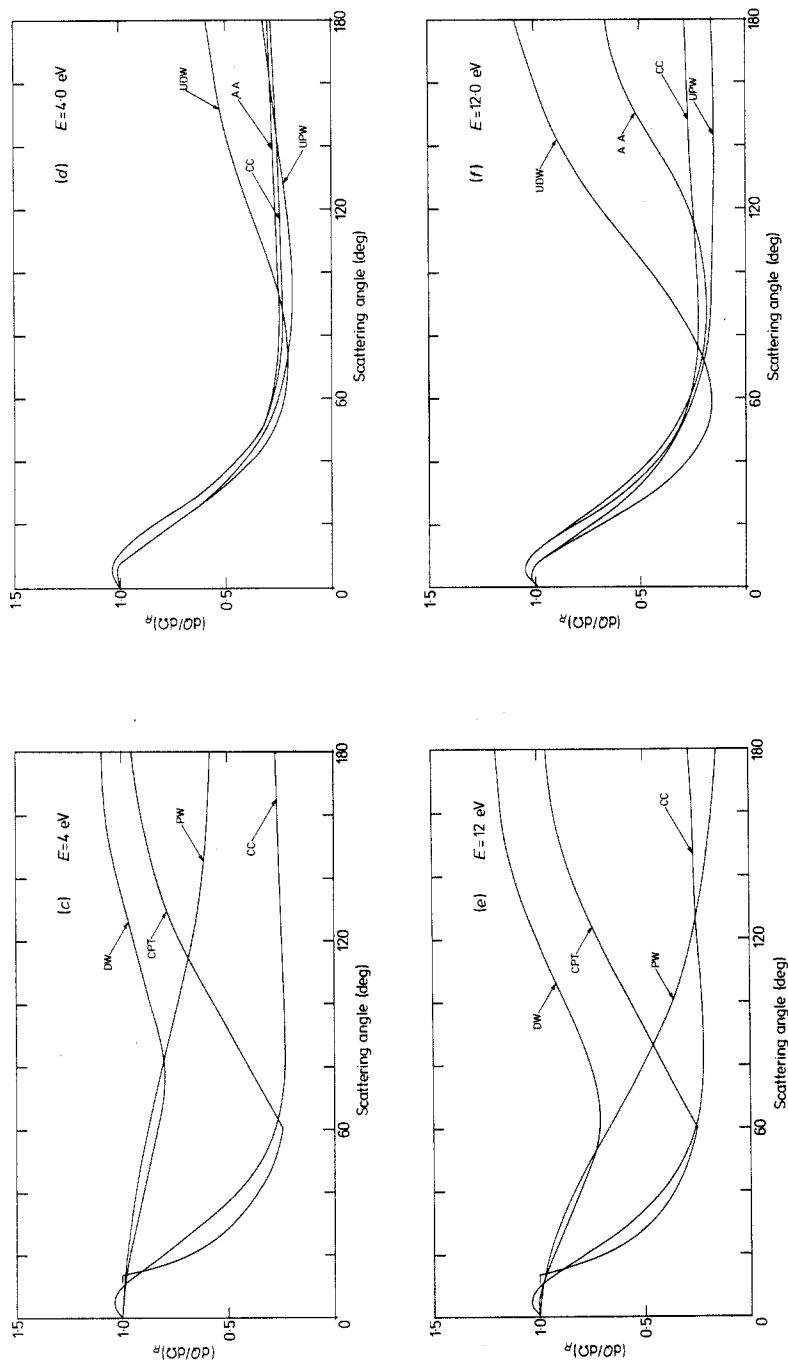


Figure 1. (a) The reduced cross section at 5.4 eV compared with experimental data (Vuskovic *et al* 1978). (b) As (a) but at 20 eV.





**Figure 2.** (a) A comparison of reduced cross sections by various theoretical methods at 0.5 eV. CPT denoted the classical perturbation theory of Dickinson (1977). (b) A comparison of reduced cross sections at 0.5 eV. (c) As (a) but at energy = 4.0 eV. (d) As (b) but at energy = 4.0 eV. (e) As (a) but at energy = 12.0 eV. (f) As (b) but at energy = 12.0 eV.

**Table 5.** Momentum-transfer cross sections for individual final states ( $\pi a_0^2$ )<sup>†</sup>.

Energy (eV)	$j' = 0$	$j' = 1$	$j' = 2$	$j' = 3$	$j' = 4$
0.5	67	75	25	17	6.1
(0.54)	(54.0)	(65.3)	(26.7)	(25.1)	
1.0	28	35	13	11	3.5
2.0	9.4	13	7.8	6.9	1.9
	(35.1)	(19.7)	(13.0)	(4.15)	
4.0	2.9	4.7	5.0	3.6	0.8
5.4	1.7	3.2	4.1	2.5	0.6
8.0	0.9	2.3	3.0	1.5	0.3

<sup>†</sup> Bracketed values are the cross sections computed using a static-exchange model by Collins and Norcross (1977).

#### 4. Conclusions

The results show that the plane-wave and distorted-wave approximations are not adequate for evaluating angular distributions and momentum-transfer cross sections and that the unitarised versions of these approximations are not generally good either. Equation (17), however, provides a more rapid means, at the energies considered, of evaluating the close-coupling results and the analytic approximation to this is very easy to compute and provides fairly accurate results.

It is more difficult to assess the accuracy of the model. A necessary criterion for any model potential is that it should be capable of reproducing the affinity of the negative ion in a bound-state calculation and the present model is adequate in this regard. Collins and Norcross (1977a,b) have computed cross sections using a static Hartree–Fock potential with a model exchange interaction. Some results of this more elaborate procedure are compared in table 5 with the present results, in which it appears that at 2.0 eV the momentum-transfer cross sections are very different. No bound-state data are available using this method however, and no experimental data have been obtained at this energy.

On the theoretical side there is perhaps as great a need to examine the effects of competing processes as to refine model potentials. Experimentally there is a need both for more experimental spectroscopic data on negative polar molecular ions and for more scattering data particularly at low energies and large scattering angles. An experiment which permitted individual rotational transitions to be resolved would provide the most searching test of all.

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