Fermilab Library
0 1160 0037752 7

IFT

Instituto de Física Teórica
Universidade Estadual Paulista

FERMILAB
JUL 2 · 195

June/94

IFT–P.022/94

The effect of positronium formation in positron-alkali-atom scattering

Hasi Ray, A. S. Ghosh

Department of Theoretical Physics
Indian Association for the Cultivation of Science
Jadavpur
Calcutta 700032
India

and

Sadhan K. Adhikari

Instituto de Física Teórica
Universidade Estadual Paulista
Rua Pamplona, 145
01405-900 – São Paulo, S.P.
Brazil

NAME	DATE	M.S.

RETURN TO FERMILAB LIBRARY

Instituto de Física Teórica
Universidade Estadual Paulista
Rua Pamplona, 145
01405-900 – São Paulo, S.P.
Brazil

Telephone: 55 (11) 251-5155
Telefax: 55 (11) 288-8224
Telex: 55 (11) 31870 UJMFBR
Electronic Address: LIBRARY@IFT.UESP.ANSP.BR
47553::LIBRARY

The effect of positronium formation in positron-alkali-atom scattering

H. Ray[(a)], Sadhan K. Adhikari[(b)], and A. S. Ghosh[(a)]

[(a)] *Department of Theoretical Physics, Indian Association for the Cultivation of Science Calcutta 700032, India*

[(b)] *Instituto de Física Teórica, Universidade Estadual Paulista 01405 São Paulo, São Paulo, Brasil*

We study e^+-Na, e^+-K, and e^+-Rb scattering using the close coupling approach in the static and coupled static expansion schemes. We calculate partial wave elastic scattering phase shifts and total elastic and Ps formation cross sections up to an incident positron energy of 100 eV. The effect of the positronium formation channel on the elastic channel is found to be strong in all cases up to an incident positron energy of 10 eV. We also make an estimate of the total cross section which exhibits a minimum as a function of energy at low energies.

PACS numbers: 34.90.+q, 34.40.+n

To appear in Chemical Physics Letters

The close coupling approximation (CCA) scheme provides a practical framework for dealing with electron-atom and positron-atom scattering. Unlike the variational calculations, CCA deals with rearrangement and elastic channels in an unified way and provides results for ionization and positronium (Ps) formation. This approach has been frequently used in e^+-H and e^+-He scattering[1–7].

Recently, there has been experimental[8, 9] and theoretical activities in positron-alkali-metal-atom scattering[10–18]. The CCA scheme has been employed in the theoretical studies. However, due to technical difficulties it is not easy to include the rearrangement positronium formation channels in the case of these large atoms. Hence most of the CCA calculations have neglected these channels. There has been some calculations including the Ps formation channel employing simple atomic wave functions[18]. Even in these calculations a systematic study of the effect of the Ps formation channel in positron-alkali-metal-atom scattering has not been made. In the present letter we make such a study of the Ps formation channel in the CCA treatment of positron-sodium, positron-potassium and positron-rubidium scattering employing realistic atomic wave functions. It is expected that any meaningful CCA calculation of positron-alkali-metal-atom scattering should include the Ps formation channel, as this channel is already open at the elastic scattering threshold.

In a recent investigation we studied e^+-Li and e^+-Na scattering in S and P waves using the CCA approach in the static and coupled static expansion schemes[19]. The term static refers to the inclusion of only the ground state of the target atom in the expansion scheme, whereas coupled static refers to the inclusion of the ground state of the positronium atom in addition to the ground state of the target atom in the expansion scheme of the CCA approach. The effect of the Ps formation channel on the elastic channel was found to be strong in both cases. In the case of the lithium atom the effect was dramatic; the inclusion of the Ps formation channel transformed the purely repulsive efective e^+-Li S wave (static) potential to a predominantly attractive (coupled static) potential. In this case, we found that in the static model $\delta(0) - \delta(\infty) = 0$, whereas in the coupled static model $\delta(0) - \delta(\infty) = \pi$, where $\delta(E)$ is the S wave phase shift at energy E. According to Levinson theorem this suggests a bound or continuum bound state of the system. This means that the inclusion of the Ps formation channel in the CCA approach to the elastic e^+-Li scattering will result in strong attraction. In the case of e^+-Na scattering the effect of the Ps formation channel on S and P wave elastic scattering was less pronounced and no change in $\delta(0) - \delta(\infty)$ was observed.

In this Letter we perform a complete study of e^+-Li, e^+-Na, e^+-K, and e^+-Rb scattering in the static and coupled static schemes of the CCA approach. We calculate total elastic and Ps formation cross sections up to an incident positron energy of 100 eV. The effect of the positronium formation on the elastic channel is found to be strong in all cases up to an incident positron energy of 10 eV. However, the effect of the Ps formation channel on S and P wave elastic positron-alkali-metal-atom scattering phase shifts is less pronounced as one passes from the lighter to the heavier alkali atoms. In the case of e^+-Li scattering the present results and conclusions are in agreements with the previously published results,[10, 19] and here we present only new results in the cases of e^+-Na, e^+-K, and e^+-Rb scattering.

We also calculate the partial wave summed elastic and Ps formation cross sections at

various energies. Experimentally, the results for total cross section is available. Estimate is made for the total cross section using previously published results for excitation cross sections and present elastic and Ps formation cross sections.

In the following we give some details of the positron-alkali-metal-atom scattering equations. In the CCA approach the total wave function for the positron-alkali-metal-atom system is written as[10]

$$\Psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_n,\vec{x}) = \sum_i \Phi_i(\vec{r}_1,\vec{r}_2,...,\vec{r}_n)F_i(\vec{x}) + \sum_\nu \Phi^+_{1s}(\vec{r}_1,\vec{r}_2...,\vec{r}_{n-1})\eta_\nu(\rho)G_\nu(\vec{R}), \quad (1)$$

with

$$\vec{\rho} = (\vec{x} - \vec{r}_n), \qquad \vec{R} = (\vec{r}_n + \vec{x})/2, \quad (2)$$

where $\vec{r}_j (j = 1,2,...,n)$ are the coordinates of the atomic electrons and $\vec{x}$ is the positron coordinate. Here $\Phi_i(\vec{r}_1,\vec{r}_2,...,\vec{r}_n)$ and $\eta_\nu(\vec{\rho})$ are the ith and νth eigenstates of the alkali-metal and positronium atom systems, respectively. The ground state wave function of the alkali-metal-ion is described by $\Phi^+_{1s}(\vec{r}_1,\vec{r}_2,...,\vec{r}_{n-1})$, $F_i(\vec{x})$ describes the motion of the incident positron and $G_\nu(\vec{R})$ describes the relative motion between the positronium and the alkali-metal-ion. In our treatment we include at most only one term in each sum of Eq. (1), e.g., the ground states of both alkali-metal and positronium atoms. In the static scheme only one term in the first sum of Eq. (1) is included, in the coupled static scheme one term in each sum of this equation is included.

We shall be working with the usual coupled scattering integral Lippmann-Schwinger type equations of the CCA approach which are written in the following form:[1 7]

$$f_{\beta\alpha}(\vec{k}',\vec{k}) = f^B_{\beta\alpha}(\vec{k}',\vec{k}) - \frac{1}{4\pi^2\mu_\nu}\sum_\nu \int d\vec{k}'' \frac{f^B_{\beta\nu}(\vec{k}',\vec{k}'')f_{\nu\alpha}(\vec{k}'',\vec{k})}{E + i0 - E_n}. \quad (3)$$

Here $f_{\beta\alpha}(\vec{k}',\vec{k})$ is the scattering amplitude for transition from channel α to channel β, $\vec{k}$ and $\vec{k}'$ are the relevant relative momenta in these channels, μ_ν is the reduced mass in channel ν, $f^B_{\beta\alpha}(\vec{k}',\vec{k})$ is the corresponding Born amplitude. The partial wave expansion of $f_{\beta\alpha}(\vec{k}',\vec{k})$ from the initial state $|nlm>$ of the target atom to the final state $< n'l'm'|$ of the target atom is given by

$$f_{\beta\alpha}(\vec{k}',\vec{k}) = \frac{1}{(kk')^{1/2}}\sum_{JM}\sum_{L,M_L}\sum_{L',M_{L'}} < L'l'M_{L'}m'|JM >< LlM_Lm|JM >$$
$$\times T^J_{\beta\alpha}(\tau'k',\tau k)Y^*_{L'M_{L'}}(\hat{k}')Y_{LM_L}(\hat{k}), \quad (4)$$

where L and M_L are the orbital angular momentum and projection of the incident projectile state, n, l and m are the principal quantum number, orbital angular momentum and projection of the initial state of the target atom, and J and M are the total angular momentum and projection, $< LlM_Lm|JM >$ is the usual Clebsch-Gordan coefficient. A similar partial wave expansion holds for the Born term. Also, τ stands for the collective quantum numbers (n,l,m).

After partial wave analysis the coupled integral equations become

$$T^J_{\beta\alpha}(\tau'k',\tau k) = B^J_{\beta\alpha}(\tau'k',\tau k) + \frac{1}{2\pi^2}\sum_\nu \int k''^2 dk'' \frac{B^J_{\beta\nu}(\tau'k',\tau''k'')T^J_{\nu\alpha}(\tau''k'',\tau k)}{k''^2 - k^2_\alpha - i0}. \quad (5)$$

The elastic scattering phase shift for the elastic channel denoted by suffix 1 is defined by

$$\delta_J = \frac{1}{2}\arctan\left[\frac{Re(T^J_{11})}{2\pi - Im(T^J_{11})}\right], \quad (6)$$

where T^J_{11} is the on-shell elastic t matrix element.

Next we illustrate some details of the positron-lithium system. The Born martix element for the elastic channel is given by

$$f^B_{11}(\vec{k}_f,\vec{k}_i) = -\frac{1}{2\pi}\int e^{i\vec{k}.\vec{x}}\Phi^*_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)\left[\frac{Z}{x} - \frac{1}{|\vec{x}-\vec{r}_1|} - \frac{1}{|\vec{x}-\vec{r}_2|} - \frac{1}{|\vec{x}-\vec{r}_3|}\right]$$
$$\times \Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{x}. \quad (7)$$

In this equation Z is the number of atomic electrons and $\vec{k} = \vec{k}_i - \vec{k}_f$. The lithium wave function is given by

$$\Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \mathcal{A}[u_{1s}(\vec{r}_1)u_{1s}(\vec{r}_2)u_{2s}(\vec{r}_3)] \quad (8)$$

where $\mathcal{A}$ denotes the proper antisymmetrizer for electrons, and the atomic orbitals for the $1s$ and the $2s$ electrons are given by

$$u_{ns}(\vec{r}) = \sum_{i=1}^{6} a_i(ns)r^{(m_i-1)}e^{-\lambda_i r}Y_{00}(\hat{r}). \quad (9)$$

The transition Born matrix element to the Ps formation channel, denoted by suffix 2, is given by

$$f^B_{21}(\vec{k}_f,\vec{k}_i) = -\frac{1}{\pi}\int e^{i\vec{\rho}.\vec{x}}e^{-i\vec{k}_f.\vec{r}_3/2}\eta^*_{1s}(|\vec{x}-\vec{r}_3|)\Phi^*_{Li^+}(\vec{r}_1,\vec{r}_2)\left[\left(\frac{Z}{x} - \frac{Z}{r_3}\right) - \left(\frac{1}{|\vec{x}-\vec{r}_1|} - \frac{1}{|\vec{r}_3-\vec{r}_1|}\right)\right.$$
$$\left. - \left(\frac{1}{|\vec{x}-\vec{r}_2|} - \frac{1}{|\vec{r}_3-\vec{r}_2|}\right)\right]\Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{x}. \quad (10)$$

In this equation $\vec{\rho} = \vec{k}_i - \vec{k}_f/2$. The lithium ion wave function is taken to be given by

$$\Phi_{Li^+}(\vec{r}_1,\vec{r}_2) = \mathcal{A}[u^+_{1s}(\vec{r}_1)u^+_{1s}(\vec{r}_2)] \quad (11)$$

where the atomic orbitals are given by

$$u^+_{1s}(\vec{r}) = \sum_{i=1}^{4} a^+_i(1s)e^{-\lambda_i r}Y_{00}(\hat{r}). \quad (12)$$

The constants for these wave functions are taken from Ref.[20]. In the calculation it is assumed that only the $2s$ electron participates in the Ps formation, so that the diagonal Born term $f^B_{22} = 0$.

Similar calculations have been carried out for the other atoms of the alkali series. The wave functions for these atoms are also taken from Clementi and Roetti[20].

The resulting partial wave scattering integral equation for the t matrix is solved by the standard matrix inversion technique without any further approximation[21].

The results of e^+-Li scattering have already appeared in the literature[10, 19] and the present calculation agrees with the previous ones. Here we present results for the other cases. In Figs. 1 (a) and 1 (b) we exhibit results for S and P wave phase shifts, respectively, for the e^+-K scattering for the static and the coupled static approaches. Similar results for e^+-Rb scattering are shown in Figs. 2 (a) and 2 (b). The results for e^+-Li and e^+-Na scattering phase shifts have appeared recently.[19] We find that in all four cases at low energies ($<$ 10 eV) the static and coupled static phase shifts are different showing the relevance of the Ps formation channel in the CCA approach. However, the difference is less in the case of heavier alkali atoms than in the case of lighter alkali atoms.

In Fig. 3 we exhibit the partial wave summed elastic and Ps formation cross sections for e^+-Na scattering using the static and coupled static CCA approaches. Note that there is no Ps formation in the static approach. In the partial wave sum at low energies some 7 partial waves were included whereas at higher energies some 15 partial waves were included. Convergence was achieved in all cases. In Figs. 4 and 5 we show the same results for e^+-K and e^+-Rb scattering. In all cases, we find that the Ps formation channel has a strong effect on the results of elastic scattering. Hence in any realistic calculation using the CCA approach it is extremely important to include the Ps formation channel. This casts doubt on some analyses of positron-alkali-metal-atom scattering in the CCA approach neglecting the Ps formation channel.[12, 15, 16]

It is instructive to estimate the total positron-alkali-metal-atom cross section in the case of sodium, potassium, and rubidium in the presence of the Ps formation channel in a CCA approach. Similar estimate has appeared in the case of the lithium.[10] Recent experiment has revealed[8, 9] that the total cross section has a minimum near the lowest excitation threshold in the case of potassium and rubidium. Previous CCA calculation of e^+-Li scattering including the Ps formation channel has demonstrated a minimum in the total cross section near the lowest excitation threshold.[10] The CCA calculations neglecting the Ps formation channel highly overestimates[12, 15, 16] the elastic cross sections at low energies, and consequently, there is no minimum in the total cross section. The total cross section is given by

$$\sigma_t = \sigma_{el} + \sigma_{Ps} + \sigma_{exc} + \sigma_{ion}, \tag{13}$$

where el, Ps, exc, and ion stands for elastic, Ps formation, excitation, and ionization, respectively. In the present estimate the partial wave summed elastic and Ps formation cross sections are taken from this study. The excitation cross sections are taken from the theoretical calculations of the York university group.[15, 16] The ionization cross sections are expected to be small[22] and are neglected. The present estimates of the total cross section in the cases of sodium, potassium, and rubidium are exhibited in Table 1 together with the present results for elastic and Ps formation cross sections.

In all three cases the present estimate for the total cross section exhibits a minimum

near the lowest excitation threshold(s), as one can see in Table 1. Similar minima have been observed in the recent measurements of the total cross section in the cases of e^+-K, and e^+-Rb scattering.[9] However, the present estimates of the total cross section, though much smaller than those of the York university group[15, 16] and of Sarkar et al.,[12] are larger than the experimental results. Though we do not have a complete explanation of this fact some explanatory remarks are in order. The present coupled static calculation while compared with the CCA calculation of the York university group neglecting the Ps formation channel reveals that the inclusion of the Ps formation channel highly reduces the elastic cross section. It is likely that the inclusion of the Ps formation channel in a fully convergent calculation using Eq. (1) may similarly reduce the excitation cross sections. This has been observed by Basu and Ghosh[10] in their study of positron-lithium scattering. They reported results for 2s-2p excitation cross sections for e^+-Li scattering using the two following basis sets: (a) Li(2s,2p), and (b) Li(2s,2p)+Ps(1s). They found that below the incident energy of 10 eV, the excitation cross sections obtained using basis (b) were appreciably less than those obtained employing the basis (a). Consequently, it is expected that after a fully convergent multichannel CCA calculation including many states of the target and the positronium atom in Eq. (1), the excitation cross sections and the total cross section of the alkali-atom-series might get reduced in agreement with experiment.

The present phase shifts are in fair agreement with previous calculations.[10, 19] However, in previous calculations phase shifts were not plotted. Also, a quantitative comparison of results of various calculations is not to the point, because different approximations and wave-functions were employed in various calculations. For example, the atomic wave functions used by Basu and Ghose[10] are different from those employed in the present calculation. However, the qualitative features of these two calculations are similar whenever results are available. Also, the calculation of Ghosh et al.[11, 12] and Ward et al.[15, 16] did not include the Ps formation channel. As we are studying the importance of the Ps formation channel, it is not fair to compare with these two calculations.

In conclusion, we have demonstrated the strong effect of the Ps formation channel on the elastic channel observables in a CCA calculation of the positron-alkali-metal-atom scattering. We have exhibited this effect on the S and P wave elastic phase shifts and on the partial wave summed elastic cross sections and calculated the Ps formation cross sections. We also made estimates for the total cross sections for e^+-Na, e^+-K, and e^+-Rb scattering and found a minimum in this cross section near the lowest scattering threshold(s) in agreement with experimental finding[9]. However, the present estimate for the total cross section uses the excitation cross sections of the York university group calculated in the CCA approach neglecting the Ps formation channel and are large compared to the experimental results. A multichannel CCA calculation including the Ps formation channel should be performed in the future to see if agreement with experimental results is improved.

The work is supported in part by the Conselho Nacional de Desenvolvimento - Científico e Tecnológico (CNPq) and Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) of Brasil. The work is partially supported by the Department of Science and Technology (D.S.T.), Government of India under project SP/S2/K-46/89. H. R. is thankful to D.S.T. for a Research Associateship.

REFERENCES

[1] M. Basu, M. Mukherjee, and A. S. Ghosh, J. Phys. B 22 (1989) 2195.

[2] M. Mukherjee, M. Basu, and A. S. Ghosh, J. Phys. B 23 (1990) 75.

[3] W. C. Fon and D. F. Gallahar, J. Phys. B 5 (1972) 943.

[4] J. W. Humberston, J. Phys. B 17 (1984) 2353.

[5] R. J. Drachman, Phys. Rev. A 12 (1975) 340.

[6] S. E. A. Wakid and R. W. LaBahn, Phys. Rev. A 6 (1972) 2039.

[7] P. Mandal, A. S. Ghosh, and N. C. Sil, J. Phys. B 8 (1975) 2377.

[8] C. K. Kwan, W. E. Kauppila, R. A. Lukaszew, S. P. Parikh, T. S. Stein, Y. J. Wan, and M. S. Dababneh, Phys. Rev. A 44 (1991) 1620.

[9] S. P. Parikh, W. E. Kauppila, C. K. Kwan, R. A. Lukaszew, D. Przybyia, T. S. Stein, and S. Zhou, Phys. Rev. A 47 (1993) 1535.

10] M. Basu and A. S. Ghosh, Phys. Rev. A 43 (1991) 4746.

11] P. Khan, S. Dutta, and A. S. Ghosh, J. Phys. B 20 (1987) 2927.

12] K. P. Sarkar, M. Basu, and A. S. Ghosh, J. Phys. B 21 (1988) 1649.

13] M. S. T. Watts and J. W. Humberston, J. Phys. B 25 (1992) L491.

14] S. L. Willis and M. R. C. McDowell, J. Phys. B 15 (1982) L31.

15] S. J. Ward, M. Horbatsch, R. P. McEachran, and A. D. Stauffer, J. Phys. B 22 (1989) 1845.

.6] R. P. McEachran, M. Horbatsch, and S. J. Ward, J. Phys. B 24 (1991) 1107.

7] M. A. Abdel Raouf, J. Phys. B 21 (1988) 2331.

8] S. Guha and A. S. Ghosh, Phys. Rev. A 23 (1981) 743.

9] S. K. Adhikari, A. S. Ghosh, and H. Ray, Chem. Phys. Lett., in press.

0] E. Clementi and C. Roetti, At. Data and Nucl. Data Tables 14 (1979) 187.

1] See, for example, S. K. Adhikari and K. L. Kowalski, Dynamical Collision Theory and Its Applications, Academic Press, Boston, 1991.

2] M. Basu and A. S. Ghosh, J. Phys. B 19 (1986) 1249.

Table Caption: The present coupled static calculation of partial wave summed elastic and Ps formation cross sections together with estimate for total cross section (πa_0^2) for e^+-Na, e^+-K, and e^+-Rb scattering. The excitation cross sections are taken from Refs. [15] (Na and K) and [16] (Rb). In the case of Rb the excitation cross sections are obtained by the method of interpolation between two energies.

Table 1

	e^+-Na			e^+-K			e^+-Rb		
E(eV)	σ_{3s3s}	σ_{3sPs}	σ_t	σ_{1s1s}	σ_{4sPs}	σ_t	σ_{5s5s}	σ_{5sPs}	σ_t
0.1	168	30	198	191	7	198	193	9	202
1	134	34	168	138	6	144	133	10	143
1.5	121	33	154	122	6	128	117	10	127
2	110	32	142	116	7	203	101	10	
2.5	100	30	130	107	7	240	89	10	156
3	91	28	119	98	7	248	79	10	
3.5	83	26	119	91	6	248	73	10	250
4	76	24	185	84	5	244	64	10	
5	65	20	175	72	4	228	53	9	
7	49	15	144	54	3	196	38	6	188
10	32	8	118	35	1	156	28	4	150
20	12	1	68	17	0	100	17	1	113
30	7	0	48	12	0	74	14	0	84
50	5	0	34	9	0	52	11	0	61

Figure Caption

1.(a) S wave and (b) P wave static (full line) and coupled static (dashed line) elastic scattering phase shifts in radians at various energies for positron-potassium scattering.

2. (a) S wave and (b) P wave static (full line) and coupled static (dashed line) elastic scattering phase shifts in radians at various energies for positron-rubidium scattering.

3. Total static (full line), total coupled static (dotted line), and total Ps formation (dashed line) cross sections at various energies for positron-sodium scattering. Note that there is no Ps formation in the static model.

4. Same as Fig. 3 for positron-potassium scattering.

5. Same as Fig. 3 for positron-rubidium scattering.

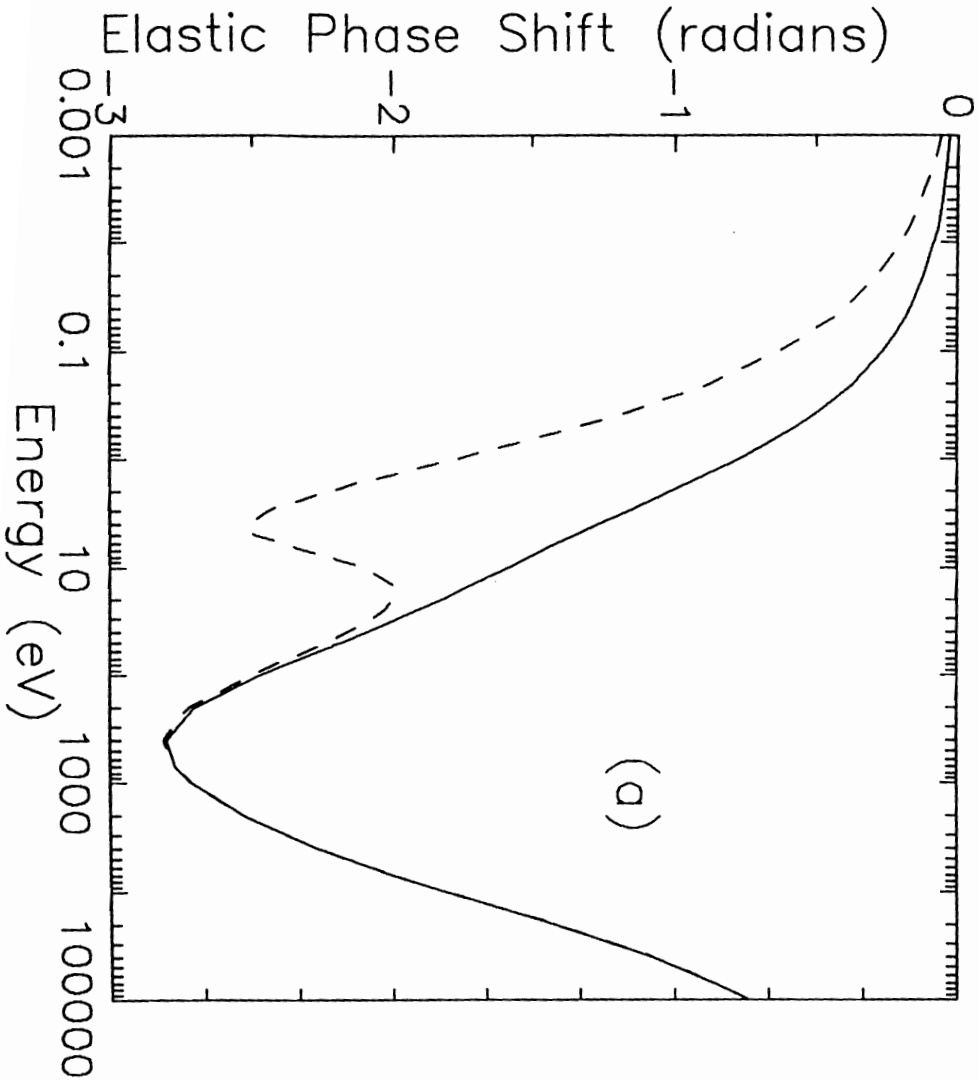

Figure 1, Ray et al, Chem. Phys. Lett.

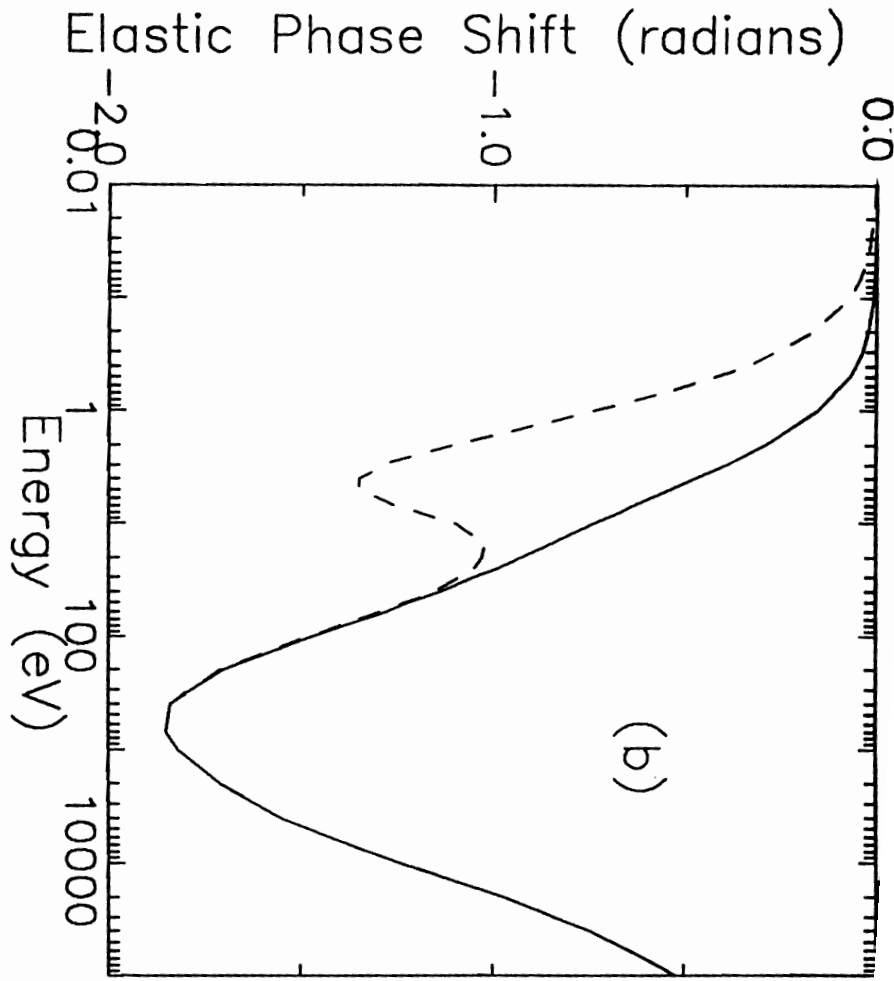

Figure 1, Ray et al, Chem. Phys. Lett.

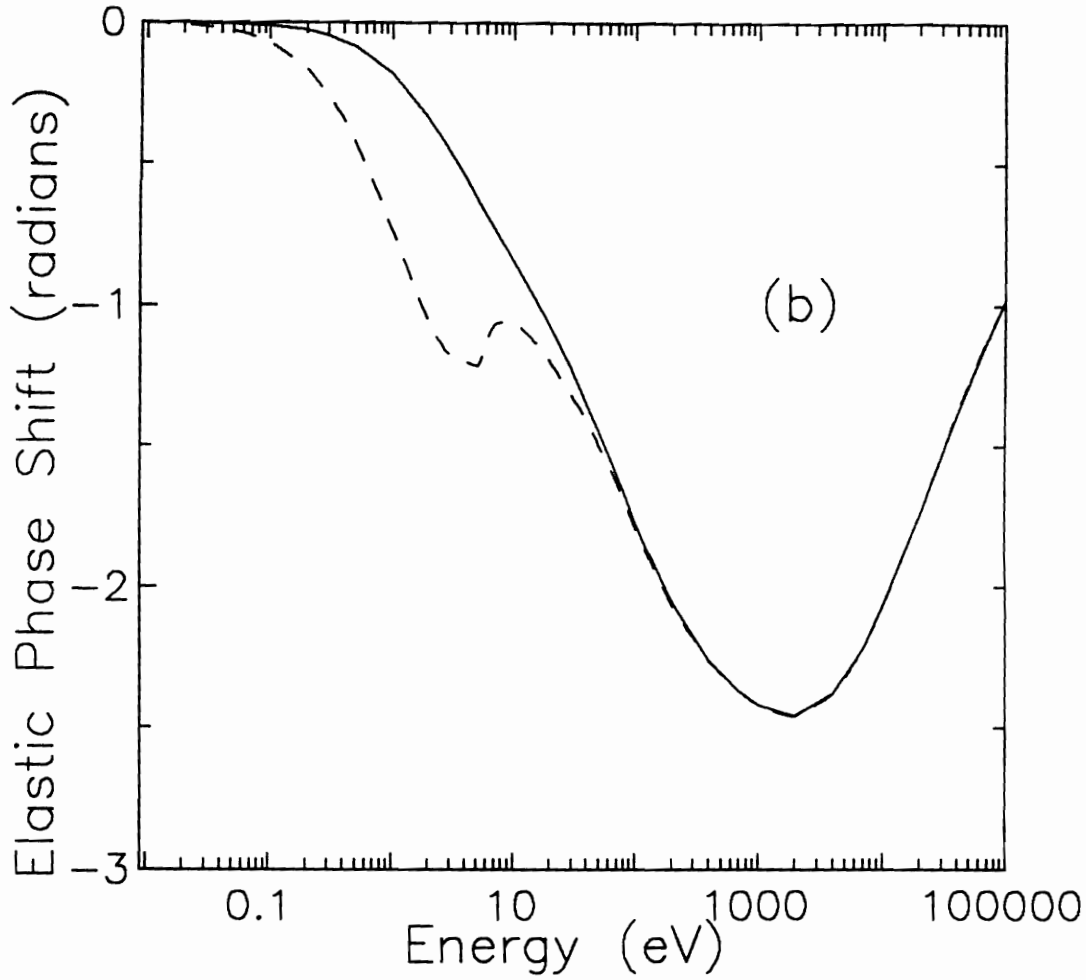

Figure 2, Ray et al., Chem. Phys. Lett.

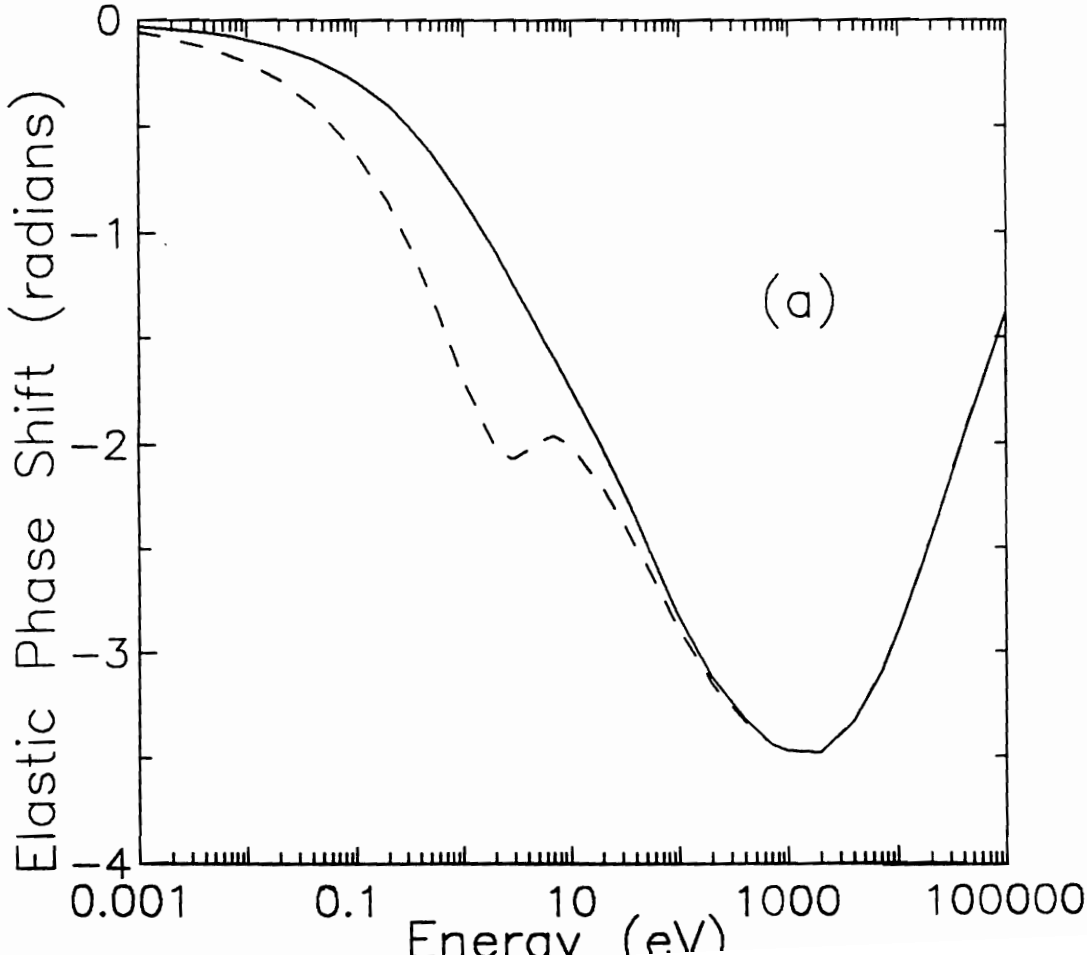

Figure 2, Ray et al., Chem. Phys. Lett.

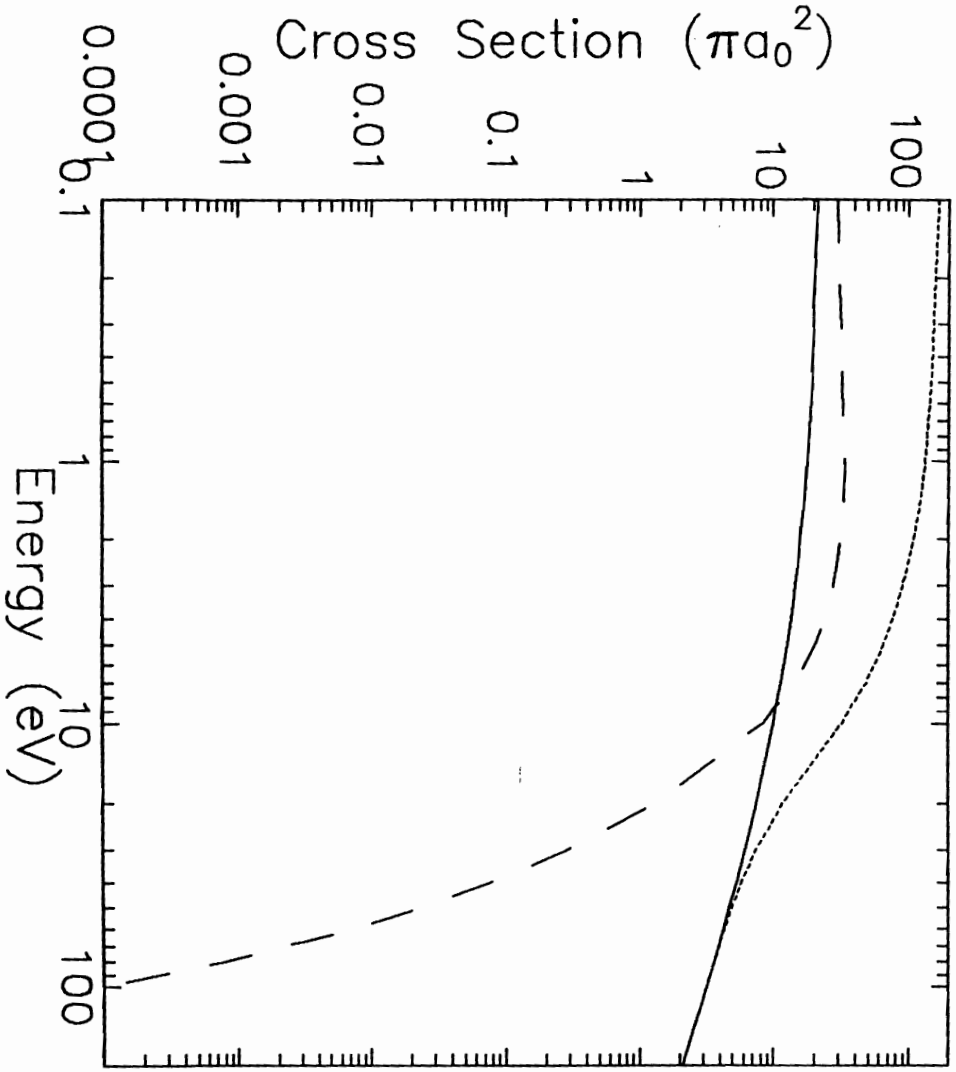

Figure 3, Ray et al., Chem. Phys. Lett.

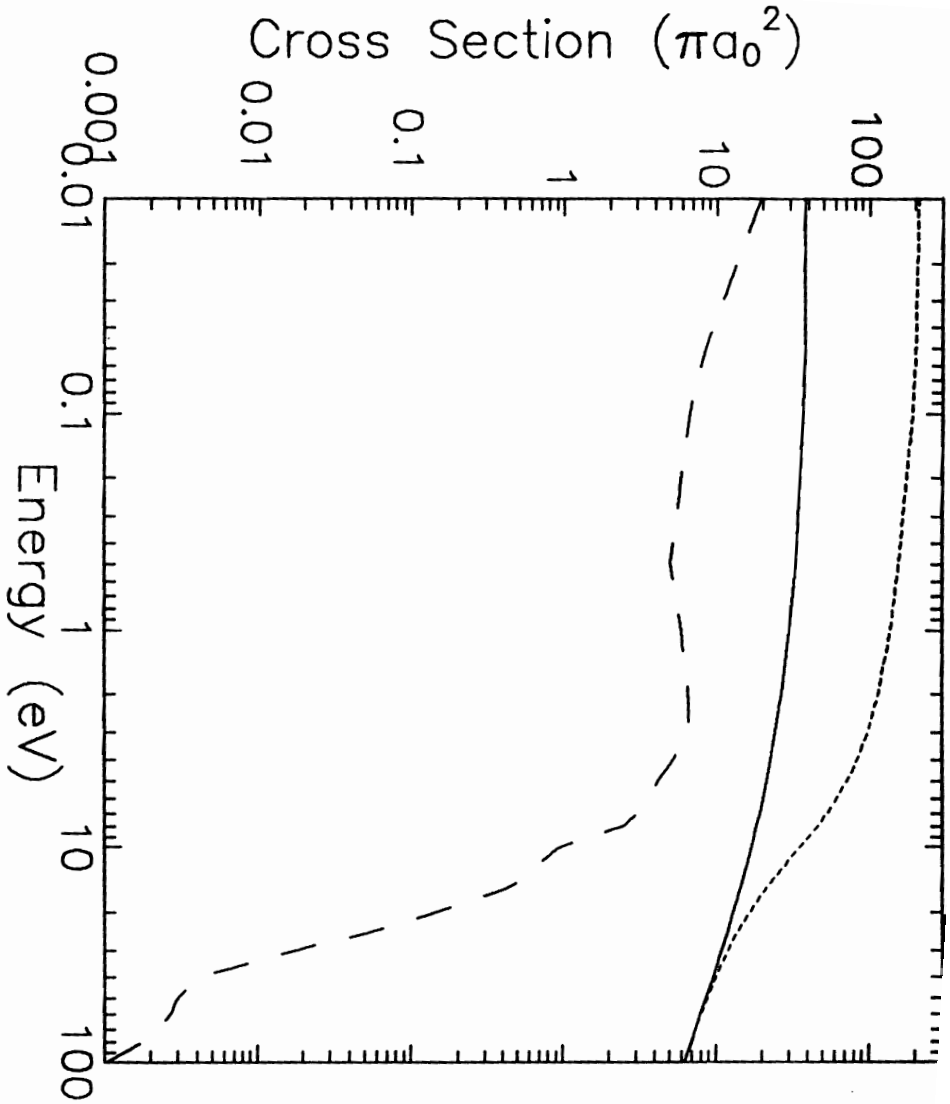

Figure 4, Ray et al., Chem. Phys. Lett.

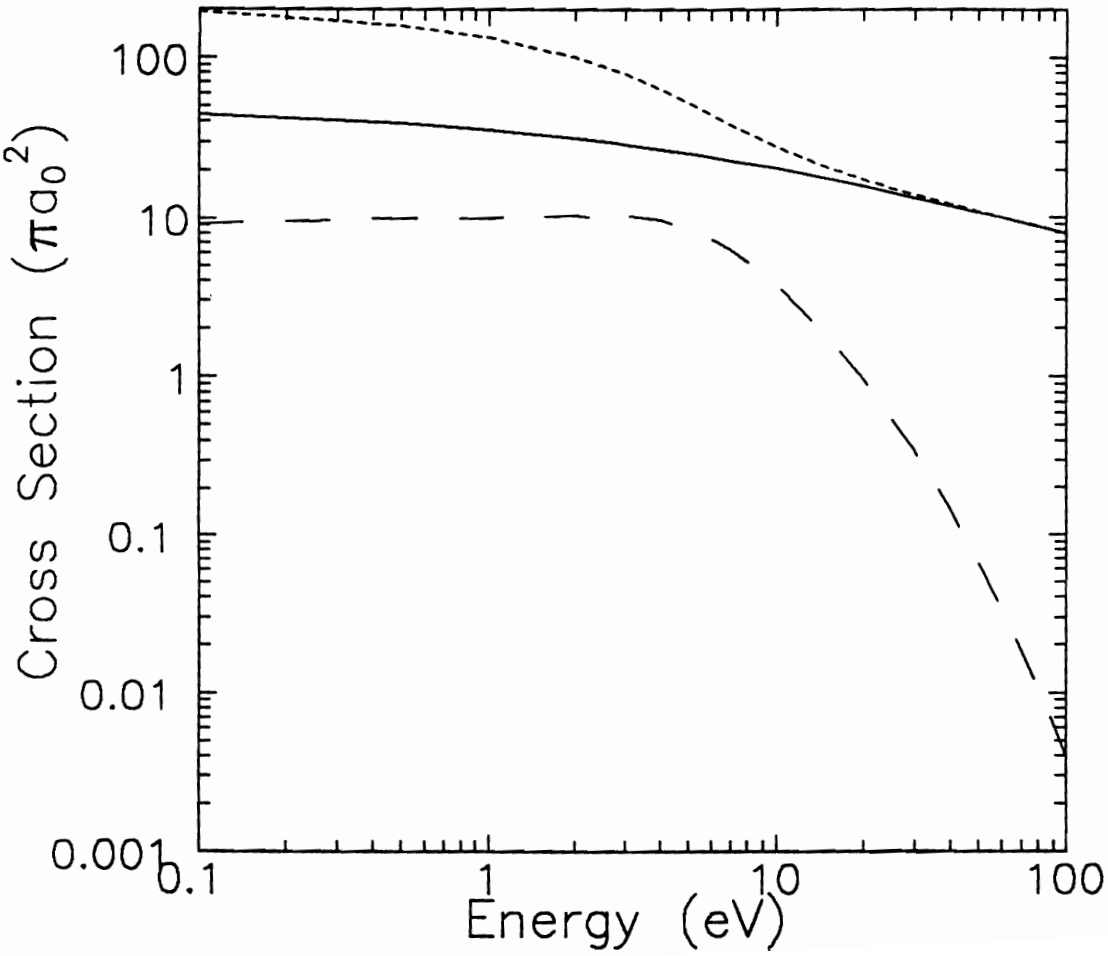

Figure 5, Ray et al., Chem. Phys. Lett.