RESONANT ELECTRON CAPTURE CROSS-SECTION FOR PIII

Abdelkrim Mekki* and Ibraheem Nasser

Department of Physics
King Fahd University of Petroleum & Minerals
Dhahran, Saudi Arabia

الخلاصـة :

تـمّ حساب كلٍّ من المقاطع المستعرضة ومعاملات المعدلات المصاحبة لإثارة المستوى $3s \rightarrow 3p$ لأيوم الفوسفور(+٢) الشبيه بالألومنيوم . وأضيف أيضاً للحسابات مقدار مساهمة مستوى الإثارة الأول $3s3p^2$.

وقد تـمّ بالتفصيل حساب الاحتمالات الانتقالية للإنبعاث الإشعاعي وكذلك لإنبعاث (أوجيه) للإليكترونات الخاصة بالمدارات المنخفضة . وقد استخدم لحساب هذه الاحتمالات التقريب الزاوي المغزلي مع استخدام الدوال غير النسبية المسماة (هارترى فوك) . ووضعت النتائج في جداول حتى يتم مقارنتها مع القياسات المعملية بالمستقبل .

ABSTRACT

Cross-sections and rate coefficients associated with the $3s \rightarrow 3p$ excitation for the Al-like P^{2+} are calculated. Contributions from the multiplets of the first excited states $3s3p^2$ are also included. Explicit calculations of the Auger and radiative transitions probabilities are evaluated at low n. These probabilities were calculated using single-configuration, non-relativistic, Hartree–Fock wavefunctions in LS coupling. Results were tabulated to facilitate comparison with future experimental measurements.

PACS codes: 34.80 KW; 34.80 DP; 31.80 TZ; 30.80 DZ.

*Address for correspondence:
KFUPM Box 1453
King Fahd University of Petroleum & Minerals
Dhahran 31261
Saudi Arabia

RESONANT ELECTRON CAPTURE CROSS-SECTION FOR P III

INTRODUCTION

It is well-known that the electric power generation that burns coal and oil produces a large amount of CO_2 and many other elements, such as P and S. These elements play a dominant role in the pollution of the atmosphere and may cause global warming through the "Greenhouse Effect". Most damage is done by pollutants through slow chemical reactions involving neutral atoms and molecules and/or molecular ions. However, also present are some ionic species of elements such as F, P, S, Cl, and so forth.

The work reported here is a continuation of the comprehensive study of a series of ionized species of elements, such as C, F, O, and N, which are assumed to be related to industrial pollution control and the "Greenhouse Effect" [1–4]. No data is available in the literature concerning the phosphorus ion, and this motivated the present study. We will present a detailed theoretical calculation of the dielectronic recombination (DR) cross-sections and rate coefficients associated with the $3s \to 3p$ excitation for the Al-like P^{2+}.

The DR process is described for the ground state ($i = 3s^2 3p$) as

$$(3s^2 3p = i) + k_c l_c \to (3s3p^2 nl = d), \quad (3s \to 3p, \Delta n_t = 0; \quad \Delta l = 1) \qquad (1a)$$

and for the excited state ($3s3p^2$) by

$$(3s3p^2 = i') + k_c' l_c' \to (3s3p^2 nl = d), \quad (3s \to 3p, \Delta n_t = 0; \Delta l = 0) \qquad (1b)$$

then, ($1a$) and ($1b$) stabilize by radiative decay

$$(3s3p^2 nl = d) \to (3s^2 pnl = f) + \gamma(3p \to 3s)$$
$$\to (3s3p^2 n'l' = f') + \gamma(nl \to n'l') \qquad (2)$$

(Explicit reference to the core electrons and the state multiplicity of P^{2+} is omitted for simplicity). In our notation, "i", "d", and "f", are the initial, intermediate, and final states respectively.

Due to the great need to study the individual contribution of each state multiplicity separately, our present work concentrates on the excitation modes represented by ($1a$) and ($1b$). Preliminary studies of other transitions such as $(3s^2 3p)\ ^2P \to (3s^2 3d)\ ^2D$ showed that their contribution to the total cross section was small and it will be neglected in the present calculation [4]. As seen from Figure 1, the levels $4p$ (d_1) and $4s$ (d_2) are close to the thresholds but their contribution to DR is only about 5 to 10 percent.

The calculation procedure adopted in this report in evaluating the DR cross-sections and rates is identical to that used by Nasser and Hahn [5]. The Hartree–Fock scheme of approximation with single configuration and in LS coupling is employed in which states are coupled sequentially with the core states coupled first. The energies of the excited states are calculated explicitly for $n \le 10$, using Cowan's RCG code [6], and adjusted, using the Grotrian Tables [7] or experimental values when available. This is a crucial step, especially when new channels are opened by Auger. All Auger and radiative transition probabilities are calculated explicitly, using Cowan's RCG code [6]. In all cases, the states with $n > 10$ are calculated by extrapolation, using the n^{-3} scale for some of the radiative and Auger transitions, A_r and A_a, respectively.

For convenience, the various channels in the DR process are defined as

$$i_1 = (3s^2 3p)^2 P,$$

$$i_2 = (3s3p^2)^4 P, \quad d_1 = (i_2) nl,$$

$$i_3 = (3s3p^2)^2 D, \quad d_2 = (i_3) nl,$$

$$i_4 = (3s3p^2)^2 S, \quad d_3 = (i_4) nl,$$

$$i_5 = (3s3p^2)^2 P, \quad d_4 = (i_5) nl.$$

RESULTS

Ionization energies of all terms of the single excited state configuration $3s3p^2$ relative to the $(3s^23p)$ ^2P target ground state for P^{2+} are given in Table 1. The core radiative rates A_r $(3p \rightarrow 3s)$ are also given in unit of s^{-1}. These are the dominant radiative rates for large n. Energy levels relevant to the DR process for the P^{2+} ion are given in Figure 1, from which all possible radiative transitions for the individual intermediate states may be determined.

In $\Delta n = 0$, $\Delta l = 1$ excitation mode, the rates' curves exhibit a double-peak, as shown in Figure 2 at $kT = 0.02$ Ry and 0.6 Ry with the corresponding rates 4.3×10^{-12} cm^3/s and 1.0×10^{-10} cm^3/s, respectively. The first peak comes from the transitions $(i_3)3d$ and $4s$. The other transitions significantly contribute to the second peak. The contributions from the states $(i_2)nl$ with small n and l ($n \leq 20$, $l \leq 2$), and $(i_4)nl$ are small and blend in with the other series. The cross-sections are given in Table 2 as a function of the continuum energy e_c (Ry) for the initial state i_1. The individual contribution from each multiplet of the excited states is given. As shown in Table 2, the

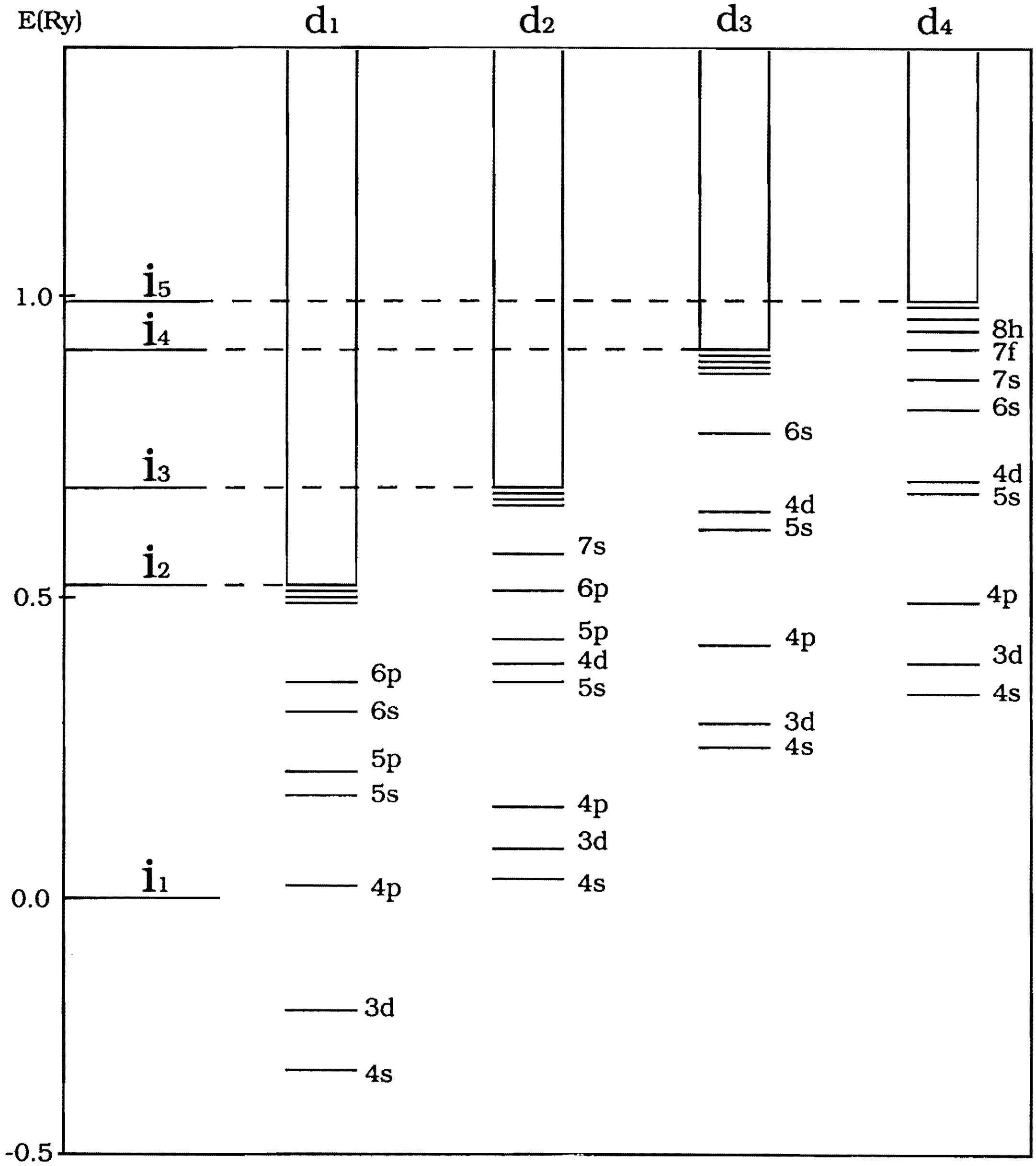

Figure 1. Energy Levels Relevant to the DR Process for the P^{2+} Ions are Given. From these all possible radiative transitions for the individual intermediate resonance states may be determined.

contributions from the states d_1, d_2, d_3, and d_4 to the total cross-sections are 1%, 30%, 6%, and 63%, respectively. The series of the core state (^2P) is the largest due to the ^2P core radiative rate (see Table 1). Although the ^2D has the largest statistical weight, the corresponding cross-sections are smaller because the ^2D core radiative rate is smaller than the ^2P core radiative rate by a factor of 10.

The DR cross-sections for the inter-multiplets excitation ($\Delta n = 0$, $\Delta l = 0$) at low energy are presented for the metastable state i_2, and also for other excited states of P^{2+}, i_3, and i_4. These levels are quite separate, as shown in Table 1. Although the excited states populations may be small in locally thermalized plasmas, except for metastable states, the corresponding rates could be very large at small energies of e_c. Therefore, it is of interest to estimate the rates of the excited states.

Table 1. Energies of all Terms of the Single Excited State Configuration $3s3p^2$ Relative to the $(3s^23p)^2P$ Target Ground State for P^{2+} in Ry. The radiative transition probabilities $A_r(3p \rightarrow 3s)$ are also given in s^{-1}. The numbers in brackets represent powers of 10.

i	ΔE (Ry)	$A_r(s^{-1})$
$i_1 = (3s^23p)^2P$	0.00	–
$i_2 = (3s\ 3p^2)^4P$	0.52	–
$i_3 = (3s\ 3p^2)^2D$	0.68	1.70 (+9)
$i_4 = (3s\ 3p^2)^2S$	0.91	3.08 (+9)
$i_5 = (3s\ 3p^2)^2P$	0.99	1.42 (+10)

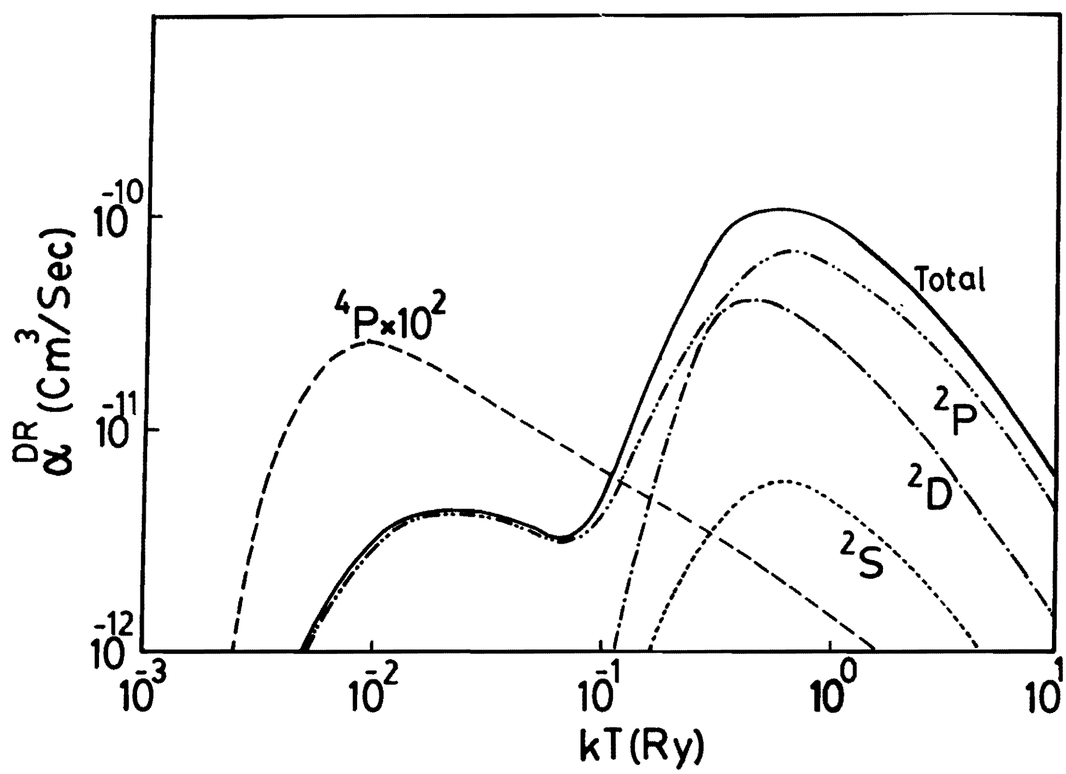

Figure 2. DR Rates as a Function of kT *(Ry) for the Excited States* ^4P, ^2D, ^2S, *and* ^2P *of* P^{2+} *in* $\Delta n = 0$, *and* $\Delta l = 1$ *Mode of Excitation.*

Table 2. Values of $\bar{\sigma}^{DR}$ *vs* e_c (Ry) for the Excited States ^4P, ^2D, ^2S, ^2P of P^{2+} in $\Delta n = 0$, and $\Delta l = 1$ Modes of Excitation, with $\Delta e_c = 0.02$ Ry.

e_c	^4P	^2D	^2S	^2P
0.02	1.60 (–20)			
0.04		2.39 (–19)		
0.06		2.54 (–19)		
0.16		3.87 (–20)		
0.18	1.73 (–21)			
0.20	0.68 (–20)			
0.24	0.57 (–21)		0.67 (–20)	
0.30			2.28 (–20)	
0.32	2.04 (–21)			0.50 (–19)
0.34	2.28 (–22)	1.00 (–20)		
0.36		4.83 (–20)		
0.38	1.02 (–21)			1.86 (–19)
0.40	1.25 (–22)	1.66 (–20)	0.95 (–20)	
0.42	0.67 (–21)	0.63 (–19)		
0.44	5.71 (–22)			
0.46	7.45 (–22)			
0.48	4.56 (–22)	4.30 (–20)		0.77 (–18)
0.50	0.53 (–22)	0.64 (–19)		
0.52		0.63 (–19)		
0.54		2.65 (–20)		
0.56		1.73 (–19)	2.24 (–21)	
0.58		1.90 (–19)	0.68 (–20)	
0.60		2.02 (–19)		
0.62		0.57 (–18)	1.94 (–20)	
0.64		3.16 (–18)		
0.66		9.81 (–18)		2.08 (–20)
0.68			1.81 (–21)	0.79 (–19)
0.70			4.37 (–21)	
0.72			1.54 (–20)	1.78 (–19)
0.74			2.22 (–20)	
0.78			5.82 (–21)	1.58 (–20)
0.80			2.35 (–20)	0.62 (–19)
0.82			4.33 (–20)	3.51 (–19)
0.84			1.81 (–19)	
0.86			1.50 (–18)	2.19 (–19)
0.88			0.86 (–18)	3.18 (–19)
0.90				4.90 (–19)
0.92				6.38 (–19)
0.94				2.42 (–18)
0.96				1.34 (–17)
0.98				1.25 (–17)
Total	3.11 (–20)	1.50 (–17)	2.73 (–18)	3.14 (–17)

Table 3. Values of $\bar{\sigma}^{DR}$ *vs* e_c (Ry) for the Initial States i_2, i_3, and i_4 of P^{2+} in $\Delta n = 0$, and $\Delta l = 0$ Modes of Excitation, with $\Delta e_c = 0.02$ Ry.

e_c	i_2	i_3	i_4
0.01		4.78 (−19)	1.92 (−18)
0.03	1.43 (−19)	1.85 (−20)	2.20 (−18)
0.05	1.18 (−20)	1.00 (−19)	2.53 (−17)
0.07	0.87 (−19)	0.71 (−19)	3.30 (−19)
0.09	1.03 (−19)	0.85 (−20)	
0.11	1.75 (−19)	1.53 (−19)	
0.13	3.63 (−18)	1.64 (−20)	
0.15	4.73 (−19)	1.36 (−19)	
0.17		2.85 (−19)	
0.19	0.56 (−20)	1.43 (−18)	
0.21	1.37 (−20)	3.67 (−18)	
0.23		4.10 (−20)	
0.25	3.78 (−21)	1.05 (−19)	
0.27	2.66 (−20)	4.46 (−19)	
0.29	0.97 (−20)	2.43 (−18)	
0.31	8.51 (−21)		
0.33	3.26 (−20)		
0.35	4.00 (−19)		
0.37	2.92 (−20)		
0.39	0.79 (−19)		
0.41	3.41 (−20)		
0.43	5.12 (−19)		
0.45	0.92 (−18)		
0.47			
Total	0.68 (−17)	0.94 (−17)	2.98 (−17)

The DR cross-sections for this mode of excitation for all initial states (i_2, i_3, and i_4) are given in Table 3. As shown in Table 3, the DR cross-sections of the excited states' multiples are in the same magnitude as the ground state i_1 and also contribute significantly at low values of e_c. So, including the excited states in the calculations could be important—especially if the excited states are highly populated, as in the metastable state i_2. The contributions from i_4 are large due to the core radiative transition and the small amount of energy involved in the excitation.

Figure 3 represents the rates for the excited states multiplets i_2, i_3, and i_4 as functions of kT(Ry). The initial state i_4 has a peak at $kT = 0.05$ Ry, with the value of 2.2×10^{-10} cm^3/s. State i_2 has a peak at $kT = 0.1$ Ry, with the value of 2.6×10^{-11} cm^3/s. There is a double-peak in i_3 at $kT = 0.006$ Ry and $kT = 0.2$ Ry, with the values 9.6×10^{-12} cm^3/s, and 3.2×10^{-11} cm^3/s, respectively.

Finally, the configuration mixing (CM) of the initial state i and the intermediate state d with states such as $3p^3$, $3s3p4s$, $3s3p3d$, *etc*., which may refine our results, was not included in the present calculation. This is due to the fact that the method of selection of the configurations to be mixed is still poorly understood [8]. The usual way of mixing all the configurations which lie near the state of interest does not give correct widths for A_r and A_a. The total widths may change as much as an order of magnitude as some crucial states are mixed [8]. Therefore, further refinements and tests of the mixing procedure should be performed before it is included in our calculations.

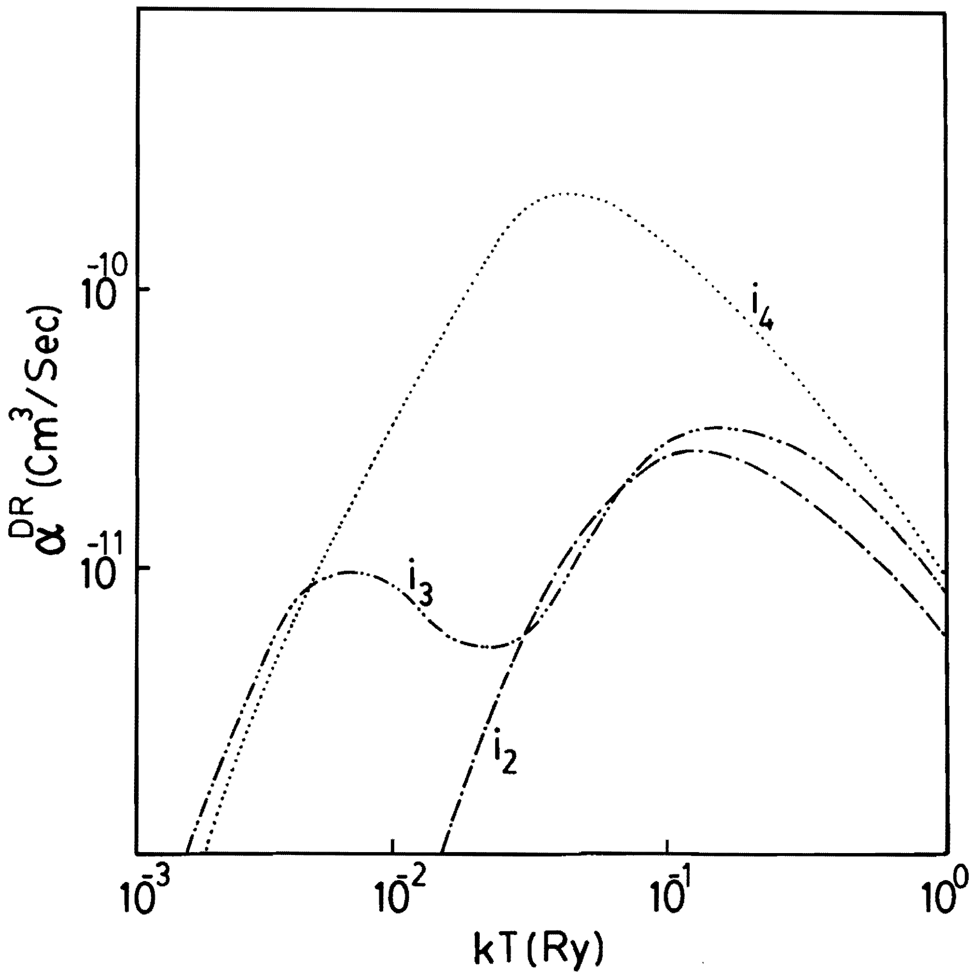

Figure 3. DR Rates as a Function of kT *(Ry) for the Initial States* i_2, i_3, i_4 *of* P^{2+} *in* $\Delta n = 0$, *and* $\Delta l = 0$ *Mode of Excitation.*

ACKNOWLEDGEMENT

This work was carried out at the KFUPM Computer Center using the Cowan atomic structure code.

REFERENCES

[1] I. Nasser and Y. Hahn, *J. Phys. B: At. Mol. Opt. Phys.*, **25** (1992), p. 521.
[2] I. Nasser, R. Bellantone, and Y. Hahn, *Phys. Rev. A*, **43** (1991), p. 4854.
[3] R. Bellantone, Y. Hahn, and D. J. McLaughlin, *Physica Scripta*, **43** (1991), p. 379.
[4] A. Al-Mulhem and I. Nasser, *Phys. Rev. A*, **46** (1992), p. 2945.
[5] I. Nasser and Y. Hahn, *Phys. Rev. A*, **39** (1989), p. 401.
[6] R. Cowan, in *The Theory of Atomic Structure and Spectra*. Berkeley: University of California Press, 1985.
[7] S. Bashkin and J. O. Stoner, Jr., in *Atomic Energy Levels and Grotrian Diagrams*. Amsterdam: North-Holland, 1977.
[8] Y. Hahn and I. Nasser, *Zeit. Fur Phy. D*, **27** (1993), p. 203.

Paper Received 5 March 1994; Accepted 24 April 1994.