Radiative Recombination Rate Coefficients for Sequence of Ions

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Abstract

The electron-ion collisional radiative recombination for electron temperatures (10-10^9) K^o have been investigated, using a new analytic fitting formula. Ionization balance in the low ionization stages of systems is important in a variety of astrophysical plasmas. Accurate recombination rates are needed but are difficult to compute in a detailed quantum mechanical treatment. The main difficulty lies in the complexity of strong electron-electron correlation. We present the electron-ion recombination rate coefficients for the electron interacting with (C_{I}, C_{II}, N_{II}, O_{III}, F_{IV}, Ne_{V}, Si_{IX}, S_{XI}) ions sequence. Our results of radiative recombination rates coefficients have compared with the available data in which depend the close coupling approximation using the R-matrix method employing a unified treatment, that considers the infinite number of states of the recombined ion and incorporates both the radiative recombination and the dielectronic recombination processes in a self-consistent manner.

Keywords: Electron-Ion collision; Recombination rate; Temperature of electron.

معاملات معدل اعادة الاتحاد المشع لمتسلسلة ايونات

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كلية العلوم / جامعة البصرة

الخلاصة

يتناول البحث عملية تصادم الالكترون والايون لاعادة الاتحاد المشع ولمدى درجة حرارة الالكترون (١٠- ١٠^٩) كلفن باستخدام صيغة جديدة لطريقة التلائم التحليلي. عملية التوازن الايوني في مراحل التأين المتدنية للأنظمة تكون ذات اهمية في بلازما فيزياء الفضاء. ان معدلات اعادة الاتحاد الدقيقة تكون مطلوبة ولكن من الصعب استحصالها من خلال معالجة كمية مفصلة. ان صعوبة ذلك تظهر اساسا في مدى تعقيد الارتباط الالكترون مع الالكترون. في هذا البحث نتناول معاملات معدل اعادة الاتحاد لتفاعل الالكترون مع متسلسلة ايونات $(C_I, C_{II}, N_{II}, O_{III}, F_{IV}, Ne_V, Si_{IX}, S_{XI})$. كانت النتائج المستحصلة لمعاملات الاتحاد المشع قد قورنت مع ما متوفر من قراءات نظرية استخدم فيها الباحثون تقريب الازدواج المغلق بالاستعانة بطريقة مصفوفة – R وبتطبيق المعالجة الموحدة والتي تفترض عدد غير المحدد من الحالات للايونات المعاد اتحادها وتدمج كل من الاتحاد المشع والاتحاد ثنائي الالكترون في عملية توافق ذاتي.

كلمات مفتاحية:تصادم الكترون-ايون، معدل اعادة الاتحاد، حرارة الالكترون.

1.Introduction

The charge changing in electron-ion collisions are critically important in plasmas whether of astrophysical nature or man made, as they play their vital role in determining the plasma properties and ionization balances. One needs atomic collisions data, such as recombination cross section, rate coefficients, and resonance energy positions for modeling and diagnosing the state of high-temperature plasmas[1].

Radiative recombination process involves a free-bound electronic transition with radiation spread over the recombination continuum. It is the inverse of photoionization without autoionization and favors high energy gaps with transitions to low $n \approx 1,2,3$ and low angular momentum states $\ell \approx 0,1,2$ at higher electron energies[2].

Electron-ion recombination is a highly exothermic mechanism in which a free electron is captured by an ion after collision. At low and moderate electron densities there are two most important recombination channels through which an ion can recombine with a free electron, namely radiative recombination (RR) and dielectronic recombination (DR). The radiative recombination is a non-resonant process and categorized as a direct mode mechanism, while dielectronic recombination proceeds in an indirect resonant mode involving two stapes. In both these channels the excess energy and momentum of the recombining electron are carried away by a photon [1].

Electron-ion recombination is proceeds via the following four processes [2]:

(a). radiative recombination (RR)

$$e^- + A^+(i) \rightarrow A(n\ell) + hv$$

(b). three-body collisional-radiative recombination

$$e^- + A^+ + e^- \rightarrow A + e^-$$

$$e^- + A^+ + M \rightarrow A + M$$

Where the third body can be an electron or a neutral gas.

(c). dielecronic recombination (DR)

$$e^- + A^{Z+}(i) \leftrightarrow [A^{Z+}(k) - e^-]_{n\ell} \rightarrow A^{(Z-1)+}_{n'\ell'}(f) + hv$$

(d). dissociative recombination (DSR)

$$e^- + AB^+ \rightarrow A + B^*$$

Electron recombination with unbond ions can proceeds only via (a) and (b), while (c) and (d) provide additional pathways for ions with at least one electron initially or for molecular ions AB^+. Calculations for electron-ion recombination usually treated the radiative and the dielectronic recombination (RR and DR).

A new and modified fitting formula putted by Badnell [3] to calculate the total radiative recombination rate coefficients (RRC) for both ground and metastable initial levels. In a recent work [4] we published a research to calculate the radiative rate coefficient for carbon ions using a formula putted by Verner & Ferland [5]. In the present work we calculate radiative recombination rate coefficients (RRC) for (C I , C II, N II, O III, F IV, Ne V, Si IX, S XI) ions, as a function of electron temperature (T). The results we have present were compared with Nahar [6] data.

Calculations for electron-ion recombination usually treated the radiative and dielectronic recombination (RR and DR) processes separately using different approximations[7-8], valid in different temperature regions and are thus susceptible to inconsistencies and inaccuracies when simply added together to obtain the total recombination rate. Furthermore, they are not, in general, consistent with the photoionization cross sections, which are usually calculated in some other approximation. Ionization balance calculations in photoionization models of radiatively ionized astrophysical plasma sources were subject to large uncertainties, particularly for complex atomic systems [7].

Many investigations [8-13] on RRC were been carried out by many researchers using different theoretical models. Nahar's [6] work reports in detail the calculations for RRC for many systems using the new unified treatment, which is dealing with the two recombination processes, RR and DR, and yields a single set of unified recombination rate coefficients over a wide range of temperatures for all practical purposes.

2. Theory

A modified fitting formula of radiative recombination rate coefficient for electron-ion recombination putted by Badnell [3], who have calculated partial final-state resolved radiative recombination rate coefficients from the initial ground and metastable levels for all isoelectronic sequences[3] :

$$\alpha_{RR}(T) = A \times \left[\sqrt{T/T_0}\,(1+\sqrt{T/T_0})^{1-B}\,(1+\sqrt{T/T_1})^{1+B}\right]^{-1} \quad \text{....... (1)}$$

Where, for low-charge ions, B is replaced as

$$B \to B + C\exp(-T_2/T) \quad \text{........ (2)}$$

Here, $T_{0,1,2}$ are in units of temperature (K^o) and the rate coefficient $\alpha_{RR}(T)$ is in units $cm^3\ s^{-1}$, while *B* and *C* are dimensionless. A non-linear least-square fit was used to determine the coefficients (*A*, *B*, $T_{0,1}$; *C*, T_2). Table (1) we present these coefficients for ions under investigation.

Table (1): Fitting coefficients for modified formula of RRC.

Ion	A	B	T_0	T_1	C	T_2
C I	2.995(-9)*	0.7849	6.670(-3)	1.943(6)	0.1597	4.955(4)
C II	2.067(-9)	0.8012	1.643(-1)	2.172(6)	0.0427	6.341(4)
N II	2.410(-9)	0.7948	1.231(-1)	3.016(6)	0.0774	1.016(5)
O III	2.501(-9)	0.7844	5.235(-1)	4.470(6)	0.0447	1.642(5)
F IV	2.236(-9)	0.7725	1.828	5.982(6)	0.0319	2.529(5)
Ne V	1.127(-9)	0.7556	1.311(1)	8.047(6)	0.0250	2.771(5)
Si IX	1.688(-9)	0.7390	5.549(1)	1.716(7)	0.000	0.000
S XI	1.702(-9)	0.7301	1.138(2)	2.253(7)	0.000	0.000

* The number 2.995(-9) denote to 2.995×10^{-9} .

The authors [2] used a formula for $\alpha_{CR}(T_e)$(radiative recombination rate coefficient) which is depend in its structure on electron density range $10^9 cm^{-3} \le n_e \le 10^{13} cm^{-3}$ and electron temperature (T_e) $2.5K \le T_e \le 4000 K^o$.

$$\alpha_{CR}(T_e) = \left[3.8\times10^{-9} T_e^{-4.5} n_e + 1.55\times10^{-10} T_e^{-0.63} + 6\times10^{-9} T_e^{-2.18} n_e^{0.37}\right] \quad .... (3)$$

The first term is the pure collisional rate, the second term is the radiative cascade contribution, and the third term arises from collisional-radiative coupling.

It is necessary to mention that, first: equation(1) is the dependent formula in our calculations of recombination rate coefficient, while equation(3) is used also for the same purpose by other researchers but we didn't depend it. Second: the simple $\alpha(T)$ with the subscript (RR) is our dependent one, while the subscript for other researchers may take the form (R) or (CR) or any form, in general it all gives the same meaning which is the recombination rate coefficient.

3. Results & Discussion

Recombination between electrons and positive ions has been studied in a wide range over a period of years. In this paper we present theoretical investigation of (C $_{\text{I}}$, C $_{\text{II}}$, N $_{\text{II}}$, O $_{\text{III}}$, F $_{\text{IV}}$, Ne $_{\text{V}}$, Si $_{\text{IX}}$, S $_{\text{XI}}$) recombination rate coefficients.

Figures (1-8) shows the final results for the $e^- + ion$ recombination rate coefficients, $\alpha_{RR}(T)$. All the results have compared with the theoretical data of Nahar [6], where in figures (1) & (2) the agreement between our data of RRC with Nahar's, are very good arriving to the temperature $\log T = 4$, for C $_{\text{I}}$ & C $_{\text{II}}$ ions respectively. In figures (3) & (4) the agreement are good until $\log T = 4.5$, for N$_{\text{II}}$ & O$_{\text{III}}$ ions respectively. In figures (5) & (6) the comparison for RRC with Nahar data shows for (F $_{\text{IV}}$) acceptable agreement with small peak appears at $\log T = 5.3$ for Nahar, whereas for (Ne $_{\text{V}}$) the agreement aren't good. Finally, in figures (7) & (8) the RRC calculations showed not good agreement for (Si $_{\text{IX}}$) and very good for (S $_{\text{XI}}$) ion.

In all figures we see that our data for RRC the electron-ion recombination starts high at low temperature mainly through non-resonant recombination, decreases with temperature to a minimum before the rising of RRC for the calculations which we compare with it at high temperatures appears as "bump", as noticed in (C $_{\text{I}}$, C $_{\text{II}}$, N $_{\text{II}}$, O $_{\text{III}}$) ions, when the resonant recombination becomes dominant, after this $\alpha_R(T)$ falls smoothly. The reason of this action is that our method doesn't include the DR part which is responsible for the resonant, and also the use of the unified method of (RR + DR) by Nahar. In addition to the prominent high-temperature resonant (DR) bump, $\alpha_R(T)$ of Nahar often exhibits a slight low-temperature small bump owing to the low energy autoionizing resonances, as seen in (Ne $_{\text{V}}$) and (Si $_{\text{IX}}$) ions.

The order of dominant states, and their fractional percentage contributions to the radiative recombination rate coefficient, varies with temperature, primarily because of detailed autoionization structures of resonances in the corresponding photoionization cross sections. Some uncertainty in the state-specified recombination rate coefficients might exist in the limits of very low and very high temperatures. At very low temperatures the coefficients are very sensitive to the exact positions and width of the resonances. For very high temperatures the uncertainty may arise from the fact that the DR contributions of the highly excited core levels are not considered.

4. Conclusions

In this paper an investigation carried out to calculate the radiative recombination rate coefficients for sequences of ions. The RRC curves have seen to decay smoothly with temperature up to a certain temperature in some ions. The peaks for $\alpha_R(T)$ rises not in our graphs but in Nahar graphs because of the dominance of DR at higher temperatures, which we hasn't include in the dependent formula. An interesting feature of the recombination rate coefficient of all the ions we had investigate is the disappearances of the "bump", in contradiction with the comparison data where the resonant part of DR has been included. From all this we conclude that the "bump" action happen at a certain temperatures and not for all the region of high temperatures even if the dielectronic recombination part is included.

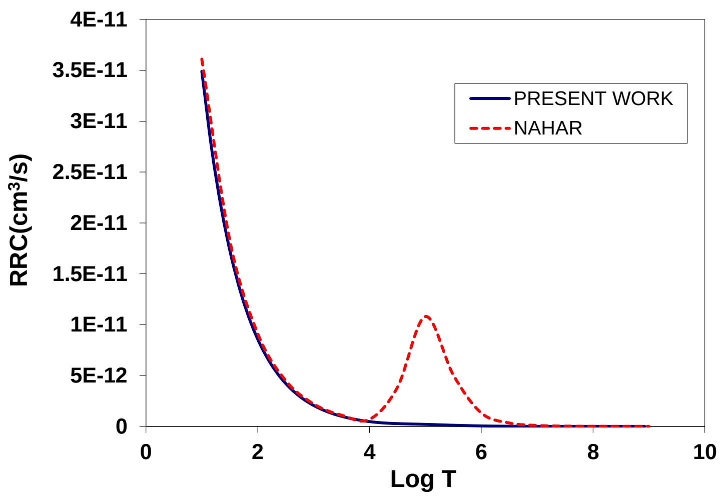

FIG1:RADIATIVE RECOMBINATION RATE FOR (C I) ION

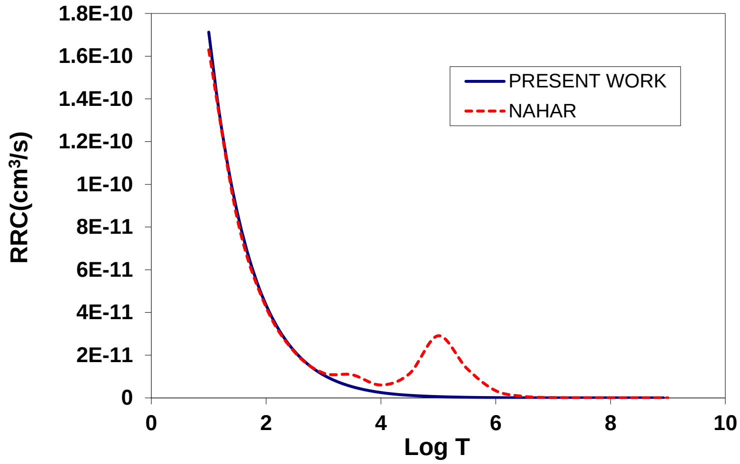

FIG2:RADIATIVE RECOMBINATION RATE FOR (C II) ION

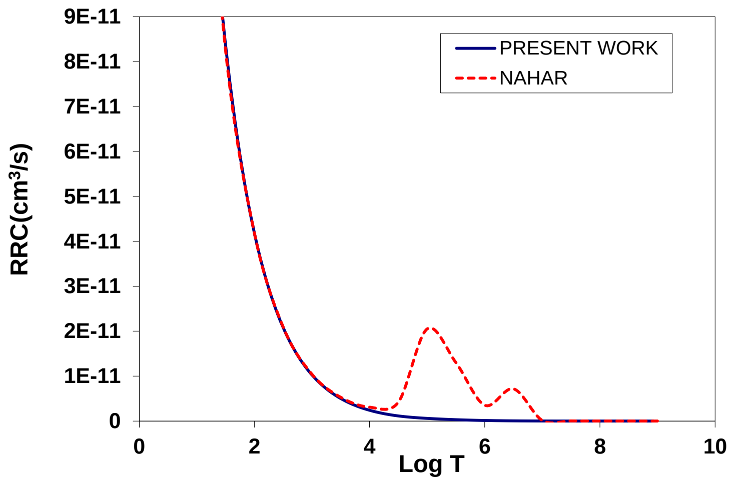

FIG3:RADIATIVE RECOMBINATION RATE FOR (N II) ION

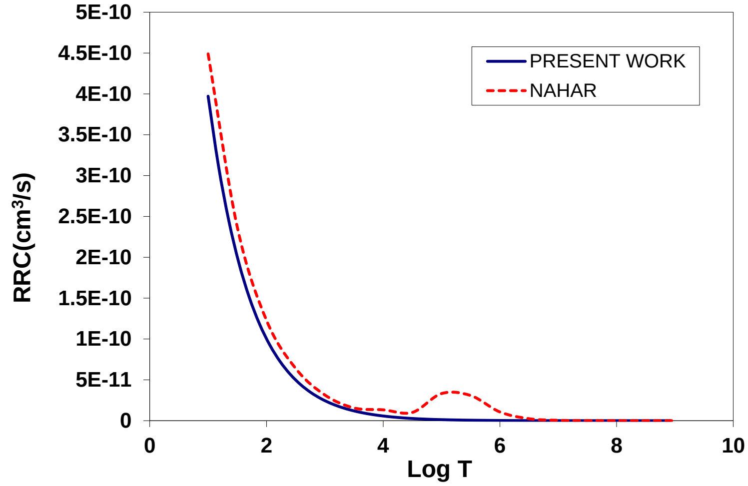

FIG4:RADIATIVE RECOMBINATION RATE FOR (O III) ION

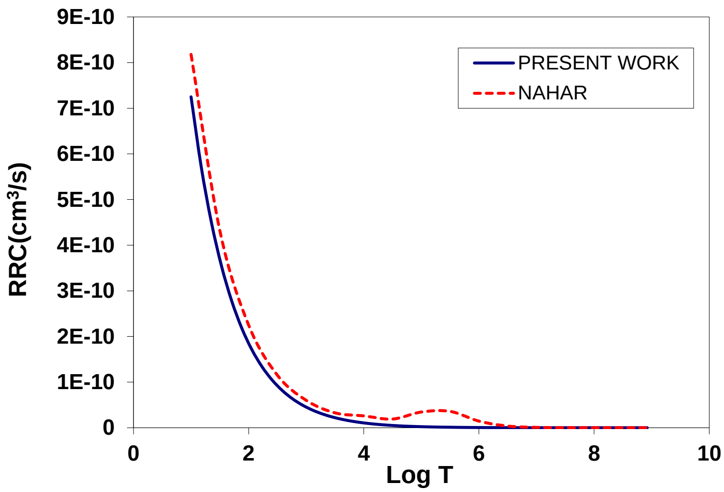

FIG5:RADIATIVE RECOMBINATION RATE FOR (F IV) ION

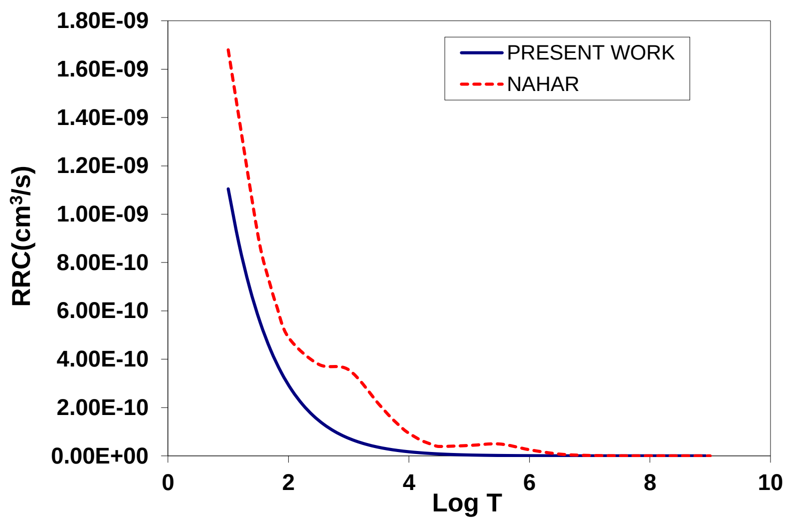

FIG6:RADIATIVE RECOMBINATION RATE FOR (Ne V) ION

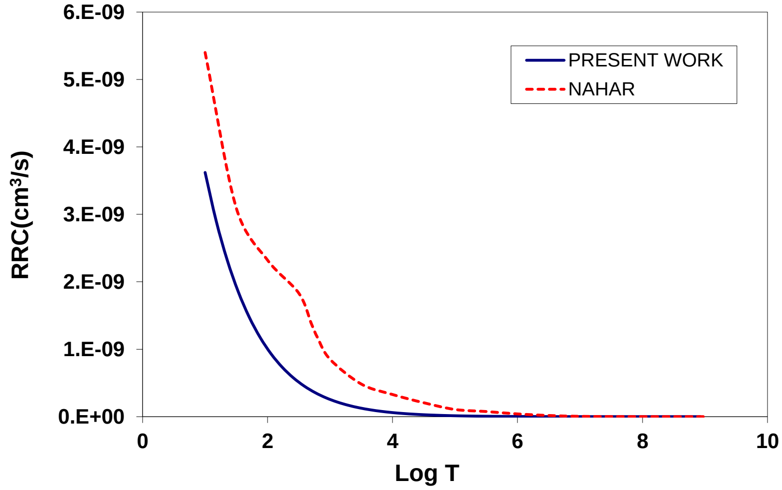

FIG7:RADIATIVE RECOMBINATION RATE FOR (Si IX) ION

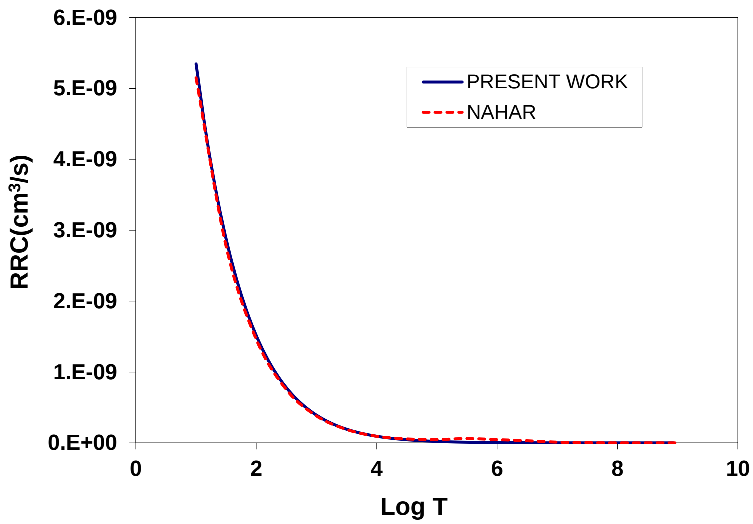

FIG8:RADIATIVE RECOMBINATION RATE FOR (S XI) ION

5. References

[1] S. Ali, (2012), "Electron-ion recombination data for plasma applications", PhD thesis; Stockholm University.

[2] M.R. Flannery, (1996), "Electron-ion and ion-ion recombination", atomic, molecular, optical phys. Handbook, 605-629.

[3] N.R. Badnell, (2006), "Radiative recombination data for modeling dynamic finite-density plasmas", Astrophy. J. Suppl. Series 167, 334-342.

[4] A.A. Khalaf, (2013), "Radiative recombination rate and photoionization cross sections for (C IV, C V and C VI) Ions", Al-Qadisiyah J. for Sci., 18, 113-121.

[5] D.A.Verner, G.J. Ferland, (1996), "Atomic data for asrtrophysics. I. Radiative recombination rates for H-like, He-like, Li-like and Na-like ions over a broad range of temperature", Astrophy. J. 103, 467-481.

[6] S.N. Nahar, (1995), "Electron-ion recombination rate coefficients for Si I, Si II, S II, S III, C II and C-like ions C I, N II, O III, F IV, Ne V, Na VI, Mg VII, Al VIII, Si IX, and S XI", Astrophy. J. Suppl. Series 101, 423-434.

[7] S.N Nahar, M.A. Bautista, A.K. Pradhan, (1997), "Electron-ion recombination of neutral iron", Astrophy. J. 479, 497-503.

[8] S. Schippers, A. Muller, (2001), "Storage ring measurement of the C IV recombination rate coefficient", Astrophy. J. 555, 1027-1037.

[9] K. Seon, U. Nam, W. Han, H. Park, B. Cheon, (2003), "Ionization balance for Ni Ions under coronal equilibrium", J. of Korean Phys. Soc., 43, 365-371.

[10] H.Beyer, (1989), "Heavy-ion coaling and radiative recombination", J. De phys., 50, 471-488.

[11] S.N. Nahar, M.A. Bautista, (1999), "Electron-ion recombination of Fe V", ApJS 120, 327-334.

[12]J. Stevefelt, J. Boulmer, J.F. Delpech, (1975), "Collisional-radiative recombination in cold plasmas", Phys. Rev. A 12, 1246-1251.

[13] A.K. Pradhan, S.N. Nahar, H.L. Zhang, (2001), "Unified electron recombination of Ne-like Fe XVII: Implication for modeling x-ray plasmas" Astrophy. J. 549, L265-L268.