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T P DONALDSON
N J PEACOCK

CULHAM LABORATORY
Abingdon Oxfordshire

1975

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TABLES FOR THE COMPUTATION OF DIELECTRONIC RECOMBINATION COEFFICIENTS

T P Donaldson*

and

N J Peacock

Culham Laboratory, Abingdon, Oxon, OX14 3DB, UK
(Euratom-UKAEA Fusion Assoc.)

ABSTRACT

Two sets of tables are presented which enable the rapid calculation of hydrogenic ion dielectronic recombination coefficients for ions of charge $Z \leqslant 17$ and for ions of charge $Z > 17$.

(Submitted for publication in J.Quant.Spectr.Rad.Transfer)

* Queen's University of Belfast, Belfast, BT7 1NN.

October 1975

1. INTRODUCTION

The purpose of this paper is to present a set of tables from which hydrogenic ion dielectronic recombination coefficients can be rapidly calculated using a simple procedure. Two sets of tables were produced, one applicable to ions of charge, $z \leq 17$ and the other for $z > 17$. The physical assumptions made can be extended to compute tables for helium-like and many electron ions.

Dielectronic recombination is the consequence of inverse auto-ionisation (resonance capture) followed by a stabilising decay, where an ion of species X, charge +z and valence electron state nl recombines with an incident electron of energy E and angular momentum l"+1 resulting in an ion of charge (z-1) and valence electron state n"ℓ". In equation 1(a) the effect of collisions is isolated and in equation 1(b) the effect of stabilisation is isolated.

$$X^{+(z)}\ (n\ell) + e^{-}(E\ell''+1) \rightarrow X^{+(z-1)}\ (n'\ell+1;\ n''\ell'') \qquad 1(a)$$

$$X^{+(z-1)}(n'\ell + 1;\ n''\ell'') \rightarrow X^{+(z-1)}\ (n\ell;\ n''\ell'') + h\nu \quad . \qquad 1(b)$$

For incident electrons of energies E→E+dE, the dielectronic recombination coefficient is expressed in the following formula, BURGESS (1):

$$\alpha_d = \frac{A(n'\ell+1;\ n''\ell'' \rightarrow n\ell;n''\ell'')C_1(kT_e)^{-3/2}\exp(-E/kT_e)EQ(\ n\ell;E\ell''+1 \rightarrow n'\ell+1;n''\ell'')dE}{A(n'\ell+1;n''\ell'' \rightarrow n\ell;n''\ell'') + C_2\omega(n\ell)EQ(n\ell;E\ell''+1 \rightarrow n'\ell+1;n''\ell'')dE/\omega(n'\ell+1;n''\ell'')} \qquad (2)$$

where $C_1 = 4(2\pi m)^{-\frac{1}{2}}$, $C_2 = 16\pi mh^{-3}$, $A(j\rightarrow i)$ is the spontaneous decay rate from level j to level i, process (1b), kT_e is the electron temperature, $Q(i\rightarrow j)$ is the collisional excitation partial cross-section from level i to level j, (process 1a), dE is the width of the electron energy spectrum and $\omega(i)$ is the statistical weight of level i. For a more detailed derivation of this formula see ANSARI et al. (2). The total dielectronic recombination coefficient is given by:

$$\alpha_d(tot) = \sum_{n'n''\ell''} \alpha_d(n'\ell+1;n''\ell'') \quad . \qquad (3)$$

2.1 COMPUTATIONAL DETAILS

To simplify the computations, an uncoupled electron model was adopted to describe the resulting helium-like ion. This can be justified by the quantum mechanical treatment to be found in SHORE (3), TREFFTZ (4). The incident electron energies are specified by:

$$E = E_{n'\ell+1} - E_{n\ell} - z^2/(n'')^2 \tag{4}$$

$$dE = \frac{2z^2}{(n'')^3} \quad . \tag{5}$$

The collision cross section, Q, was calculated at threshold using the Coulomb-Born approximation.

$$Q = \frac{8\pi}{\sqrt{3}} \frac{1}{E} \frac{f(n'\ell+1 \to n\ell)}{(E_{n'\ell+1} - E_{n\ell})} g_{\ell''+1}(E_{th}) \pi a_o^2 \tag{6}$$

where $E_{n\ell}$ is the energy of the state $n\ell$, in Rydbergs, $f(i \to j)$ is the emission oscillator strength from level i to level j, $g_{\ell''+1}(E_{th})$ is the partial free-bound Gaunt factor evaluated at threshold for an incident electron with angular momentum $\ell''+1$ and threshold energy $E_{th} = E_{n'\ell+1} - E_{n\ell}$, calculated from collision strengths tabulated by BURGESS et al. (5) , and a_o is the first Bohr radius. The A coefficient was assumed independent of the captured electron:

$$A(n'\ell+1; n''\ell'' \to n\ell; n''\ell'') = A(n'\ell+1 \to n\ell) \quad . \tag{7}$$

Recombinations involving excitation and decay of the core electron from and to the ground state were found to be the only significant contributions to the recombination coefficient $\alpha_d(\text{tot})$, so that:

$$A(n'\ell+1 \to n\ell) = A(n'p \to 1s) \tag{8}$$

$$Q(n\ell; E\ell''+1 \to n'\ell+1; n''\ell'') = Q(1s; E\ell''+1 \to n'p) \quad . \tag{9}$$

2.2 COMPUTATION OF THE TABLES

The approximation enabling the computation of tables for low z applies when n'' is sufficiently small that the first term in the denominator of equation (2) is an order of magnitude less than the second term. Then equation (2) reduces to the following form, BATES et al. (6) , BURGESS (1), where dielectronic recombination is only sensitive to core stabilisation.

$$\alpha_d = \frac{C_1}{C_2} A(n'\ell+1 \to n\ell) \frac{\omega(n'\ell+1)\omega(n''\ell'')}{\omega(n\ell)} (kT_e)^{-3/2} \exp(-E/kT_e) \quad . \tag{10}$$

Comparison of the terms in the denominatior of equation (2) leads to the following condition for the validity of equation (10):

$$\frac{(z+1)^6}{z^2} < \frac{9.4\times10^6}{(n'')^3}\,\frac{g_{\ell''+1}(E_{th})}{(2\ell''+1)} \quad . \qquad (11)$$

Since there is a maximum value of n'' that can satisfy condition (11) a termination value n''_t must be used when equation (10) is summed over n'' in equation (3). The main ℓ'' contribution to the summation of equation (3) was found to be ℓ''=2. Substitution of this value in equation (11) gives n''_t in terms of z

$$(n_t'')^3 \sim 4\times10^5\,\frac{z^2}{(z+1)^6} \quad . \qquad (12)$$

It is possible to make the approximation because the maximum value of α_d in α_d (tot) is reached with n'' < 4, so that for $Z \leqslant 8$ the main contributions to α_d(tot) are from values of n'' where equation (10) is valid. Equation (10) was summed in equation (3) by expressing the total dielectronic recombination coefficient as the product of two functions Θ,ϕ.

$$\alpha_d(\text{tot}) = C_3(kT_e)^{-3/2}(z+1)^4\Theta(\Delta_z,n_t')\phi(\Delta_{z-1},n_t''), \qquad (13)$$

where $C_3 = \frac{C_1}{C_2}\,2\,\frac{\omega(n'\ell+1)}{\omega(n\ell)}\,1.5\,\chi_H^2h^2c^2 = 7.9\times10^{-12}$ (kT_e in electron volts);

$\Delta_z = \frac{\chi_z}{kT_e}$, where χ_z is the ionisation potential of an ion charge z and χ_H is the ionisation potential of hydrogen

$$\Theta(\Delta,n_t') = \sum_{n'=2}^{n_t'} f(n'\ell+1\to n\ell)(1-1/n'^2)^2\,\exp(-\Delta(1-1/n'^2)) \qquad (14)$$

$$\phi(\Delta,n_t'') = \sum_{n''=2}^{n_t''} \exp(\Delta/(n'')^2) \sum_{\ell''=0}^{L} (2\ell''+1) \qquad (15)$$

where $L = \ell''; \; \ell'' < 3$

$L = 3 \; ; \; \ell'' \geqslant 3$.

The summation over ℓ'' was terminated at $\ell''=3$ since the only significant contributions to the summation in (3) are from $\ell''\leqslant 3$. Otherwise the terms of the summation in equation (15) would diverge for large values of n''. The summation over n' can be terminated at $n_t' = 4$, within the accuracy of this approximation, since the main inner electron contributions are from $n' \leqslant 4$.

By comparison of values for α_d(tot) obtained using this approximation with values calculated using the complete formula, equation (12) was found to overestimate the value of n_t'' required. A better formula for n_t'' was obtained empirically by the comparison of equations (2) and (10) for a range of z and kT_e:

$$(n_t'')^{3\cdot 5} = 1.46\times 10^6 \frac{z^2}{(z+1)^6} \qquad 1 < z \leqslant 17 \quad . \tag{16}$$

Given values of z, kT_e and $n_t' = 4$, n_t'' can be determined from (16) and the corresponding values of Θ and ϕ obtained from tables I and II.

For $z > 17$ the opposite inequality to (11) is satisfied by all values of n'', since $n_t'' < 2$, and a second approximation can be made, where dielectronic recombination is only sensitive to the collisional excitation of the core.

$$\alpha_d = C_1 E Q(n\ell;E\ell''+1\rightarrow n'\ell+1;n''\ell'')dE(kT_e)^{-3/2} \exp(-E/kT_e) \; . \tag{17}$$

The total dielectronic recombination coefficient is expressed as the product of functions β, γ.

$$\alpha_d(\text{tot}) = C_4(kT_e)^{-3/2} \frac{z^2}{(z+1)^2} \beta(\Delta_z, n_t')\gamma(\Delta_{z-1}, n_t'') \tag{18}$$

where

$$C_4 = \frac{16(\pi a_o \chi_H)^2}{\sqrt{3}} = 3.16\times 10^{-5} \quad (kT_e \text{ in electron volts})$$

$$\beta(\Delta, n_t') = \sum_{n'=2}^{n_t'} \frac{f(n'\ell+1\rightarrow n\ell)}{(1-1/n'^2)} \exp(-\Delta(1-1/n'^2)) \tag{19}$$

$$\gamma(\Delta, n_t'') = \sum_{n''=2}^{n_t''} \frac{\exp(\Delta/n''^2)}{n''^3} \sum_{\ell''=1}^{n''} g_{\ell''+1}(E_{th}) \tag{20}$$

Given values of z, kT_e, $n'_t = 4$ and $n_t'' = 10$, within the accuracy of the approximation, the corresponding values of β and γ can be obtained from tables III and IV.

3. CONCLUSIONS

The preceding sections indicate two separate physical regimes of dielectronic recombination, $z \leq 17$, where the coefficient is sensitive to core stabilisation and $z > 17$ where the coefficient is sensitive to the collisional excitation of the core.

Comparisons of the values of α_d(tot) calculated from the tables are made, in Figure (1), with values calculated from equation (2), for HeII, FIX, AXVIII and FeXXVI. Such comparisons show that for the range $1 \leq z < 8$ the approximation expressed in equation (13) was found to give values of α_d(tot) numerically accurate to better than 20% for $z = 7$, with the accuracy increasing for lower z to better than 2% for $z = 1$. For the range $8 \leq z \leq 17$ the accuracy is reduced to 25% for $z = 8$ and better than 35% for $z = 17$, since in this range $2 \leq n_t'' \leq 4$.

For $z > 17$ the approximation expressed in equation (18) is numerically accurate to better than 50%, because the opposite inequality to (11) is satisfied by all values of n", since $n_t'' \leq 2$. When $z > 22$ the accuracy of this approximation increases to better than 20% and when $z > 30$ to better than 10%.

It should be noted that the limit of validity of the approximation is reached for $\Delta > 10$, since above this value the exponential term in equation (2) is so heavily weighted towards low n" levels that the only significant contribution to α_d(tot) is from n"=2, where the approximation for E given in equation (4) is least accurate. However, for large Δ the magnitude of α_d(tot) is insignificant relative to other recombination coefficients.

In computation of tables for ions other than hydrogenic the appropriate f values can be substituted, but the energy levels must still be assumed hydrogenic. This is a reasonable approximation for most ions, since the significant contributions to α_d(tot) come from values of $n' < n''$.

These tables are particularly useful when high density and temperature plasma typical of laser-generated plasma conditions, ($N_e > 10^{17}\,cm^{-3}$ and $kT_e > 100$ eV) are under consideration, for which purpose they were originally intended, DONALDSON (7). In this case the termination value n_t can be set equal to the thermal limit i.e. the maximum principle quantum level that is significantly populated under these conditions, which is generally less than the value of n_t obtained from equation (16), so that the approximation is still valid.

ACKNOWLEDGEMENTS

One of us, T.P.D., wishes to acknowledge Professor P.K. Carroll and the Spectroscopy Group in the Physics Department of University College, Dublin where a part of this work was carried out during the tenure of a National Science Council of Ireland post-doctoral fellowship. We gratefully acknowledge Dr H.P. Summers for some useful comments on the manuscript.

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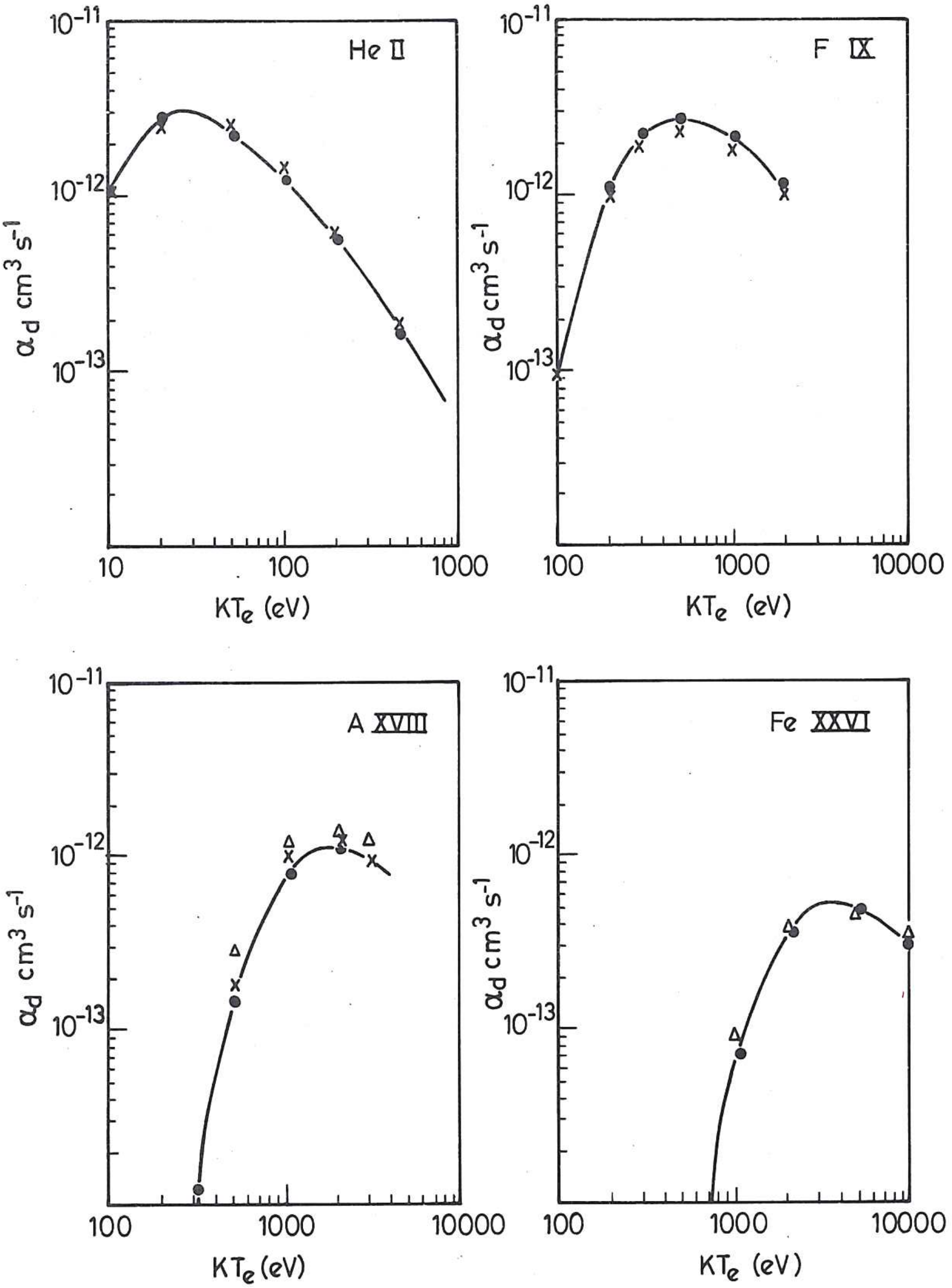

Fig.1 Comparison of dielectronic recombination coefficients calculated from the tables with coefficients calculated from the complete formula in equation (2). x computed from equation (13), Δ computed from equation (18), . computed from equation (2).

Table I: Values of the Function $\theta(\Delta, n_t')$

n_t \ Δ	0.1	0.2	0.5	1.0	2.0	5.0	10.0
2	7.240-2	6.717-2	5.363-2	3.686-2	1.741-2	1.835-3	4.316-5
3	9.146-2	8.461-2	6.699-2	4.543-2	2.093-2	2.080-3	4.603-5
4	9.919-2	9.165-2	7.231-2	4.875-2	2.224-2	2.158-3	4.676-5
5	1.031-1	9.518-2	7.496-2	5.039-2	2.286-2	2.193-3	4.705-5
6	1.053-1	9.721-2	7.647-2	5.132-2	2.322-2	2.212-3	4.719-5
7	1.067-1	9.847-2	7.741-2	5.190-2	2.343-2	2.223-3	4.728-5
8	1.076-1	9.932-2	7.804-2	5.228-2	2.358-2	2.231-3	4.733-5
9	1.083-1	9.991-2	7.848-2	5.255-2	2.368-2	2.237-3	4.737-5
10	1.088-1	1.003-1	7.880-2	5.275-2	2.375-2	2.240-3	4.740-5

Table II: Values of the Function $\phi(\Delta,n_t'')$

n_t \ Δ	0.1	0.2	0.5	1.0	2.0	5.0	10.0
2	4.101	4.205	4.533	5.136	6.595	1.396+1	4.873+1
3	1.320+1	1.341+1	1.405+1	1.519+1	1.784+1	2.965+1	7.607+1
4	2.226+1	2.252+1	2.333+1	2.477+1	2.803+1	4.195+1	9.288+1
5	3.129+1	3.159+1	3.251+1	3.414+1	3.778+1	5.294+1	1.063+2
6	4.032+1	4.064+1	4.164+1	4.340+1	4.730+1	6.328+1	1.182+2
7	4.934+1	4.968+1	5.073+1	5.258+1	5.667+1	7.325+1	1.292+2
8	5.835+1	5.871+1	5.980+1	6.172+1	6.596+1	8.298+1	1.398+2
9	6.736+1	6.773+1	6.886+1	7.083+1	7.518+1	9.255+1	1.499+2
10	7.637+1	7.675+1	7.790+1	7.992+1	8.436+1	1.020+2	1.599+2
11	8.538+1	8.576+1	8.694+1	8.900+1	9.351+1	1.114+2	1.697+2
12	9.439+1	9.478+1	9.597+1	9.806+1	1.026+2	1.207+2	1.793+2
13	1.034+2	1.038+2	1.050+2	1.071+2	1.117+2	1.300+2	1.889+2
14	1.124+2	1.128+2	1.140+2	1.162+2	1.208+2	1.392+2	1.983+2
15	1.214+2	1.218+2	1.230+2	1.252+2	1.299+2	1.484+2	2.077+2
16	1.304+2	1.308+2	1.321+2	1.342+2	1.390+2	1.576+2	2.171+2
17	1.394+2	1.398+2	1.411+2	1.433+2	1.481+2	1.668+2	2.264+2
18	1.484+2	1.488+2	1.501+2	1.523+2	1.571+2	1.759+2	2.357+2
19	1.574+2	1.578+2	1.591+2	1.613+2	1.662+2	1.850+2	2.449+2
20	1.664+2	1.668+2	1.681+2	1.703+2	1.752+2	1.941+2	2.542+2

Table III: Values of the Function $\beta(\Delta, n_t')$

n_t \ Δ	0.1	0.2	0.5	1.0	2.0	5.0	10.0
2	1.716-1	1.592-1	1.271-1	8.738-2	4.127-2	4.350-3	1.023-4
3	1.988-1	1.840-1	1.462-1	9.957-2	4.629-2	4.699-3	1.064-4
4	2.081-1	1.926-1	1.526-1	1.036-1	4.787-2	4.794-3	1.073-4
5	2.125-1	1.966-1	1.556-1	1.055-1	4.858-2	4.833-3	1.076-4
6	2.150-1	1.988-1	1.572-1	1.065-1	4.896-2	4.854-3	1.078-4
7	2.165-1	2.001-1	1.583-1	1.071-1	4.919-2	4.866-3	1.079-4
8	2.174-1	2.010-1	1.589-1	1.075-1	4.934-2	4.874-3	1.079-4
9	2.181-1	2.016-1	1.594-1	1.078-1	4.945-2	4.880-3	1.080-4
10	2.186-1	2.021-1	1.597-1	1.080-1	4.952-2	4.883-3	1.080-4

Table IV: Values of the Function $\gamma(\Delta, n_t'')$

n_t \ Δ	0.1	0.2	0.5	1.0	2.0	5.0	10.0
2	4.536-2	4.650-2	5.013-2	5.680-2	7.293-2	1.544-1	5.389-1
3	6.641-2	6.780-2	7.214-2	8.007-2	9.894-2	1.907-1	6.022-1
4	7.584-2	7.728-2	8.180-2	9.004-2	1.096-1	2.035-1	6.197-1
5	8.068-2	8.214-2	8.672-2	9.506-2	1.148-1	2.094-1	6.269-1
6	8.348-2	8.495-2	8.955-2	9.793-2	1.177-1	2.126-1	6.305-1
7	8.524-2	8.671-2	9.133-2	9.973-2	1.196-1	2.145-1	6.327-1
8	8.642-2	8.789-2	9.252-2	1.009-1	1.208-1	2.158-1	6.341-1
9	8.725-2	8.872-2	9.335-2	1.018-1	1.216-1	2.167-1	6.350-1
10	8.785-2	8.933-2	9.395-2	1.024-1	1.222-1	2.173-1	6.357-1
11	8.830-2	8.978-2	9.441-2	1.028-1	1.227-1	2.178-1	6.362-1
12	8.865-2	9.013-2	9.476-2	1.032-1	1.231-1	2.182-1	6.365-1
13	8.893-2	9.041-2	9.503-2	1.035-1	1.233-1	2.184-1	6.368-1
14	8.915-2	9.063-2	9.525-2	1.037-1	1.236-1	2.187-1	6.371-1
15	8.933-2	9.080-2	9.543-2	1.039-1	1.237-1	2.189-1	6.372-1
16	8.947-2	9.095-2	9.558-2	1.040-1	1.239-1	2.190-1	6.374-1
17	8.960-2	9.107-2	9.570-2	1.041-1	1.240-1	2.191-1	6.375-1
18	8.970-2	9.118-2	9.581-2	1.042-1	1.241-1	2.192-1	6.376-1
19	8.979-2	9.127-2	9.590-2	1.043-1	1.242-1	2.193-1	6.377-1
20	8.986-2	9.134-2	9.597-2	1.044-1	1.243-1	2.194-1	6.378-1