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SEVERAL EXPANSION FORMULAE OF THE COMPLEMENTARY INCOMPLETE GAMMA FUNCTION AND POSSIBLE APPLICATIONS

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ABSTRACT

The complementary incomplete Gamma function, defined by Euler's integral $\int_x^\infty e^{-t}t^{a-1}\,dt$, appears in many physicochemical problems. In this paper, several expansion formulae of the above integral are presented. Some properties of these asymptotic series are discussed from the point of view of the possibilities of their application to kinetics problems.

INTRODUCTION

The complementary incomplete Gamma function, or Prym's function [1,2], is defined by Euler's integral [1—5]

$$\Gamma(a, x) = \int_x^\infty e^{-t}t^{a-1}\,dt \tag{1}$$

This integral is an entire function of a. It is defined for $t \geqslant x$ and has a pole at $t = 0$ [5]. In physicochemical problems, the branch for x being positive is usually considered. For the complementary incomplete Gamma function, the following recurrence relation exists

$$\Gamma(a + 1, x) = a\Gamma(a, x) + e^{-x}x^a \tag{2}$$

This type of function appears in many kinetics problems [6—19] and other types of problem [20—22]. Since integrals expressed by eqn. (1) can not be resolved exactly, many expansion series have been proposed in the literature [3,4]. In this paper, several of them are reviewed. An attempt is also made to show the advantages and disadvantages of the application of these asymptotic series, as well as the possibilities of their application to physicochemical problems.

EXPANSION SERIES OF $\int_x^\infty e^{-t}t^{a-1}\,dt$-TYPE INTEGRAL

The values of some of Euler's integrals can be calculated based on asymptotic series for $\Gamma(0, x)$. If a admits integer values, any complementary incom-

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plete Gamma function can be expressed by $\Gamma(0, x)$, based on the recurrence relation (2). In the literature, two series of the above type have been proposed.

A. The convergent series based on Taylor's asymptotic expansion formulae [1—5]

$$\Gamma(0, x) = -\gamma - \ln x + \sum_{n=1}^{\infty} \frac{(-1)^{n-1} x^n}{n \cdot n!} \tag{3}$$

where $\gamma = \lim_{n \to \infty} (1 + \frac{1}{2} + \frac{1}{3} + ... + 1/n - \ln n)$ is the Euler's constant [4].

If $a = -1$

$$\Gamma(-1, x) = \frac{e^{-x}}{x} + \gamma + \ln x - x + \frac{x^2}{2 \cdot 2!} - ... + \frac{(-1)^n x^n}{n \cdot n!} \tag{4}$$

In this work, $\gamma = 0.577215664901533$ was used [23].

Although the above series has often been discussed in the literature [14,20,21,24—28], they have never been applied in solid state reaction kinetics.

B. The convergent series of $\Gamma(0, x)$ expressed by Tshebysheff's polynomial [29]

$$\Gamma(0, x) = \frac{e^{-x}}{x} \left(0.9999965 - \frac{0.9989710}{x} + \frac{1.9487646}{x^2} - \frac{4.9482092}{x^3} + \frac{11.7850792}{x^4} - \frac{20.4523840}{x^5} + \frac{21.1491469}{x^6} - \frac{9.5240410}{x^7}\right) \tag{5}$$

The maximum error of the series in the bracket is 0.35×10^{-5}. In the case $a = -1$

$$\Gamma(-1, x) = \frac{e^{-x}}{x} \left(0.0000035 + \frac{0.9989710}{x} - \frac{1.9487646}{x^2} + ...\right) \tag{6}$$

The above series has been introduced into kinetics by Flynn and Wall [30], based on ref. 23, and its properties has been investigated by Norwisz and Hajduk [28]. Until now, however, eqns. (5) and (6) have not been in practical use.

Other asymptotic series of the complementary incomplete Gamma function reviewed in this work can be presented in such a way to allow the calculation of numerical values of $\Gamma(a, x)$ for any real values of a.

C. Semi-divergent series through integration by parts [3]

$$\Gamma(a, x) = e^{-x} x^{a-1} \sum_{n=0}^{\infty} \frac{(-1)^n b_n}{x^n} \tag{7}$$

where $b_0 = 1$

$b_n = (1 - a)(2 - a) ... (n - a)$

For $a = -1$

$$\Gamma(-1, x) = \frac{e^{-x}}{x^2}\left[1 - \frac{2!}{x} + \frac{3!}{x^2} - \ldots + \frac{(n+1)!}{x^n}\right] \tag{8}$$

Since the above series presents a fairly simple form, its application in many physicochemical problems has been considered [8,14,20—22,24—26, 28,30—35]. In most cases, the above series has been used in the form of eqn. (8). Vallet [8] has proposed the application of eqn. (7) for $a = -3/2$ and $a = -2$. The properties of this series has been investigated by Saint-Georges and Garnaud [15], Chen [22] and Biegun and Czanderna [33]. It is also worth noting that eqn. (8) has became the basis of several integral methods proposed in solid state reaction kinetics [12,32,35].

D. Schlömilch's divergent series [4]

$$\Gamma(a, x) = e^{-x}x^a \sum_{n=0}^{\infty} \frac{A_n(1-a)}{x(x+1)\ldots(x+n)} \tag{9}$$

where $A_0(1-a) = 1$

$$A_n(1-a) = \sum_{s=0}^{s=n-1} (-1)^{s+1} C_n^{n-1-s}(1-a)(2-a)\ldots(1+s-a)$$

The method for the determination of the value of the function C_n^{n-1-s} can be found in ref. 4. The following relationship may be useful, however, during calculations.

$$x(x+1)\ldots(x+n-1) = C_n^0 x^n + C_n^1 x^{n-1} + \ldots + C_n^{n-1} x \tag{10}$$

Therefore, in the case $n = 6$

$$\begin{aligned} A_6(1-a) = &-C_6^5(1-a) + C_6^4(1-a)(2-a) - C_6^3(1-a)(2-a)(3-a) \\ &+ C_6^2(1-a)\ldots(4-a) - C_6^1(1-a)\ldots(5-a) \\ &+ C_6^0(1-a)\ldots(6-a) \end{aligned} \tag{11}$$

and from relationship (10), one obtains

$$x(x+1)\ldots(x+5) = x^6 + 15x^5 + 85x^4 + 225x^3 + 274x^2 + 120x. \tag{12}$$

Substituting appropriate coefficients of polynomial (12) into eqn. (11), it is possible to calculate A_6 for any real a value. Listed below are the values for $A_n(1-a)$ for the first 10 terms of Schlömilch's series in the cases $a = 0$ and $a = -1$.

For $a = 0$

$A_0(1) = 1$; $A_1(1) = -1$; $A_2(1) = 1$; $A_3(1) = -2$; $A_4(1) = 4$; $A_5(1) = -14$;

$A_6(1) = 38$; $A_7(1) = -216$; $A_8(1) = 600$; $A_9(1) = -6240$.

For $a = -1$

$A_0(2) = 1$; $A_1(2) = -2$; $A_2(2) = 4$; $A_3(2) = -10$; $A_4(2) = 30$; $A_5(2) = -108$;

$A_6(2) = 444$; $A_7(2) = -2112$; $A_8(2) = 11040$; $A_9(2) = -65712$.

Therefore

$$\Gamma(-1, x) = \frac{e^{-x}}{x^2}\left[1 - \frac{2}{x+1} + \frac{4}{(x+1)(x+2)} - \ldots\right] \tag{13}$$

The Schlömilch's series has been introduced into solid state reaction kinetics by Van Krevelen et al. [7]. Although the above series has often been applied in kinetics problems [7,11,14,17,24–26,28,30,31,36], its properties have not been investigated till now.

E. Tricomi's divergent series [3,37]

$$\Gamma(1 + a, x) = \frac{e^{-x}}{x^{1+a}} \sum_{n=0}^{\infty} \frac{B_n}{(x - a)^{n+1}} \tag{14}$$

where

$$B_n = \frac{d^n}{dt^n}\left\{e^{-at}(1 + t)^a]\right\}_{t=0}$$

Differentiation of the above function leads to rather cumbersome equations allowing the calculation of B_n. However, this problem may be simplified if one uses the following numbers of Pascal's triangle

n													
0							1						
1						–1		1					
2					1		–2		1				
3				–1		3		–3		1			
4			1		–4		6		–4		1		
5		–1		5		–10		10		–5		1	
6	1		–6		15		–20		15		–6		1

(15)

For example, coefficient B_6 can be expressed by the equation

$$\begin{aligned} B_6 &= 1a^6 - 6a^6 + 15a^5(a-1) - 20a^4(a-1)(a-2) \\ &+ 15a^3(a-1)(a-2)(a-3) - 6a^2(a-1)(a-2)(a-3)(a-4) \\ &+ 1a(a-1)(a-2)\ldots(a-5). \end{aligned} \tag{16}$$

In the case where $a = -2$, which corresponds to $\Gamma(-1, x)$, the following values of B_n were found: $B_0 = 1$; $B_1 = 0$; $B_2 = 2$; $B_3 = -4$; $B_4 = 24$; $B_5 = -128$; $B_6 = 880$; $B_7 = -6816$; $B_8 = 60\,032$; $B_9 = -589\,312$; $B_{10} = 6384\,384$.

Therefore

$$\Gamma(-1, x) = \frac{e^{-x}}{x}\left[\frac{1}{x+2} + \frac{2}{(x+2)^3} - \frac{4}{(x+2)^4} + \ldots\right] \tag{17}$$

The last three asymptotic series of the complementary incomplete Gamma function presented in this communication can be expressed by a continued fraction expansion.

F. The continued fraction developed by Legendre [3,4]

$$\Gamma(a,x) = \cfrac{e^{-x}\,x^{a}}{x + \cfrac{1-a}{1 + \cfrac{1}{x + \cfrac{2-a}{1 + \cfrac{2}{x + \cfrac{3-a}{1 + \ddots}}}}}} \tag{18}$$

G. The Schlömilch's continued fraction [4]

$$\Gamma(a,x) = \cfrac{e^{-x}\,x^{a}}{x-a + \cfrac{1x}{x-1-a + \cfrac{2x}{x-2-a + \cfrac{3x}{x-3-a + \ddots}}}} \tag{19}$$

H. The continued fraction expansion proposed by Nielsen [4] based on the work of Tannery [38]

$$\Gamma(a,x) = \cfrac{e^{-x}\,x^{a}}{x+1-a - \cfrac{1(1-a)}{x+3-a - \cfrac{2(2-a)}{x+5-a - \cfrac{3(3-a)}{x+7-a - \ddots}}}} \tag{20}$$

SELECTED PROPERTIES OF ASYMPTOTIC SERIES REVIEWED IN THIS WORK

In physicochemical problems, values of x which represent the lower integration limit in eqn. (1) correspond to some function of physicochemical parameters. In solid state reaction kinetics, x describes the ratio E/RT (E = apparent activation energy; R = constant; T = temperature). Since values of x can not be generally predicted, it is important to know ranges for the lower integration limit in which certain asymptotic series can be applied.

Another problem appears when requirements with respect to the level of accuracy of calculations have to be taken into account. In this work, we applied a very simple criterion of accuracy which could be helpful during comparison of the properties of several expansion series. This criterion requires that one obtains identical values of $\Gamma(a, x)$ up to n significant digits. Therefore, in performing calculations of the values of the integral expressed by eqn. (1), a number of terms (or truncated parts) of any expansion formula should be taken such that identical numerical values are obtained at the assumed level of accuracy (i.e. up to n significant digits). In many cases, when only values of Euler's integral for the given value of x are necessary, accuracy up to 5 significant digits is sufficient. If it is necessary to know the

TABLE 1

Selected values of $\int_x^\infty e^{-t}t^{-2}\,dt$ integral calculated based on the asymptotic series presented in this work

Calculations were performed on a TI 59 calculator. Values of $\Gamma(-1, x)$ are presented in computer notation, for example: 4.6031-01 = 4.6031 × 10^{-1}.

x	Symbol of the expansion series									
	A [eqn. (4)]		B [eqn. (6)]		C [eqn. (8)]			D [eqn. (13)]		
	$\Gamma(-1, x)$	N *	$\Gamma(-1, x)$	N *	$\Gamma(-1, x)$	N *	ν **	$\Gamma(-1, x)$	N *	ν **
0.6	4.6031-01	9								
1	1.4850-01	11								
2	1.8767-02	16						1.87 -02	10	1.806
3	3.5473-03	20						3.55 -03	9	1.558
4	7.9956-04	23						7.996 -04	10	1.432
5	1.9929-04	26	1.99 -04	7				1.9929-04	10	1.352
6	5.3043-05	31	5.30 -05	7				5.304 -05	8	1.298
7	1.4787-05	34	1.479 -05	7				1.4787-05	8	1.259
8	4.267 -06	38	4.267 -06	7				4.2672-06	9	1.228
9	1.26 -06	41	1.2648-06	7				1.2648-06	10	1.205
10			3.830 -07	7				3.8302-07	8	1.185
11			1.1804-07	7	1.18 -07	5	1.166	1.1804-07	7	1.169
12			3.691 -08	6	3.69 -08	6	1.157	3.6910-08	9	1.156
13			1.1685-08	7	1.17 -08	5	1.143	1.1685-08	6	1.145
14			3.7387-09	7	3.74 -09	5	1.134	3.7386-09	7	1.135
15			1.2073-09	6	1.207 -09	6	1.127	1.2072-09	6	1.126
16			3.9298-10	7	3.930 -10	9	1.119	3.9296-10	6	1.119
17			1.2883-10	6	1.288 -10	6	1.112	1.2883-10	7	1.112
18			4.2503-11	7	4.2501-11	9	1.106	4.2501-11	6	1.106
19			1.4102-11	6	1.4101-11	8	1.101	1.4101-11	5	1.101
20			4.7026-12	6	4.7024-12	10	1.096	4.7024-12	6	1.096
25			2.0628-14	6	2.0628-14	7	1.077	2.0628-14	5	1.077
30			9.7652-17	6	9.7656-17	7	1.065	9.7656-17	5	1.065
35			4.8752-19	5	4.8756-19	6	1.056	4.8756-19	5	1.056
40			2.5312-21	5	2.5315-21	5	1.049	2.5315-21	4	1.049
45			1.3544-23	5	1.3546-23	4	1.044	1.3546-23	4	1.044
50			7.4223-26	5	7.4236-26	4	1.039	7.4236-26	5	1.039

TABLE 1 (continued)

x	Symbol of the expansion series											
	E [eqn. (17)]			F $a = -1$ [eqn. (18)]			G $a = -1$ [eqn. (19)]			H $a = -1$ [eqn. (20)]		
	$\Gamma(-1, x)$	N *	ν **	$\Gamma(-1, x)$	N *	ν **	$\Gamma(-1, x)$	N *	ν **	$\Gamma(-1, x)$	N *	ν **
0.6				4.6031-01	20	1.472				4.6031-01	24	0.7643
1				1.4850-01	11	1.239				1.4850-01	16	0.8258
2				1.8767-02	8	1.082				1.8767-02	8	0.9014
3				3.5473-03	6	1.040				3.5473-03	6	0.9357
4				7.9956-04	6	1.023				7.9956-04	7	0.9545
5				1.9929-04	5	1.014				1.9929-04	4	0.9660
6				5.3043-04	4	1.010				5.3043-05	5	0.9736
7	1.48 -05	2	0.9759	1.4787-05	4	1.007	1.48 -05	4	0.9772	1.4787-05	4	0.9786
8	4.27 -06	4	0.9819	4.2672-06	4	1.005	4.27 -06	6	0.9823	4.2672-06	4	0.9827
9	1.265 -06	6	0.9854	1.2648-06	4	1.004	1.265 -06	6	0.9853	1.2648-06	3	0.9856
10	3.830 -07	7	0.9878	3.8302-07	3	1.003	3.830 -07	7	0.9891	3.8302-07	3	0.9878
11	1.180 -07	5	0.9896	1.1804-07	3	1.002	1.180 -07	3	0.9902	1.1804-07	4	0.9895
12	3.691 -08	5	0.9909	3.6910-08	3	1.002	3.691 -08	5	0.9910	3.6910-08	4	0.9909
13	1.1685-08	6	0.9920	1.1685-08	2	1.002	1.1685-08	6	0.9920	1.1685-08	3	0.9920
14	3.7386-09	7	0.9929	3.7386-09	3	1.001	3.7386-09	7	0.9929	3.7386-09	3	0.9929
15	1.2072-09	5	0.9937	1.2072-09	2	1.001	1.2072-09	5	0.9937	1.2072-09	3	0.9937
16	3.9296-10	6	0.9944	3.9296-10	3	1.001	3.9296-10	6	0.9944	3.9296-10	3	0.9944
17	1.2883-10	6	0.9949	1.2883-10	2	1.001	1.2883-10	6	0.9949	1.2883-10	3	0.9949
18	4.2501-11	5	0.9954	4.2501-11	2	1.001	4.2501-11	5	0.9954	4.2501-11	3	0.9954
19	1.4101-11	4	0.9958	1.4101-11	2	1.001	1.4101-11	4	0.9958	1.4101-11	3	0.9958
20	4.7024-12	5	0.9961	4.7024-12	3	1.001	4.7024-12	5	0.9962	4.7024-12	3	0.9962
25	2.0628-14	4	0.9974	2.0628-14	2	1.000	2.0628-14	4	0.9974	2.0628-14	3	0.9974
30	9.7656-17	4	0.9981	9.7656-17	2	1.000	9.7656-17	4	0.9981	9.7656-17	3	0.9982
35	4.8756-19	4	0.9986	4.8756-19	2	1.000	4.8756-19	4	0.9986	4.8756-19	2	0.9986
40	2.5315-21	3	0.9989	2.5315-21	2	1.000	2.5315-21	3	0.9989	2.5315-21	2	0.9989
45	1.3546-23	3	0.9991	1.3546-23	2	1.000	1.3546-23	3	0.9991	1.3546-23	2	0.9991
50	7.4236-26	4	0.9993	7.4236-26	2	1.000	7.4236-26	4	0.9993	7.4236-26	2	0.9993

* N = number of terms (for the expansion series A, B, C, D, E), or truncated parts (for the continued fraction expansion F, G, H) necessary to obtain values of $\Gamma(-1, x)$ with an accuracy indicated in the preceding column.

** $\nu = \Gamma_1(-1, x)/\Gamma_N(-1, x)$; ν describes the ratio of the value of the first term (for the expansion series C, D, E) or the first truncated part (for the continued fraction expansion F, G, H) to the value of $\Gamma(-1, x)$ listed in the first column for the given series.

difference between values of Euler's integral [e.g. $\Gamma(a, x_1) - \Gamma(a, x_2)$], higher accuracy may be required.

For the purpose of the comparison of the properties of the expansion series reviewed in this work it was necessary to choose the value of a. We assume $a = -1$, because this case corresponds to the p(x) function applied widely in solid state reaction kinetics.

Selected values of $\Gamma(-1, x)$, as well as other parameters are listed in Table 1. For a given expansion series, either two or three kinds of information are presented in this table. In the first column, the values of $\Gamma(-1, x)$ are listed. These values have been calculated with an arbitrarily assumed accuracy of 5 significant digits. In most cases, it was impossible to apply certain expansion formula in the whole range of x. Usually, expansion series have lower (or upper) limits for x beyond which they can not be used. These limits change with changes in the level of accuracy. So, if the level of accuracy is lower (for example down to 3 significant digits) the range for x in which the given expansion series can be applied is larger. When it was impossible to calculate values of $\Gamma(-1, x)$ to 5 significant digits, the range of x was extended such that values of $\Gamma(-1, x)$ could be obtained with an accuracy of 3 significant digits. In the second column, numbers of terms (or truncated parts) are shown. These have to be taken into account if one wants to obtain values of $\Gamma(-1, x)$ with the accuracy indicated in the first column of the given series. For some expansion series, the ratio of the value of the first term (or the first truncated part) to the value of $\Gamma(-1, x)$ listed in the first column are presented in the third column.

DISCUSSION

The information listed in Table 1 allows us to compare the properties of the series reviewed in this work from the point of view of the possibilities of their applications.

Series A can be used in problems where fairly low values of the lower integration limit [x in eqn. (1)] can be expected. It is shown in Table 1 that an accuracy of 5 significant digits can not be attained for x values exceeding 7. Also, it may be seen that a relatively large number of terms in this series has to be taken into account if one intends to obtain a certain level of accuracy [26]. Therefore, series A can not, in practice, be applied in solid state reaction kinetics. On the other hand, this series is probably the best possible for calculation of $\Gamma(a, x)$ for fairly low x values (e.g. $0 < x < \pi$ [5,39]). It is worth mentioning that series A has been applied as the basis for the construction of tables of values for the exponential integral [i.e. $\Gamma(0, x)$] for low values of x [39,40].

Although series B has been mentioned by some authors [28,30], it has never been in practical use. As may be seen in Table 1, a relatively large number of terms in this series has to be taken into account if one wants to obtain an accuracy of 5 significant digits. Furthermore, in many cases, calculated values of $\Gamma(-1, x)$ based on this series differ from those obtained from other series. Moreover, the method of calculating the coefficients of Tshebysheff's polynomial presents rather difficult problems [29]. Therefore, this series can not be recommended for use in solid state reaction kinetics. An additional inconvenience is that both series A and B can be applied only for integer a.

There is no doubt that series C is the most widely applied in solid state reaction kinetics. It is the basis for several integral methods [12,32,35]. This series has also been recommended for calculation of the values of the $\Gamma(-1, x)$ function (see, for example, refs. 21, 23, 25 and 32). As may be seen in Table 1, however, series C has rather uninteresting properties. An accuracy of 5 significant digits can be obtained for $x > 18$. Also, the coefficient ν differs significantly from 1, so taking only the first term of this series results in the relatively large error in the $\Gamma(-1, x)$ function. The properties of series C have been investigated by Biegun and Czanderna [33]. They found that series C is semi-divergent, i.e. it becomes divergent in its higher terms. The maximum accuracy is obtained for $N = x - 1$ and the terms of this series with N higher than $x - 1$ cannot therefore be used for calculations. Chen [22] has shown that, by adding one half of the next term in the series, the possible error reduces to half its previous value. However, introducing the correction proposed by Chen creates additional technical problems during calculations. Moreover, calculation of b_n coeffients of this series becomes more difficult for non-integer a values.

Series D based on Schlömilch's approximation [4] has better properties compared with series C. However, calculation of $A_n(1 - a)$ presents a difficult problem, especially for higher terms of this series. The calculations become even more difficult if one intends to apply series D for non-integer a.

As is shown in Table 1, series E and G have similar properties. It was found that both series are semi-divergent, similar to series C. Also, both series allow the calculation of values of $\Gamma(-1, x)$ with approximately the same accuracy. In the case of series E, the same problem appears as for series D, namely the necessity of calculating B_n coefficients.

Lastly, the data in Table 1 shows that both series F and H have the best properties among those reviewed in this paper. They can be used in the whole range of x (i.e. $x > 0$). The values of Euler's integral calculated based on these series step asymptotically toward an accurate value of the $\Gamma(a, x)$ function. Both series can be applied with equal ease for any real a value. Based on these continued fraction expansion series, up to 10 truncated parts are necessary to obtain an accuracy better than 5 significant digits for $x > 2$. Since the latter case describes all problems in solid state reaction kinetics, both F and H series can be recommended for application therewith. It is also worth mentioning that now that computation hardware has been improved, the application of series F and H does not create any difficulties, despite the fact that eqns. (18) and (20) seem to be complicated. As Varhegyi [17] has mentioned, proper computer programs for series F can be written in a very few lines. From our experience, it is easier to write programs for series F or H than, for example, series D. Calculations of $\Gamma(a, x)$ can also be performed on programable calculators (e.g. TI 59 with an accuracy up to 9 significant digits).

As may be seen in Table 1, taking only the first truncated part of the Legendre series $e^{-x}x^{-1}[(x + 1)/(x + 3)]$, the values of $\Gamma(-1, x)$ can be obtained with an error less than 1% for $x > 7$. This level of accuracy is sufficient for the application of only the above form in most kinetics problems [26].

In this paper we reviewed 8 selected expansion series of the complementary incomplete Gamma function. In the literature, one can find other series [4,26] or approximation formulae [17,24—26,28,31,41—46] for the calculation of $\Gamma(a, x)$. We did not consider any approximation formulae because values of $\Gamma(-1, x)$ obtained based on them are less accurate than those calculated based on an asymptotic series. Also, it was found that the properties of the series proposed by Nielsen (ref. 4, Vol. 2, p. 47) and very similar series proposed by Van Tets [26] are no better than the properties of the series reviewed in this work. Moreover, Van Tets [26] did not show a method of calculating the coefficients for his series.

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