Studies on Rydberg Orbitals. V. Supplementary Tables of the Basic Formulae for the One-Electron Perturbation Calculation of Molecular Rydberg States

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General expressions have been given of the one-electron perturbation energy of a hydrogenic Rydberg orbital experienced in a cluster of point charges of any geometry.[1] In order to apply these results to the Rydberg states of a given molecule it is convenient to use the wavefunctions of real form. As analytical expressions for the s, p and d orbitals are given in Ref. 1, the results for the f orbital will be given in this paper. Thus only a brief description of the theory is necessary here.[2]

Consider a hydrogenic orbital

$$(n,\ l,\ m)=R_{nl}(r)\ \theta_{lm}(\theta)\ \Phi_m(\phi)\ . \tag{1}$$

Let the spherical harmonics

$$\begin{aligned} &Y_{lm}=\theta_{lm}\Phi_m \\ &\theta_{lm}(\theta)=(-1)^{(m+|m|)/2}\sqrt{\frac{2l+1}{2}\frac{(l-|m|)\,!}{(l+|m|)\,!}}\,P_l^{|m|}(\cos\theta) \\ &\Phi_m(\phi)=\exp(im\phi)/\sqrt{2\pi} \end{aligned} \tag{2}$$

be transformed into real forms as

$$\begin{aligned} &S_{l0}=Y_{l0} \\ &S_{lM}=(Y_{l-M}+(-1)^M Y_{lM})/\sqrt{2} \\ &S_{l-M}=i(Y_{l-M}-(-1)^M Y_{lM})/\sqrt{2} \end{aligned} \qquad (M>0) \tag{3}$$

For convenience' sake a cartesian naming system $l\gamma$, like px and dz^2, is adopted for the angular part of the wavefunction

$$(n,\ l,\ \gamma)=R_{nl}(r)\ \Omega_{l\gamma}(\theta,\ \phi)\ . \tag{4}$$

Corresponding relations between $\Omega_{l\gamma}$ and S_{lM} are given in Table I.

Since the radial part of the wavefunction is hydrogenic, unperturbed energy of the orbital $|nl\gamma\rangle$ in a spherical potential

$$h^{\circ} = -\Delta/2 - 1/r \tag{5}$$

is given in atomic units as

$$\varepsilon^{\circ}(nl\gamma,\ nl\gamma) = \langle nl\gamma | h^{\circ} | nl\gamma \rangle = -1/2n^2 \tag{6}$$

and the basis set $|nl\gamma\rangle$ is orthonormal to each other

$$\langle nl\gamma | n'l'\gamma' \rangle = \delta(n,\ n')\ \delta(l,\ l')\ \delta(\gamma,\ \gamma')\ . \tag{7}$$

If the point charge is displaced to a point A (See Fig. 1 for explanation) the first order perturbation energy of $|nl\gamma\rangle$ is given by

$$\varepsilon_a'(nl\gamma,\ nl\gamma) = \langle nl\gamma | h_a' | nl\gamma \rangle\ , \tag{8}$$

where

$$h_a' = 1/r - 1/r_a\ . \tag{9}$$

By the use of the Neumann expansion h_a' can be expressed as

$$h_a' = \begin{cases} -\left\{\sum\limits_{k=0} \dfrac{r^k}{d^{k+1}} P_k(\cos\lambda) - \dfrac{1}{r}\right\} & (r \leqq d) \\ -\left\{\sum\limits_{k=0} \dfrac{d^k}{r^{k+1}} P_k(\cos\lambda) - \dfrac{1}{r}\right\}\ . & (r > d) \end{cases} \tag{10}$$

Define the following integral $T_k^{nl,\,n'l'}$

$$T_k^{nl,\,n'l'}(d) = \begin{cases} \left\langle R_{nl}(r) \left| \dfrac{1}{d} - \dfrac{1}{r} \right| R_{n'l'}(r) \right\rangle_{r \leqq d} & (k=0) \\ \left\langle R_{nl}(r) \left| \dfrac{r^k}{d^{k+1}} \right| R_{n'l'}(r) \right\rangle_{r \leqq d} & \\ \quad + \left\langle R_{nl}(r) \left| \dfrac{d^k}{r^{k+1}} \right| R_{n'l'}(r) \right\rangle_{r > d}\ . & (k=1,\ 2,\ \cdots) \end{cases} \tag{11}$$

Then one gets

$$\varepsilon_a'(nl\gamma,\ n'l'\gamma') = -\sum_{k=0} C_k^{l\gamma,\,l'\gamma'}\ T_k^{nl,\,n'l'}\ . \tag{12}$$

The general expressisns of the coefficient $C_k^{l\gamma,\,l'\gamma'}$ are given as eqs. (37)-(40) in Ref. 1, where the analytical expressions for all the combinations of s, p and d orbitals are also given. Table II gives the result for the case with $l = l' = f$. Interaction of f with s, p and d orbitals is thought to be smaller and omitted from the table.

Since the hydrogenic R_{nl} function is expressed as the Laguerre's polynomial, the $T_k^{nl,\,n'l'}$ integrals can be obtained as closed forms. The results for $n \leqq 6$ and $l \leqq 3$ are given in Table III. Note, however, the following transformation[3)]

$$x = d/n . \tag{13}$$

References

1) H. Hosoya: International J. Quantum Chem., in press (1972).
2) References on this subject are given in Ref. 1.
3) In Ref. 1 the same integrals are given in terms of $T_k^{nl,nl}(d)$ for smaller n and l values, while for higher members $T_k^{nl,nl}(x)$ expressions are simpler in their coefficients.

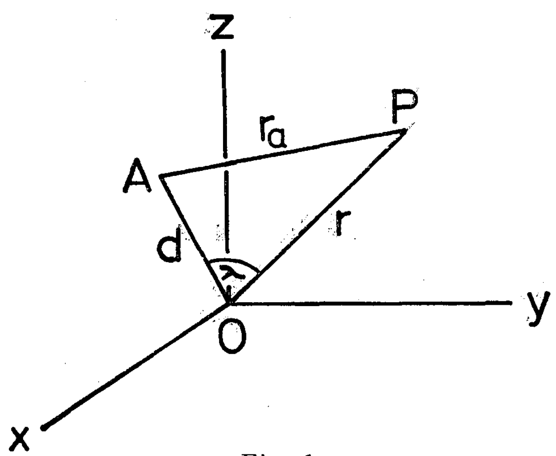

Fig. 1.

Table I. $\Omega_{\ell\gamma}$ functions.

ℓ	γ	$S_{\ell M} = \sum Y_{\ell M}$ a)	$\Omega_{\ell\gamma}$
s		(0 0)	$1/\sqrt{4\pi}$
p	z	(1 0)	$\sqrt{3/4\pi}\ \cos\theta$
	x	$[(1\ -1) - (1\ 1)]/\sqrt{2}$	$\sqrt{3/4\pi}\ \sin\theta\cdot\cos\phi$
	y	$[(1\ -1) + (1\ 1)]i/\sqrt{2}$	$\sqrt{3/4\pi}\ \sin\theta\cdot\sin\phi$
d	z^2	(2 0)	$\sqrt{5/16\pi}\ 3\cos^2\theta - 1$
	zx	$[(2\ -1) - (2\ 1)]/\sqrt{2}$	$\sqrt{15/4\pi}\ \sin\theta\cdot\cos\theta\cdot\cos\phi$
	zy	$[(2\ -1) + (2\ 1)]i/\sqrt{2}$	$\sqrt{15/4\pi}\ \sin_\theta\cdot\cos\theta\cdot\sin\phi$
	x^2-y^2	$[(2\ -2) + (2\ 2)]/\sqrt{2}$	$\sqrt{15/16\pi}\ \sin^2\theta\cdot\cos2\phi$
	xy	$[(2\ -2) - (2\ 2)]i/\sqrt{2}$	$\sqrt{15/16\pi}\ \sin^2\theta\cdot\sin2\phi$
f	z^3	(3 0)	$\sqrt{7/16\pi}\ (\cos^3\theta - 3\cos\theta$
	z^2x	$[(3\ -1) - (3\ 1)]/\sqrt{2}$	$\sqrt{21/32\pi}\ (5\cos^2\theta - 1)\sin\theta\cdot\cos\phi$
	z^2y	$[(3\ -1) + (3\ 1)]i/\sqrt{2}$	$\sqrt{21/32\pi}\ (5\cos^2\theta - 1)\sin\theta\cdot\sin\phi$
	$(x^2-y^2)z$	$[(3\ -2) + (3\ 2)]/\sqrt{2}$	$\sqrt{105/16\pi}\ \sin^2\theta\cdot\cos\theta\cdot\cos2\phi$
	xyz	$[(3\ -2) - (3\ 2)]i/\sqrt{2}$	$\sqrt{105/16\pi}\ \sin^2\theta\cdot\cos\theta\cdot\sin2\phi$
	x^3	$[(3\ -3) - (3\ 3)]/\sqrt{2}$	$\sqrt{35/32\pi}\ \sin^3\theta\cdot\cos3\phi$
	y^3	$[(3\ -3) + (3\ 3)]i/\sqrt{2}$	$\sqrt{35/32\pi}\ \sin^3\theta\cdot\sin3\phi$

a) $(\ell\ m) = Y_{\ell m}(\theta,\phi) = \Theta_{\ell m}(\theta)\Phi_m(\phi)$. See eq. (2).

Table II. The $C_k^{f\gamma f\gamma'}$ coefficients.[a]

γ	γ'	C_0	C_2	C_4	C_6
z^3	z^3	1	$(2/15)A$	$6aB$	$20bG$
z^2x	z^2x	1	$(1/10)(A+2\cdot s\alpha 2\cdot c2\beta)$	$a(H+4C\cdot s\alpha 2\cdot c2\beta)$	$-15b(G-7I\cdot s\alpha 2\cdot c2\beta)$
z^2y	z^2y	1	$(1/10)(A-2\cdot s\alpha 2\cdot c2\beta)$	$a(H-4C\cdot s\alpha 2\cdot c2\beta)$	$-15b(G+7I\cdot s\alpha 2\cdot c2\beta)$
$(x^2-y^2)z$	$(x^2-y^2)z$	1	0	$-7a(B-5\cdot s\alpha 4\cdot c4\beta)$	$6b(G+21I\cdot s\alpha 4\cdot c4\beta)$
xyz	xyz	1	0	$-7a(B+5\cdot s\alpha 4\cdot c4\beta)$	$6b(G-21I\cdot s\alpha 4\cdot c4\beta)$
x^3	x^3	1	$-(1/6)A$	$3aB$	$-b(G-231\cdot s\alpha 6\cdot c6\beta)$
y^3	y^3	1	$-(1/6)A$	$3aB$	$-b(G+231\cdot s\alpha 6\cdot c6\beta)$
z^2x	z^2y	0	$(1/5)s\alpha 2\cdot s2\beta$	$(1/66)C\cdot s\alpha 2\cdot s2\beta$	$(175/2288)I\cdot s\alpha 2\cdot s2\beta$
$(x^2-y^2)z$	xyz	0	0	$(35/264)s\alpha 4\cdot s4\beta$	$(105/1144)J\cdot s\alpha 4\cdot s4\beta$
x^3	y^3	0	0	0	$(35/208)s\alpha 6\cdot s6\beta$
z^3	z^2x	0	$(\sqrt{2}/5\sqrt{3})c\alpha\cdot s\alpha\cdot c\beta$	$(5/22\sqrt{6})D\cdot c\alpha\cdot s\alpha\cdot c2\beta$	$(175/286\sqrt{6})H\cdot c\alpha\cdot s\alpha 2\cdot c2\beta$
z^3	z^2y	0	$(\sqrt{2}/5\sqrt{3})c\alpha\cdot s\alpha\cdot s\beta$	$(5/22\sqrt{6})D\cdot c\alpha\cdot s\alpha\cdot s2\beta$	$(175/286\sqrt{6})H\cdot c\alpha\cdot s\alpha 2\cdot s2\beta$
z^3	$(x^2-y^2)z$	0	$-(1/\sqrt{15})s\alpha 2\cdot c2\beta$	$-(\sqrt{5}/44\sqrt{3})C\cdot s\alpha 2\cdot c2\beta$	$(35\sqrt{5}/572\sqrt{3})I\cdot s\alpha 2\cdot c2\beta$
z^3	xyz	0	$-(1/\sqrt{15})s\alpha 2\cdot s2\beta$	$-(\sqrt{5}/44\sqrt{3})C\cdot s\alpha 2\cdot s2\beta$	$(35\sqrt{5}/572\sqrt{3})I\cdot s\alpha 2\cdot s2\beta$
z^3	x^3	0	0	$-(7\sqrt{5}/22\sqrt{2})c\alpha\cdot s\alpha 3\cdot c3\beta$	$(35\sqrt{5}/572\sqrt{2})J\cdot c\alpha\cdot s\alpha 3\cdot c3\beta$
z^3	y^3	0	0	$-(7\sqrt{5}/22\sqrt{2})c\alpha\cdot s\alpha 3\cdot s3\beta$	$(35\sqrt{5}/572\sqrt{2})J\cdot c\alpha\cdot s\alpha 3\cdot s3\beta$
z^2x	$(x^2-y^2)z$	0	$(1/\sqrt{10})c\alpha\cdot s\alpha\cdot c\beta$	$c(R\cdot c\beta+S\cdot c3\beta)$	$-d(T\cdot c\beta-U\cdot c3\beta)$
z^2x	xyz	0	$(1/\sqrt{10})c\alpha\cdot s\alpha\cdot s\beta$	$c(R\cdot s\beta+S\cdot s3\beta)$	$-d(T\cdot s\beta-U\cdot s3\beta)$
z^2y	$(x^2-y^2)z$	0	$-(1/\sqrt{10})c\alpha\cdot s\alpha\cdot s\beta$	$-c(R\cdot s\beta-S\cdot s3\beta)$	$d(T\cdot s\beta+U\cdot s3\beta)$
z^2y	xyz	0	$(1/\sqrt{10})c\alpha\cdot s\alpha\cdot c\beta$	$c(R\cdot c\beta-S\cdot c3\beta)$	$-d(T\cdot c\beta+U\cdot c3\beta)$
z^2x	x^3	0	$-(1/6\sqrt{15})s\alpha 2\cdot c2\beta$	$e(V\cdot c2\beta-W\cdot c4\beta)$	$-f(X\cdot c2\beta-Y\cdot c4\beta)$
z^2x	y^3	0	$-(1/6\sqrt{15})s\alpha 2\cdot s2\beta$	$e(V\cdot s2\beta-W\cdot s4\beta)$	$-f(X\cdot s2\beta-Y\cdot s4\beta)$
z^2y	x^3	0	$(1/6\sqrt{15})s\alpha 2\cdot s2\beta$	$-e(V\cdot s2\beta+W\cdot s4\beta)$	$f(X\cdot s2\beta+Y\cdot s4\beta)$
z^2y	y^3	0	$-(1/6\sqrt{15})s\alpha 2\cdot c2\beta$	$e(V\cdot c2\beta+W\cdot c4\beta)$	$-f(X\cdot c2\beta+Y\cdot c4\beta)$
$(x^2-y^2)z$	x^3	0	$(\sqrt{15}/7\sqrt{2})c\alpha\cdot s\alpha\cdot c\beta$	$-gD\cdot c\alpha\cdot s\alpha\cdot c\beta$	$h(T\cdot c\beta+Z\cdot c5\beta)$
$(x^2-y^2)z$	y^3	0	$(\sqrt{15}/7\sqrt{2})c\alpha\cdot s\alpha\cdot s\beta$	$-gD\cdot c\alpha\cdot s\alpha\cdot s\beta$	$h(T\cdot s\beta+Z\cdot s5\beta)$
xyz	x^3	0	$-(\sqrt{15}/7\sqrt{2})c\alpha\cdot s\alpha\cdot s\beta$	$gD\cdot c\alpha\cdot s\alpha\cdot s\beta$	$-h(T\cdot s\beta-Z\cdot s5\beta)$
xyz	y^3	0	$(\sqrt{15}/7\sqrt{2})c\alpha\cdot s\alpha\cdot c\beta$	$-gD\cdot c\alpha\cdot s\alpha\cdot c\beta$	$h(T\cdot c\beta-Z\cdot c5\beta)$

a) $\langle n\ell\gamma|h_a'|n'\ell'\gamma'\rangle = -\sum_k C_k^{\ell\gamma\ell'\gamma'} T_k^{n\ell,n'\ell'}$.

$\langle n\ell\gamma|h_a'|n'\ell'\gamma'\rangle = \langle n'\ell'\gamma'|h_a'|n\ell\gamma\rangle$.

Abbreviations: $s\alpha = \sin\alpha$, $c\alpha = \cos\alpha$, $s2\alpha = \sin 2\alpha$, $c\alpha 2 = \cos^2\alpha$, etc.

$A = 3\cdot c\alpha 2 - 1$, $B = 35\cdot c\alpha 4 - 30\cdot c\alpha 2 + 3$, $C = 7\cdot c\alpha 2 - 1$,

$D = 7\cdot c\alpha 2 - 3$, $G = 231\cdot c\alpha 6 - 315\cdot c\alpha 4 + 105\cdot c\alpha 2 - 5$,

$H = 33\cdot c\alpha 4 - 30\cdot c\alpha 2 + 5$, $I = 33\cdot c\alpha 4 - 18\cdot c\alpha 2 + 1$,

$J = 11\cdot c\alpha 2 - 1$, $K = 11\cdot c\alpha 2 - 3$, $R = 4D\cdot s\alpha$, $S = 7\cdot c\alpha\cdot s\alpha 3$,

$T = H\cdot c\alpha\cdot s\alpha$, $U = 3K\cdot c\alpha\cdot s\alpha 3$, $V = 6C\cdot s\alpha 2$, $W = 7\cdot s\alpha 4$,

$X = I\cdot s\alpha 2$, $Y = 3J\cdot s\alpha 4$, $Z = 33\cdot c\alpha\cdot s\alpha 5$,

$a = 1/264$, $b = 5/6864$, $c = \sqrt{5}/66\sqrt{2}$, $d = 35\sqrt{5}/1144\sqrt{2}$,

$e = \sqrt{5}/88\sqrt{3}$, $f = 35\sqrt{5}/2288\sqrt{3}$, $g = 5/22\sqrt{6}$, $h = 35/1144\sqrt{6}$.

Table III. The $T_k^{n\ell,n\ell}$ integrals.[a)]

i) ℓ = s.	
$T_0^{1s,1s}(x)$	$= (1/x - 1) - e^{-2x}(1/x + 1)$
$T_0^{2s,2s}(x)$	$= (1/2x - 1/4) - e^{-2x}(1/2x + 3/4 + x/2 + x^2/2)$
$T_0^{3s,3s}(x)$	$= (1/3x - 1/9) - e^{-2x}(1/3x + 5/9 + 4x/9 + 4x^2/9 - 4x^3/27 + 4x^4/27)$
$T_0^{4s,4s}(x)$	$= (1/4x - 1/16) - e^{-2x}(1/4x + 7/16 + 3x/8 + 3x^2/8 - x^3/4 + 3x^4/8 - 5x^5/36 + x^6/36)$
$T_0^{5s,5s}(x)$	$= (1/5x - 1/25) - e^{-2x}(1/5x + 9/25 + 8x/25 + 8x^2/25 - 8x^3/25 + 16x^4/25 - 512x^5/1125 + 24x^6/125 - 44x^7/1125 + 4x^8/1125)$
$T_0^{6s,6s}(x)$	$= (1/6x - 1/36) - e^{-2x}(1/6x + 11/36 + 5x/18 + 5x^2/18 - 10x^3/27 + 25x^4/27 - 26x^5/27 + 50x^6/81 - 94x^7/405 + 7x^8/135 - 38x^9/6075 + 2x^{10}/6075)$
ii) ℓ = p.	
$T_0^{2p,2p}(x)$	$= (1/2x - 1/4) - e^{-2x}(1/2x + 3/4 + x/2 + x^2/6)$
$T_2^{2p,2p}(x)$	$= 15/4x^3 - e^{-2x}(15/4x^3 + 15/2x^2 + 15/2x + 5 + 5x/2 + 5x^2/6)$
$T_0^{3p,3p}(x)$	$= (1/3x - 1/9) - e^{-2x}(1/3x + 5/9 + 4x/9 + 2x^2/9 + 2x^3/27 + 2x^4/27)$
$T_2^{3p,3p}(x)$	$= 20/3x^3 - e^{-2x}(20/3x^3 + 40/3x^2 + 40/3x + 80/9 + 40x/9 + 5x^2/3 + 10x^3/27 + 10x^4/27)$
$T_0^{4p,4p}(x)$	$= (1/4x - 1/16) - e^{-2x}(1/4x + 7/16 + 3x/8 + 5x^2/24$

$$+ x^3/12 + 13x^4/120 - x^5/20 + x^6/60)$$

$$T_2^{4p,4p}(x) = 75/8x^3 - e^{-2x}(75/8x^3 + 75/4x^2 + 75/4x + 25/2 + 25x/4 + 29x^2/12 + 2x^3/3 + 2x^4/3 - x^5/4 + x^6/12)$$

$$T_0^{5p,5p}(x) = (1/5x - 1/25) - e^{-2x}(1/5x + 9/25 + 8x/25 + 14x^2/75 + 2x^3/25 + 2x^4/15 - 152x^5/1125 + 32x^6/375 - 8x^7/375 + 8x^8/3375)$$

$$T_2^{5p,5p}(x) = 12/x^3 - e^{-2x}(12/x^3 + 24/x^2 + 24/x + 16 + 8x + 47x^2/15 + 14x^3/15 + 14x^4/15 - 32x^5/45 + 4x^6/9 - 8x^7/75 + 8x^8/675)$$

$$T_0^{6p,6p}(x) = (1/6x - 1/36) - e^{-2x}(1/6x + 11/36 + 5x/18 + x^2/6 + 2x^3/27 + 7x^4/45 - 34x^5/135 + 134x^6/567 - 314x^7/2835 + 83x^8/2835 - 34x^9/8505 + 2x^{10}/8505)$$

$$T_2^{6p,6p}(x) = 175/12x^3 - e^{-2x}(175/12x^3 + 175/6x^2 + 175/6x + 175/9 + 175x/18 + 23x^2/6 + 32x^3/27 + 32x^4/27 - 37x^5/27 + 34x^6/27 - 46x^7/81 + 4x^8/27 - 34x^9/1701 + 2x^{10}/1701)$$

iii) ℓ = d.

$$T_0^{3d,3d}(x) = (1/3x - 1/9) - e^{-2x}(1/3x + 5/9 + 4x/9 + 2x^2/9 + 2x^3/27 + 2x^4/135)$$

$$T_2^{3d,3d}(x) = 14/3x^3 - e^{-2x}(14/3x^3 + 28/3x^2 + 28/3x + 56/9 + 28x/9 + 11x^2/9 + 10x^3/27 + 2x^4/27)$$

$$T_4^{3d,3d}(x) = 105/x^5 - e^{-2x}(105/x^5 + 210/x^4 + 210/x^3 + 140/x^2 + 70/x + 28 + 28x/3 + 8x^2/3 + 2x^3/3 + 2x^4/15)$$

$$T_0^{4d,4d}(x) = (1/4x - 1/16) - e^{-2x}(1/4x + 7/16 + 3x/8 + 5x^2/24$$

$$+ x^3/12 + x^4/40 + x^5/180 + x^6/180)$$

$$T_2^{4d,4d}(x) = 63/8x^3 - e^{-2x}(63/8x^3 + 63/4x^2 + 63/4x + 21/2$$
$$+ 21x/4 + 25x^2/12 + 2x^3/3 + x^4/6 + x^5/36 + x^6/36)$$

$$T_4^{4d,4d}(x) = 2835/8x^5 - e^{-2x}(2835/8x^3 + 2835/4x^4 + 2835/4x^3$$
$$+ 945/2x^2 + 945/4x + 189/2 + 63x/2 + 9x^2 + 9x^3/4$$
$$+ 19x^4/40 + x^5/20 + x^6/20)$$

$$T_0^{5d,5d}(x) = (1/5x - 1/25) - e^{-2x}(1/5x + 9/25 + 8x/25$$
$$+ 14x^2/75 + 2x^3/25 + 2x^4/75 + 8x^5/1125 + 32x^6/2625$$
$$+ 8x^7/1575 + 8x^8/7875)$$

$$T_2^{5d,5d}(x) = 54/5x^3 - e^{-2x}(54/5x^3 + 108/5x^2 + 108/5x + 72/5$$
$$+ 36x/5 + 43x^2/15 + 14x^3/15 + 26x^4/105 + 16x^5/315$$
$$+ 12x^6/175 - 8x^7/315 + 8x^8/1575)$$

$$T_4^{5d,5d}(x) = 3969/5x^5 - e^{-2x}(3969/5x^5 + 7938/5x^4 + 7938/5x^3$$
$$+ 5292/5x^2 + 2646/5x + 5292/25 + 1764x/25$$
$$+ 504x^2/25 + 126x^3/25 + 38x^4/35 + 136x^5/875$$
$$+ 136x^6/875 - 8x^7/175 + 8x^8/875)$$

$$T_0^{6d,6d}(x) = (1/6x - 1/36) - e^{-2x}(1/6x + 11/36 + 5x/18 + x^2/6$$
$$+ 2x^3/27 + 7x^4/270 + x^5/135 + 61x^6/2835 - 11x^7/567$$
$$+ 47x^8/5670 - 13x^9/8505 + x^{10}/8505)$$

$$T_2^{6d,6d}(x) = 163/12x^3 - e^{-2x}(163/12x^3 + 163/6x^2 + 163/6x$$
$$+ 163/9 + 163x/18 + 65x^2/18 + 32x^3/27 + 61x^4/189$$
$$+ x^5/14 + 72x^6/567 - 19x^7/189 + 72x^8/1701$$
$$- 13x^9/1701 + x^{10}/1701)$$

$$T_4^{6d,6d}(x) = 1470/x^5 - e^{-2x}(1470/x^5 + 2940/x^3 + 1960/x^2 + 980/x$$

$$+ 392 + 392x/3 + 112x^2/3 + 28x^3/3 + 853x^4/420$$

$$+ 23x^5/70 + 23x^6/70 - 37x^7/189 + 151x^8/1890$$

$$- 13x^9/945 + x^{10}/945)$$

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iv) ℓ = f.

$$T_0^{4f,4f}(x) = (1/4x - 1/16) - e^{-2x}(1/4x + 7/16 + 3x/8 + 5x^2/24$$

$$+ x^3/12 + x^4/40 + x^5/180 + x^6/1260)$$

$$T_2^{4f,4f}(x) = 45/8x^3 - e^{-2x}(45/8x^3 + 45/4x^2 + 45/4x + 15/2$$

$$+ 15x/4 + 251x^2/168 + 41x^3/84 + 11x^4/84 + x^5/36$$

$$+ x^6/252)$$

$$T_4^{4f,4f}(x) = 1485/8x^5 - e^{-2x}(1485/8x^5 + 1485/4x^4 + 1485/4x^3$$

$$+ 495/2x^2 + 495/4x + 99/2 + 33x/2 + 33x^2/7 + 33x^3/28$$

$$+ x^4/40 + x^5/20 + x^6/140)$$

$$T_6^{4f,4f}(x) = 135135/16x^7 - e^{-2x}(135135/16x^7 + 135135/8x^6$$

$$+ 135135/8x^5 + 45045/4x^4 + 45045/8x^3 + 9009/4x^2$$

$$+ 3003/4x + 429/2 + 429x/8 + 143x^2/12 + 143x^3/60$$

$$+ 13x^4/30 + 13x^5/180 + 13x^6/1260)$$

$$T_0^{5f,5f}(x) = (1/5x - 1/25) - e^{-2x}(1/5x + 9/25 + 8x/25 + 14x^2/75$$

$$+ 2x^3/25 + 2x^4/75 + 8x^5/1125 + 4x^6/2625 + 2x^7/7875$$

$$+ 2x^8/7875)$$

$$T_2^{5f,5f}(x) = 9/x^3 - e^{-2x}(9/x^3 + 18/x^2 + 18/x + 12 + 6x$$

$$+ 503x^2/210 + 83x^3/105 + 23x^4/105 + 16x^5/315$$

$$+ x^6/105 + 2x^7/1575 + 2x^8/1575)$$

$$T_4^{5f,5f}(x) = 5643/10x^5 - e^{-2x}(5643/10x^5 + 5643/5x^4 + 5643/5x^3$$

$$+ 3762/5x^2 + 1881/5x + 3762/25 + 1254x/25$$

$$+ 2508x^2/175 + 627x^3/175 + 139x^4/175 + 136x^5/875$$

$$+ 22x^6/875 + 2x^7/875 + 2x^8/875)$$

$$T_6^{5f,5f}(x) = 216216/5x^7 - e^{-2x}(216216/5x^7 + 432432/5x^6$$

$$+ 432432/5x^5 + 288288/5x^4 + 144144/5x^3 + 288288/25x^2$$

$$+ 96096/25x + 27456/25 + 6864x/25 + 4576x^2/75$$

$$+ 4576x^3/375 + 832x^4/375 + 416x^5/1125 + 143x^6/2625$$

$$+ 26x^7/7875 + 26x^8/7875)$$

$$T_0^{6f,6f}(x) = (1/6x - 1/36) - e^{-2x}(1/6x + 11/36 + 5x/18 + x^2/6$$

$$+ 2x^3/27 + 7x^4/270 + x^5/135 + x^6/567 + x^7/2835$$

$$+ 13x^8/17010 - x^9/3645 + x^{10}/25515)$$

$$T_2^{6f,6f}(x) = 145/12x^3 - e^{-2x}(145/12x^3 + 145/6x^2 + 145/6x$$

$$+ 145/9 + 145x/18 + 811x^2/252 + 403x^3/378$$

$$+ 113x^4/378 + x^5/14 + 7x^6/486 + 4x^7/1701 + x^8/243$$

$$- x^9/729 + x^{10}/5103)$$

$$T_4^{6f,6f}(x) = 2365/2x^5 - e^{-2x}(2365/2x^5 + 2365/x^4 + 2365/x^3$$

$$+ 4730/3x^2 + 2365/3x + 946/3 + 946x/9 + 1892x^2/63$$

$$+ 473x^3/63 + 2099x^4/1260 + 23x^5/70 + x^6/18$$

$$+ 19x^7/2835 + 7x^8/810 - x^9/405 + x^{10}/2835)$$

$$T_6^{6f,6f}(x) = 135135/x^7 - e^{-2x}(135135/x^7 + 270270/x^6 + 270270/x^5$$

$$+ 180180/x^4 + 90090/x^3 + 36036/x^2 + 12012/x + 3432$$

$$+ 858x + 572x^2/3 + 572x^3/15 + 104x^4/15 + 52x^5/45$$

$$+ 1469x^6/8505 + 26x^7/1701 + 26x^8/1701 - 13x^9/3645$$

$$+ 13x^{10}/25515)$$

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a) $x = d/n$.