

Tables Useful for the Calculation of the Molecular Integrals. I.¹

Eiichi Ishiguro (石黒英一)

Department of Physics, Faculty of Science,
Ochanomizu University, Tokyo.

Katsunori Hijikata, Tadashi Arai and Masataka Mizushima²

Introduction and Summary.

Under the guidance of Prof. M. Kotani (University of Tokyo), we are now studying many problems of molecular structures and carrying out the numerical calculations in order to obtain quantitative results.

Because the numerical tables thus obtained seem to be useful for other problems in these fields of physics, we consider it worth while to put the parts of it into printed form.

Exponential functions over thirty figures are given in Tab. I. Tab. II is the functions defined by James and Coolidge, namely

$$Z(m, n, j, k, p) = \frac{1}{4\pi^2} \iiint \iiint e^{-\alpha(\lambda_1 + \lambda_2)} \lambda_1^m \lambda_2^n \mu_1^j \mu_2^k \rho^p d\lambda_1 d\lambda_2 d\mu_1 d\mu_2 d\varphi_1 d\varphi_2.$$

In this paper we give $Z(m, n, j, k, p)$ for $\alpha = 1.5$, $p = 0$ only, while for $\alpha = 1.5$, $p = -1$ and

$$X(m, n, j, k, p) = Z(m+2, n, j, k, p) - Z(m, n, j+2, k, p), \quad p = 0, -1,$$

will be given in part II. These tables are useful for the calculation of the quadrupole moment, polarizability, magnetic shielding and other problems in Hydrogen molecules.

Table I.

x	e^x						
0.01	1.01005	01670	84168	05754	21654	56902	86003
0.02	1.02020	13400	26755	81016	01439	20483	1514
0.03	1.03045	45339	53516	85561	24399	53831	1981
0.04	1.04081	07741	92388	22675	70447	57916	8547
0.05	1.05127	10963	76024	03969	75176	36335	6452
0.06	1.06183	65465	45359	62222	46848	77168	3723
0.07	1.07250	81812	54216	47905	31039	49889	1146
0.08	1.08328	70676	74958	55443	59877	58674	8885
0.09	1.09417	42837	05210	35787	28976	23544	8360
0.10	1.10517	09180	75647	62481	17078	26490	2467

¹ Contributions from Department of Physics, Faculty of Science, Ochanomizu University No. 3.

² Department of Physics, Faculty of Science, University of Tokyo, Tokyo.

x	e^{-x}						
0.01	0.99004	98337	49168	05357	39059	77180	03656
0.02	0.98019	86733	06755	30222	08141	04225	3089
0.03	0.97044	55335	48508	17693	25283	51959	1944
0.04	0.96078	94391	52323	20943	92106	91323	2459
0.05	0.95122	94245	00714	00909	14253	19779	6522
0.06	0.94176	45335	84248	70953	71527	83271	1497
0.07	0.93239	38199	05948	22885	79726	32484	9679
0.08	0.92311	63463	86635	73291	07598	49572	3889
0.09	0.91393	11852	71228	18674	73535	46499	5207
0.10	0.90483	74180	35959	57316	42490	59446	4366

x	e^x						
0.1	1.10517	09180	75647	62481	17078	26490	2467
0.2	1.22140	27581	60169	83392	10719	94639	6742
0.3	1.34985	88075	76003	10398	37443	13328	0073
0.4	1.49182	46976	41270	31782	48529	52837	2223
0.5	1.64872	12707	00128	14684	86507	87314	1636
0.6	1.82211	88003	90508	97487	53676	68162	8645
0.7	2.01375	27074	70476	52162	45493	88583	0653
0.8	2.22554	09284	92467	60457	95375	31395	0768
0.9	2.45960	31111	56949	66380	01265	63602	4707
1.0	2.71828	18284	59045	23536	02874	71352	6625

x	e^{-x}						
0.1	0.90483	74180	35959	57316	42490	59446	4366
0.2	0.81873	07530	77981	85866	99355	08619	0394
0.3	0.74081	82206	81717	86606	68737	79317	8169
0.4	0.67032	00460	35639	30074	44329	25147	8261
0.5	0.60653	06597	12633	42360	37995	34991	1805
0.6	0.54881	16360	94026	43262	84589	17232	5679
0.7	0.49658	53037	91409	51470	48000	93397	5290
0.8	0.44932	89641	17221	59143	01023	85015	5628
0.9	0.40656	96597	40599	11188	34542	39645	6260
1.0	0.36787	94411	71442	32159	55237	70161	4609

x	e^x							
1	2.	71828	18284	59045	23536	02874	71352	663
2	7.	38905	60989	30650	22723	04274	60575	01
3	20.	08553	69231	87667	74092	85296	54581	7
4	54.	59815	00331	44239	07811	02612	02860	9
5	148.	41315	91025	76603	42111	55800	40552	
6	403.	42879	34927	35122	60838	71805	43388	
7	1096.	63315	84284	58599	26372	02382	8812	
8	2980.	95798	70417	28274	74359	20994	5289	
9	8103.	08392	75753	84007	70999	66894	3276	
10	22026.	46579	48067	16516	95790	06452	782	

x	e^{-x}						
1	0.36787	94411	71442	32159	55237	70161	4609
2	0.13533	52832	36612	69189	39994	94972	4844
3	0.04978	70683	67863	94297	93424	15650	0618
4	0.01831	56388	88734	18029	37180	21273	2412
5	0.00673	79469	99085	46709	66360	48423	1484
6	0.00247	87521	76666	35842	30451	67430	8167
7	0.00091	18819	65554	51620	80031	36084	4093
8	0.00033	54626	27902	51183	88213	89125	7809
9	0.00012	34098	04086	67954	94976	36690	7300
10	0.00004	53999	29762	48485	15355	91515	5606

Table II.

n	$Z(0.n.0.0.0)$	$Z(1.n.0.0.0)$	$Z(2.n.0.0.0)$
0	0.08851 03437 6		
1	0.14751 72396 1	0.24586 20660 1	
2	0.28519 99965 9	0.47533 33276 3	0.91897 77667 5
3	0.65891 03368 2	1.09818 38948 6	2.12315 55300 7
4	1.84560 45755 5	3.07600 76259 1	5.94694 80767 6
5	6.24052 55955 8	10.40087 59926 4	20.10836 02524 4
6	25.05061 27261 5	41.75102 12101 8	80.71864 10063 5
7	116.99136 97322 3	194.98561 62204 4	376.97219 13595 3
8	624.04248 22491 9	1040.07080 37486 5	2010.80355 39140 6
n	$Z(3.n.0.0.0)$	$Z(4.n.0.0.0)$	$Z(5.n.0.0.0)$
3	4.90522 13970 6		
4	13.73950 07290 6	38.48427 31863 9	
5	46.45724 61004 7	130.12651 51968 4	439.99557 62517 2
6	186.48789 47388 0	522.35166 53628 9	1766.22283 06024 8
7	870.93575 22545 6	2439.48670 91014 5	8248.61373 50738
8	4645.64958 76326 9	13012.44138 24147	43998.84709 20383
n	$Z(6.n.0.0.0)$	$Z(7.n.0.0.0)$	$Z(8.n.0.0.0)$
6	7089.94193 51360 3		
7	33111.44631 00276	1 54637.07314 98612	
8	1 76619.43175 05076	8 24848.05350 27246	43 99813.66116 13140
n	$Z(0.n.0.2.0)$	$Z(1.n.0.2.0)$	$Z(2.n.0.2.0)$
0	0.02950 34479 2		
1	0.04917 24132 0	0.08195 40220 0	
2	0.09506 66655 2	0.15844 44425 4	0.30632 59222 5
3	0.21963 67789 4	0.36606 12982 9	0.70771 85100 2
4	0.61520 15251 8	1.02533 58753 0	1.98231 60256 2
5	2.08017 51985 3	3.46695 86642 1	6.70278 67508 1
6	8.35020 42420 5	13.91700 70700 6	26.90621 36687 8
7	38.99712 32440 7	64.99520 54068 1	125.65739 71198 4
8	208.01416 07497 3	346.69026 79162 2	670.26735 13046 8

n	$Z(3.n.0.2.0)$			$Z(4.n.0.2.0)$			$Z(5.n.0.2.0)$		
3	1.63507	37990	2						
4	4.57983	35763	5	12.82809	10621	3			
5	15.48574	87001	6	43.37550	50656	1	146.66519	20839	1
6	62.16263	15796	0	174.11722	17876	3	588.74094	35341	6
n	$Z(6.n.0.2.0)$								
6	2363.31397	83786	8						
n	$Z(0.n.0.4.0)$			$Z(1.n.0.4.0)$			$Z(2.n.0.4.0)$		
0	0.01770	20687	5						
1	0.02950	34479	2	0.04917	24132	0			
2	0.05703	99993	2	0.09506	66655	3	0.18379	55533	5
3	0.13178	20673	6	0.21963	67789	7	0.42463	11060	1
4	0.36912	09151	1	0.61520	15251	8	1.18938	96153	5
5	1.24810	51191	2	2.08017	51985	3	4.02167	20504	9
6	5.01012	25452	3	8.35020	42420	4	16.14372	82012	7
7	23.39827	39464	5	38.99712	32440	9	75.39443	82719	1
n	$Z(3.n.0.4.0)$			$Z(4.n.0.4.0)$			$Z(5.n.0.4.0)$		
3	0.98104	42794	1						
4	2.74790	01458	1	7.69685	46372	8			
5	9.29144	92200	9	26.02530	30393	7	87.99911	52503	4
6	37.29757	89477	6	104.47033	30725	8	353.24456	61205	0
n	$Z(6.n.0.4.0)$								
6	1417.98838	70272	1						
n	$Z(0.n.0.6.0)$			$Z(1.n.0.6.0)$			$Z(2.n.0.6.0)$		
0	0.01264	43348	2						
1	0.02107	38913	7	0.03512	31522	9			
2	0.04074	23566	6	0.06790	47610	9	0.13128	25381	1
3	0.09413	00481	2	0.15688	34135	5	0.30330	79328	7
4	0.26365	77965	1	0.43942	96608	4	0.84956	40109	7
5	0.89150	36565	1	1.48583	94275	2	2.87262	28932	1
6	3.57865	89608	8	5.96443	16014	5	11.53123	44294	8
n	$Z(3.n.0.6.0)$			$Z(4.n.0.6.0)$			$Z(5.n.0.6.0)$		
3	0.70074	59138	7						
4	1.96278	58184	4	5.49775	33123	4			
5	6.63674	94429	2	18.58950	21709	8	62.85651	08931	0
6	26.64112	78198	3	74.62166	64804	1	252.31754	72289	3
n	$Z(6.n.0.6.0)$								
6	1012.84884	78765	8						

n	$Z(0.n.2.2.0)$	$Z(1.n.2.2.0)$	$Z(2.n.2.2.0)$
0	0.00983 44826 4		
1	0.01639 08044 0	0.02731 80073 3	
2	0.03168 88885 1	0.05281 48141 8	0.10210 86407 5
3	0.07321 22596 5	0.12202 04327 6	0.23590 61700 1
4	0.20506 71750 6	0.34177 86251 0	0.66077 20085 3
5	0.69339 17328 4	1.15565 28880 7	2.23426 22502 7
6	2.78340 14140 2	4.63900 23566 9	8.96873 78895 9
7	12.99904 10813 6	21.66506 84689 4	41.88579 90399 5
8	69.33805 35832 5		
n	$Z(3.n.2.2.0)$	$Z(4.n.2.2.0)$	
3	0.54502 45996 7		
4	1.52661 11921 2	4.27603 03540 4	
5	5.16191 62333 9	14.45850 16885 4	
6	20.72087 71932 0	58.03907 39292 1	
7	96.77063 91394 0		
n	$Z(0.n.2.4.0)$	$Z(1.n.2.4.0)$	$Z(2.n.2.4.0)$
0	0.00590 06895 8		
1	0.00983 44826 4	0.01639 08044 0	
2	0.01901 33331 1	0.03168 88885 1	0.06126 51844 5
3	0.04392 73557 9	0.07321 22596 6	0.14154 37020 0
4	0.12304 03050 4	0.20506 71750 6	0.39646 32051 2
5	0.41693 59397 1	0.69339 17328 4	1.34055 73501 6
6	1.67004 08484 1	2.78340 14140 1	5.38124 27337 6
7	7.79942 46488 2	12.99904 10813 6	
n	$Z(3.n.2.4.0)$	$Z(4.n.2.4.0)$	
3	0.32701 47598 0		
4	0.91596 67152 7	2.56561 82124 3	
5	3.09714 97400 3	8.67510 10131 2	
6	12.43252 63159 2		
7	58.06238 34836 4		
n	$Z(0.n.2.6.0)$	$Z(1.n.2.6.0)$	$Z(2.n.2.6.0)$
0	0.00421 47782 7		
1	0.00702 46304 6	0.01170 77174 3	
2	0.01358 09522 2	0.02263 49203 6	0.04376 08460 4
3	0.03137 66827 1	0.05229 44711 8	0.10110 26442 9
4	0.08788 59321 7	0.14647 65536 1	0.28318 80036 6
5	0.29716 78855 0	0.49527 98091 7	0.95754 09644 0
6	1.19288 63202 9	1.98814 38671 5	
n	$Z(3.n.2.6.0)$		
3	0.23358 19712 9		
4	0.65426 19394 8		
5	2.21224 98143 1		
6	8.88037 59399 4		

n	$Z(0. n. 2. 8. 0)$	$Z(1. n. 2. 8. 0)$	$Z(2. n. 2. 8. 0)$
0	0.00327 81608 8		
1	0.00546 36014 7	0.00910 60024 5	
2	0.01056 29628 4	0.01760 49380 6	0.03403 62135 8
3	0.02440 40865 5	0.04067 34775 9	0.07863 53900 0
4	0.06835 57250 2		
n	$Z(3. n. 2. 8. 0)$		
3	0.18167 48665 6		
4	0.59887 03973 7		
n	$Z(0. n. 4. 4. 0)$	$Z(1. n. 4. 4. 0)$	$Z(2. n. 4. 4. 0)$
0	0.00354 04137 5		
1	0.00590 06895 8	0.00983 44826 4	
2	0.01140 79998 6	0.01901 33331 1	0.03675 91106 7
3	0.02635 64134 7	0.04392 73557 9	0.08492 62212 0
4	0.07382 41830 2	0.12304 03050 4	0.23787 79230 7
5	0.24962 10238 2	0.41603 50397 0	0.80433 44101 0
6	1.00202 45090 5	1.67004 08484 1	
7		7.79942 46488 2	
n	$Z(3. n. 4. 4. 0)$	$Z(4. n. 4. 4. 0)$	
3	0.19620 88558 8		
4	0.54958 00291 6	1.53937 09274 6	
5	1.85828 98440 2		
6	7.45951 57895 5		
n	$Z(0. n. 4. 6. 0)$	$Z(1. n. 4. 6. 0)$	$Z(2. n. 4. 6. 0)$
0	0.00252 88669 6		
1	0.00421 47782 7	0.00702 46304 6	
2	0.00814 85713 3	0.01358 09522 2	0.02625 65076 2
3	0.01882 60096 2	0.03137 66827 1	0.06066 15365 7
4	0.05273 15593 0	0.08788 59321 7	0.16991 28021 9
5		0.29716 78855 0	
6		1.19288 63202 9	
n	$Z(3. n. 4. 6. 0)$		
4	0.14014 91827 7		
5	0.39255 71636 9		
n	$Z(0. n. 4. 8. 0)$	$Z(1. n. 4. 8. 0)$	
0	0.00196 68965 3		
1	0.00327 81608 8	0.00546 36014 7	
2	0.00633 77777 0	0.01056 29628 4	
3		0.02440 40865 5	
4		0.06835 57250 2	

n	$Z(0.n.6.6.0)$	$Z(1.n.6.6.0)$	$Z(2.n.6.6.0)$
0	0.00180 63335 5		
1	0.00301 05559 1	0.00501 75931 8	
2	0.00582 04080 9	0.00970 06801 6	0.01875 46483 0
3		0.02241 19162 2	
4		0.06277 56658 3	

In conclusion we wish to express our thanks to Miss A. Uno, K. Horie, M. Iwano, K. Nagai, S. Nakadate and H. Nishikubo for their assistance.