

# Tables Useful for the Calculation of the Molecular Integrals II<sup>1</sup>

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In part II we shall give the following numerical tables:

Table III:

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

$$\alpha = 1.5, \quad p = -1.$$

Table IV, V:

$$C_\tau^\nu(k) = \frac{1}{2} \int_{-1}^1 P_\tau^\nu(\mu) (1 - \mu^2)^{\frac{\nu}{2}} \mu^k d\mu,$$

Table VI, VII:

$$\bar{C}_\tau^\nu(k) = C_\tau^\nu(k) - C_\tau^\nu(k+2).$$

Table III

<i>n</i>	<i>Z</i> (0. <i>n</i> . 0. 0. -1)	<i>Z</i> (1. <i>n</i> . 0. 0. -1)	<i>Z</i> (2. <i>n</i> . 0. 0. -1)
0	0.06025 69845 6		
1	0.09008 88734 6	0.13670 38045 1	
2	0.15087 20345 8	0.23302 26822 3	0.40584 02092 6
3	0.29265 47237 3	0.46073 58980 0	0.82173 70715 1
4	0.67676 15371 7	1.08487 57920 0	1.98011 62347 3
5	1.89274 10700 6	3.07878 83906 4	5.72971 15456 0
6	6.38005 65288 8	10.48424 01602 2	19.79337 85372 9
7	25.51823 67291 9	42.19945 78497 8	80.43475 23799 2
8	118.77139 78588	197.12534 57200	377.97732 03104
<i>n</i>	<i>Z</i> (3. <i>n</i> . 0. 0. -1)	<i>Z</i> (4. <i>n</i> . 0. 0. -1)	<i>Z</i> (5. <i>n</i> . 0. 0. -1)
3	1.70913 90781 7		
4	4.23042 22857 4	10.76439 42453 5	
5	12.53199 87552 7	32.70142 17611 0	101.76563 91338 2
6	44.09112 81519 8	117.46086 41323	373.26772 73417
7	181.52936 75123	491.29738 43702	1588.01176 8774
8	860.56735 42142	2355.80763 6907	7715.42025 4490

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$n$	$Z(6.n.0.0.-1)$	$Z(7.n.0.0.-1)$	
6	1395.82124 50075		
7	6038.26311 9647	26524.79446 182	
8	29743.50632 8714	I 32420.79585 23	

  

$n$	$Z(0.n.0.2.-1)$	$Z(1.n.0.2.-1)$	$Z(2.n.0.2.-1)$
0	0.02008 56615 2		
1	0.03002 96244 9	0.04556 79348 4	
2	0.05029 06781 9	0.07767 42274 1	0.13528 00697 5
3	0.09755 15745 8	0.15357 86326 7	0.27391 23571 7
4	0.22558 71790 6	0.36162 52640 0	0.66003 87449 1
5	0.63091 36900 2	1.02626 27968 8	1.90990 38485 3
6	2.12668 55096 3	3.49474 67200 7	6.59779 28457 6
7	8.50607 89097 3	14.06648 59499 3	26.81 58 41266 4
8	39.59046 59529 2	65.70844 85733 2	125.99244 01034 2

  

$n$	$Z(3.n.0.2.-1)$	$Z(4.n.0.2.-1)$	
3	0.56971 30260 6		
4	1.41014 07619 1	3.58813 14151 2	
5	4.17733 29184 2	10.90047 39203 7	
6	14.69704 27173 3	39.15362 13774 4	

  

$n$	$Z(0.n.0.4.-1)$	$Z(1.n.0.4.-1)$	$Z(2.n.0.4.-1)$
0	0.01205 13969 1		
1	0.01801 77746 9	0.02734 07609 0	
2	0.03017 44069 2	0.04660 45364 5	0.08116 80418 5
3	0.05853 09447 5	0.09214 71796 0	0.16434 74143 0
4	0.13535 23074 3	0.21697 51584 0	0.39602 32469 5
5	0.37854 82140 1	0.61575 76781 3	1.14594 23091 2
6	1.27601 13057 8	2.09684 80320 4	3.95867 57074 6
7	5.10364 73458 4	8.43989 15699 6	16.08695 04759 8

  

$n$	$Z(3.n.0.4.-1)$	$Z(4.n.0.4.-1)$	
3	0.34182 78156 3		
4	0.84608 44571 5	2.15287 88490 7	
5	2.50639 97510 5	6.54028 43522 6	

  

$n$	$Z(0.n.0.6.-1)$	$Z(1.n.0.6.-1)$	$Z(2.n.0.6.-1)$
0	0.00860 81406 5		
1	0.01286 98390 7	0.01952 91149 3	
2	0.02155 31478 0	0.03328 89546 0	0.05797 71727 5
3	0.04180 78176 8	0.06581 94140 0	0.11739 10102 2
4	0.09668 02196 0	0.15498 22560 0	0.28287 37478 2
5	0.27039 15814 4	0.43982 69129 5	0.81853 02208 0
6	0.91143 66469 8	1.49774 85943 2	2.82762 55053 3

$n$	$Z(3.n.0.6.-1)$	$Z(4.n.0.6.-1)$	
3	0.24416 27254 5		
4	0.60434 60408 2	1.53777 06064 8	
5		4.67163 16801 6	
$n$	$Z(0.n.0.8.-1)$	$Z(1.n.0.8.-1)$	$Z(2.n.0.8.-1)$
0	0.00669 52205 1		
1	0.01000 98748 3	0.01518 93116 1	
2	0.01676 35594 0	0.02589 14091 4	0 04509 33565 8
3	0.03251 71915 3	0.05119 28775 6	0.09130 41190 6
4	0.07519 57263 5	0.12054 17546 7	0.22001 29149 7
$n$	$Z(0.n.1.1.-1)$	$Z(1.n.1.1.-1)$	$Z(2.n.1.1.-1)$
0	0.00623 00042 7		
1	0.00883 28489 3	0.01289 53968 9	
2	0.01371 04351 1	0.02076 54892 0	0.03500 85624 9
3	0.02397 46933 4	0.03791 66578 7	0.06743 03480 6
4	0.04864 23743 9	0.08056 86640 2	0.15158 94730 6
5	0.11714 82931 9	0.20270 80353 4	0.40219 72524 8
6	0.33803 38371 6	0.60657 31172 4	1.25871 75581 1
7			4.60580 46880 5
8			19.46335 12860 8
$n$	$Z(3.n.1.1.-1)$	$Z(4.n.1.1.-1)$	
3	0.13804 92087 7		
4	0.33059 05223 5	0.84429 21039 9	
5	0.93048 13604 3	2.52288 63620 3	
6	3.03264 54396 7	8.74523 48076 8	
7	11.66619 79285 6		
$n$	$Z(0.n.1.3.-1)$	$Z(1.n.1.3.-1)$	$Z(2.n.1.3.-1)$
0	0.00373 80025 6		
1	0.00529 97093 6	0.00773 72381 4	
2	0.00822 62610 7	0.01245 92935 2	0.02100 51374 9
3	0.01438 48160 0	0.02274 99947 2	0.04045 82088 4
4	0.02918 54246 3	0.04834 11984 1	0.09095 36838 4
5	0 07028 89759 1	0.12162 48212 1	0.24131 83514 9
6	0.20282 03023 0	0.36394 38703 5	0.75523 05348 7
7	0.69782 35297 0	1.28643 69982 3	2.76348 28128 3
8	2.82383 98632		11.67801 07716 5
$n$	$Z(3.n.1.3.-1)$	$Z(4.n.1.3.-1)$	$Z(5.n.1.3.-1)$
3	0.08282 95252 6		
4	0 19835 43134 1	0.50657 52624 0	
5	0 55828 88162 6	1.51373 18172 2	4.78372 66285 0
6	1.83758 72638 0	5.24714 08846 1	
7	6.99971 87571 4		

$n$	$Z(0. n. 1. 5. -1)$	$Z(1. n. 1. 5. -1)$	$Z(2. n. 1. 5. -1)$
0	0.00267 00018 3		
1	0.00378 55066 8	0.00552 65986 7	
2	0.00587 59007 6	0.00889 94953 7	0.01500 36696 4
3	0.01027 48685 7	0.01624 99962 3	0.02889 87206 0
4	0.02084 67318 8	0.03452 94274 4	0.06496 69170 3
5	0.05020 64113 7	0.08687 48722 9	0.17237 02510 6
6	0.14487 16445 0	0.25995 99073 9	0.53945 03820 5
7	0.49844 53783 6		1.97391 62948 8

  

$n$	$Z(3. n. 1. 5. -1)$	$Z(4. n. 1. 5. -1)$	
3	0.05916 39466 1		
4	0.14168 16524 3	0.36183 94731 4	
5	0.39877 77259 0	1.08123 70123 0	
6	1.31256 23312 8		

  

$n$	$Z(0. n. 1. 7. -1)$	$Z(1. n. 1. 7. -1)$	$Z(2. n. 1. 7. -1)$
0	0.00207 66680 9		
1	0.00294 42829 8	0.00429 84656 3	
2	0.00457 01450 4	0.00692 18297 3	0.01166 95208 3
3	0.00799 15644 5	0.01263 88859 6	0.02247 67826 9
4	0.01621 41248 0	0.02685 62213 4	0.05052 98243 5
5	0.03904 94310 6		0.13406 57508 3

  

$n$	$Z(3. n. 1. 7. -1)$		
3	0.04601 64029 2		
4	0.11019 68407 8		

  

$n$	$Z(0. n. 1. 9. -1)$	$Z(1. n. 1. 9. -1)$	$Z(2. n. 1. 9. -1)$
0	0.00169 90920 7		
1	0.00240 89588 0	0.00351 69264 2	
2	0.00373 92095 8	0.00566 33152 4	0.00954 77897 7
3			0.01839 00949 3

  

$n$	$Z(0. n. 2. 2. -1)$	$Z(1. n. 2. 2. -1)$	$Z(2. n. 2. 2. -1)$
0	0.00745 66106 4		
1	0.01106 18447 3	0.01670 17008 0	
2	0.01833 54210 2	0.02826 84460 8	0.04907 25664 9
3	0.03511 90693 6	0.05537 64320 0	0.09884 62163 4
4	0.08009 29719 0	0.12897 88617 5	0.23649 48383 9
5	0.22102 83571 3	0.36191 36820 4	0.67856 05746 3
6	0.73659 50826 2	1.21956 48559 7	2.32341 50168 7
7	2.91994 65872 4	4.86502 92223	9.36233 20853 0
8	13.50001 81411		

$n$	$Z(3. n. 2. 2. -1)$	$Z(4. n. 2. 2. -1)$	
3	0.20544 42947 0		
4	0.50707 60673 0	1.29221 51475 6	
5	1.49473 96012 1	3.92131 55386 4	
6	5.22500 75981 8	14.03574 45242 4	
7	21.35781 65153		
$n$	$Z(0. n. 2. 4. -1)$	$Z(1. n. 2. 4. -1)$	$Z(2. n. 2. 4. -1)$
0	0.00466 97524 0		
1	0.00690 76133 8	0.01040 99205 6	
2	0.01140 54456 7	0.01757 23057 2	0.03046 67653 0
3	0.02174 04959 1	0.03430 16303 2	0.06124 71262 5
4	0.04931 50751 0	0.07955 68588 7	0.14613 51119 3
5	0.13537 45613 5	0.22224 63448 7	0.41791 73055 2
6	0.44907 98842 8	0.74579 15862 5	1.42597 34848 2
7	1.77371 88825 2	2.96432 62520	
$n$	$Z(3. n. 2. 4. -1)$	$Z(4. n. 2. 4. -1)$	
3	0.12726 25646 7		
4	0.31376 74209 5	0.80005 88623 3	
5	0.92314 82651 7	2.42680 12685 2	
6	3.21883 14226 7		
7	13.12014 65128 0		
$n$	$Z(0. n. 2. 6. -1)$	$Z(1. n. 2. 6. -1)$	$Z(2. n. 2. 6. -1)$
0	0.00341 32303 9		
1	0.00504 13534 3	0.00758 99829 7	
2	0.00830 71409 1	0.01279 42017 3	0.02216 80170 4
3	0.01579 44234 0	0.02492 80578 2	0.04451 75490 8
4	0.03572 47726 1	0.05768 72570 6	0.10606 40517 3
5	0.09779 03799 3	0.16077 04589 0	0.30279 05201 2
6	0.32359 78676 3	0.53828 47333 0	
$n$	$Z(3. n. 2. 6. -1)$		
3	0.09248 75413 7		
4	0.22789 80707 5		
5	0.66982 99134 0		
6	2.33242 99303 8		
$n$	$Z(0. n. 2. 8. -1)$	$Z(1. n. 2. 8. -1)$	$Z(2. n. 2. 8. -1)$
0	0.00269 31887 3		
1	0.00397 41824 6	0.00597 97033 8	
2	0.00654 04965 5	0.01007 10981 6	0.01744 27612 3
3	0.01241 59595 0	0.01959 97800 4	0.03500 56744 0
4	0.02803 32699 0		

<i>n</i>	$Z(3.n.2.8.-1)$		
3	0.07271 96004 9		
4	0.17912 42139 5		
<i>n</i>	$Z(0.n.3.3.-1)$	$Z(1.n.3.3.-1)$	$Z(2.n.3.3.-1)$
0	0.00235 23874 1		
1	0.00332 92446 8	0.00485 57532 7	
2	0.00515 46614 2	0.00780 72913 7	0.01315 79668 1
3	0.00898 28723 1	0.01422 34467 8	0.02532 05847 5
4	0.01814 69956 5	0.03013 03657 6	0.05682 75154 7
5	0.04349 06537 7	0.07552 21124 3	0.15040 24431 5
6	0.12486 76327 4	0.22505 43214 5	0.46923 73624 3
7	0.42763 97547	0.79219 91886	1.71101 82165
<i>n</i>	$Z(3.n.3.3.-1)$	$Z(4.n.3.3.-1)$	
3	0.05186 70290 3		
4	0.12418 00468 3	0.31751 83407 2	
5	0.34911 94656 9	0.94893 42077	
6	1.14681 84830	3.28644 39817	
<i>n</i>	$Z(0.n.3.5.-1)$	$Z(1.n.3.5.-1)$	$Z(2.n.3.5.-1)$
0	0.00172 37631 8		
1	0.00243 73252 0	0.00355 30818 5	
2	0.00376 87680 0	0.00570 82697 3	0.00961 87399 1
3	0.00655 60130 4	0.01038 71643 5	0.01850 10763 3
4	0.01321 44178 7	0.02196 83758 7	0.04148 60450 8
5	0.03158 74781 8	0.05495 51674 9	0.10965 70756 8
6	0.09045 12660 0	0.16340 70547 0	0.34155 80531 2
7	0.30900 68236		
<i>n</i>	$Z(3.n.3.5.-1)$	$Z(4.n.3.5.-1)$	
3	0.03790 87172 0		
4	0.09075 06127 4	0.23218 49986 4	
5	0.25498 46088	0.69395 90044	
<i>n</i>	$Z(0.n.3.7.-1)$	$Z(1.n.3.7.-1)$	$Z(2.n.3.7.-1)$
0	0.00136 22283 0		
1	0.00192 50445 6	0.00280 54237 3	
2	0.00297 42587 6	0.00450 49170 5	0.00759 02261 7
3	0.00516 82536 6	0.00819 15360 7	0.01459 51024 9
4	0.01040 27455 0	0.01730 76013 3	0.03270 98851 6
5	0.02482 67613 0		0.08639 09698 5
<i>n</i>	$Z(3.n.3.7.-1)$		
3	0.02991 06296 6		
4	0.07159 87430		

$n$	$Z(0. n. 3. 9. -1)$		
0	0.00112 67421 2		
1	0.00159 16596 8		
2	0.00245 78381 2		
3	0.00426 77300 9		

$n$	$Z(0. n. 4. 4. -1)$	$Z(1. n. 4. 4. -1)$	$Z(2. n. 4. 4. -1)$
0	0.00298 72660 7		
1	0.00440 02508 7	0.00661 32103 0	
2	0.00722 42364 2	0 01111 97198 1	0.01924 48390 7
3	0.01367 23810 0	0.02159 28196 8	0.03857 55287 1
4	0.03076 47850 8	0.04976 72665 0	0.09166 70141 3
5	0.08378 15215 8	0.13810 18800 7	0.26085 88481 1
6	0.27600 01204	0.46049 99413	

$n$	$Z(3. n. 4. 4. -1)$	$Z(4. n. 4. 4. -1)$	
3	0.08012 64330 1		
4	0.19724 10620 7	0.50339 86416	
5	0.57866 61273		
6	2.01005 23700		

$n$	$Z(0. n. 4. 6. -1)$	$Z(1. n. 4. 6. -1)$	$Z(2. n. 4. 6. -1)$
0	0.00221 17826 7		
1	0.00325 05129 6	0.00487 80233 3	
2	0.00532 00637 3	0.00818 45988 0	0.01415 13167 1
3	0.01002 90158 8	0.01584 76316 6	0.02832 06942 0
4	0.02246 57403 4	0.03639 86777 4	0.06714 73546 9
5		0.10062 77679 7	
6		0.33434 46109	

$n$	$Z(3. n. 4. 6. -1)$		
3	0.05881 55679 1		
4	0.14465 70460 6		

$n$	$Z(0. n. 4. 8. -1)$	$Z(1. n. 4. 8. -1)$	
0	0.00176 04147 0		
1	0.00258 34333 9	0.00387 33243 4	
2	0.00421 99540 4	0.00649 00837 4	
3		0.01254 36540 8	
4		0.02874 61183 8	

$n$	$Z(0.n.5.5.-1)$	$Z(1.n.5.5.-1)$	$Z(2.n.5.5.-1)$
0	0.00128 26255 8		
1	0.00181 09356 3	0.00263 78502 5	
2	0.00279 44098 0	0.00423 25898 0	0.00713 02515 5
3	0.00484 73270 9	0.00768 75632 3	0.01370 43871 7
4	0.00973 52975 1	0.01621 73633 9	0.03068 75920 2
5	0.02317 50015 3	0.04044 09265 2	

  

$n$	$Z(3.n.5.5.-1)$
3	
4	0.06724 12640 4

  

$n$	$Z(0.n.5.7.-1)$	$Z(1.n.5.7.-1)$	$Z(2.n.5.7.-1)$
0	0.00102 49657 1		
1	0.00144 45540 5	0.00210 31244 6	
2	0.00222 61552 4	0.00337 19396 4	0.00567 94631 4
3	0.00385 47178 7	0.00611 71897 9	0.01091 08542 7

  

$n$	$Z(0.n.6.6.-1)$	$Z(1.n.6.6.-1)$	$Z(2.n.6.6.-1)$
0	0.00165 14795 3		
1	0.00242 03105 5	0.00362 56297 9	
2	0.00394 62520 0	0.00606 74464 3	0.01047 85371 6
3		0.01170 68907 8	

Table IV  $C_{\tau^0}(k)$ 

$\tau \backslash k$	0	1	2	3	4	5	6	7	8	9
0	1	0	$\frac{1}{3}$	0	$\frac{1}{5}$	0	$\frac{1}{7}$	0	$\frac{1}{9}$	0
1	0	$\frac{1}{3}$	0	$\frac{1}{5}$	0	$\frac{1}{7}$	0	$\frac{1}{9}$	0	$\frac{1}{11}$
2	0	0	$\frac{2}{15}$	0	$\frac{4}{35}$	0	$\frac{2}{21}$	0	$\frac{8}{99}$	0
3	0	0	0	$\frac{2}{35}$	0	$\frac{4}{63}$	0	$\frac{2}{33}$	0	$\frac{8}{143}$
4	0	0	0	0	$\frac{8}{315}$	0	$\frac{8}{231}$	0	$\frac{16}{429}$	0
5	0	0	0	0	0	$\frac{8}{693}$	0	$\frac{8}{429}$	0	$\frac{16}{715}$
6	0	0	0	0	0	0	$\frac{16}{3003}$	0	$\frac{64}{6435}$	0
7	0	0	0	0	0	0	0	$\frac{16}{6435}$	0	$\frac{64}{12155}$
8	0	0	0	0	0	0	0	0	$\frac{128}{109395}$	0
9	0	0	0	0	0	0	0	0	0	$\frac{128}{230945}$



Table V  $C_{\tau}^1(k)$ 

$\tau \backslash k$	0	1	2	3	4	5	6	7	8
1	$\frac{2}{3}$	0	$\frac{2}{15}$	0	$\frac{2}{35}$	0	$\frac{2}{63}$	0	$\frac{2}{99}$
2	0	$\frac{2}{5}$	0	$\frac{6}{35}$	0	$\frac{2}{21}$	0	$\frac{2}{33}$	0
3	0	0	$\frac{8}{35}$	0	$\frac{16}{105}$	0	$\frac{8}{77}$	0	$\frac{96}{1287}$
4	0	0	0	$\frac{8}{63}$	0	$\frac{80}{693}$	0	$\frac{40}{429}$	0
5	0	0	0	0	$\frac{16}{231}$	0	$\frac{80}{1001}$	0	$\frac{32}{429}$
6	0	0	0	0	0	$\frac{16}{429}$	0	$\frac{112}{2145}$	0
7	0	0	0	0	0	0	$\frac{128}{6435}$	0	$\frac{3584}{109395}$

Table VI  $\bar{C}_{\tau}^0(k)$ 

$\tau \backslash k$	0	1	2	3	4	5	6
0	$\frac{2}{3}$	0	$\frac{2}{15}$	0	$\frac{2}{35}$	0	$\frac{2}{63}$
1	0	$\frac{2}{15}$	0	$\frac{2}{35}$	0	$\frac{2}{63}$	0
2	0	0	$\frac{2}{105}$	0	$\frac{2}{105}$	0	$\frac{10}{693}$
3	0	0	0	$-\frac{2}{315}$	0	$\frac{2}{693}$	0
4	0	0	0	0	$-\frac{32}{3465}$	0	$-\frac{16}{3003}$
5	0	0	0	0	0	$-\frac{64}{9009}$	0

Table VII  $\bar{C}_{\tau}^1(k)$ 

$\tau \backslash k$	0	1	2	3	4	5	6
1	$\frac{8}{15}$	0	$\frac{8}{105}$	0	$\frac{8}{315}$	0	$\frac{8}{693}$
2	0	$\frac{8}{35}$	0	$\frac{8}{105}$	0	$\frac{8}{231}$	0
3	0	0	$\frac{8}{105}$	0	$\frac{8}{165}$	0	$\frac{24}{819}$
4	0	0	0	$\frac{8}{693}$	0	$\frac{200}{9009}$	0
5	0	0	0	0	$-\frac{32}{3003}$	0	$\frac{16}{3003}$

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