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Wave Functions for Quadrupole Antishielding Factors*

Supplement to the paper: "Quadrupole Antishielding
Factors of Ions", Phys. Rev. 132, 1637 (1963).

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INTRODUCTION

The purpose of this paper is to present tables of the
perturbed wave functions which have been recently obtained in a
calculation of the quadrupole antishielding factors γ_{∞} for the
following ions: F^- , Br^- , Rb^+ , Pr^{3+} , and Tm^{3+} . The wave functions
 $v_1'(nl \rightarrow l)$ which are tabulated represent the effect of the per-
turbation due to a nuclear quadrupole moment Q on the wave functions
of the outer electrons of the ion core.

The functions $v_1'(nl \rightarrow l)$ are the solutions of the following
equation:

* Work performed under the auspices of the U.S. Atomic Energy Commission

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$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V_0 - E_0 \right] v_1'(nl \rightarrow l) = u_0' \left(\frac{1}{r^3} - \left\langle \frac{1}{r^3} \right\rangle_{nl}^{(1)} \right)$$

where u_0' is r times the unperturbed radial wave function for the nl shell; u_0' is normalized according to:

$$\int_0^\infty u_0'^2 dr = 1. \quad (2)$$

In Eq. (1), V_0 and E_0 are the unperturbed (spherical) effective potential and the unperturbed eigenvalue for the state nl . $v_1'(nl \rightarrow l)$ is completely determined by Eq. (1) and by the orthogonality condition:

$$\int_0^\infty u_0' v_1'(nl \rightarrow l) dr = 0. \quad (3)$$

We note that $v_1'(nl \rightarrow l)$ is the same as the function $u_1'(nl \rightarrow l)$ of reference 1. We use the notation v_1' in order to be consistent with the notation of three previous tabulations³ of perturbed wave functions pertaining to the effect of the nuclear quadrupole moment.

According to a method previously employed by the author,²⁻⁴ $V_0 - E_0$ is obtained from the unperturbed wave function u_0' by means of the relation:

$$V_0 - E_0 = \frac{1}{u_0'} \frac{d^2 u_0'}{dr^2} - \frac{l(l+1)}{r^2}. \quad (4)$$

The method of solution of Eq. (1) has been described in reference 1. The unperturbed wave functions u_0' used in this work were the Hartree-Fock functions^{5,6} for F^- , Br^- , and Rb^+ , and the Hartree functions⁷ for Pr^{3+} and Tm^{3+} .

The contribution to the total antishielding factor γ_∞ due to the $nl \rightarrow l$ mode of excitation of the nl shell is given by:

$$\gamma_\infty(nl \rightarrow l) = C_{\ell\ell}^{(2)} \int_0^\infty u_0' v_1'(nl \rightarrow l) r^2 dr, \quad (5)$$

where the coefficient $C_{\ell\ell}^{(2)}$ represents the effect of the integration over the angular variables and the summation over magnetic substates. For a completed p shell, $C_{11}^{(2)} = 48/25$; for a completed d shell, $C_{22}^{(2)} = 16/7$.

The resulting functions $v_1'(np \rightarrow p)$ and $v_1'(nd \rightarrow d)$ are presented in Tables I-VII. In Tables II-V pertaining to Br^- and Rb^+ , we have also given the unperturbed functions $u_0'(3p)$, $u_0'(3d)$, and $u_0'(4p)$ of Watson and Freeman,⁶ which were used in the calculations. We have also listed the values of $\langle r_8^{-3} \rangle_{nl}$ (in units a_H^{-3}), $\gamma_\infty(nl \rightarrow l)$, and $J(nl \rightarrow l)$ defined by :

$$J(nl \rightarrow l) = \int_0^\infty u_0' v_1'(nl \rightarrow l) r^{-3} dr. \quad (6)$$

As previously discussed in reference 8, $J(nl \rightarrow l)$ enters into the calculation of the second-order quadrupole effect for the hyperfine structure.

It is estimated that the accuracy of the functions $v_1'(nl \rightarrow l)$ and of the resulting values of $\gamma_\infty(nl \rightarrow l)$ is generally within 3%. The estimated accuracy of $J(nl \rightarrow l)$ is generally within 10%, with the exception of the two cases: $Rb^{+4}p \rightarrow p$ and $Tm^{3+}5p \rightarrow p$, where the uncertainty of the values of $v_1'(nl \rightarrow l)$ near $r = 0$ is somewhat greater ($\sim 35\%$ for $Rb^{+4}p \rightarrow p$, and up to a factor of ~ 1.8 for $Tm^{3+}5p \rightarrow p$). The resulting uncertainty of $J(np \rightarrow p)$ is $\sim 30\%$ for both cases. However, the perturbed wave functions at large r are known with considerably greater precision, and as a result the values of $\gamma_\infty(np \rightarrow p)$ for these two cases have been determined to $\leq 6\%$. Specifically, $|\gamma_\infty(4p \rightarrow p)|$ for Rb^{+4} , which is given as 43.8 in Table I of reference 1, may be as low as 42.0, although this is considered unlikely. Similarly, for $|\gamma_\infty(5p \rightarrow p)|$ of Tm^{3+} which is given as 67.2, an upper limit is 72.

TABLE I. Wave function $v_1'(2p \rightarrow p)$ for F^- .

r	$v_1'(2p \rightarrow p)$	r	$v_1'(2p \rightarrow p)$
0.01	+0.108	1.4	-0.594
0.02	0.234	1.6	-1.066
0.03	0.369	1.8	-1.407
0.04	0.512	2.0	-1.643
0.05	0.658	2.2	-1.795
0.06	0.805	2.4	-1.882
0.08	1.101	2.6	-1.919
0.10	1.386	2.8	-1.918
0.12	1.656	3.0	-1.887
0.14	1.903	3.2	-1.836
0.16	2.131	3.4	-1.771
0.18	2.334	3.6	-1.693
0.20	2.514	3.8	-1.611
0.22	2.667	4.0	-1.524
0.24	2.803	4.5	-1.303
0.26	2.914	5.0	-1.091
0.28	3.004	5.5	-0.901
0.30	3.078	6.0	-0.733
0.35	3.187	6.5	-0.592
0.40	3.200	7.0	-0.474
0.45	3.143	7.5	-0.376
0.50	3.025	8.0	-0.297
0.55	2.864	8.5	-0.234
0.60	2.670	9.0	-0.183
0.7	2.223	9.5	-0.143
0.8	1.746	10.0	-0.111
0.9	1.274	11.0	-0.068
1.0	0.821	12.0	-0.041
1.1	0.406		
1.2	+0.034		
		$\langle r^{-3} \rangle_{2p}$	6.401
		γ_{∞}	-23.30
		J	+50.88

TABLE II. Wave functions $v_1'(3p \rightarrow p)$ and $v_1'(3d \rightarrow d)$ for Br^- . The unperturbed wave functions $u_0'(3p)$ and $u_0'(3d)$ of Watson and Freeman⁶ are also listed.

r	$v_1'(3p \rightarrow p)$	$v_1'(3d \rightarrow d)$	$u_0'(3p)$	$u_0'(3d)$
0.01	+ 2.77	+0.0187	+0.0398	+0.0006
0.02	5.36	+0.0773	0.1338	0.0043
0.03	7.21	0.171	0.2526	0.0132
0.04	8.26	0.292	0.3766	0.0281
0.05	8.55	0.436	0.4927	0.0494
0.06	8.17	0.597	0.5930	0.0770
0.07	7.25	0.767	0.6727	0.1105
0.08	5.90	0.943	0.7299	0.1492
0.09	4.24	1.116	0.7641	0.1924
0.10	+ 2.36	1.287	0.7761	0.2394
0.12	- 1.71	1.608	0.7397	0.3415
0.14	- 5.76	1.882	0.6368	0.4500
0.16	- 9.41	2.102	0.4854	0.5598
0.18	-12.46	2.263	0.3023	0.6671
0.20	-14.80	2.365	+0.1020	0.7691
0.22	-16.42	2.413	-0.1036	0.8636
0.24	-17.39	2.412	-0.3056	0.9493
0.26	-17.79	2.369	-0.4972	1.0256
0.28	-17.68	2.289	-0.6740	1.0919
0.30	-17.14	2.178	-0.8329	1.1484
0.35	-14.53	1.803	-1.1449	1.2484
0.40	-10.86	1.353	-1.3378	1.2967
0.45	- 6.93	0.883	-1.4296	1.3034
0.50	- 3.22	0.433	-1.4437	1.2787
0.55	- 0.01	+0.022	-1.4027	1.2317
0.60	+ 2.57	-0.336	-1.3255	1.1699
0.7	6.34	-0.903	-1.1117	1.0233
0.8	8.10	-1.258	-0.8934	0.8698

TABLE II (cont'd).

r	$v_1'(3p \rightarrow p)$	$v_1'(3d \rightarrow d)$	$u_0'(3p)$	$u_0'(3d)$
0.9	8.40	-1.443	-0.6899	0.7252
1.0	7.86	-1.501	-0.5195	0.5964
1.1	6.92	-1.473	-0.3840	0.4855
1.2	5.85	-1.389	-0.2799	0.3921
1.4	3.77	-1.136	-0.1450	0.2517
1.6	2.31	-0.873	-0.0743	0.1595
1.8	1.40	-0.649	-0.0385	0.1007
2.0	0.855	-0.472	-0.0205	0.0636
2.2	0.526	-0.340	-0.0112	0.0404
2.4	0.317	-0.243	-0.0062	0.0258
2.6	0.190	-0.173	-0.0033	0.0166
2.8		-0.123		0.0107
3.0		-0.086		0.0069
3.2		-0.060		0.0045
3.4		-0.042		0.0029
3.6		-0.029		0.0019
<hr/>				
$\langle r^{-3} \rangle_{nl}$	181.3	23.08	----	-----
γ_∞	-4.51	-1.627	----	-----
J	+4545	+66.50	----	-----

TABLE III. Wave function $v_1'(4p-p)$ for Br^- .

r	$v_1'(4p-p)$	$u_0'(4p)$
0.01	+0.68	+0.00940
0.02	1.35	0.03190
0.03	1.86	0.06023
0.04	2.17	0.08973
0.05	2.30	0.1173
0.06	2.26	0.1409
0.07	2.08	0.1594
0.08	1.77	0.1725
0.09	1.37	0.1798
0.10	+0.91	0.1817
0.12	-0.13	0.1707
0.14	-1.20	0.1435
0.16	-2.19	0.1047
0.18	-3.04	0.0585
0.20	-3.71	+0.0086
0.22	-4.18	-0.0418
0.24	-4.46	-0.0905
0.26	-4.57	-0.1357
0.28	-4.52	-0.1763
0.30	-4.33	-0.2114
0.35	-3.38	-0.2733
0.40	-1.98	-0.2991
0.45	-0.36	-0.2936
0.50	+1.28	-0.2635
0.55	2.84	-0.2154
0.60	4.24	-0.1549
0.7	6.56	-0.0152
0.8	8.10	+0.1292
0.9	9.00	0.2637

TABLE III(cont'd).

r	$v_1'(4p+p)$	$u_0'(4p)$
1.0	9.34	0.3813
1.1	9.22	0.4791
1.2	8.75	0.5572
1.4	7.17	0.6598
1.6	5.22	0.7047
1.8	3.26	0.7091
2.0	+1.46	0.6871
2.2	-0.100	0.6497
2.4	-1.390	0.6046
2.6	-2.426	0.5568
2.8	-3.238	0.5093
3.0	-3.854	0.4638
3.2	-4.306	0.4211
3.4	-4.616	0.3814
3.6	-4.804	0.3447
3.8	-4.894	0.3109
4.0	-4.899	0.2798
4.5	-4.643	0.2130
5.0	-4.137	0.1597
5.5	-3.528	0.1182
6.0	-2.911	0.0863
6.5	-2.338	0.0624
7.0	-1.836	0.0447
7.5	-1.420	0.0317
8.0	-1.080	0.0224
8.5	-0.816	0.0156
9.0	-0.605	0.0109
9.5	-0.451	0.0075
10.0	-0.332	0.0052
$\langle r^{-3} \rangle_{4p}$	10.244	-----
γ_∞	-118.7	-----
J	+281.5	-----

TABLE IV. Wave functions $v_1'(3p \rightarrow p)$ and $v_1'(3d \rightarrow d)$ for Rb^+ .

The unperturbed wave functions $u_0'(3p)$ and $u_0'(3d)$ of Watson and Freeman⁶ are also listed.

r	$v_1'(3p \rightarrow p)$	$v_1'(3d \rightarrow d)$	$u_0'(3p)$	$u_0'(3d)$
0.01	+ 3.28	+0.0247	+0.0470	+0.0008
0.02	6.27	0.1015	0.1561	0.0057
0.03	8.29	0.2218	0.2918	0.0171
0.04	9.33	0.3746	0.4302	0.0361
0.05	9.43	0.5552	0.5565	0.0632
0.06	8.74	0.7534	0.6616	0.0980
0.07	7.41	0.9596	0.7410	0.1397
0.08	5.62	1.1683	0.7929	0.1876
0.09	3.49	1.3728	0.8174	0.2406
0.10	+ 1.17	1.568	0.8161	0.2976
0.12	- 3.80	1.923	0.7456	0.4199
0.14	- 8.50	2.207	0.6033	0.5472
0.16	-12.56	2.416	0.4121	0.6735
0.18	-15.74	2.547	+0.1923	0.7942
0.20	-18.00	2.604	-0.0393	0.9062
0.22	-19.37	2.597	-0.2695	1.0073
0.24	-19.99	2.534	-0.4890	1.0964
0.26	-19.92	2.422	-0.6911	1.1728
0.28	-19.29	2.271	-0.8718	1.2365
0.30	-18.20	2.091	-1.0289	1.2880
0.35	-14.11	1.555	-1.3169	1.3677
0.40	- 9.23	0.976	-1.4686	1.3881
0.45	- 4.46	+0.418	-1.5127	1.3639
0.50	- 0.28	-0.082	-1.4798	1.3084
0.55	+ 3.09	-0.508	-1.3968	1.2325
0.60	5.63	-0.852	-1.2843	1.1448
0.7	8.46	-1.335	-1.0272	0.9573
0.8	9.22	-1.563	-0.7807	0.7773
0.9	8.70	-1.612	-0.5731	0.6185

TABLE IV (cont'd).

r	$v_1'(3p \rightarrow p)$	$v_1'(3d \rightarrow d)$	$u_0'(3p)$	$u_0'(3d)$
1.0	7.54	-1.545	-0.4104	0.4850
1.1	6.19	-1.413	-0.2887	0.3763
1.2	4.92	-1.253	-0.2007	0.2897
1.4	2.97	-0.912	-0.0954	0.1691
1.6	1.67	-0.631	-0.0454	0.0977
1.8	0.934	-0.424	-0.0220	0.0565
2.0	0.515	-0.281	-0.0108	0.0328
2.2	0.279	-0.184	-0.0052	0.0191
2.4	0.151	-0.119	-0.0023	0.0112
2.6		-0.076		0.0066
2.8		-0.049		0.0039
3.0		-0.031		0.0023
3.2		-0.020		0.0013
$\langle r^{-3} \rangle_{n\ell}$	228.1	30.61	-----	-----
γ_{∞}	-3.93	-1.231	-----	-----
J	+6006	+89.70	-----	-----

TABLE V. Wave function $v_1'(4p \rightarrow p)$ for Rb^+ .

r	$v_1'(4p \rightarrow p)$	$u_0'(4p)$	r	$v_1'(4p \rightarrow p)$	$u_0'(4p)$
0.01	+0.97	+0.01404	1.2	6.84	0.7895
0.02	1.83	0.04668	1.4	3.57	0.8459
0.03	2.40	0.08719	1.6	+0.67	0.8285
0.04	2.66	0.12843	1.8	-1.61	0.7684
0.05	2.65	0.1659	2.0	-3.23	0.6878
0.06	2.40	0.1967	2.2	-4.26	0.6008
0.07	1.96	0.2196	2.4	-4.83	0.5157
0.08	1.38	0.2340	2.6	-5.04	0.4370
0.09	+0.70	0.2400	2.8	-4.99	0.3665
0.10	-0.03	0.2379	3.0	-4.76	0.3047
0.12	-1.54	0.2130	3.2	-4.42	0.2515
0.14	-2.93	0.1662	3.4	-4.02	0.2061
0.16	-4.10	0.1049	3.6	-3.60	0.1679
0.18	-4.96	+0.0356	3.8	-3.17	0.1360
0.20	-5.50	-0.0361	4.0	-2.76	0.1095
0.22	-5.73	-0.1062	4.5	-1.83	0.06235
0.24	-5.70	-0.1713	5.0	-1.15	0.03459
0.26	-5.43	-0.2293	5.5	-0.700	0.01882
0.28	-4.95	-0.2790	6.0	-0.415	0.01011
0.30	-4.31	-0.3195	6.5	-0.241	0.00540
0.35	-2.20	-0.3801	7.0	-0.138	0.00288
0.40	+0.22	-0.3874	7.5	-0.078	0.00154
0.45	2.61	-0.3519	8.0	-0.047	0.00083
0.50	4.76	-0.2849	8.5	-0.027	0.00045
0.55	6.55	-0.1970	9.0	-0.016	0.00024
0.60	7.93	-0.0968			
0.7	9.78	+0.1150	$\langle r^{-3} \rangle_{4p}$	20.21	-----
0.8	10.49	0.3151	γ_∞	-42.0	-----
0.9	10.34	0.4861	J	+516	-----
1.0	9.54	0.6217			
1.1	8.30	0.7218			

TABLE VI. Wave functions $v_1'(4p \rightarrow p)$ and $v_1'(5p \rightarrow p)$ for Pr^{3+} .

r	$v_1'(4p \rightarrow p)$	$v_1'(5p \rightarrow p)$	r	$v_1'(4p \rightarrow p)$	$v_1'(5p \rightarrow p)$
0.01	+ 6.15	+1.86	1.2	-11.65	-16.65
0.02	10.32	2.80	1.4	- 7.96	-11.15
0.03	10.30	2.62	1.6	- 4.89	- 4.88
0.04	7.78	1.61	1.8	- 2.81	+ 0.42
0.05	+ 3.63	+0.11	2.0	- 1.542	4.39
0.06	- 1.30	-1.56	2.2	- 0.823	7.03
0.07	- 6.31	-3.25	2.4	- 0.431	8.49
0.08	-10.92	-4.60	2.6	- 0.223	9.09
0.09	-14.81	-5.63	2.8	- 0.114	9.03
0.10	-17.81	-6.31	3.0	- 0.058	8.58
0.12	-20.85	-6.58	3.2	- 0.030	7.83
0.14	-20.42	-5.69	3.4	- 0.015	7.00
0.16	-17.23	-4.17	3.6		6.12
0.18	-12.11	-2.20	3.8		5.27
0.20	- 5.83	+0.03	4.0		4.49
0.22	+0.92	2.29	4.5		2.743
0.24	7.52	4.47	5.0		1.585
0.26	13.61	6.34	5.5		0.880
0.28	18.91	7.82	6.0		0.471
0.30	23.29	8.90	6.5		0.244
0.35	30.12	10.89	7.0		0.122
0.40	31.31	10.70	7.5		0.061
0.45	28.39	8.60	8.0		0.031
0.50	22.95	5.18	<hr/>		
0.55	16.36	+1.26	$\langle r^{-3} \rangle_{nl}$	285.6	40.10
0.60	+ 9.66	-2.71	γ_{∞}	-8.81	-69.7
0.7	- 1.73	-10.27	<hr/>		
0.8	- 9.12	-15.65			
0.9	-12.82	-18.58			
1.0	-13.84	-19.38			
1.1	-13.18	-18.59			

TABLE VII. Wave functions $v_1'(4p \rightarrow p)$ and $v_1'(5p \rightarrow p)$ for Tm^{3+} .

r	$v_1'(4p \rightarrow p)$	$v_1'(5p \rightarrow p)$	r	$v_1'(4p \rightarrow p)$	$v_1'(5p \rightarrow p)$
0.01	+8.53	+ 4.36	1.4	-4.65	- 3.20
0.02	15.16	6.30	1.6	-2.278	+ 3.63
0.03	13.76	6.14	1.8	-1.065	8.18
0.04	8.30	4.36	2.0	-0.482	10.74
0.05	+0.66	+ 1.61	2.2	-0.215	11.78
0.06	-7.55	- 1.53	2.4	-0.095	11.78
0.07	-15.05	- 4.52	2.6	-0.042	11.09
0.08	-21.11	- 7.12	2.8	-0.018	10.01
0.09	-25.31	- 9.10	3.0		8.76
0.10	-27.48	-10.34	3.2		7.49
0.12	-26.32	-10.65	3.4		6.27
0.14	-19.76	- 8.67	3.6		5.16
0.16	-9.97	- 5.06	3.8		4.19
0.18	+1.06	- 0.73	4.0		3.36
0.20	11.86	+ 3.71	4.5		1.85
0.22	21.39	7.77	5.0		0.97
0.24	29.10	11.14	5.5		0.493
0.26	34.72	13.67	6.0		0.250
0.28	38.29	15.35	6.5		0.125
0.30	40.05	16.20	7.0		0.063
0.35	38.51	15.33			
0.40	30.74	10.98			
0.45	20.33	+ 4.67			
0.50	9.83	- 2.24			
0.55	+0.69	- 8.85			
0.60	-6.52	-14.62			
0.7	-15.33	-22.47			
0.8	-17.99	-25.31			
0.9	-17.05	-24.27			
1.0	-14.56	-21.04			
1.1	-11.61	-16.72			
1.2	-8.84	-11.99			
			$\langle r^{-3} \rangle_{nl}$	518.2	61.87
			γ_{∞}	-6.79	-67.2

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