Experimental and theoretical study of core-excited 3pnd Rydberg series of Mg

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Experimental and theoretical study of core-excited $3pnd$ Rydberg series of Mg

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The energies and widths of $(3p_{j_c}nd_j)_3$, $(3p_{j_c}nf_j)_2$ and $(3p_{j_c}nf_j)_4$ core-excited Rydberg states calculated with the present theoretical approach are compared to available experimental data [1, 2] in Tables I, II, III, and IV below.

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	Term value / cm^{-1}			Quantum defect		
	E_{exp} [2]	E_{th}	ΔE	δ_{exp} [2]	δ_{th}	$\Delta\delta$
$3p_{3/2}9d_{3/2}$	95616.9	95621.9	-5.0	1.224	1.214	0.011
$9d_{5/2}$	95737.0	95738.2	-1.2	0.954	0.951	0.003
$10d_{3/2}$	96005.1	96007.4	-2.3	1.230	1.223	0.007
$10d_{5/2}$	96082.5	96084.3	-1.8	0.982	0.976	0.006
$11d_{3/2}$	96279.6	96281.6	-2.0	1.241	1.233	0.008
$11d_{5/2}$	96329.7	96332.7	-3.0	1.022	1.009	0.013
$12d_{3/2}$	96481.0	96483.2	-2.2	1.257	1.245	0.012
$12d_{5/2}$	96514.3	96516.3	-2.0	1.064	1.053	0.011
$13d_{3/2}$	96634.1	96634.9	-0.8	1.272	1.266	0.005
$13d_{5/2}$	96654.6	96655.4	-0.8	1.118	1.113	0.005
$14d_{3/2}$	96749.9	96749.5	0.4	1.315	1.320	-0.004
$14d_{5/2}$	96789.6	96792.4	-2.8	0.929	0.901	0.028
$15d_{3/2}$	96853.5	96854.2	-0.7	1.226	1.219	0.008
$15d_{5/2}$	96873.7	96874.2	-0.5	0.979	0.973	0.006
$16d_{3/2}$	96938.8	96940.3	-1.5	1.082	1.062	0.021
$16d_{5/2}$	96961.1	96958.5	2.6	0.733	0.776	-0.043
$17d_{3/2}$	96985.1	96986.4	-1.3	1.328	1.307	0.022
$17d_{5/2}$	97006.9	97008.1	-1.2	0.932	0.910	0.021
$18d_{3/2}$	97049.7	97051.2	-1.5	1.056	1.024	0.032
$18d_{5/2}$	97063.0	97063.7	-0.7	0.753	0.738	0.015
$19d_{3/2}$	97086.1	97086.6	-0.5	1.19	1.18	0.01
$19d_{5/2}$	97095.8	97096.3	-0.5	0.93	0.92	0.01
$20d_{3/2}$	97124.7	97125.5	-0.8	1.10	1.08	0.02
$20d_{5/2}$	97132.5	97133.3	-0.8	0.86	0.83	0.02
$21d_{3/2}$	97156.9	97157.2	-0.3	1.02	1.02	0.01
$21d_{5/2}$	97164.3	97163.9	0.4	0.75	0.77	-0.02
$22d_{3/2}$	97174.9	97174.2	0.7	1.34	1.37	-0.03
$22d_{5/2}$	97183.4	97183.2	0.2	0.99	1.00	-0.01
$23d_{3/2}$	97198.1	97197.4	0.7	1.34	1.37	-0.04
$23d_{5/2}$	97204.5	97205.0	-0.5	1.03	1.01	0.02
$24d_{3/2}$	97222.5	97223.2	-0.7	1.11	1.08	0.03
$24d_{5/2}$	97226.9	97226.8	0.1	0.86	0.87	-0.01
$25d_{3/2}$	97242.1	97241.9	0.2	0.96	0.98	-0.02
$25d_{5/2}$	97245.9	97245.1	0.8	0.71	0.77	-0.06
$26d_{3/2}$	97253.9	97254.4	-0.5	1.17	1.15	0.03
$26d_{5/2}$	97256.1	97257.1	-1.0	1.02	0.95	0.07
$27d_{3/2}$	97269.6	97269.8	-0.2	1.00	0.99	0.01
$27d_{5/2}$	97271.8	97271.8	0.0	0.82	0.83	-0.01
$28d_{3/2}$	97280.1	97280.1	-0.0	1.12	1.12	-0.01
$28d_{5/2}$	97283.8	97283.6	0.2	0.78	0.81	-0.03
$29d_{3/2}$	97291.4	97291.8	-0.4	1.06	1.03	0.03
$29d_{5/2}$	97294.6	97294.5	0.1	0.73	0.75	-0.02

TABLE I. Comparison of the term values and quantum defects of $(3p_{3/2}nd_{3/2,5/2})_3$ resonances measured by Dai *et al.* [1] with the results of the present calculations. The quoted uncertainty of the experimental term values is 0.4 cm^{-1}.

	Term value / cm^{-1}			Quantum defect		
	$E_{\rm exp}$ [2]	$E_{\rm th}$	ΔE	$\delta_{\rm exp}$ [2]	$\delta_{\rm th}$	$\Delta\delta$
$3p_{1/2}9d_{5/2}$	95507.6	95508.9	-1.3	1.262	1.259	0.003
$10d_{5/2}$	95913.5	95914.5	-1.0	1.230	1.227	0.003
$11d_{5/2}$	96199.6	96200.0	-0.4	1.192	1.190	0.002
$12d_{5/2}$	96410.8	96409.0	1.8	1.135	1.145	-0.011
$13d_{5/2}$	96569.1	96567.5	1.6	1.072	1.084	-0.012
$14d_{5/2}$	96688.7	96692.0	-3.3	1.023	0.990	0.033
$15d_{5/2}$	96763.5	96764.5	-1.0	1.207	1.196	0.011
$16d_{5/2}$	96834.7	96835.5	-0.8	1.268	1.258	0.011
$17d_{5/2}$	96901.8	96902.6	-0.8	1.181	1.167	0.014
$18d_{5/2}$	96958.3	96958.5	-0.2	1.052	1.047	0.005
$19d_{5/2}$	96993.8	96993.8	0.0	1.21	1.21	-0.00
$20d_{5/2}$	97028.8	97029.1	-0.3	1.23	1.22	0.01
$21d_{5/2}$	97063.8	97063.7	0.1	1.08	1.08	-0.00
$22d_{5/2}$	97087.1	97086.6	0.5	1.18	1.21	-0.02
$23d_{5/2}$	97109.6	97109.6	0.0	1.19	1.19	-0.00
$24d_{5/2}$	97132.9	97133.3	-0.4	1.00	0.98	0.02
$25d_{5/2}$	97145.5	97145.6	-0.1	1.27	1.26	0.01
$26d_{5/2}$	97163.5	97163.9	-0.4	1.09	1.06	0.03
$27d_{5/2}$	97173.8	97174.2	-0.4	1.33	1.31	0.03
$28d_{5/2}$	97189.1	97189.0	0.1	1.06	1.08	-0.01
$29d_{5/2}$	97197.4	97197.4	0.0	1.29	1.30	-0.01

TABLE II. Comparison of the term values and quantum defects of $(3p_{1/2}nd_{5/2})_3$ resonances measured by Dai *et al.* [1] with the results of the present calculations. The quoted uncertainty of the experimental term values is 0.4 cm^{-1}.

	Term value / cm^{-1}			Quantum defect		
	$E_{\rm exp}$ [2]	$E_{\rm th}$	ΔE	$\delta_{\rm exp}$ [2]	$\delta_{\rm th}$	$\Delta\delta$
$3p_{1/2}9f_{5/2}$	95970.29	95970.85	-0.56	0.050	0.048	0.002
$10f_{5/2}$	96232.69	96233.24	-0.55	0.046	0.044	0.002
$11f_{5/2}$	96426.30	96426.81	-0.51	0.043	0.040	0.003
$12f_{5/2}$	96573.76	96573.84	-0.08	0.035	0.035	0.000
$13f_{5/2}$	96688.05	96688.54	-0.49	0.030	0.025	0.005
$14f_{5/2}$	96782.21	96782.47	-0.26	-0.022	-0.025	0.003
$16f_{5/2}$	96908.45	96909.44	-0.99	0.060	0.042	0.018
$17f_{5/2}$	96957.77	96959.23	-1.46	0.064	0.032	0.032
$19f_{5/2}$	97033.35	97034.86	-1.51	0.094	0.048	0.046
$3p_{3/2}9f_{5/2}$	96062.89	96063.45	-0.56	0.047	0.045	0.002
$10f_{5/2}$	96323.42	96323.33	0.09	0.050	0.051	-0.001
$11f_{5/2}$	96515.16	96515.63	-0.47	0.059	0.057	0.002
$12f_{5/2}$	96661.98	96661.45	0.53	0.061	0.066	-0.005
$13f_{5/2}$	96782.16	96782.47	-0.31	0.004	0.002	0.002
$14f_{5/2}$	96868.43	96868.44	-0.01	0.045	0.046	-0.001
$15f_{5/2}$	96940.20	96940.44	-0.24	0.061	0.059	0.002
$16f_{5/2}$	96999.50	96997.54	1.96	0.070	0.107	-0.038
$17f_{5/2}$	97047.97	97049.86	-1.89	0.094	0.054	0.040
$3p_{3/2}9f_{7/2}$	96080.76	96081.81	-1.05	-0.012	-0.015	0.003
$10f_{7/2}$	96337.51	96337.83	-0.32	-0.014	-0.015	0.001
$11f_{7/2}$	96526.94	96527.39	-0.45	-0.012	-0.014	0.002
$12f_{7/2}$	96672.09	96671.98	0.11	-0.018	-0.016	-0.002
$13f_{7/2}$	96783.81	96784.24	-0.43	-0.012	-0.016	0.003
$14f_{7/2}$	96873.18	96873.23	-0.05	-0.014	-0.014	-0.001
$15f_{7/2}$	96944.27	96945.15	-0.88	-0.001	-0.013	0.012
$17f_{7/2}$	97051.01	97052.88	-1.87	0.027	-0.013	0.040

TABLE III. Comparison of the term values and quantum defects of $(3p_{j_c}nd_j)_2$ resonances measured by Lyons *et al.* [2] with the results of the present calculations. The quoted uncertainty of the experimental term values is 0.05 cm^{-1}. The experimental quantum defects were calculated from the experimental term values of [2] and the threshold energies given by NIST [3], and differ slightly from those reported by Lyons *et al.* [2]. Resonances are labeled with jj-coupled configurations, instead of the jk-coupled configurations used in [2].

	Term value / cm^{-1}			Quantum defect			Width / cm^{-1}		
	E_{exp} [2]	E_{th}	ΔE	δ_{exp} [2]	δ_{th}	$\Delta\delta$	Γ_{exp} [2]	Γ_{th}	$\Delta\Gamma$
$3p_{1/2}9f_{7/2}$	95967.83	95969.31	-1.48	0.058	0.054	0.005	6.48(1.30)	7.93	-1.45
$10f_{7/2}$	96231.89	96231.27	0.62	0.050	0.053	-0.003	5.60(1.12)	6.18	-0.58
$11f_{7/2}$	96424.39	96424.74	-0.35	0.054	0.052	0.002	4.90(0.98)	4.88	0.02
$12f_{7/2}$	96571.94	96571.72	0.22	0.050	0.051	-0.002	3.69(0.74)	3.96	-0.27
$13f_{7/2}$	96686.31	96686.10	0.21	0.047	0.049	-0.002	3.43(0.69)	3.37	0.06
$14f_{7/2}$	96778.00	96777.31	0.69	0.031	0.039	-0.009	4.95(0.99)	3.60	1.35
$15f_{7/2}$	96848.72	96848.84	-0.12	0.060	0.058	0.002	1.62(0.50)	1.63	-0.01
$16f_{7/2}$	96907.94	96908.76	-0.82	0.070	0.055	0.015	1.55(0.50)	1.57	-0.02
$17f_{7/2}$	96957.11	96958.32	-1.21	0.078	0.052	0.026	1.38(0.50)	1.44	-0.06
$18f_{7/2}$	96999.49	97000.25	-0.76	0.057	0.038	0.019	3.60(0.72)	1.79	1.81
$19f_{7/2}$	97033.17	97034.56	-1.39	0.099	0.057	0.042	0.73(0.50)	0.88	-0.15
$3p_{3/2}9f_{5/2}$	96065.66	96066.98	-1.32	0.038	0.034	0.004	11.53(2.31)	11.71	-0.18
$10f_{5/2}$	96326.73	96326.84	-0.11	0.035	0.035	0.000	9.25(1.85)	8.54	0.71
$11f_{5/2}$	96518.26	96519.03	-0.77	0.041	0.036	0.004	6.28(1.26)	6.42	-0.14
$12f_{5/2}$	96665.55	96665.12	0.43	0.034	0.038	-0.004	5.26(1.05)	4.96	0.30
$13f_{5/2}$	96778.31	96779.48	-1.17	0.043	0.032	0.011	5.05(1.01)	3.67	1.38
$14f_{5/2}$	96869.47	96869.08	0.39	0.032	0.038	-0.006	3.07(0.61)	3.12	-0.05
$15f_{5/2}$	96941.58	96941.74	-0.16	0.040	0.039	0.001	2.13(0.50)	2.54	-0.41
$16f_{5/2}$	97000.40	97001.51	-1.11	0.053	0.034	0.019	2.64(0.53)	1.97	0.67
$17f_{5/2}$	97049.01	97050.53	-1.52	0.071	0.039	0.032	1.73(0.50)	1.75	-0.02
$18f_{5/2}$	97090.85	97091.94	-1.09	0.063	0.036	0.026	2.15(0.50)	1.42	0.73
$3p_{3/2}9f_{7/2}$	96050.34	96050.79	-0.45	0.088	0.086	0.001	3.63(0.73)	3.95	-0.32
$10f_{7/2}$	96314.82	96314.91	-0.09	0.089	0.089	0.000	2.54(0.51)	2.47	0.07
$11f_{7/2}$	96509.75	96509.98	-0.23	0.091	0.090	0.001	1.19(0.50)	1.58	-0.39
$12f_{7/2}$	96658.25	96658.00	0.25	0.090	0.093	-0.003	0.54(0.50)	0.91	-0.37
$13f_{7/2}$	96771.41	96771.75	-0.34	0.110	0.108	0.003		1.4(-6)	
$14f_{7/2}$	96865.43	96864.99	0.44	0.082	0.088	-0.007	1.48(0.50)	1.09	0.39
$15f_{7/2}$	96938.06	96938.27	-0.21	0.093	0.092	0.002	0.95(0.50)	0.61	0.34
$16f_{7/2}$	96996.76	96997.52	-0.76	0.120	0.108	0.012	0.37(0.50)	2.9(-4)	0.37
$17f_{7/2}$	97046.97	97048.20	-1.23	0.116	0.091	0.025	1.19(0.50)	0.49	0.70
$18f_{7/2}$	97088.30	97089.11	-0.81	0.130	0.111	0.019	0.59(0.50)	4.2(-3)	0.59

TABLE IV. Comparison of the term values, quantum defects and widths of $(3p_{j_c}nd_j)_4$ resonances measured by Lyons *et al.* [2] with the results of the present calculations. The quoted uncertainty of the experimental term values is 0.05 cm^{-1}. The experimental quantum defects were calculated from the term values of [2] and the threshold energies given by NIST [3], and differ slightly from those reported by Lyons *et al.* [2]. The numbers in parenthesis in the column displaying the experimental widths give the quoted experimental uncertainties in cm^{-1}. Those in the column showing the calculated widths represent the power of 10 associated with the value (*e.g.*, $1.4(-6) = 1.4 \times 10^{-6}$). Resonances are labeled with jj-coupled configurations, instead of the jk-coupled configurations used in [2].