

Two-electron binding energies  $E_{\text{val}}$  in a.u. and energy differences  $\Delta$  ( $\text{cm}^{-1}$ ) for low-lying levels of Mg.

Config.	Level	CI		CI+MBPT		Experiment	
		$E_{\text{val}}$	$\Delta$	$E_{\text{val}}$	$\Delta$	$E_{\text{val}}$	$\Delta$
$3s^2$	$^1S_0$	0.819907	—	0.833556	—	0.833518 <sup>1</sup>	—
$3s\ 4s$	$^3S_1$	0.635351	40505	0.645853	41196	0.645809	41197.4
$3s\ 4s$	$^1S_0$	0.624990	42779	0.635283	43516	0.635303	43503.1
$3s\ 3d$	$^1D_2$	0.613603	45278	0.621830	46469	0.622090	46403.1
$3s\ 3p$	$^3P_0^o$	0.724170	21012	0.733896	21879	0.733961	21850.4
$3s\ 3p$	$^3P_1^o$	0.724077	21032	0.733796	21901	0.733869	21870.4
$3s\ 3p$	$^3P_2^o$	0.723889	21073	0.733596	21945	0.733684	21911.1
$3s\ 3p$	$^1P_1^o$	0.662255	34601	0.674226	34975	0.673813	35051.4

<sup>1</sup>Two-electron binding energy of the ground state is determined as a sum of the first two ionization potentials IP (Mg) and IP ( $\text{Mg}^+$ ), where IP (Mg) =  $61669.1\ \text{cm}^{-1}$  and IP ( $\text{Mg}^+$ ) =  $121267.4\ \text{cm}^{-1}$ .

Two-electron binding energies in a.u. and energy differences in  $\text{cm}^{-1}$  for the low-lying levels of Ca.

Config.	Level	CI <sup>1</sup>		CI+MBPT		Experiment	
		$E_{\text{val}}$	$\Delta$	$E_{\text{val}}$	$\Delta$	$E_{\text{val}}$	$\Delta$
$4s^2$	$^1S_0$	0.636590	—	0.661274	—	0.660927 <sup>2</sup>	—
$4s\ 3d$	$^3D_1$	0.528838	23649	0.567744	20527	0.568273	20335.3
$4s\ 3d$	$^3D_2$	0.528868	23642	0.567656	20547	0.568209	20349.2
$4s\ 3d$	$^3D_3$	0.528820	23653	0.567517	20577	0.568110	20371.0
$4s\ 3d$	$^1D_2$	0.528824	23652	0.559734	22285	0.561373	21849.6
$4s\ 5s$	$^3S_1$	0.498205	30372	0.517490	31557	0.517223	31539.5
$4s\ 4p$	$^3P_0^o$	0.574168	13700	0.591521	15309	0.591863	15157.9
$4s\ 4p$	$^3P_1^o$	0.573942	13750	0.591274	15363	0.591625	15210.1
$4s\ 4p$	$^3P_2^o$	0.573486	13850	0.590774	15473	0.591143	15315.9
$4s\ 4p$	$^1P_1^o$	0.530834	23211	0.553498	23654	0.553159	23652.3

<sup>1</sup>Note that on the CI stage the order of  $D$ -states is incorrect. <sup>2</sup>For the ground state  $E_{\text{val}} = \text{IP}(\text{Ca}) + \text{IP}(\text{Ca}^+)$ , where  $\text{IP}(\text{Ca}) = 49304.8\ \text{cm}^{-1}$  and  $\text{IP}(\text{Ca}^+) = 95752.2\ \text{cm}^{-1}$

Two-electron binding energies in a.u. and energy differences in  $\text{cm}^{-1}$  for the low-lying levels of Sr.

Config.	Level	CI		CI+MBPT		Experiment	
		$E_{\text{val}}$	$\Delta$	$E_{\text{val}}$	$\Delta$	$E_{\text{val}}$	$\Delta$
$5s^2$	$^1S_0$	0.586538	—	0.614409	—	0.614601 <sup>1</sup>	—
$5s\ 4d$	$^3D_1$	0.497148	19619	0.532110	18063	0.531862	18159.1
$5s\ 4d$	$^3D_2$	0.497077	19635	0.531809	18129	0.531590	18218.8
$5s\ 4d$	$^3D_3$	0.496941	19664	0.531298	18242	0.531132	18319.3
$5s\ 4d$	$^1D_2$	0.494339	20235	0.522311	20213	0.522792	20149.7
$5s\ 6s$	$^3S_1$	0.460940	27566	0.481533	29162	0.482291	29038.8
$5s\ 5p$	$^3P_0^o$	0.529636	12489	0.548754	14410	0.549366	14317.5
$5s\ 5p$	$^3P_1^o$	0.528850	12662	0.547896	14598	0.548514	14504.4
$5s\ 5p$	$^3P_2^o$	0.527213	13021	0.546079	14997	0.546718	14898.6
$5s\ 5p$	$^1P_1^o$	0.491616	20833	0.515901	21621	0.515736	21698.5

<sup>1</sup>For the ground state  $E_{\text{val}} = \text{IP}(\text{Sr}) + \text{IP}(\text{Sr}^+)$ , where  $\text{IP}(\text{Sr}) = 45925.6 \text{ cm}^{-1}$  and  $\text{IP}(\text{Sr}^+) = 88964.0 \text{ cm}^{-1}$ .

	Mg		Ca		Sr	
	CI	CI+MBPT	CI	CI+MBPT	CI	CI+MBPT
${}^1P_1^o(nsnp) \rightarrow {}^1S_0(ns^2)$						
L-gauge	4.09	4.03	5.20	4.91	5.63	5.28
V-gauge	4.06	4.04	5.11	4.93	5.48	5.32
Final value		4.03(2)		4.91(7)		5.28(9)
Experiment		4.15(10)		4.967(9)		5.57(6)
		4.06(10)		4.99(4)		5.40(8)
		4.12(6)		4.93(11)		
${}^1P_1^o(nsnp) \rightarrow {}^1D_2(nsm d)^8$						
L-gauge	4.43	4.62		1.16	1.75	1.92
V-gauge	4.47	4.59				
Final value		4.62(5)		1.2(3)		1.9(4)
Experiment						1.24(18)
${}^1P_1^o(nsnp) \rightarrow {}^3S_1(ns(n+1)s)$						
L-gauge	0.0088	0.0097	0.035	0.043	0.15	0.19
V-gauge	0.0089	0.0101	0.035	0.045	0.15	0.20
Final value		0.0098(10)		0.043(5)		0.19(2)
${}^3P_1^o(nsnp) \rightarrow {}^1S_0(ns^2)$						
L-gauge	0.0055	0.0064	0.027	0.034	0.12	0.16
V-gauge	0.0062	0.0062	0.030	0.032	0.13	0.17
Final value		0.0064(7)		0.034(4)		0.160(15)
Experiment		0.0053(3)		0.0357(4)		0.1555(16)
		0.0056(4)		0.0352(10)		0.1510(18)
		0.0061(10)		0.0357(16)		0.1486(17)
${}^3P_1^o(nsnp) \rightarrow {}^1D_2(nsm d)^1$						
L-gauge	0.0052	0.0049		0.059	0.33	0.19
V-gauge	0.0050	0.0047		0.061	0.36	0.18
Final value		0.0048(5)		0.059(6)		0.19(2)
${}^3P_2^o(nsnp) \rightarrow {}^1D_2(nsm d)^1$						
L-gauge	0.0039	0.0031		0.028	0.15	0.10
V-gauge	0.0041	0.0032		0.024	0.16	0.06
Final value		0.0035(4)		0.028(3)		0.10(2)

$^1m$  corresponds to the valence  $d$ -shell and equals 3 for Mg and Ca and 4 for Sr.