

Atomic % Calculations when Peaks have Doublet Pairs

See CasaXPS document "Relative Sensitivity Factors for Doublet Pairs"

Element	Atomic #	Doublet Pair	Scofield Sensitivity	Scofield Sum	Kratos Sensitivity Relative to F1s	Kratos Sensitivity Relative to C1s	Peaks to use for Atomic % Calculation
Sc	21	2p 1/2	2.17				
		2p 3/2	4.21	6.38	1.88	6.74	Use Both Peaks
Ti	22	2p 1/2	2.59				
		2p 3/2	5.22	7.81	2.00	7.19	Use Both Peaks
V	23	2p 1/2	3.29				
		2p 3/2	6.37	9.66	2.12	7.61	Use only the 2p 3/2 peak
Cr	24	2p 1/2	3.98				
		2p 3/2	7.69	11.67	2.43	8.73	Use only the 2p 3/2 peak
Mn	25	2p 1/2	4.74				
		2p 3/2	9.17	13.91	2.66	9.56	Use only the 2p 3/2 peak
Fe	26	2p 1/2	5.60				
		2p 3/2	10.80	16.40	2.96	10.65	Use only the 2p 3/2 peak
Co	27	2p 1/2	6.54				
		2p 3/2	12.60	19.14	3.59	12.91	Use only the 2p 3/2 peak
Ni	28	2p 1/2	7.57				
		2p 3/2	14.60	22.17	4.04	14.55	Use only the 2p 3/2 peak
Cu	29	2p 1/2	8.70				
		2p 3/2	16.70	25.40	5.32	19.14	Use only the 2p 3/2 peak
Zn	30	2p 1/2	9.80				
		2p 3/2	18.90	28.70	5.59	20.10	Use only the 2p 3/2 peak
Ga	31	2p 1/2	11.10				
		2p 3/2	21.40	32.50	5.58	20.08	Use only the 2p 3/2 peak
Rb	37	3d 3/2	1.72				
		3d 5/2	2.49	4.21	1.54	5.55	Use Both Peaks
Sr	38	3d 3/2	2.06				
		3d 5/2	2.99	5.05	1.84	6.62	Use Both Peaks
Y	39	3d 3/2	2.44				
		3d 5/2	3.54	5.98	2.18	7.82	Use Both Peaks
Zr	40	3d 3/2	2.87				
		3d 5/2	4.17	7.04	2.58	9.27	Use Both Peaks
Nb	41	3d 3/2	3.35				
		3d 5/2	4.86	8.21	2.92	10.51	Use Both Peaks
Mo	42	3d 3/2	3.88				
		3d 5/2	5.62	9.50	3.32	11.95	Use Both Peaks
Ru	44	3d 3/2	5.10				
		3d 5/2	7.39	12.49	4.27	15.37	Use Both Peaks
Rh	45	3d 3/2	5.80				
		3d 5/2	8.39	14.19	4.82	17.35	Use Both Peaks
Pd	46	3d 3/2	6.56				
		3d 5/2	9.48	16.04	5.36	19.28	Use Both Peaks
Ag	47	3d 3/2	7.38				
		3d 5/2	10.70	18.08	5.99	21.54	Use Both Peaks
Cd	48	3d 3/2	8.27				
		3d 5/2	12.00	20.27	6.62	23.82	Use Both Peaks
In	49	3d 3/2	9.22				
		3d 5/2	13.30	22.52	7.27	26.13	Use Both Peaks
Sn	50	3d 3/2	10.30				
		3d 5/2	14.80	25.10	7.88	28.33	Use Both Peaks
Sb	51	3d 3/2	11.40				
		3d 5/2	16.40	27.80	8.63	31.03	Use Both Peaks
Te	52	3d 3/2	12.50				
		3d 5/2	18.10	30.60	9.51	34.20	Use Both Peaks
I	53	3d 3/2	13.80				
		3d 5/2	19.90	33.70	10.34	37.21	Use Both Peaks

Element	Atomic #	Doublet Pair	Scofield Sensitivity	Scofield Sum	Kratos Sensitivity Relative to F1s	Kratos Sensitivity Relative to C1s	Peaks to use for Atomic % Calculation
Xe	54	3d 3/2	15.10				
		3d 5/2	21.80	36.90	11.07	39.81	Use Both Peaks
Cs	55	3d 3/2	16.50				
		3d 5/2	23.80	40.30	11.74	42.21	Use Both Peaks
Ba	56	3d 3/2	17.90				
		3d 5/2	25.80	43.70	12.45	44.78	Use Both Peaks
La	57	3d 3/2	19.50				
		3d 5/2	28.10	47.60	9.12	32.81	Use only the 3d 5/2 peak
Ce	58	3d 3/2	21.10				
		3d 5/2	30.50	51.60	8.81	31.68	Use only the 3d 5/2 peak
Pr	59	3d 3/2	22.70				
		3d 5/2	32.90	55.60	7.63	27.44	Use only the 3d 5/2 peak
Nd	60	3d 3/2	24.30				
		3d 5/2	35.30	59.60	5.67	20.40	Use only the 3d 5/2 peak
Sm	62	3d 3/2	28.00				
		3d 5/2	40.40	68.40	6.02	21.65	Use only the 3d 5/2 peak
Eu	63	3d 3/2	29.90				
		3d 5/2	43.20	73.10	2.47	8.87	Use only the 3d 5/2 peak
Gd	64	4d 3/2	4.26				
		4d 5/2	6.14	10.40	2.48	8.94	Use Both Peaks
Tb	65	4d 3/2	4.46				
		4d 5/2	6.41	10.87	2.48	8.91	Use Both Peaks
Dy	66	4d 3/2	4.69				
		4d 5/2	6.74	11.43	2.47	8.90	Use Both Peaks
Ho	67	4d 3/2	4.92				
		4d 5/2	7.08	12.00	2.47	8.88	Use only the 4d 5/2 peak
Er	68	4d 3/2	5.15				
		4d 5/2	7.41	12.56	2.46	8.86	Use only the 4d 5/2 peak
Yb	70	4d 3/2	5.61				
		4d 5/2	8.07	13.68	2.45	8.82	Use only the 4d 5/2 peak
Lu	71	4d 3/2	5.87				
		4d 5/2	8.45	14.32	2.44	8.78	Use only the 4d 5/2 peak
Hf	72	4f 5/2	3.32				
		4f 7/2	4.20	7.52	2.64	9.49	Use Both Peaks
Ta	73	4f 5/2	3.80				
		4f 7/2	4.82	8.62	3.08	11.09	Use Both Peaks
W	74	4f 5/2	4.32				
		4f 7/2	5.48	9.80	3.52	12.67	Use Both Peaks
Re	75	4f 5/2	4.88				
		4f 7/2	6.20	11.08	3.96	14.25	Use Both Peaks
Os	76	4f 5/2	5.48				
		4f 7/2	6.96	12.44	4.46	16.05	Use Both Peaks
Ir	77	4f 5/2	6.12				
		4f 7/2	7.78	13.90	5.02	18.06	Use Both Peaks
Pt	78	4f 5/2	6.80				
		4f 7/2	8.65	15.45	5.58	20.05	Use Both Peaks
Au	79	4f 5/2	7.54				
		4f 7/2	9.58	17.12	6.25	22.48	Use Both Peaks
Hg	80	4f 5/2	8.32				
		4f 7/2	10.60	18.92	6.92	24.87	Use Both Peaks
Tl	81	4f 5/2	9.14				
		4f 7/2	11.60	20.74	8.39	30.19	Use Both Peaks
Pb	82	4f 5/2	10.00				
		4f 7/2	12.70	22.70	8.33	29.96	Use Both Peaks
Bi	83	4f 5/2	10.90				
		4f 7/2	13.90	24.80	9.14	32.88	Use Both Peaks
Th	90	4f 5/2	18.80				
		4f 7/2	23.90	42.70	12.73	45.77	Use Both Peaks