

Element, Wavelength and Order	Use?	# IECs	IEC	k1	k2	Calc-in-fit?
As 189.042 {479}	☒	1	Fe	-0.000064	0.000000	No
Ti 190.856 {477}	☒	5	Mo	-0.002450	0.000000	No
			Co	0.002248	0.000000	No
			Ti	-0.000500	0.000000	No
			Mn	0.000370	0.000000	No
			V	-0.012340	0.000000	No
Pb 220.353 {453}	☒	6	Mo	-0.001480	0.000000	No
			Al	-0.000075	0.000000	No
			Cu	0.001400	0.000000	No
			Fe	0.000030	0.000000	No
			Mn	0.000340	0.000000	No
			Ni	0.000630	0.000000	No
Se 196.090 {472}	☒	3	Fe	-0.000308	0.000000	No
			Mn	0.000470	0.000000	No
			Co	-0.000630	0.000000	No
Sb 206.833 {463}	☒	4	Cr	0.010700	0.000000	No
			V	-0.001168	0.000000	No
			Mo	-0.002850	0.000000	No
			Ni	-0.000440	0.000000	No
Al 396.152 { 85}	☒	1	Mo	0.037230	0.000000	No
Ba 493.409 { 68}	☐	None				
Be 234.861 {144}	☒	3	Mo	-0.000320	0.000000	No
			Fe	0.000010	0.000000	No
			Mn	-0.000047	0.000000	No
Cd 214.438 {457}	☒	1	Fe	0.000040	0.000000	No
Ca 373.690 { 90}	☐	None				
Cr 267.716 {126}	☒	1	Mn	0.000160	0.000000	No
Co 228.616 {448}	☒	2	Ti	0.001840	0.000000	No
			Mo	-0.001230	0.000000	No
Cu 324.754 {104}	☒	4	Co	-0.000796	0.000000	No
			Fe	-0.000100	0.000000	No
			Mn	0.000345	0.000000	No
			Ni	0.000895	0.000000	No
Fe 259.837 {130}	☐	None				
Mn 257.610 {131}	☒	1	Ni	0.000897	0.000000	No
Mg 279.079 {121}	☐	None				
Ni 231.604 {446}	☐	None				
Ag 328.068 {103}	☒	3	Fe	-0.000100	0.000000	No
			Mn	0.000146	0.000000	No
			V	-0.000889	0.000000	No
Na 818.326 { 41}	☐	None				
V 292.402 {115}	☒	2	Mo	-0.008480	0.000000	No
			Cr	-0.002220	0.000000	No
Zn 206.200 {464}	☐	None				
Zn 213.856 {158}	☒	1	Ni	0.007280	0.000000	No
K 769.896 { 44}	☐	None				
P 177.495 {490}	☒	2	Ni	0.001640	0.000000	No
			Cu	-0.012530	0.000000	No
B 249.678 {135}	☒	3	Co	0.002880	0.000000	No
			V	-0.002000	0.000000	No
			Fe	-0.001360	0.000000	No
Mo 202.030 {467}	☐	None				
S 182.034 {485}	☒	2	Mo	-0.008000	0.000000	No
			Mn	0.002700	0.000000	No

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Si 251.611 {134}	☒	2	Mo	0.010520	0.000000	No
			Ti	0.005650	0.000000	No
Sn 189.989 {478}	☐	None				
Ti 336.121 {100}	☒	1	Ni	-0.001000	0.000000	No
Li 670.784 { 50}	☐	None				
Y 224.306 {450}*	☐	None				
Y 360.073 { 94}*	☐	None				
Y 371.030 { 91}*	☐	None				
Y 224.306 {150}*	☐	None				
In 230.606 {446}*	☐	None				
Sr 407.771 { 83}	☐	None				