

## SFAC table for SHELX Copper Radiation

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H						
SFAC H	0.493002	10.510900	0.322912	26.125700	0.140191	3.142360 =
	0.040810	57.799702	0.003038	0.000000	0.000000	0.62 0.32
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He						
SFAC HE	0.873400	9.103700	0.630900	3.356800	0.311200	22.927601 =
	0.178000	0.982100	0.006400	0.000000	0.000000	1.34 0.93
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Li						
SFAC LI	1.128200	3.954600	0.750800	1.052400	0.617500	85.390503 =
	0.465300	168.261002	0.037700	0.001000	0.000000	2.27 1.23
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Be						
SFAC BE	1.591900	43.642700	1.127800	1.862300	0.539100	103.483002 =
	0.702900	0.542000	0.038500	0.003000	0.001000	3.67 0.90
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B						
SFAC B	2.054500	23.218500	1.332600	1.021000	1.097900	60.349800 =
	0.706800	0.140300	-0.193200	0.008000	0.004000	6.19 0.82
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C						
SFAC C	2.310000	20.843901	1.020000	10.207500	1.588600	0.568700 =
	0.865000	51.651199	0.215600	0.017000	0.009000	10.67 0.77
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N						
SFAC N	12.212600	0.005700	3.132200	9.893300	2.012500	28.997499 =
	1.166300	0.582600	-11.529000	0.029000	0.018000	18.37 0.75
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O						
SFAC O	3.048500	13.277100	2.286800	5.701100	1.546300	0.323900 =
	0.867000	32.908901	0.250800	0.047000	0.032000	30.48 0.73
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F						
SFAC F	3.539200	10.282500	2.641200	4.294400	1.517000	0.261500 =
	1.024300	26.147600	0.277600	0.069000	0.053000	49.99 0.72
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Ne						
SFAC NE	3.955300	8.404200	3.112500	3.426200	1.454600	0.230600 =
	1.125100	21.718399	0.351500	0.097000	0.083000	74.02 0.71
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Na						
SFAC NA	4.762600	3.285000	3.173600	8.842200	1.267400	0.313600 =
	1.112800	129.423996	0.676000	0.129000	0.124000	112.20 1.54
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Mg						
SFAC MG	5.420400	2.827500	2.173500	79.261101	1.226900	0.380800 =
	2.307300	7.193700	0.858400	0.165000	0.177000	160.70 1.36
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Al						
SFAC AL	6.420200	3.038700	1.900200	0.742600	1.593600	31.547199 =
	1.964600	85.088600	1.115100	0.204000	0.246000	225.80 1.18
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Si						
SFAC SI	6.291500	2.438600	3.035300	32.333698	1.989100	0.678500 =
	1.541000	81.693703	1.140700	0.244000	0.330000	304.70 1.11
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P						
SFAC P	6.434500	1.906700	4.179100	27.157000	1.780000	0.526000 =
	1.490800	68.164497	1.114900	0.283000	0.434000	404.80 1.06
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S						
SFAC S	6.905300	1.467900	5.203400	22.215099	1.437900	0.253600 =
	1.586300	56.172001	0.866900	0.319000	0.557000	512.50 1.02

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CL  
SFAC CL 11.460400 0.010400 7.196400 1.166200 6.255600 18.519400 =  
1.645500 47.778400 -9.557400 0.348000 0.702000 685.30 0.99

CL(-1)  
SFAC CL 18.291500 0.006600 7.208400 1.171700 6.533700 19.542400 =  
2.338600 60.448601-16.378000 0.348000 0.702000

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Ar  
SFAC AR 7.484500 0.907200 6.772300 14.840700 0.653900 43.898300 =  
1.644200 33.392899 1.444500 0.366000 0.872000

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K  
SFAC K 8.218600 12.794900 7.439800 0.774800 1.051900213.186996 =  
0.865900 41.684101 1.422800 0.365000 1.066000

K(+1)  
SFAC K 7.957800 12.633100 7.491700 0.767400 6.359000 -0.002000 =  
1.191500 31.912800 -4.997800 0.365000 1.066000

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Ca  
SFAC CA 8.626600 10.442100 7.387300 0.659900 1.589900 85.748398 =  
1.021100178.436996 1.375100 0.341000 1.286000

Ca(+2)  
SFAC CA 15.634800 -0.007400 7.951800 0.608900 8.437200 10.311600 =  
0.853700 25.990499-14.875000 0.341000 1.286000

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Sc  
SFAC SC 9.189000 9.021300 7.367900 0.572900 1.640900136.108002 =  
1.468000 51.353100 1.332900 0.285000 1.533000

Sc(+2)  
SFAC SC 13.400800 0.298540 8.027300 7.962900 1.659430 -0.286040 =  
1.579360 16.066200 -6.666700 0.285000 1.533000

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Ti  
SFAC TI 9.759500 7.850800 7.355800 0.500000 1.699100 35.633801 =  
1.902100116.105003 1.280700 0.189000 1.807000

Ti(+2)  
SFAC TI 9.114230 7.524300 7.621740 0.457585 2.279300 19.536100 =  
0.087899 61.655800 0.897155 0.189000 1.807000

Ti(+3)  
SFAC TI 17.734400 0.220610 8.738160 7.047160 5.256910 -0.157620 =  
1.921340 15.976800-14.652000 0.189000 1.807000

Ti(+4)  
SFAC TI 19.511400 0.178847 8.234730 6.670180 2.013410 -0.292630 =  
1.520800 12.946400-13.280000 0.189000 1.807000

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V  
SFAC V 10.297100 6.865700 7.351100 0.438500 2.070300 26.893801 =  
2.057100102.477997 1.219900 0.035000 2.110000

V(+2)  
SFAC V 10.106000 6.881800 7.354100 0.440900 2.288400 20.300400 =  
0.022300115.122002 1.229800 0.035000 2.110000

V(+3)  
SFAC V 9.431410 6.395350 7.741900 0.383349 2.153430 15.190800 =  
0.016865 63.969002 0.656565 0.035000 2.110000

V(+4)  
SFAC V 15.688700 0.679003 8.142080 5.401350 2.030810 9.972780 =  
-9.576000 0.940464 1.714300 0.035000 2.110000

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Cr  
SFAC CR 10.640600 6.103800 7.353700 0.392000 3.324000 20.262600 =  
1.492200 98.739899 1.183200 -0.198000 2.443000

Cr(+2)  
SFAC CR 9.540340 5.660780 7.750900 0.344261 3.582740 13.307500 =  
0.509107 32.422401 0.616898 -0.198000 2.443000

Cr(+3)  
SFAC CR 9.680900 5.594630 7.811360 0.334393 2.876030 12.828800 =  
0.113575 32.876099 0.518275 -0.198000 2.443000

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Mn  
SFAC MN 11.281900 5.340900 7.357300 0.343200 3.019300 17.867399 =  
2.244100 83.754303 1.089600 -0.568000 2.808000

Mn(+2)  
SFAC MN 10.806100 5.279600 7.362000 0.343500 3.526800 14.343000 =  
0.218400 41.323502 1.087400 -0.568000 2.808000

Mn(+3)  
SFAC MN 9.845210 4.917970 7.871940 0.294393 3.565310 10.817100 =  
0.323613 24.128099 0.393974 -0.568000 2.808000

Mn(+4)  
SFAC MN 9.962530 4.848500 7.970570 0.283303 2.760670 10.485200 =  
0.054447 27.573000 0.251877 -0.568000 2.808000

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Fe  
SFAC FE 11.769500 4.761100 7.357300 0.307200 3.522200 15.353500 =  
2.304500 76.880501 1.036900 -1.179000 3.204000

Fe(+2)  
SFAC FE 11.042400 4.653800 7.374000 0.305300 4.134600 12.054600 =  
0.439900 31.280899 1.009700 -1.179000 3.204000

Fe(+3)  
SFAC FE 11.176400 4.614700 7.386300 0.300500 3.394800 11.672900 =  
0.072400 38.556599 0.970700 -1.179000 3.204000

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Co  
SFAC CO 12.284100 4.279100 7.340900 0.278400 4.003400 13.535900 =  
2.348800 71.169197 1.011800 -2.464000 3.608000

Co(+2)  
SFAC CO 11.229600 4.123100 7.388300 0.272600 4.739300 10.244300 =  
0.710800 25.646601 0.932400 -2.464000 3.608000

Co(+3)  
SFAC CO 10.338000 3.909690 7.881730 0.238668 4.767950 8.355830 =  
0.725591 18.349100 0.286667 -2.464000 3.608000

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Ni  
SFAC NI 12.837600 3.878500 7.292000 0.256500 4.443800 12.176300 =  
2.380000 66.342102 1.034100 -2.956000 0.509000

Ni(+2)  
SFAC NI 11.416600 3.676600 7.400500 0.244900 5.344200 8.873000 =  
0.977300 22.162600 0.861400 -2.956000 0.509000

Ni(+3)  
SFAC NI 10.780600 3.547700 7.758680 0.223140 5.227460 7.644680 =  
0.847114 16.967300 0.386044 -2.956000 0.509000

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Cu						
SFAC CU	13.338000	3.582800	7.167600	0.247000	5.615800	11.396600 =
	1.673500	64.812599	1.191000	-2.019000	0.589000	
Cu(+2)						
SFAC CU	11.947500	3.366900	7.357300	0.227400	6.245500	8.662500 =
	1.557800	25.848700	0.890000	-2.019000	0.589000	
Cu(+3)						
SFAC CU	11.816800	3.374840	7.111810	0.244078	5.781350	7.987600 =
	1.145230	19.896999	1.144310	-2.019000	0.589000	
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Zn						
SFAC ZN	14.074300	3.265500	7.031800	0.233300	5.165200	10.316300 =
	2.410000	58.709702	1.304100	-1.612000	0.678000	
Zn(+2)						
SFAC ZN	11.971900	2.994600	7.386200	0.203100	6.466800	7.082600 =
	1.394000	18.099501	0.780700	-1.612000	0.678000	
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Ga						
SFAC GA	15.235400	3.066900	6.700600	0.241200	4.359100	10.780500 =
	2.962300	61.413502	1.718900	-1.354000	0.777000	
Ga(+3)						
SFAC GA	12.692000	2.812620	6.698830	0.227890	6.066920	6.364410 =
	1.006600	14.412200	1.535450	-1.354000	0.777000	
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Ge						
SFAC GE	16.081600	2.850900	6.374700	0.251600	3.706800	11.446800 =
	3.683000	54.762501	2.131300	-1.163000	0.886000	
Ge(+4)						
SFAC GE	12.917200	2.537180	6.700030	0.205855	6.067910	5.479130 =
	0.859041	11.603000	1.455720	-1.163000	0.886000	
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As						
SFAC AS	16.672300	2.634500	6.070100	0.264700	3.431300	12.947900 =
	4.277900	47.797199	2.531000	-1.011000	1.006000	
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Se						
SFAC SE	17.000601	2.409800	5.819600	0.272600	3.973100	15.237200 =
	4.354300	43.816299	2.840900	-0.879000	1.139000	
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Br						
SFAC BR	17.178900	2.172300	5.235800	16.579599	5.637700	0.260900 =
	3.985100	41.432800	2.955700	-0.767000	1.283000	
Br(-1)						
SFAC BR	17.171801	2.205900	6.333800	19.334499	5.575400	0.287100 =
	3.727200	58.153500	3.177600	-0.767000	1.283000	
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Kr						
SFAC KR	17.355499	1.938400	6.728600	16.562300	5.549300	0.226100 =
	3.537500	39.397202	2.825000	-0.665000	1.439000	
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Rb						
SFAC RB	17.178400	1.788800	9.643500	17.315100	5.139900	0.274800 =
	1.529200	164.934006	3.487300	-0.574000	1.608000	
Rb(+1)						
SFAC RB	17.581600	1.713900	7.659800	14.795700	5.898100	0.160300 =
	2.781700	31.208700	2.078200	-0.574000	1.608000	
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Sr						
SFAC SR	17.566299	1.556400	9.818400	14.098800	5.422000	0.166400 =
	2.669400	132.376007	2.506400	-0.465000	1.820000	
Sr(+2)						
SFAC SR	18.087400	1.490700	8.137300	12.696300	2.565400	24.565100 =
	-34.193001	-0.013800	41.402500	-0.465000	1.820000	

Y  
SFAC Y 17.775999 1.402900 10.294600 12.800600 5.726290 0.125599 =  
3.265880104.353996 1.912130 -0.386000 2.025000

Y(+2)  
SFAC Y 17.926800 1.354170 9.153100 11.214500 1.767950 22.659901 =  
-33.108002 -0.013190 40.260201 -0.386000 2.025000

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Zr  
SFAC ZR 17.876499 1.276180 10.948000 11.916000 5.417320 0.117622 =  
3.657210 87.662697 2.069290 -0.314000 2.245000

Zr(+2)  
SFAC ZR 18.166800 1.214800 10.056200 10.148300 1.011180 21.605400 =  
-2.647900 -0.102760 9.414540 -0.314000 2.245000

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Nb  
SFAC NB 17.614201 1.188650 12.014400 11.766000 4.041830 0.204785 =  
3.533460 69.795700 3.755910 -0.248000 2.482000

Nb(+2)  
SFAC NB 19.881201 0.019175 18.065300 1.133050 11.017700 10.162100 =  
1.947150 28.338900-12.912000 -0.248000 2.482000

Nb(+3)  
SFAC NB 17.916300 1.124460 13.341700 0.028781 10.799000 9.282060 =  
0.337905 25.722799 -6.393400 -0.248000 2.482000

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Mo  
SFAC MO 3.702500 0.277200 17.235600 1.095800 12.887600 11.004000 =  
3.742900 61.658401 4.387500 -0.191000 2.735000

Mo(+2)  
SFAC MO 21.166401 0.014734 18.201700 1.030310 11.742300 9.536590 =  
2.309510 26.630699-14.421000 -0.191000 2.735000

Mo(+3)  
SFAC MO 21.014900 0.014345 18.099199 1.022380 11.463200 8.788090 =  
0.740625 23.345200-14.316000 -0.191000 2.735000

Mo(+4)  
SFAC MO 17.887100 1.036490 11.175000 8.480610 6.578910 0.058881 =  
0.000000 0.000000 0.344941 -0.191000 2.735000

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Tc  
SFAC TC 19.130100 0.864132 11.094800 8.144870 4.649010 21.570700 =  
2.712630 86.847198 5.404280 -0.145000 3.005000

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Ru  
SFAC RU 19.267401 0.808520 12.918200 8.434670 4.863370 24.799700 =  
1.567560 94.292801 5.378740 -0.105000 3.296000

Ru(+2)  
SFAC RU 18.563801 0.847329 13.288500 8.371640 9.326020 0.017662 =  
3.009640 22.886999 -3.189200 -0.105000 3.296000

Ru(+3)  
SFAC RU 18.500299 0.844582 13.178700 8.125340 4.713040 0.364950 =  
2.185350 20.850401 1.423570 -0.105000 3.296000

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Rh  
SFAC RH 19.295700 0.751536 14.350100 8.217580 4.734250 25.874901 =  
1.289180 98.606201 5.328000 -0.077000 3.605000

Rh(+2)  
SFAC RH 18.878500 0.764252 14.125900 7.844380 3.325150 21.248699 =  
-6.198900 -0.010360 11.867800 -0.077000 3.605000

Rh(+3)  
SFAC RH 18.854500 0.760825 13.980600 7.624360 2.534640 19.331699 =  
-5.652600 -0.010200 11.283500 -0.077000 3.605000

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Pd  
SFAC PD 19.331900 0.698655 15.501700 7.989290 5.295370 25.205200 =  
0.605844 76.898598 5.265930 -0.059000 3.934000

Pd(+2)  
SFAC PD 19.170099 0.696219 15.209600 7.555730 4.322340 22.505699 =  
0.000000 0.000000 5.291600 -0.059000 3.934000

Pd(+3)  
SFAC PD 19.249300 0.683839 14.790000 7.148330 2.892890 17.914400 =  
-7.949200 0.005127 13.017400 -0.059000 3.934000

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Ag  
SFAC AG 19.280800 0.644600 16.688499 7.472600 4.804500 24.660500 =  
1.046300 99.815598 5.179000 -0.060000 4.282000

Ag(+1)  
SFAC AG 19.181200 0.646179 15.971900 7.191230 5.274750 21.732599 =  
0.357534 66.114700 5.215720 -0.060000 4.282000

Ag(+2)  
SFAC AG 19.164301 0.645643 16.245600 7.185440 4.370900 21.407200 =  
0.000000 0.000000 5.214040 -0.060000 4.282000

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Cd  
SFAC CD 19.221399 0.594600 17.644400 6.908900 4.461000 24.700800 =  
1.602900 87.482498 5.069400 -0.079000 4.653000

Cd(+2)  
SFAC CD 19.151400 0.597922 17.253500 6.806390 4.471280 20.252100 =  
0.000000 0.000000 5.119370 -0.079000 4.653000

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In  
SFAC IN 19.162399 0.547600 18.559601 6.377600 4.294800 25.849899 =  
2.039600 92.802902 4.939100 -0.126000 5.045000

In(+3)  
SFAC IN 19.104500 0.551522 18.110800 6.324700 3.788970 17.359501 =  
0.000000 0.000000 4.996350 -0.126000 5.045000

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Sn  
SFAC SN 19.188900 5.830300 19.100500 0.503100 4.458500 26.890900 =  
2.466300 83.957100 4.782100 -0.194000 5.459000

Sn(+2)  
SFAC SN 19.109400 0.503600 19.054800 5.837800 4.564800 23.375200 =  
0.487000 62.206100 4.786100 -0.194000 5.459000

Sn(+4)  
SFAC SN 18.933300 5.764000 19.713100 0.465500 3.418200 14.004900 =  
0.019300 -0.758300 3.918200 -0.194000 5.459000

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Sb  
SFAC SB 19.641800 5.303400 19.045500 0.460700 5.037100 27.907400 =  
2.682700 75.282501 4.590900 -0.287000 5.894000

Sb(+2)  
SFAC SB 18.975500 0.467196 18.933001 5.221260 5.107890 19.590200 =  
0.288753 55.511299 4.696260 -0.287000 5.894000

Sb(+4)  
SFAC SB 19.868500 5.448530 19.030199 0.467973 2.412530 14.125900 =  
0.000000 0.000000 4.692630 -0.287000 5.894000

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Te  
SFAC TE 19.964399 4.817420 19.013800 0.420885 6.144870 28.528400 =  
2.523900 70.840302 4.352000 -0.418000 6.352000

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I  
SFAC I 20.147200 4.347000 18.994900 0.381400 7.513800 27.766001 =  
2.273500 66.877602 4.071200 -0.579000 6.835000

I(-1)  
SFAC I 20.233200 4.357900 18.997000 0.381500 7.806900 29.525900 =  
2.886800 84.930397 4.071400 -0.579000 6.835000

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Xe  
SFAC XE 20.293301 3.928200 19.029800 0.344000 8.976700 26.465900 =  
1.990000 64.265800 3.711800 -0.783000 7.348000

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Cs  
SFAC CS 20.389200 3.569000 19.106199 0.310700 10.662000 24.387899 =  
1.495300213.904007 3.335200 -1.022000 7.904000

Cs(+1)  
SFAC CS 20.352400 3.552000 19.127800 0.308600 10.282100 23.712799 =  
0.961500 59.456501 3.279100 -1.022000 7.904000

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Ba  
SFAC BA 20.336100 3.216000 19.297001 0.275600 10.888000 20.207300 =  
2.695900167.201996 2.773100 -1.334000 8.460000

Ba(+2)  
SFAC BA 20.180700 3.213670 19.113600 0.283310 10.905400 20.055799 =  
0.776340 51.745998 3.029020 -1.334000 8.460000

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La  
SFAC LA 20.577999 2.948170 19.599001 0.244475 11.372700 18.772600 =  
3.287190133.123993 2.146780 -1.716000 9.036000

La(+2)  
SFAC LA 20.248899 2.920700 19.376301 0.250698 11.632300 17.821100 =  
0.336048 54.945301 2.408600 -1.716000 9.036000

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Ce  
SFAC CE 21.167101 2.812190 19.769501 0.226836 11.851300 17.608299 =  
3.330490127.112999 1.862640 -2.170000 9.648000

Ce(+2)  
SFAC CE 20.803600 2.776910 19.559000 0.231540 11.936900 16.540800 =  
0.612376 43.169201 2.090130 -2.170000 9.648000

Ce(+3)  
SFAC CE 20.323500 2.659410 19.818600 0.218850 12.123300 15.799200 =  
0.144583 62.235500 1.591800 -2.170000 9.648000

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Pr  
SFAC PR 22.044001 2.773930 19.669701 0.222087 12.385600 16.766899 =  
2.824280143.643997 2.058300 -2.939000 10.535000

Pr(+2)  
SFAC PR 21.372700 2.645200 19.749100 0.214299 12.132900 15.323000 =  
0.975180 36.406502 1.771320 -2.939000 10.535000

Pr(+3)  
SFAC PR 20.941299 2.544670 20.053900 0.202481 12.466800 14.813700 =  
0.296689 45.464298 1.242850 -2.939000 10.535000

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Nd  
SFAC ND 22.684500 2.662480 19.684700 0.210628 12.774000 15.885000 =  
2.851370137.903000 1.984860 -3.431000 10.933000

Nd(+2)  
SFAC ND 21.961000 2.527220 19.933901 0.199237 12.120000 14.178300 =  
1.510310 30.871700 1.475880 -3.431000 10.933000

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Pm  
SFAC PM 23.340500 2.562700 19.609501 0.202088 13.123500 15.100900 =  
2.875160132.720993 2.028760 -4.357000 11.614000

Pm(+2)  
SFAC PM 22.552700 2.417400 20.110800 0.185769 12.067100 13.127500 =  
2.074920 27.449100 1.194990 -4.357000 11.614000

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Sm  
SFAC SM 24.004200 2.472740 19.425800 0.196451 13.439600 14.399600 =  
2.896040128.007004 2.209630 -5.696000 12.320000

Sm(+2)  
SFAC SM 23.150400 2.316410 20.259899 0.174081 11.920200 12.157100 =  
2.714880 24.824200 0.954586 -5.696000 12.320000

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Eu  
SFAC EU 24.627399 2.387900 19.088600 0.194200 13.760300 13.754600 =  
2.922700123.174004 2.574500 -7.718000 11.276000

Eu(+2)  
SFAC EU 24.006300 2.277830 19.950399 0.173530 11.803400 11.609600 =  
3.872430 26.515600 1.363890 -7.718000 11.276000

Eu(+3)  
SFAC EU 23.749701 2.222580 20.374500 0.163940 11.850900 11.311000 =  
3.265030 22.996599 0.759344 -7.718000 11.276000

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Gd  
SFAC GD 25.070900 2.253410 19.079800 0.181951 13.851800 12.933100 =  
3.545450101.398003 2.419600 -9.242000 11.946000

Gd(+2)  
SFAC GD 24.346600 2.135530 20.420799 0.155525 11.870800 10.578200 =  
3.714900 21.702900 0.645089 -9.242000 11.946000

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Tb  
SFAC TB 25.897600 2.242560 18.218500 0.196143 14.316700 12.664800 =  
2.953540115.362000 3.582240 -9.498000 9.242000

Tb(+2)  
SFAC TB 24.955900 2.056010 20.327101 0.149525 12.247100 10.049900 =  
3.773000 21.277300 0.691967 -9.498000 9.242000

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Dy  
SFAC DY 26.507000 2.180200 17.638300 0.202172 14.559600 12.189900 =  
2.965770111.874001 4.297280-10.423000 9.748000

Dy(+2)  
SFAC DY 25.539499 1.980400 20.286100 0.143384 11.981200 9.349720 =  
4.500730 19.580999 0.689690-10.423000 9.748000

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Ho  
SFAC HO 26.904900 2.070510 17.294001 0.197940 14.558300 11.440700 =  
3.638370 92.656601 4.567960-12.255000 3.704000

Ho(+2)  
SFAC HO 26.129601 1.910720 20.099400 0.139358 11.978800 8.800180 =  
4.936760 18.590799 0.852795-12.255000 3.704000

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Er  
SFAC ER 27.656300 2.073560 16.428499 0.223545 14.977900 11.360400 =  
2.982330105.703003 5.920460 -9.733000 3.937000

Er(+2)  
SFAC ER 26.722000 1.846590 19.774799 0.137290 12.150600 8.362250 =  
5.173790 17.897400 1.176130 -9.733000 3.937000

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Tm  
SFAC TM 28.181900 2.028590 15.885100 0.238849 15.154200 10.997500 =  
2.987060102.960999 6.756210 -8.488000 4.181000

Tm(+2)  
SFAC TM 27.308300 1.787110 19.332001 0.136974 12.333900 7.967780 =  
5.383480 17.292200 1.639290 -8.488000 4.181000

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Yb  
SFAC YB 28.664101 1.988900 15.434500 0.257119 15.308700 10.664700 =  
2.989630100.417000 7.566720 -7.701000 4.432000

Yb(+2)  
SFAC YB 28.120899 1.785030 17.681700 0.159970 13.333500 8.183040 =  
5.146570 20.389999 3.709830 -7.701000 4.432000

Yb(+2)  
SFAC YB 27.891701 1.732720 18.761400 0.138790 12.607200 7.644120 =  
5.476470 16.815300 2.260010 -7.701000 4.432000

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Lu  
SFAC LU 28.947599 1.901820 15.220800 9.985190 15.100000 0.261033 =  
3.716010 84.329803 7.976280 -7.133000 4.693000

Lu(+2)  
SFAC LU 28.462799 1.682160 18.121000 0.142292 12.842900 7.337270 =  
5.594150 16.353500 2.975730 -7.133000 4.693000

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Hf  
SFAC HF 29.143999 1.832620 15.172600 9.599900 14.758600 0.275116 =  
4.300130 72.028999 8.581540 -6.715000 4.977000

Hf(+2)  
SFAC HF 28.813101 1.591360 18.460100 0.128903 12.728500 6.762320 =  
5.599270 14.036600 2.396990 -6.715000 4.977000

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Ta  
SFAC TA 29.202400 1.773330 15.229300 9.370460 14.513500 0.295977 =  
4.764920 63.364399 9.243540 -6.351000 5.271000

Ta(+2)  
SFAC TA 29.158701 1.507110 18.840700 0.116741 12.826800 6.315240 =  
5.386950 12.424400 1.785550 -6.351000 5.271000

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W  
SFAC W 29.081800 1.720290 15.430000 9.225900 14.432700 0.321703 =  
5.119820 57.056000 9.887500 -6.048000 5.577000

W(+2)  
SFAC W 29.493601 1.427550 19.376301 0.104621 13.054400 5.936670 =  
5.064120 11.197200 1.010740 -6.048000 5.577000

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Re  
SFAC RE 28.762100 1.671910 15.718900 9.092270 14.556400 0.350500 =  
5.441740 52.086102 10.472000 -5.790000 5.891000

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Os  
SFAC OS 28.189400 1.629030 16.155001 8.979480 14.930500 0.382661 =  
5.675890 48.164700 11.000500 -5.581000 6.221000

Os(+2)  
SFAC OS 30.419001 1.371130 15.263700 6.847060 14.745800 0.165191 =  
5.067950 18.003000 6.498040 -5.581000 6.221000

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Ir						
SFAC IR	27.304899	1.592790	16.729601	8.865530	15.611500	0.417916 =
	5.833770	45.001099	11.472200	-5.391000	6.566000	
Ir(+2)						
SFAC IR	30.415600	1.343230	15.862000	7.109090	13.614500	0.204633 =
	5.820080	20.325399	8.279030	-5.391000	6.566000	
Ir(+3)						
SFAC IR	30.705799	1.309230	15.551200	6.719830	14.232600	0.167252 =
	5.536720	17.491100	6.968240	-5.391000	6.566000	
<hr/>						
Pt						
SFAC PT	27.005899	1.512930	17.763901	8.811740	15.713100	0.424593 =
	5.783700	38.610298	11.688300	-5.233000	6.925000	
Pt(+2)						
SFAC PT	29.842899	1.329270	16.722401	7.389790	13.215300	0.263297 =
	6.352340	22.942600	9.853290	-5.233000	6.925000	
Pt(+3)						
SFAC PT	30.961201	1.248130	15.982900	6.608340	13.734800	0.168640 =
	5.920340	16.939199	7.395340	-5.233000	6.925000	
<hr/>						
Au						
SFAC AU	16.881901	0.461100	18.591299	8.621600	25.558201	1.482600 =
	5.860000	36.395599	12.065800	-5.096000	7.297000	
Au(+1)						
SFAC AU	28.010900	1.353210	17.820400	7.739500	14.335900	0.356752 =
	6.580770	26.404301	11.229900	-5.096000	7.297000	
Au(+3)						
SFAC AU	30.688601	1.219900	16.902901	6.828720	12.780100	0.212867 =
	6.523540	18.659000	9.096800	-5.096000	7.297000	
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Hg						
SFAC HG	20.680901	0.545000	19.041700	8.448400	21.657499	1.572900 =
	5.967600	38.324600	12.608900	-4.990000	7.686000	
Hg(+1)						
SFAC HG	25.085300	1.395070	18.497299	7.651050	16.888300	0.443378 =
	6.482160	28.226200	12.020500	-4.990000	7.686000	
Hg(+2)						
SFAC HG	29.564100	1.211520	18.059999	7.056390	12.837400	0.284738 =
	6.899120	20.748199	10.626800	-4.990000	7.686000	
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Tl						
SFAC TL	27.544600	0.655150	19.158400	8.707510	15.538000	1.963470 =
	5.525930	45.814899	13.174600	-4.883000	8.089000	
Tl(+1)						
SFAC TL	21.398500	1.471100	20.472300	0.517394	18.747801	7.434630 =
	6.828470	28.848200	12.525800	-4.883000	8.089000	
Tl(+2)						
SFAC TL	30.869499	1.100800	18.384100	6.538520	11.932800	0.219074 =
	7.005740	17.211399	9.802700	-4.883000	8.089000	
<hr/>						
Pb						
SFAC PB	31.061701	0.690200	13.063700	2.357600	18.441999	8.618000 =
	5.969600	47.257900	13.411800	-4.818000	8.505000	
Pb(+1)						
SFAC PB	21.788601	1.336600	19.568199	0.488383	19.140600	6.772700 =
	7.011070	23.813200	12.473400	-4.818000	8.505000	
Pb(+2)						
SFAC PB	32.124401	1.005660	18.800301	6.109260	12.017500	0.147041 =
	6.968860	14.714000	8.084280	-4.818000	8.505000	

Bi  
SFAC BI 33.368900 0.704000 12.951000 2.923800 16.587700 8.793700 =  
6.469200 48.009300 13.578200 -4.776000 8.930000

Bi(+1)  
SFAC BI 21.805300 1.235600 19.502600 6.241490 19.105301 0.469999 =  
7.102950 20.318501 12.471100 -4.776000 8.930000

Bi(+2)  
SFAC BI 33.536400 0.916540 25.094601 0.390420 19.249701 5.714140 =  
6.915550 12.828500 -6.799400 -4.776000 8.930000

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Po  
SFAC PO 34.672600 0.700999 15.473300 3.550780 13.113800 9.556420 =  
7.025880 47.004501 13.677000 -4.756000 9.383000

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AT  
SFAC AT 35.316299 0.685870 19.021099 3.974580 9.498870 11.382400 =  
7.425180 45.471500 13.710800 -4.772000 9.843000

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Rn  
SFAC RN 35.563099 0.663100 21.281601 4.069100 8.003700 14.042200 =  
7.443300 44.247299 13.690500 -4.787000 10.317000

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Fr  
SFAC FR 35.929901 0.646453 23.054701 4.176190 12.143900 23.105200 =  
2.112530150.645004 13.724700 -4.833000 10.803000

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Ra  
SFAC RA 35.763000 0.616341 22.906401 3.871350 12.473900 19.988701 =  
3.210970142.324997 13.621100 -4.898000 11.296000

Ra(+1)  
SFAC RA 35.215000 0.604909 21.670000 3.576700 7.913420 12.601000 =  
7.650780 29.843599 13.543100 -4.898000 11.296000

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Ac  
SFAC AC 35.659698 0.589092 23.103201 3.651550 12.597700 18.599001 =  
4.086550117.019997 13.526600 -4.994000 11.799000

Ac(+1)  
SFAC AC 35.173599 0.579689 22.111200 3.414370 8.192160 12.918700 =  
7.055450 25.944300 13.463700 -4.994000 11.799000

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Th  
SFAC TH 35.564499 0.563359 23.421900 3.462040 12.747300 17.830900 =  
4.807030 99.172203 13.431400 -5.091000 12.330000

Th(+2)  
SFAC TH 35.100700 0.555054 22.441799 3.244980 9.785540 13.466100 =  
5.294440 23.953300 13.376000 -5.091000 12.330000

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Pa  
SFAC PA 35.884701 0.547751 23.294800 3.415190 14.189100 16.923500 =  
4.172870105.250999 13.428700 -5.216000 12.868000

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U  
SFAC U 36.022800 0.529300 23.412800 3.325300 14.949100 16.092699 =  
4.188000100.612999 13.396600 -5.359000 13.409000

U(+2)  
SFAC U 35.574699 0.520480 22.525900 3.122930 12.216500 12.714800 =  
5.370730 26.339399 13.309200 -5.359000 13.409000

U(+3)  
SFAC U 35.371498 0.516598 22.532600 3.050530 12.029100 12.572300 =  
4.798400 23.458200 13.267100 -5.359000 13.409000

U(+4)  
SFAC U 34.850899 0.507079 22.758400 2.890300 14.009900 13.176700 =  
1.214570 25.201700 13.166500 -5.359000 13.409000

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Np  
SFAC NP 36.187401 0.511929 23.596399 3.253960 15.640200 15.362200 =  
4.185500 97.490799 13.357300 -5.529000 13.967000

Np(+2)  
SFAC NP 35.707401 0.502322 22.613001 3.038070 12.989800 12.144900 =  
5.432270 25.492800 13.254400 -5.529000 13.967000

Np(+3)  
SFAC NP 35.510300 0.498626 22.578699 2.966270 12.776600 11.948400 =  
4.921590 22.750200 13.211600 -5.529000 13.967000

Np(+4)  
SFAC NP 35.013599 0.489810 22.728600 2.810990 14.388400 12.330000 =  
1.756690 22.658100 13.113000 -5.529000 13.967000

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Pu  
SFAC PU 36.525398 0.499384 23.808300 3.263710 16.770700 14.945500 =  
3.479470105.980003 13.381200 -5.712000 14.536000

Pu(+2)  
SFAC PU 35.840000 0.484938 22.716900 2.961180 13.580700 11.533100 =  
5.660160 24.399200 13.199100 -5.712000 14.536000

Pu(+3)  
SFAC PU 35.649300 0.481422 22.646000 2.890200 13.359500 11.316000 =  
5.188310 21.830099 13.155500 -5.712000 14.536000

Pu(+4)  
SFAC PU 35.173599 0.473204 22.718100 2.738480 14.763500 11.553000 =  
2.286780 20.930300 13.058200 -5.712000 14.536000

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Am  
SFAC AM 36.670601 0.483629 24.099199 3.206470 17.341499 14.313600 =  
3.493310102.273003 13.359200 -5.930000 15.087000

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Cm  
SFAC CM 36.648800 0.465154 24.409599 3.089970 17.399000 13.434600 =  
4.216650 88.483398 13.288700 -6.176000 15.634000

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Bk  
SFAC BK 36.788101 0.451018 24.773600 3.046190 17.891899 12.894600 =  
4.232840 86.002998 13.275400 -6.498000 16.316999

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Cf  
SFAC CF 36.918499 0.437533 25.199499 3.007750 18.331699 12.404400 =  
4.243910 83.788101 13.267400 -6.798000 16.930000