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He³ AND Ne²⁰ CLASSICAL ATOMIC SCATTERING CROSS
SECTIONS FOR $\theta_{\text{Lab}} = 90^\circ$ and 138° USING THE
MOLIERE APPROXIMATION OF THE THOMAS-FERMI
POTENTIAL

MASTER

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Moliere Approximation of the
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ABSTRACT

The Moliere approximation to the Thomas-Fermi screening function has been used in a screened Coulomb potential to calculate tables of differential scattering cross sections for laboratory scattering angles of 90° and 138° . Data are provided for incident ions of $^3\text{He}^+$ and $^{20}\text{Ne}^+$ as a function of energy (0.05 - 5.0 keV) and target atom.

Atomic scattering cross sections are one of the important parameters in determining the relative and absolute sensitivities of low energy ion scattering spectroscopy. Repulsive potential of the screened Coulomb type $\left(V(r) = Z_1 Z_2 \frac{e^2}{r} \phi \left(\frac{r}{a} \right) \right)$ where Z_1 and Z_2 are the atomic numbers of the colliding atoms, e is the electronic charge, r is the distance between the two nuclei and a is the electronic screening length $\left(a = \frac{0.467 \text{\AA}}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \right)$ and $\phi(r/a)$ is the particular form of the screening function) are usually used to describe the interaction between the incoming ion and target atoms. The various forms of the screening function (e.g. Bohr, Moliere, etc.) differ in the strength of the screening as a function of separation between incoming ion and target atom. Bingham (1) has tabulated the atomic scattering parameters for the screened Coulomb potential using the Bohr screening function while Robinson (2) has tabulated them for the Bohr, Sommerfield, and Moliere screening functions. These tables are such that they can be easily applied to a wide variety of pairs of atoms, large energy range, and a range of center of mass scattering angles. However, in low energy ion scattering spectroscopy one is interested in one or two ions scattered from a wide variety of target atoms through a fixed angle in the lab system. In this case the interpolation of the tables can become quite tedious. For routine use, one would like to have a table of differential scattering cross sections as a function of incident ion energy and atomic number, and the target

atomic number, for the laboratory scattering angles of interest. Up until now, the only such table is one which gives the screened Coulomb cross sections based on the Bohr screening function for $\text{He}^{3,4}$ and Ne^{20} at a laboratory scattering angle of 90° (3). Over the past few years the Moliere approximation to the Thomas Fermi screening function has been favored because it gives a better fit to the experimental ion scattering results. The present paper provides the low energy ion scattering spectroscopist with a set of tables of differential scattering cross sections based on the Moliere approximation. The cross sections were calculated using a modified version of a computer program due to Y. S. Chen of Bell Laboratories. Values are reported for every target atomic number, Z , up to 15 and for every fifth target atomic number above 15. Results are given for the incident He^3 and Ne^{20} ions with energies between 500 eV and 5000 eV at laboratory scattering angles of 90° and 138° . Values for other energies or target atomic numbers can easily be obtained by interpolation.

In addition to the table, plots of the differential scattering cross sections as a function of energy, scattering angle, and projectile and target atomic number are provided in Figures 1-3 to graphically illustrate their dependence on these parameters.

Figure 4 shows the Z dependence of the ratio of the Moliere to Bohr values. As can be seen from this figure, the ratio decreases as the atomic number decreases. These data indicate that the Moliere approximation predicts a much

stronger Z dependence of the relative sensitivity than the Bohr screening function. This strong Z dependency more closely follows what is found experimentally. Because of their agreement with experiments, the cross sections listed in these tables can be used in estimating relative sensitivity factors for semiquantitative analysis with low energy ion scattering.

Figure 1. Energy dependence of the differential scattering cross sections for He^3 and Ne^{20} scattered through 90° and 138° from $^{45}\text{Rh}^{102.9}$.

Figure 2. Differential scattering cross sections versus laboratory scattering angle for 2 keV Ne²⁰ scattered from ₄₅Rh^{102.9}.

Figure 3.
Z dependence of
the differential
scattering cross
section for 2 keV
He³ and Ne²⁰ for
laboratory scatter-
ing angles of
90° and 138°

Figure 4. Ratio of the differential scattering cross sections calculated from the Moliere and Bohr screening function as a function of atomic number.

(TABLE I

Differential scattering cross sections
 ($\text{\AA}^2/\text{steradian}$) as a function of energy
 for He^3 and Ne^{20} at $\theta_{\text{Lab}} = 90^\circ$ and 138°

<u>Energy (eV)</u>	<u>He³</u>	
	<u>90°</u>	<u>138°</u>
	<u><u>³Li 6.939</u></u>	
500	.00267	.00065
1000	.000938	.00026
1500	.000483	.00013
2000	.000293	.000083
2500	.000202	.000054
3000	.000147	.000039
3500	.000112	.000029
4000	.0000882	.000023
4500	.0000711	.000019
5000	.0000586	.000015

	<u><u>⁹Be 9.012</u></u>	
500	.00415	.0012
1000	.00153	.00045
1500	.000800	.000241
2000	.000505	.000151
2500	.000350	.000103
3000	.000256	.0000754
3500	.000195	.0000573
4000	.000154	.0000452
4500	.000124	.0000367
5000	.000103	.0000302

Energy (eV)

90°

He³

138°

5B10.811

500	.00552	.0018
1000	.00213	.000690
1500	.00117	.000370
2000	.000730	.000231
2500	.000510	.000159
3000	.000380	.000117
3500	.000293	.0000900
4000	.000233	.0000710
4500	.000189	.0000578
5000	.000157	.0000479

6C12.0112

500	.00700	.0024
1000	.00279	.000930
1500	.00150	.000496
2000	.000990	.000315
2500	.000694	.000220
3000	.000512	.000162
3500	.000393	.000125
4000	.000311	.0000982
4500	.000257	.0000810
5000	.000216	.0000675

7N14.007

500	.00846	.00299
1000	.00342	.00128
1500	.00194	.000645
2000	.00125	.000414
2500	.000876	.000290
3000	.000664	.000210
3500	.000519	.000166
4000	.000416	.000133
4500	.000340	.000109
5000	.000284	.0000904

Energy (eV) 90° He³ 138°

8O 15.999

500	.00979	.00356
1000	.00407	.00143
1500	.00234	.000797
2000	.00153	.000517
2500	.00110	.000364
3000	.000824	.000271
3500	.000639	.000211
4000	.000510	.000169
4500	.000417	.000139
5000	.000353	.000116

9F 18.998

500	.0110	.00418
1000	.00481	.00171
1500	.00271	.000965
2000	.00184	.000627
2500	.00131	.000445
3000	.000974	.000333
3500	.000742	.000260
4000	.000628	.000209
4500	.000520	.000172
5000	.000437	.000144

Energy (eV) 90° He³ 138° 90° Ne²⁰

11Na 22.990

500	.0137	.00528	
1000	.00608	.00222	.0113
1500	.00360	.00128	.00754
2000	.00240	.000848	.00551
2500	.00174	.000603	.00442
3000	.00134	.000458	.00356
3500	.00106	.000360	.00307
4000	.000855	.000290	.00263
4500	.000704	.000240	.00226
5000	.000590	.000202	.00204

<u>Energy (eV)</u>	<u>90°</u>	<u>He³</u>	<u>138°</u>	<u>90°</u>	<u>Ne²⁰</u>
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¹²Mg^{24.32}

500	.0149	.00578		
1000	.00667	.00247	.0139	
1500	.00401	.00143	.00942	
2000	.00266	.000958	.00695	
2500	.00197	.000690	.00558	
3000	.00151	.000519	.00452	
3500	.00119	.000411	.00388	
4000	.000964	.000334	.00334	
4500	.000794	.000276	.00289	
5000	.000683	.000233	.00259	

¹³Al^{26.982}

500	.0161	.00631	.0348	
1000	.00725	.00274	.0182	
1500	.00441	.00160	.0122	
2000	.00297	.00107	.00910	
2500	.00221	.000774	.00721	
3000	.00169	.000590	.00596	
3500	.00133	.000466	.00506	
4000	.00109	.000378	.00431	
4500	.000916	.000314	.00382	
5000	.000760	.000265	.00340	

¹⁴Si^{28.086}

500	.0172	.00679	.0387	
1000	.00781	.00296	.0204	
1500	.00479	.00176	.0137	
2000	.00327	.00119	.0103	
2500	.00243	.000850	.00809	
3000	.00186	.000656	.00673	
3500	.00146	.000521	.00563	
4000	.00122	.000425	.00494	
4500	.00102	.000312	.00434	
5000	.000872	.000297	.00382	

<u>Energy (eV)</u>	<u>90°</u>	<u>He³</u> <u>138°</u>	<u>90°</u>	<u>Ne²⁰</u> <u>138°</u>
<u><u>15P^{30.974}</u></u>				
500	.0184	.00731	.0449	.0110
1000	.00837	.00324	.0239	.0045
1500	.00517	.00192	.0161	.0030
2000	.00358	.00130	.0120	.0023
2500	.00265	.00094	.00953	.0018
3000	.00202	.00072	.00793	.00155
3500	.00163	.000578	.00672	.00133
4000	.00135	.000471	.00573	.00114
4500	.00114	.000391	.00513	.00102
5000	.000964	.000331	.00457	.000857

<u><u>20Ca^{40.08}</u></u>				
500	.0234	.00955	.0642	.016
1000	.0110	.00442	.0352	.010
1500	.00692	.00270	.0239	.0067
2000	.00498	.00186	.0181	.00496
2500	.00368	.00139	.0143	.00397
3000	.00295	.00107	.0121	.00300
3500	.00240	.000860	.0101	.00279
4000	.00198	.000710	.00896	.00243
4500	.00165	.000600	.00791	.00215
5000	.00143	.000510	.00699	.00191

<u><u>25Mn^{54.938}</u></u>				
500	.0281	.0117	.0819	.027
1000	.0136	.00553	.0462	.015
1500	.00868	.00346	.0319	.0107
2000	.00627	.00243	.0243	.00810
2500	.00479	.00182	.0191	.00638
3000	.00383	.00143	.0163	.00539
3500	.00311	.00116	.0137	.00459
4000	.00259	.000965	.0122	.00400
4500	.00224	.000816	.0108	.00353
5000	.00194	.000700	.00955	.00315

<u>Energy (eV)</u>	<u>90°</u>	<u>He³</u>	<u>138°</u>	<u>90°</u>	<u>Ne²⁰</u>	<u>138°</u>
<u><u>30Zn^{65.37}</u></u>						
500	.0322		.0136	.0942		.034
1000	.0158		.00654	.0540		.0198
1500	.0103		.00415	.0374		.0136
2000	.00745		.00295	.0289		.0103
2500	.00579		.00224	.0235		.00833
3000	.00465		.00177	.0194		.00695
3500	.00378		.00145	.0169		.00594
4000	.00323		.00122	.0147		.00518
4500	.00279		.00104	.0129		.00458
5000	.00242		.000889	.0117		.00411

<u><u>35Br^{79.909}</u></u>						
500	.0359		.0153	.105		.042
1000	.0179		.00749	.0607		.0251
1500	.0117		.00479	.0435		.0167
2000	.00857		.00345	.0332		.0127
2500	.00673		.00264	.0272		.00998
3000	.00542		.00211	.0228		.00858
3500	.00446		.00174	.0197		.00734
4000	.00384		.00155	.0170		.00620
4500	.00332		.00124	.0154		.00670
5000	.00288		.00108	.0138		.00510

<u><u>40Zr^{91.22}</u></u>						
500	.0393		.0169	.113		.048
1000	.0197		.00838	.0669		.0275
1500	.0131		.00542	.0485		.0192
2000	.00967		.00393	.0374		.0146
2500	.00761		.00302	.0304		.0118
3000	.00614		.00243	.0258		.00982
3500	.00511		.00201	.0221		.00852
4000	.00441		.00169	.0194		.00755
4500	.00382		.00145	.0174		.00662
5000	.00332		.00126	.0156		.00595

<u>Energy (eV)</u>	<u>He³</u>		<u>Ne²⁰</u>	
	<u>90°</u>	<u>138°</u>	<u>90°</u>	<u>138°</u>
<u><u>45Rh^{102.905}</u></u>				
500	.0423	.0185	.120	.053
1000	.0214	.00922	.0725	.0306
1500	.0143	.00600	.0529	.0215
2000	.0106	.00438	.0412	.0165
2500	.00843	.00339	.0333	.0138
3000	.00684	.00274	.0286	.0112
3500	.00572	.00227	.0244	.00946
4000	.00496	.00192	.0216	.00846
4500	.00429	.00165	.0194	.00751
5000	.00374	.00145	.0173	.00677

<u><u>50Sn^{118.69}</u></u>				
500	.0448	.0199	.126	.058
1000	.0232	.00990	.0779	.0336
1500	.0155	.00656	.0571	.0238
2000	.0116	.00481	.0448	.0183
2500	.00922	.00375	.0360	.0149
3000	.00750	.00303	.0312	.0125
3500	.00631	.00253	.0265	.0109
4000	.00548	.00215	.0238	.00948
4500	.00475	.00186	.0212	.00844
5000	.00415	.00163	.0188	.00759

<u><u>55Cs^{132.905}</u></u>				
500	.0478	.0213	.132	.062
1000	.0249	.0107	.0822	.0363
1500	.0166	.00710	.0607	.0258
2000	.0125	.00522	.0479	.0200
2500	.00997	.00409	.0389	.0163
3000	.00814	.00333	.0335	.0137
3500	.00686	.00278	.0287	.0119
4000	.00598	.00237	.0258	.0104
4500	.00520	.00206	.0229	.00928
5000	.00454	.00181	.0205	.00836

<u>Energy (eV)</u>	<u>He³</u>		<u>Ne²⁰</u>	
	<u>90°</u>	<u>138°</u>	<u>90°</u>	<u>138°</u>
<u><u>60Nd^{144.24}</u></u>				
500	.0506	.0226	.136	.064
1000	.0266	.0114	.0858	.0385
1500	.0177	.00760	.0639	.0276
2000	.0134	.00562	.0507	.0214
2500	.0107	.00440	.0414	.0175
3000	.00876	.00360	.0357	.0148
3500	.00739	.00301	.0307	.0128
4000	.00645	.00258	.0275	.0117
4500	.00562	.00224	.0245	.00989
5000	.00492	.00192	.0220	.00905

<u><u>65Tb^{158.924}</u></u>				
500	.0531	.0239	.141	.067
1000	.0281	.0122	.0891	.0408
1500	.0188	.00810	.0670	.0294
2000	.0143	.00600	.0533	.0229
2500	.0114	.00472	.0437	.0188
3000	.00936	.00386	.0378	.0159
3500	.00789	.00324	.0326	.0137
4000	.00691	.00279	.0293	.0121
4500	.00604	.00243	.0260	.0108
5000	.00529	.00214	.0235	.00973

<u><u>70Yb^{173.04}</u></u>				
500	.0555	.0250	.144	.070
1000	.0296	.0128	.0920	.0428
1500	.0199	.00852	.0697	.0310
2000	.0151	.00636	.0558	.0243
2500	.0120	.00497	.0459	.0199
3000	.00993	.00412	.0397	.0169
3500	.00837	.00347	.0344	.0146
4000	.00735	.00298	.0309	.0129
4500	.00644	.00260	.0274	.0113
5000	.00565	.00230	.0249	.0104

<u>Energy (eV)</u>	<u>He³</u>		<u>Ne²⁰</u>	
	<u>90°</u>	<u>138°</u>	<u>90°</u>	<u>138°</u>
<u><u>75^{Re}186.2</u></u>				
500	.0577	.0260	.148	.071
1000	.0244	.0136	.0941	.0445
1500	.0209	.00903	.0721	.0324
2000	.0159	.00670	.0579	.0254
2500	.0126	.00532	.0474	.0210
3000	.0105	.00436	.0415	.0177
3500	.00882	.00369	.0359	.0154
4000	.00778	.00317	.0324	.0135
4500	.00682	.00277	.0288	.0122
5000	.00704	.00246	.0262	.0110

<u><u>80^{Hg}200.59</u></u>				
500	.0597	.0271	.151	.073
1000	.0324	.0141	.0969	.0463
1500	.0219	.00948	.0745	.0339
2000	.0167	.00706	.0600	.0267
2500	.0132	.00556	.0493	.0221
3000	.0110	.00461	.0433	.0188
3500	.00920	.00400	.0376	.0163
4000	.00819	.00336	.0339	.0144
4500	.00720	.00295	.0302	.0129
5000	.00634	.00261	.0275	.0115

<u><u>85^{At}210</u></u>				
500	.0616	.0281	.153	.077
1000	.0337	.0147	.0994	.0478
1500	.0229	.00981	.0764	.0351
2000	.0174	.00740	.0618	.0278
2500	.0138	.00587	.0511	.0230
3000	.0116	.00485	.0449	.0196
3500	.00966	.00411	.0389	.0170
4000	.00859	.00354	.0352	.0151
4500	.00757	.00310	.0315	.0135
5000	.00668	.00276	.0286	.0122

<u>Energy (eV)</u>	<u>90°</u>	<u>He³</u> <u>138°</u>	<u>90°</u>	<u>Ne²⁰</u> <u>138°</u>
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90Th^{232.038}

500	.0633	.0290	.155	.079
1000	.0349	.0153	.102	.0494
1500	.0238	.0103	.0785	.0365
2000	.0181	.00772	.0637	.0290
2500	.0143	.00614	.0528	.0240
3000	.0121	.00507	.0465	.0205
3500	.0101	.00430	.0404	.0179
4000	.00898	.00372	.0366	.0158
4500	.00792	.00327	.0327	.0142
5000	.00700	.00291	.0298	.0128

95Am^{243.0}

500	.0649	.0299	.156	.080
1000	.0361	.0159	.104	.0508
1500	.0247	.0108	.0801	.0376
2000	.0188	.00800	.0652	.0299
2500	.0149	.00640	.0545	.0249
3000	.0126	.00529	.0480	.0213
3500	.0106	.00500	.0414	.0185
4000	.00935	.00390	.0378	.0164
4500	.00827	.00342	.0339	.0148
5000	.00732	.00304	.0308	.0134

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