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Supporting information for article:

High-accuracy measurement of mass attenuation coefficients and the imaginary component of the atomic form factor of zinc from 8.51 keV to 11.59 keV, and X-ray absorption fine structure with investigation of zinc theory and nanostructure

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High accuracy measurement of mass attenuation coefficients and the imaginary component of the atomic form factor of zinc from 8.51 keV to 11.59 keV, and X-ray absorption fine structure with investigation of zinc theory and nanostructure

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X-ray mass attenuation coefficients; Atomic form factor; XERT; X-ray absorption fine structure; dynamic nanostructure of zinc; Jump ratio; Jump factor

Abstract

High accuracy X-ray mass attenuation coefficients were measured from the first X-ray Extended Range Technique (XERT) -like experiment at the Australian Synchrotron. Experimentally measured mass attenuation coefficients deviate by $\approx 50\%$ from the theoretical values near the zinc absorption edge, suggesting improvements in theoretical tabulations of mass attenuation coefficients are required to bring them into better agreement with experiment. Using these values the imaginary component of

the atomic form factor of zinc was determined for all the measured photon energies. The zinc K-edge jump ratio and jump factor are determined and results raise significant questions regarding the definitions of quantities used and best practice for background subtraction prior to X-ray absorption fine structure (XAFS) analysis. The XAFS analysis shows excellent agreement between the measured and tabulated values and yield bond lengths and nanostructure of zinc with uncertainties of from 0.1% to 0.3% or 0.003Å to 0.008Å. We observed significant variation from reported crystal structure, suggesting local dynamic motion of the standard crystal lattice. XAFS is sensitive to dynamic correlated motion and *in principle* is capable of observing local dynamic motion beyond the reach of conventional crystallography. These results for the zinc absorption coefficient, XAFS and structure are the most accurate structural refinements of zinc at room temperature.

1. Supporting information

Table 1: Table S1. Mass attenuation coefficients $\left[\frac{\mu}{\rho}\right]_{tot}$ and the imaginary component f_2 of the form factor as a function of X-ray energy with one standard deviation. Relative and total percentage uncertainties in the total mass attenuation coefficient $\sigma\left[\frac{\mu}{\rho}\right]_{rel}$, $\sigma\left[\frac{\mu}{\rho}\right]_{tot}$ are presented with the latter also given in absolute units. The percentage uncertainty in $\left[\frac{\mu}{\rho}\right]_{pe}$ includes uncertainty in the measurements and in the calculations of thermal diffuse and Compton scattering attenuation.

Energy (eV)	σ_E (eV)	$\left[\frac{\mu}{\rho}\right]_{tot}$ ($\frac{cm^2}{g}$)	$\sigma\left[\frac{\mu}{\rho}\right]_{tot}$ %	$\sigma\left[\frac{\mu}{\rho}\right]_{rel}$ %	$\left[\frac{\mu}{\rho}\right]_{pe}$ ($\frac{cm^2}{g}$)	$\sigma\left[\frac{\mu}{\rho}\right]_{pe}$ %	f_2 (e/atom)
8508.98	0.165	48.672	0.023	0.0026	46.695	0.060	0.617
8549.04	0.168	48.044	0.023	0.0026	46.076	0.061	0.612
8569.06	0.170	47.623	0.023	0.0014	45.660	0.062	0.608
8589.09	0.171	47.457	0.023	0.0034	45.498	0.062	0.607
8609.12	0.173	47.022	0.023	0.0057	45.068	0.063	0.603
8629.15	0.174	46.803	0.023	0.0014	44.854	0.063	0.601
8669.20	0.177	46.259	0.023	0.0034	44.318	0.064	0.597
8709.25	0.180	45.613	0.023	0.0012	43.681	0.065	0.591
8749.31	0.183	45.015	0.023	0.0032	43.092	0.067	0.586
8789.37	0.186	44.424	0.024	0.0010	42.510	0.068	0.581
8829.42	0.189	43.875	0.023	0.0030	41.969	0.069	0.576
8869.47	0.192	43.306	0.023	0.0009	41.409	0.070	0.571
8909.53	0.195	42.747	0.023	0.0047	40.858	0.071	0.566
8949.58	0.198	42.379	0.023	0.0013	40.498	0.072	0.563
8989.64	0.201	41.638	0.023	0.0040	39.766	0.074	0.555
9029.69	0.204	41.132	0.023	0.0021	39.268	0.075	0.551
9069.75	0.207	40.615	0.023	0.0032	38.759	0.076	0.546
9109.80	0.210	40.182	0.024	0.0013	38.334	0.077	0.543
9149.86	0.212	39.536	0.023	0.0032	37.696	0.078	0.536
9189.91	0.215	39.048	0.024	0.0024	37.216	0.080	0.531

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Energy (eV)	σ_E (eV)	$[\frac{\mu}{\rho}]_{tot}$ ($\frac{cm^2}{g}$)	$\sigma_{[\frac{\mu}{\rho}]_{tot}}$	%	$[\frac{\mu}{\rho}]_{rel}$	%	$[\frac{\mu}{\rho}]_{pe}$ ($\frac{cm^2}{g}$)	$\sigma_{[\frac{\mu}{\rho}]_{pe}}$	%	$f_2(e/atom)$
9229.97	0.218	38.687	0.023	0.0043	36.864	0.080	0.529			
9270.02	0.221	38.104	0.023	0.0015	36.288	0.082	0.523			
9310.08	0.224	37.667	0.023	0.0054	35.859	0.083	0.519			
9350.13	0.227	37.144	0.023	0.0016	35.344	0.084	0.513			
9390.19	0.230	36.676	0.023	0.0029	34.883	0.085	0.509			
9413.22	0.232	36.423	0.024	0.0019	34.635	0.086	0.507			
9419.22	0.232	36.487	0.023	0.0033	34.700	0.086	0.508			
9425.23	0.233	36.425	0.024	0.0013	34.639	0.086	0.507			
9431.24	0.233	36.311	0.023	0.0021	34.527	0.086	0.506			
9437.25	0.234	36.283	0.023	0.0014	34.499	0.086	0.506			
9443.26	0.234	36.131	0.023	0.0032	34.349	0.087	0.504			
9449.27	0.234	36.178	0.023	0.0019	34.397	0.087	0.505			
9455.27	0.235	36.037	0.023	0.0034	34.257	0.087	0.503			
9461.28	0.235	36.038	0.023	0.0009	34.259	0.087	0.504			
9467.29	0.236	35.872	0.023	0.0029	34.094	0.087	0.501			
9473.30	0.236	35.827	0.023	0.0017	34.050	0.088	0.501			
9479.31	0.237	35.779	0.023	0.0045	34.003	0.088	0.501			
9485.32	0.237	35.598	0.023	0.0010	33.823	0.088	0.498			
9491.32	0.238	35.591	0.023	0.0030	33.818	0.088	0.499			
9497.33	0.238	35.504	0.023	0.0018	33.732	0.088	0.498			
9503.34	0.238	35.462	0.023	0.0035	33.691	0.088	0.497			
9509.35	0.239	35.480	0.024	0.0014	33.710	0.088	0.498			
9515.36	0.239	35.358	0.023	0.0036	33.590	0.089	0.497			
9521.36	0.240	35.299	0.023	0.0012	33.531	0.089	0.496			
9527.37	0.240	35.240	0.023	0.0024	33.474	0.089	0.496			
9533.38	0.241	35.184	0.023	0.0013	33.418	0.089	0.495			
9539.39	0.241	35.148	0.023	0.0027	33.384	0.089	0.495			
9545.40	0.242	35.040	0.024	0.0011	33.277	0.089	0.494			
9551.41	0.242	34.991	0.023	0.0051	33.229	0.089	0.493			
9557.41	0.242	35.041	0.023	0.0016	33.281	0.089	0.494			
9563.42	0.243	34.941	0.023	0.0029	33.182	0.090	0.493			
9569.43	0.243	34.973	0.023	0.0012	33.214	0.090	0.494			
9575.44	0.244	34.873	0.023	0.0045	33.116	0.090	0.493			
9581.45	0.244	34.900	0.024	0.0014	33.144	0.090	0.493			
9587.46	0.245	34.819	0.023	0.0038	33.064	0.090	0.493			
9593.46	0.245	34.765	0.023	0.0011	33.011	0.090	0.492			
9599.47	0.245	34.844	0.023	0.0029	33.091	0.090	0.494			
9605.48	0.246	34.881	0.024	0.0011	33.129	0.090	0.494			
9611.49	0.246	34.920	0.023	0.0043	33.169	0.090	0.495			
9617.50	0.247	34.962	0.024	0.0014	33.213	0.090	0.496			
9620.70	0.247	35.031	0.023	0.0031	33.282	0.089	0.497			
9621.20	0.247	35.066	0.023	0.0017	33.317	0.089	0.498			
9621.70	0.247	35.046	0.023	0.0053	33.297	0.089	0.498			
9622.20	0.247	35.078	0.024	0.0020	33.329	0.089	0.498			
9622.70	0.247	35.079	0.023	0.0029	33.331	0.089	0.498			
9623.20	0.247	35.129	0.023	0.0015	33.380	0.089	0.499			
9623.71	0.247	35.121	0.023	0.0029	33.373	0.089	0.499			
9624.21	0.247	35.196	0.024	0.0015	33.448	0.089	0.500			
9624.71	0.247	35.155	0.023	0.0043	33.407	0.089	0.500			
9625.21	0.247	35.194	0.023	0.0012	33.446	0.089	0.500			
9625.71	0.247	35.197	0.023	0.0034	33.449	0.089	0.500			
9626.21	0.247	35.222	0.023	0.0009	33.474	0.089	0.501			
9626.71	0.247	35.238	0.023	0.0028	33.491	0.089	0.501			
9627.21	0.248	35.268	0.024	0.0010	33.520	0.089	0.501			
9627.71	0.248	35.268	0.023	0.0026	33.520	0.089	0.501			
9628.21	0.248	35.314	0.023	0.0012	33.567	0.089	0.502			
9628.71	0.248	35.290	0.023	0.0032	33.542	0.089	0.502			
9629.21	0.248	35.237	0.023	0.0018	33.490	0.089	0.501			
9629.71	0.248	35.294	0.023	0.0035	33.547	0.089	0.502			
9630.21	0.248	35.276	0.023	0.0016	33.529	0.089	0.502			
9630.71	0.248	35.322	0.023	0.0029	33.575	0.089	0.502			
9631.21	0.248	35.344	0.023	0.0012	33.597	0.089	0.503			
9631.71	0.248	35.367	0.023	0.0036	33.621	0.089	0.503			
9632.22	0.248	35.396	0.023	0.0012	33.649	0.089	0.504			
9632.72	0.248	35.420	0.023	0.0022	33.674	0.088	0.504			
9633.22	0.248	35.450	0.023	0.0023	33.703	0.088	0.504			
9633.72	0.248	35.475	0.023	0.0025	33.728	0.088	0.505			
9634.22	0.248	35.488	0.023	0.0021	33.742	0.088	0.505			
9634.72	0.248	35.552	0.023	0.0030	33.805	0.088	0.506			
9635.22	0.248	35.556	0.023	0.0011	33.810	0.088	0.506			
9635.72	0.248	35.636	0.023	0.0027	33.890	0.088	0.507			
9636.22	0.248	35.649	0.023	0.0016	33.903	0.088	0.508			
9636.72	0.248	35.721	0.023	0.0024	33.975	0.088	0.509			
9637.22	0.248	35.700	0.023	0.0013	33.954	0.088	0.508			
9637.72	0.248	35.811	0.023	0.0023	34.066	0.088	0.510			
9638.22	0.248	35.814	0.023	0.0013	34.069	0.088	0.510			

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Energy (eV)	σ_E (eV)	$\left[\frac{\mu}{\rho} \right]_{tot} (\frac{cm^2}{g})$	$\sigma \left[\frac{\mu}{\rho} \right]_{tot}$	%	$\sigma \left[\frac{\mu}{\rho} \right]_{rel}$	%	$\left[\frac{\mu}{\rho} \right]_{pe} (\frac{cm^2}{g})$	$\sigma \left[\frac{\mu}{\rho} \right]_{pe}$	%	$f_2(e/atom)$
9638.72	0.248	35.930	0.023	0.0039	34.185	0.087	0.512			
9639.22	0.248	35.931	0.023	0.0013	34.186	0.087	0.512			
9639.73	0.248	36.062	0.023	0.0026	34.317	0.087	0.514			
9640.23	0.248	36.070	0.023	0.0008	34.325	0.087	0.514			
9640.73	0.249	36.180	0.023	0.0029	34.435	0.087	0.516			
9641.23	0.249	36.198	0.024	0.0020	34.453	0.087	0.516			
9641.73	0.249	36.315	0.023	0.0026	34.570	0.086	0.518			
9642.23	0.249	36.352	0.023	0.0014	34.607	0.086	0.518			
9642.73	0.249	36.478	0.023	0.0046	34.733	0.086	0.520			
9643.23	0.249	36.523	0.023	0.0016	34.778	0.086	0.521			
9643.73	0.249	36.638	0.023	0.0026	34.894	0.086	0.523			
9644.23	0.249	36.713	0.023	0.0011	34.969	0.085	0.524			
9644.73	0.249	36.824	0.023	0.0044	35.079	0.085	0.526			
9645.23	0.249	36.943	0.024	0.0022	35.198	0.085	0.527			
9645.73	0.249	37.052	0.023	0.0049	35.308	0.085	0.529			
9646.24	0.249	37.201	0.023	0.0021	35.457	0.084	0.531			
9646.74	0.249	37.342	0.023	0.0025	35.598	0.084	0.534			
9647.24	0.249	37.501	0.024	0.0015	35.757	0.084	0.536			
9647.74	0.249	37.666	0.023	0.0029	35.922	0.083	0.538			
9648.24	0.249	37.837	0.024	0.0010	36.094	0.083	0.541			
9648.74	0.249	38.018	0.023	0.0029	36.274	0.083	0.544			
9649.24	0.249	38.232	0.023	0.0016	36.488	0.082	0.547			
9649.74	0.249	38.453	0.023	0.0028	36.710	0.082	0.550			
9650.24	0.249	38.634	0.023	0.0011	36.891	0.081	0.553			
9650.74	0.249	39.001	0.023	0.0032	37.258	0.081	0.559			
9651.24	0.249	39.212	0.023	0.0011	37.469	0.080	0.562			
9651.74	0.249	39.651	0.023	0.0026	37.908	0.079	0.568			
9652.24	0.249	39.953	0.023	0.0009	38.210	0.079	0.573			
9652.74	0.249	40.472	0.023	0.0026	38.729	0.078	0.581			
9653.25	0.249	40.918	0.023	0.0010	39.175	0.077	0.588			
9653.75	0.249	41.541	0.023	0.0027	39.798	0.076	0.597			
9654.25	0.250	42.145	0.023	0.0019	40.402	0.075	0.606			
9654.75	0.250	42.987	0.023	0.0040	41.244	0.074	0.619			
9655.25	0.250	43.869	0.023	0.0040	42.127	0.072	0.632			
9655.75	0.250	45.050	0.023	0.0064	43.307	0.070	0.650			
9656.25	0.250	46.363	0.023	0.0096	44.621	0.069	0.669			
9656.75	0.250	48.188	0.023	0.0177	46.446	0.066	0.697			
9657.25	0.250	50.384	0.024	0.0227	48.642	0.064	0.730			
9657.75	0.250	53.726	0.024	0.0271	51.984	0.060	0.780			
9658.25	0.250	58.365	0.024	0.0218	56.623	0.056	0.850			
9658.75	0.250	65.880	0.025	0.0185	64.138	0.052	0.963			
9659.25	0.250	77.756	0.029	0.0137	76.015	0.048	1.141			
9659.75	0.250	97.000	0.032	0.0122	95.258	0.045	1.430			
9660.25	0.250	123.314	0.036	0.0100	121.573	0.043	1.825			
9660.75	0.250	153.021	0.033	0.0098	151.279	0.038	2.271			
9661.26	0.250	179.796	0.030	0.0096	178.055	0.035	2.673			
9661.76	0.250	200.278	0.028	0.0098	198.537	0.031	2.980			
9662.26	0.250	216.916	0.027	0.0099	215.175	0.030	3.230			
9662.76	0.250	231.009	0.027	0.0102	229.268	0.030	3.442			
9663.26	0.250	242.570	0.027	0.0104	240.829	0.030	3.616			
9663.76	0.250	251.328	0.028	0.0108	249.587	0.030	3.747			
9664.26	0.250	257.017	0.028	0.0112	255.276	0.030	3.833			
9664.76	0.250	261.512	0.028	0.0115	259.772	0.030	3.901			
9665.26	0.250	266.378	0.028	0.0119	264.637	0.031	3.974			
9665.76	0.250	273.201	0.029	0.0122	271.461	0.031	4.077			
9666.26	0.250	281.180	0.029	0.0126	279.439	0.031	4.197			
9666.76	0.250	290.040	0.030	0.0129	288.299	0.032	4.330			
9667.26	0.250	298.021	0.030	0.0130	296.281	0.032	4.450			
9667.76	0.251	305.501	0.031	0.0131	303.760	0.032	4.563			
9668.27	0.251	311.899	0.031	0.0131	310.159	0.033	4.659			
9668.76	0.251	317.850	0.032	0.0129	316.110	0.033	4.749			
9669.27	0.251	322.668	0.032	0.0124	320.928	0.033	4.821			
9669.77	0.251	326.292	0.032	0.0120	324.552	0.033	4.876			
9670.27	0.251	327.760	0.032	0.0115	326.021	0.033	4.898			
9670.77	0.251	326.300	0.032	0.0111	324.560	0.033	4.877			
9671.27	0.251	320.434	0.032	0.0108	318.694	0.033	4.789			
9671.77	0.251	312.342	0.031	0.0106	310.602	0.033	4.667			
9672.27	0.251	302.348	0.031	0.0105	300.609	0.032	4.517			
9672.77	0.251	292.177	0.030	0.0104	290.437	0.032	4.365			
9673.27	0.251	283.354	0.030	0.0103	281.615	0.031	4.232			
9673.77	0.251	276.488	0.029	0.0103	274.748	0.031	4.130			
9674.27	0.251	271.882	0.029	0.0103	270.143	0.031	4.060			
9674.77	0.251	268.794	0.029	0.0103	267.056	0.031	4.014			
9675.27	0.251	265.770	0.029	0.0103	264.031	0.031	3.969			
9675.78	0.251	264.446	0.029	0.0103	262.707	0.031	3.949			
9676.28	0.251	263.758	0.029	0.0102	262.019	0.031	3.939			

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Energy (eV)	σ_E (eV)	$[\frac{\mu}{\rho}]_{tot}$ ($\frac{cm^2}{g}$)	$\sigma_{[\frac{\mu}{\rho}]_{tot}}$	%	$[\frac{\mu}{\rho}]_{rel}$	%	$[\frac{\mu}{\rho}]_{pe}$ ($\frac{cm^2}{g}$)	$\sigma_{[\frac{\mu}{\rho}]_{pe}}$	%	$f_2(e/atom)$
9676.78	0.251	263.701	0.029	0.0103	261.962	0.031	3.939			
9677.28	0.251	264.055	0.029	0.0101	262.317	0.031	3.944			
9677.78	0.251	264.341	0.029	0.0101	262.603	0.031	3.949			
9678.28	0.251	264.352	0.029	0.0099	262.614	0.031	3.949			
9678.78	0.251	263.832	0.029	0.0099	262.094	0.031	3.941			
9679.28	0.251	262.828	0.028	0.0097	261.090	0.031	3.926			
9679.78	0.251	261.288	0.028	0.0097	259.550	0.031	3.903			
9680.28	0.251	259.323	0.028	0.0095	257.585	0.031	3.874			
9680.78	0.251	257.207	0.028	0.0096	255.469	0.030	3.843			
9681.28	0.252	255.076	0.028	0.0094	253.339	0.030	3.811			
9681.78	0.252	253.091	0.028	0.0095	251.353	0.030	3.781			
9682.28	0.252	251.428	0.028	0.0094	249.690	0.030	3.756			
9682.79	0.252	250.293	0.028	0.0095	248.556	0.030	3.739			
9683.29	0.252	249.463	0.028	0.0094	247.725	0.030	3.727			
9683.79	0.252	248.980	0.028	0.0095	247.243	0.030	3.720			
9684.29	0.252	248.797	0.028	0.0095	247.060	0.030	3.717			
9684.79	0.252	248.749	0.028	0.0096	247.012	0.030	3.717			
9685.29	0.252	248.872	0.028	0.0096	247.135	0.030	3.719			
9685.79	0.252	249.254	0.028	0.0097	247.517	0.030	3.725			
9686.29	0.252	249.760	0.028	0.0097	248.023	0.030	3.733			
9686.79	0.252	250.666	0.028	0.0099	248.930	0.030	3.746			
9687.29	0.252	251.597	0.028	0.0099	249.861	0.030	3.761			
9687.79	0.252	252.847	0.028	0.0100	251.110	0.030	3.780			
9688.29	0.252	254.156	0.028	0.0100	252.420	0.030	3.800			
9688.79	0.252	255.713	0.028	0.0102	253.977	0.030	3.823			
9689.29	0.252	257.254	0.028	0.0102	255.518	0.030	3.847			
9689.80	0.252	259.052	0.028	0.0103	257.316	0.030	3.874			
9690.29	0.252	260.823	0.028	0.0104	259.087	0.031	3.901			
9690.80	0.252	262.804	0.028	0.0105	261.068	0.031	3.931			
9691.30	0.252	264.602	0.028	0.0105	262.866	0.031	3.958			
9691.80	0.252	266.601	0.029	0.0106	264.865	0.031	3.988			
9692.30	0.252	268.482	0.029	0.0107	266.747	0.031	4.017			
9692.80	0.252	270.467	0.029	0.0107	268.732	0.031	4.047			
9693.30	0.252	272.209	0.029	0.0107	270.473	0.031	4.073			
9693.80	0.252	273.937	0.029	0.0108	272.201	0.031	4.100			
9694.30	0.252	275.389	0.029	0.0108	273.654	0.031	4.122			
9694.80	0.253	276.746	0.029	0.0109	275.011	0.031	4.142			
9695.30	0.253	277.786	0.029	0.0108	276.051	0.031	4.158			
9695.80	0.253	278.692	0.029	0.0109	276.957	0.031	4.172			
9696.30	0.253	279.296	0.029	0.0109	277.561	0.031	4.181			
9696.80	0.253	279.768	0.029	0.0109	278.033	0.031	4.189			
9697.30	0.253	279.890	0.029	0.0108	278.155	0.031	4.191			
9697.81	0.253	279.911	0.029	0.0108	278.176	0.031	4.191			
9698.31	0.253	279.760	0.029	0.0108	278.026	0.031	4.189			
9698.81	0.253	279.508	0.029	0.0106	277.774	0.031	4.186			
9699.31	0.253	279.152	0.029	0.0104	277.417	0.031	4.181			
9699.81	0.253	278.671	0.029	0.0104	276.937	0.031	4.174			
9700.31	0.253	278.190	0.029	0.0103	276.455	0.031	4.167			
9701.51	0.253	276.463	0.029	0.0103	274.729	0.031	4.141			
9703.31	0.253	272.857	0.029	0.0104	271.124	0.031	4.087			
9705.12	0.253	269.696	0.029	0.0105	267.963	0.031	4.041			
9706.92	0.253	267.840	0.029	0.0105	266.107	0.031	4.013			
9708.82	0.254	267.054	0.029	0.0105	265.322	0.031	4.002			
9710.82	0.254	267.835	0.029	0.0104	266.103	0.031	4.015			
9712.83	0.254	269.905	0.029	0.0104	268.173	0.031	4.047			
9714.83	0.254	271.851	0.029	0.0104	270.119	0.031	4.077			
9716.83	0.254	272.548	0.029	0.0105	270.816	0.031	4.089			
9718.93	0.254	271.871	0.029	0.0105	270.141	0.031	4.079			
9721.04	0.254	271.163	0.029	0.0107	269.432	0.031	4.069			
9723.24	0.255	270.873	0.029	0.0108	269.143	0.031	4.066			
9725.44	0.255	271.018	0.029	0.0109	269.289	0.031	4.069			
9727.65	0.255	271.775	0.029	0.0109	270.046	0.031	4.081			
9729.95	0.255	273.198	0.029	0.0108	271.469	0.031	4.104			
9732.25	0.255	275.314	0.029	0.0107	273.586	0.031	4.137			
9734.66	0.255	277.576	0.029	0.0105	275.849	0.031	4.172			
9737.06	0.256	278.807	0.029	0.0103	277.079	0.031	4.192			
9739.46	0.256	278.906	0.029	0.0103	277.179	0.031	4.194			
9741.96	0.256	277.365	0.029	0.0102	275.639	0.031	4.172			
9744.47	0.256	274.397	0.029	0.0102	272.671	0.031	4.128			
9746.97	0.256	270.897	0.029	0.0100	269.171	0.031	4.076			
9749.58	0.257	268.168	0.029	0.0101	266.442	0.031	4.036			
9752.18	0.257	266.777	0.029	0.0101	265.052	0.031	4.016			
9754.78	0.257	265.579	0.029	0.0103	263.854	0.031	3.999			
9757.49	0.257	264.219	0.028	0.0103	262.495	0.031	3.979			
9760.29	0.257	263.063	0.028	0.0104	261.340	0.031	3.963			
9762.99	0.258	263.024	0.028	0.0105	261.301	0.031	3.964			

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Energy (eV)	σ_E (eV)	$[\frac{\mu}{\rho}]_{tot}$ ($\frac{cm^2}{g}$)	$\sigma [\frac{\mu}{\rho}]_{tot}$	%	$[\frac{\mu}{\rho}]_{rel}$	%	$[\frac{\mu}{\rho}]_{pe}$ ($\frac{cm^2}{g}$)	$\sigma [\frac{\mu}{\rho}]_{pe}$	%	$f_2(e/atom)$
9765.80	0.258	264.655	0.028	0.0107	262.933	0.031	3.990			
9768.70	0.258	266.848	0.029	0.0107	265.126	0.031	4.024			
9771.51	0.258	269.014	0.029	0.0107	267.293	0.031	4.058			
9774.41	0.258	270.977	0.029	0.0106	269.257	0.031	4.089			
9777.41	0.259	273.313	0.029	0.0106	271.593	0.031	4.126			
9780.42	0.259	275.143	0.029	0.0105	273.424	0.031	4.155			
9783.42	0.259	275.581	0.029	0.0106	273.862	0.031	4.163			
9786.53	0.259	274.586	0.029	0.0104	272.867	0.031	4.149			
9789.63	0.259	273.362	0.029	0.0104	271.644	0.031	4.132			
9792.74	0.260	272.464	0.029	0.0102	270.746	0.031	4.119			
9795.94	0.260	271.772	0.029	0.0102	270.056	0.031	4.110			
9799.14	0.260	270.984	0.029	0.0100	269.268	0.031	4.100			
9802.35	0.260	269.850	0.029	0.0100	268.134	0.031	4.084			
9805.65	0.261	268.386	0.029	0.0099	266.671	0.031	4.063			
9809.06	0.261	266.895	0.029	0.0101	265.180	0.031	4.041			
9812.36	0.261	265.041	0.028	0.0101	263.327	0.031	4.015			
9815.77	0.261	263.025	0.028	0.0102	261.311	0.031	3.985			
9819.27	0.262	261.300	0.028	0.0102	259.587	0.031	3.960			
9822.68	0.262	261.155	0.028	0.0102	259.443	0.031	3.959			
9826.18	0.262	262.625	0.028	0.0102	260.913	0.031	3.983			
9829.79	0.262	264.513	0.028	0.0103	262.802	0.031	4.014			
9833.39	0.263	265.642	0.028	0.0102	263.932	0.031	4.032			
9837.00	0.263	266.086	0.029	0.0103	264.377	0.031	4.041			
9840.70	0.263	265.925	0.029	0.0103	264.216	0.031	4.040			
9844.41	0.263	266.038	0.029	0.0103	264.330	0.031	4.043			
9848.11	0.264	266.140	0.029	0.0102	264.432	0.031	4.046			
9851.92	0.264	266.415	0.029	0.0103	264.708	0.031	4.052			
9855.72	0.264	266.817	0.029	0.0101	265.111	0.031	4.060			
9859.53	0.265	267.005	0.029	0.0101	265.299	0.031	4.064			
9863.43	0.265	266.689	0.029	0.0099	264.985	0.031	4.061			
9867.34	0.265	266.228	0.029	0.0099	264.524	0.031	4.055			
9871.34	0.265	265.103	0.029	0.0098	263.399	0.031	4.040			
9875.35	0.266	263.439	0.028	0.0099	261.736	0.031	4.016			
9879.35	0.266	261.535	0.028	0.0098	259.833	0.031	3.988			
9883.46	0.266	259.747	0.028	0.0099	258.046	0.031	3.963			
9887.56	0.267	258.344	0.028	0.0099	256.643	0.031	3.943			
9891.77	0.267	257.498	0.028	0.0100	255.798	0.031	3.931			
9895.98	0.267	257.140	0.028	0.0099	255.441	0.031	3.928			
9900.18	0.268	257.777	0.028	0.0099	256.079	0.031	3.939			
9904.39	0.268	258.210	0.028	0.0098	256.513	0.031	3.947			
9908.69	0.268	258.677	0.028	0.0099	256.980	0.031	3.956			
9913.10	0.269	258.749	0.028	0.0098	257.053	0.031	3.959			
9917.41	0.269	258.680	0.028	0.0099	256.985	0.031	3.960			
9921.91	0.269	258.522	0.028	0.0098	256.828	0.031	3.959			
9926.32	0.270	258.374	0.028	0.0099	256.680	0.031	3.959			
9930.82	0.270	258.258	0.028	0.0097	256.565	0.031	3.959			
9935.33	0.270	258.051	0.028	0.0098	256.359	0.031	3.957			
9939.94	0.271	257.638	0.028	0.0096	255.947	0.031	3.953			
9944.54	0.271	257.312	0.028	0.0097	255.621	0.031	3.950			
9949.15	0.271	256.711	0.028	0.0095	255.021	0.031	3.942			
9953.86	0.272	256.055	0.028	0.0096	254.367	0.031	3.934			
9958.56	0.272	255.101	0.028	0.0095	253.413	0.031	3.921			
9963.27	0.272	253.900	0.028	0.0096	252.213	0.031	3.904			
9968.08	0.273	252.669	0.028	0.0094	250.983	0.031	3.887			
9972.88	0.273	251.905	0.028	0.0096	250.219	0.031	3.877			
9977.79	0.273	251.265	0.028	0.0094	249.581	0.031	3.869			
9982.69	0.274	250.942	0.028	0.0096	249.258	0.031	3.866			
9987.60	0.274	250.409	0.028	0.0094	248.727	0.031	3.860			
9992.61	0.274	250.035	0.028	0.0095	248.353	0.031	3.856			
9997.62	0.275	249.859	0.028	0.0094	248.178	0.031	3.855			
10000.12	0.275	249.949	0.028	0.0095	248.268	0.031	3.857			
10002.72	0.275	249.776	0.028	0.0095	248.096	0.031	3.856			
10007.73	0.276	249.583	0.028	0.0094	247.904	0.031	3.855			
10012.94	0.276	249.452	0.028	0.0094	247.773	0.031	3.855			
10018.04	0.276	249.150	0.028	0.0094	247.472	0.031	3.852			
10023.25	0.277	248.990	0.028	0.0094	247.313	0.031	3.851			
10028.46	0.277	248.667	0.028	0.0093	246.992	0.031	3.848			
10033.76	0.277	248.332	0.028	0.0093	246.657	0.031	3.845			
10039.07	0.278	247.798	0.028	0.0092	246.124	0.031	3.839			
10044.48	0.278	247.218	0.027	0.0093	245.545	0.031	3.832			
10049.89	0.279	246.383	0.027	0.0091	244.710	0.031	3.821			
10055.29	0.279	245.639	0.027	0.0092	243.968	0.031	3.811			
10060.70	0.279	244.808	0.027	0.0091	243.138	0.031	3.801			
10066.21	0.280	244.203	0.027	0.0092	242.534	0.031	3.793			
10071.82	0.280	243.641	0.027	0.0090	241.973	0.031	3.787			
10077.32	0.281	243.223	0.027	0.0092	241.556	0.031	3.782			

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Table of results Continued from previous page

Energy (eV)	σ_E (eV)	$\left[\frac{\mu}{\rho} \right]_{tot} (\frac{cm^2}{g})$	$\sigma \left[\frac{\mu}{\rho} \right]_{tot}$	%	$\sigma \left[\frac{\mu}{\rho} \right]_{rel}$	%	$\left[\frac{\mu}{\rho} \right]_{pe} (\frac{cm^2}{g})$	$\sigma \left[\frac{\mu}{\rho} \right]_{pe}$	%	$f_2(e/atom)$
10082.93	0.281	242.728	0.027	0.0090	241.062	0.031	3.776			
10088.64	0.281	242.391	0.027	0.0091	240.726	0.031	3.773			
10094.35	0.282	241.815	0.027	0.0089	240.150	0.031	3.766			
10100.05	0.282	241.398	0.027	0.0091	239.734	0.031	3.762			
10105.76	0.283	240.988	0.027	0.0089	239.326	0.031	3.758			
10111.57	0.283	240.662	0.027	0.0091	239.000	0.031	3.755			
10117.48	0.284	240.335	0.027	0.0089	238.675	0.031	3.752			
10123.29	0.284	239.981	0.027	0.0091	238.321	0.031	3.748			
10129.29	0.284	239.555	0.027	0.0088	237.896	0.031	3.744			
10135.20	0.285	239.170	0.027	0.0090	237.512	0.031	3.740			
10141.21	0.285	238.725	0.027	0.0087	237.068	0.031	3.735			
10147.22	0.286	238.234	0.027	0.0089	236.578	0.030	3.730			
10153.33	0.286	237.581	0.027	0.0087	235.927	0.030	3.722			
10159.44	0.287	237.199	0.027	0.0089	235.546	0.030	3.718			
10165.54	0.287	236.489	0.027	0.0086	234.836	0.031	3.709			
10171.75	0.288	235.979	0.027	0.0089	234.328	0.030	3.703			
10177.96	0.288	235.253	0.027	0.0086	233.603	0.030	3.694			
10184.17	0.288	234.878	0.027	0.0088	233.229	0.030	3.690			
10190.48	0.289	234.385	0.027	0.0085	232.737	0.030	3.685			
10196.79	0.289	233.910	0.027	0.0088	232.263	0.030	3.680			
10203.20	0.290	233.376	0.027	0.0084	231.730	0.030	3.674			
10209.60	0.290	232.814	0.027	0.0087	231.169	0.030	3.667			
10216.01	0.291	232.351	0.027	0.0083	230.707	0.030	3.662			
10222.52	0.291	231.943	0.027	0.0087	230.300	0.030	3.658			
10229.03	0.292	231.475	0.027	0.0083	229.833	0.030	3.653			
10235.54	0.292	231.023	0.027	0.0087	229.382	0.030	3.648			
10242.15	0.293	230.720	0.027	0.0082	229.080	0.030	3.645			
10248.76	0.293	230.424	0.027	0.0086	228.785	0.030	3.643			
10255.47	0.294	229.836	0.027	0.0082	228.199	0.030	3.636			
10262.18	0.294	229.441	0.027	0.0086	227.805	0.030	3.632			
10268.89	0.295	228.845	0.027	0.0081	227.210	0.030	3.625			
10275.70	0.295	228.339	0.026	0.0085	226.705	0.030	3.619			
10282.50	0.296	227.763	0.026	0.0080	226.130	0.030	3.613			
10289.31	0.296	227.336	0.026	0.0085	225.704	0.030	3.608			
10296.22	0.297	226.845	0.026	0.0079	225.214	0.030	3.603			
10303.13	0.297	226.370	0.026	0.0085	224.741	0.030	3.598			
10310.14	0.298	225.783	0.026	0.0079	224.155	0.030	3.591			
10317.15	0.298	225.402	0.026	0.0084	223.775	0.030	3.587			
10324.16	0.299	224.811	0.026	0.0078	223.185	0.030	3.580			
10331.27	0.299	224.346	0.026	0.0084	222.721	0.030	3.575			
10338.38	0.300	223.871	0.026	0.0077	222.247	0.030	3.570			
10345.49	0.300	223.399	0.026	0.0084	221.776	0.030	3.565			
10352.70	0.301	222.900	0.026	0.0076	221.278	0.030	3.559			
10359.91	0.301	222.558	0.026	0.0084	220.938	0.030	3.556			
10367.22	0.302	222.006	0.026	0.0076	220.387	0.030	3.550			
10374.53	0.302	221.517	0.026	0.0083	219.899	0.030	3.545			
10381.84	0.303	220.954	0.026	0.0075	219.337	0.030	3.538			
10389.15	0.304	220.609	0.026	0.0082	218.993	0.030	3.535			
10396.66	0.304	220.083	0.026	0.0074	218.469	0.030	3.529			
10404.07	0.305	219.640	0.026	0.0082	218.027	0.030	3.524			
10411.58	0.305	219.226	0.026	0.0073	217.614	0.030	3.520			
10419.09	0.306	218.761	0.026	0.0082	217.151	0.030	3.515			
10426.60	0.306	218.167	0.026	0.0072	216.558	0.030	3.508			
10434.21	0.307	217.750	0.026	0.0081	216.142	0.030	3.504			
10441.92	0.307	217.239	0.026	0.0071	215.632	0.030	3.498			
10449.53	0.308	216.764	0.026	0.0081	215.158	0.030	3.493			
10457.24	0.309	216.226	0.026	0.0071	214.622	0.030	3.487			
10465.05	0.309	215.841	0.026	0.0081	214.238	0.030	3.483			
10472.86	0.310	215.416	0.026	0.0070	213.814	0.030	3.479			
10480.67	0.310	214.984	0.026	0.0080	213.383	0.030	3.475			
10488.49	0.311	214.458	0.026	0.0069	212.859	0.030	3.469			
10496.40	0.311	214.020	0.026	0.0080	212.422	0.030	3.464			
10504.41	0.312	213.551	0.026	0.0068	211.954	0.030	3.459			
10512.32	0.313	213.143	0.026	0.0079	211.548	0.030	3.455			
10520.33	0.313	212.680	0.026	0.0067	211.086	0.030	3.450			
10528.44	0.314	212.169	0.026	0.0080	210.576	0.030	3.445			
10536.45	0.314	211.649	0.026	0.0066	210.057	0.030	3.439			
10544.66	0.315	211.289	0.026	0.0079	209.698	0.030	3.436			
10552.77	0.316	210.763	0.026	0.0065	209.174	0.030	3.430			
10560.98	0.316	210.289	0.026	0.0079	208.701	0.030	3.424			
10569.20	0.317	209.772	0.026	0.0064	208.186	0.030	3.419			
10577.51	0.317	209.313	0.026	0.0078	207.728	0.030	3.414			
10585.82	0.318	208.851	0.026	0.0063	207.267	0.030	3.409			
10594.13	0.319	208.390	0.026	0.0078	206.807	0.030	3.404			
10602.54	0.319	207.819	0.026	0.0062	206.238	0.030	3.397			
10610.95	0.320	207.465	0.025	0.0077	205.885	0.030	3.394			

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Energy (eV)	σ_E (eV)	$\left[\frac{\mu}{\rho} \right]_{tot} (\frac{cm^2}{g})$	$\sigma \left[\frac{\mu}{\rho} \right]_{tot}$	%	$\sigma \left[\frac{\mu}{\rho} \right]_{rel}$	%	$\left[\frac{\mu}{\rho} \right]_{pe} (\frac{cm^2}{g})$	$\sigma \left[\frac{\mu}{\rho} \right]_{pe}$	%	$f_2(e/atom)$
10619.46	0.320	206.982	0.025	0.0061	205.403	0.030	3.389			
10627.98	0.321	206.555	0.025	0.0077	204.978	0.030	3.385			
10636.49	0.322	206.131	0.025	0.0060	204.555	0.030	3.380			
10645.10	0.322	205.694	0.025	0.0077	204.119	0.030	3.376			
10653.71	0.323	205.200	0.025	0.0059	203.626	0.030	3.371			
10662.32	0.324	204.757	0.025	0.0076	203.185	0.030	3.366			
10671.04	0.324	204.206	0.025	0.0057	202.636	0.030	3.360			
10679.75	0.325	203.752	0.025	0.0076	202.183	0.030	3.355			
10688.56	0.326	203.246	0.025	0.0057	201.679	0.030	3.349			
10697.37	0.326	202.789	0.025	0.0075	201.223	0.030	3.344			
10706.18	0.327	202.300	0.025	0.0055	200.735	0.030	3.339			
10715.10	0.327	201.831	0.025	0.0075	200.267	0.030	3.334			
10724.01	0.328	201.301	0.025	0.0054	199.739	0.030	3.328			
10732.92	0.329	200.944	0.025	0.0075	199.383	0.030	3.325			
10741.93	0.329	200.440	0.025	0.0053	198.880	0.030	3.319			
10750.94	0.330	200.041	0.025	0.0074	198.483	0.030	3.315			
10759.96	0.331	199.500	0.025	0.0052	197.943	0.030	3.309			
10769.07	0.331	199.027	0.025	0.0074	197.471	0.031	3.304			
10778.28	0.332	198.553	0.025	0.0051	196.999	0.031	3.299			
10787.39	0.333	198.117	0.025	0.0074	196.564	0.031	3.294			
10796.61	0.333	197.566	0.025	0.0050	196.015	0.031	3.288			
10805.92	0.334	197.200	0.025	0.0074	195.650	0.031	3.285			
10815.13	0.335	196.660	0.025	0.0049	195.112	0.031	3.279			
10824.54	0.336	196.227	0.025	0.0073	194.679	0.031	3.274			
10833.86	0.336	195.679	0.025	0.0048	194.133	0.031	3.268			
10843.27	0.337	195.258	0.025	0.0073	193.714	0.031	3.264			
10852.68	0.338	194.747	0.025	0.0047	193.204	0.031	3.258			
10862.20	0.338	194.400	0.025	0.0073	192.858	0.031	3.255			
10871.71	0.339	193.912	0.025	0.0046	192.372	0.031	3.249			
10881.22	0.340	193.453	0.025	0.0072	191.914	0.031	3.245			
10890.83	0.340	193.114	0.025	0.0045	191.577	0.031	3.242			
10900.45	0.341	192.656	0.025	0.0072	191.121	0.031	3.237			
10910.16	0.342	192.198	0.025	0.0044	190.663	0.031	3.232			
10919.87	0.343	191.752	0.025	0.0071	190.219	0.031	3.227			
10929.59	0.343	191.215	0.025	0.0043	189.684	0.031	3.221			
10939.30	0.344	190.770	0.025	0.0071	189.240	0.031	3.216			
10949.12	0.345	190.299	0.025	0.0042	188.771	0.031	3.211			
10959.03	0.345	189.872	0.025	0.0070	188.345	0.031	3.207			
10968.94	0.346	189.292	0.025	0.0041	187.766	0.031	3.200			
10978.85	0.347	188.876	0.025	0.0070	187.352	0.031	3.196			
10988.77	0.348	188.475	0.025	0.0040	186.952	0.031	3.192			
10998.78	0.348	187.898	0.025	0.0070	186.377	0.031	3.185			
11008.80	0.349	187.420	0.025	0.0039	185.900	0.031	3.180			
11018.91	0.350	186.959	0.025	0.0069	185.441	0.031	3.175			
11029.02	0.351	186.576	0.025	0.0038	185.060	0.031	3.171			
11039.14	0.351	186.119	0.025	0.0069	184.604	0.031	3.166			
11049.35	0.352	185.634	0.025	0.0037	184.121	0.031	3.161			
11059.57	0.353	185.184	0.025	0.0068	183.671	0.031	3.156			
11069.88	0.354	184.600	0.025	0.0036	183.089	0.031	3.149			
11080.19	0.354	184.249	0.025	0.0068	182.740	0.031	3.146			
11090.51	0.355	183.795	0.025	0.0035	182.287	0.031	3.141			
11100.82	0.356	183.364	0.025	0.0069	181.858	0.031	3.137			
11111.34	0.357	182.873	0.025	0.0034	181.368	0.031	3.131			
11121.75	0.357	182.346	0.025	0.0068	180.842	0.031	3.125			
11132.26	0.358	181.838	0.025	0.0033	180.336	0.031	3.119			
11142.78	0.359	181.370	0.025	0.0067	179.870	0.031	3.114			
11153.29	0.360	180.875	0.025	0.0032	179.376	0.031	3.108			
11163.91	0.360	180.518	0.025	0.0067	179.021	0.031	3.105			
11174.52	0.361	179.938	0.025	0.0031	178.442	0.031	3.098			
11185.24	0.362	179.539	0.025	0.0068	178.045	0.031	3.094			
11195.95	0.363	179.088	0.025	0.0031	177.596	0.031	3.089			
11206.67	0.364	178.777	0.024	0.0066	177.285	0.031	3.087			
11217.48	0.364	178.332	0.024	0.0030	176.843	0.031	3.082			
11228.30	0.365	177.903	0.024	0.0066	176.415	0.031	3.078			
11239.21	0.366	177.455	0.024	0.0029	175.968	0.031	3.073			
11250.13	0.367	176.993	0.024	0.0066	175.508	0.031	3.068			
11261.04	0.368	176.589	0.024	0.0028	175.106	0.031	3.064			
11271.96	0.368	175.914	0.024	0.0066	174.432	0.031	3.055			
11282.97	0.369	175.533	0.024	0.0028	174.053	0.031	3.051			
11294.09	0.370	175.038	0.024	0.0065	173.560	0.031	3.046			
11305.20	0.371	174.436	0.024	0.0027	172.959	0.031	3.038			
11316.32	0.372	174.044	0.024	0.0064	172.569	0.031	3.034			
11327.43	0.372	173.467	0.024	0.0026	171.993	0.031	3.027			
11338.65	0.373	173.114	0.024	0.0064	171.641	0.031	3.024			
11349.86	0.374	172.609	0.024	0.0025	171.138	0.031	3.018			
11361.18	0.375	172.093	0.024	0.0066	170.624	0.031	3.012			

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Table of results Continued from previous page

Energy (eV)	σ_E (eV)	$\left[\frac{\mu}{\rho} \right]_{tot}$ ($\frac{cm^2}{g}$)	$\sigma \left[\frac{\mu}{\rho} \right]_{tot}$	%	$\sigma \left[\frac{\mu}{\rho} \right]_{rel}$	%	$\left[\frac{\mu}{\rho} \right]_{pe}$ ($\frac{cm^2}{g}$)	$\sigma \left[\frac{\mu}{\rho} \right]_{pe}$	%	$f_2(e/atom)$
11372.49	0.376	171.533	0.024		0.0026		170.065	0.031		3.005
11383.81	0.377	171.311	0.024		0.0064		169.845	0.031		3.004
11395.22	0.377	170.788	0.024		0.0024		169.323	0.032		2.998
11406.64	0.378	170.310	0.024		0.0063		168.847	0.032		2.992
11418.05	0.379	169.811	0.024		0.0023		168.349	0.032		2.987
11429.57	0.380	169.406	0.024		0.0063		167.946	0.032		2.982
11441.19	0.381	168.912	0.024		0.0022		167.454	0.032		2.977
11452.70	0.382	168.478	0.024		0.0062		167.021	0.032		2.972
11464.32	0.383	168.039	0.024		0.0022		166.584	0.032		2.967
11476.03	0.383	167.601	0.024		0.0062		166.147	0.032		2.962
11487.65	0.384	166.991	0.024		0.0021		165.539	0.032		2.955
11499.37	0.385	166.524	0.024		0.0061		165.074	0.032		2.949
11511.18	0.386	166.097	0.024		0.0021		164.648	0.032		2.945
11523.00	0.387	165.730	0.024		0.0062		164.283	0.032		2.941
11534.81	0.388	165.209	0.024		0.0020		163.763	0.032		2.935
11546.63	0.389	164.873	0.024		0.0062		163.429	0.032		2.932
11558.55	0.389	164.269	0.024		0.0020		162.827	0.032		2.924
11570.56	0.390	163.799	0.024		0.0061		162.358	0.032		2.919
11582.58	0.391	163.366	0.024		0.0019		161.926	0.032		2.914
11594.60	0.392	162.914	0.024		0.0061		161.476	0.032		2.909

Concluded