Shell-to-shell ionization cross sections of antiprotons, H^+ , He^{2+} , Be^{4+} , C^{6+} and O^{8+} on H, C, N, O, P, and S neutral atoms

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Abstract

Total ionization cross sections of H, C, N, O, P and S neutral atoms by impact of antiprotons, H^+ , He^{2+} , Be^{4+} , C^{6+} and O^{8+} . were calculated using the CDWEIS (continuum distorted wave -Eikonal Initial state) theoretical method. Cross section depending on of initial the quantum numbers n and l are reported in Tables for a range of impact energies covering from 100 keV/amu to 10 MeV/amu

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Total ionization cross sections of H, C, N, O, P and S neutral atoms by impact of \bar{p} (antiprotons), H⁺, He²⁺, Be⁴⁺, C⁶⁺ and O⁸⁺. were calculated using the CDWEIS (continuum distorted wave -Eikonal Initial state) theoretical method. The total ionization cross section of an electron in the nlm initial state, due to the interaction with a projectile of charge Z_P and impact velocity v, is given by the four-dimensional integral

$$\sigma_{nl} = \sum_{m=1}^{l} \frac{(2\pi)^2}{v^2} \int d\overrightarrow{E} \int d\overrightarrow{\eta} \left| T_{\overrightarrow{k},nlm}(\overrightarrow{E}, \overrightarrow{\eta}) \right|^2 \tag{1}$$

where $T_{\overrightarrow{k},nlm}(\overrightarrow{E},\overrightarrow{\eta})$ is the transition matrix as a function of is the component of the momentum transfer $\overrightarrow{\eta}$ perpendicular to the incident velocity \overrightarrow{v} . In our theoretical treatment we expand our final continuum wave function on the target atom in the usual form

$$\psi_{\overrightarrow{k}}^{-}(\overrightarrow{r}) = \sum_{l=0}^{l_{\text{max}}} \sum_{m=-l}^{l} R_{kl}^{-}(r) Y_l^m(\widehat{r}) Y_l^{m^*}(\widehat{k}), \tag{2}$$

We are confident with our calculations up to $l_{\text{max}} \sim 30$. As the impact velocity v increases we would require of larger l_{max} in (1). At the highest impact energies here reported we estimate a deficiency of our results of about 2-3%. The wave functions of initial bound state characterized by the quantum numbers nlm and final continuum state $\psi_{\overrightarrow{k}}^-(\overrightarrow{r})$ were obtained by using the RADIALF code developed by Salvat and co-workers using a Hartree Fock potential obtained the Depurated Inversion Model [1, 2]. Details of the calculation can be seen in [3], and for proton in Refs.[4, 5] In parallel to this article, we will be presenting ionization cross sections of biomolecules of interest by using these results along with the stoichiometric approximation [6].

The Tables that follows reports the calculated cross section σ_{nl} in atomic units

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TABLE I: Total ionization cross sections for multicharge bare ions on Hydrogen at different impact energies. Cross sections are in atomic units divided Z_P^2 , and projectile energies are in MeV/amu. To save space, throughout these tables the subindex n replaces the 10^n factor.

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
-1	1s	3.30	2.33	1.77	1.43	1.20	9.11_{-1}	6.75_{-1}	3.71_{-1}	2.59_{-1}	1.64_{-1}	1.22_{-1}	8.82_2
1	1s	4.24	2.64	1.91	1.50	1.25	9.34_{-1}	6.86_{-1}	3.73_{-1}	2.69_{-1}	1.70_{-1}	1.26_{-1}	8.82_{-2}
2	1s	3.13	2.33	1.77	1.43	1.20	9.09_{-1}	6.74_{-1}	3.70_{-1}	2.67_{-1}	1.69_{-1}	1.25_{-1}	8.81_2
4	1s	1.66	1.67	1.41	1.20	1.04	8.24_{-1}	6.29_{-1}	3.58_{-1}	2.53_{-1}	1.67_{-1}	1.24_{-1}	8.76_{-2}
6	1s	9.39_{-1}	1.22	1.12	1.00	8.94_{-1}	7.33_{-1}	5.76_{-1}	3.41_{-1}	2.53_{-1}	1.64_{-1}	1.23_{-1}	8.67_{-2}
8	1s	5.60_{-1}	9.08_{-1}	9.05_{-1}	8.42_{-1}	7.72_{-1}	6.54_{-1}	5.28_{-1}	3.23_{-1}	2.36_{-1}	1.60_{-1}	1.20_{-1}	8.55_{-2}

TABLE II: Total ionization cross sections for multicharge bare ions on Carbon at different impact energies. Cross sections are in atomic units divided \mathbb{Z}_{P}^{2} , and projectile energies are in MeV/amu

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
-1	2p	3.74	2.95	2.38	1.99	1.71	1.34	1.02	5.89_{-1}	4.21_{-1}	2.74_{-1}	2.06_{-1}	1.51_{-1}
-1	2s	1.49	1.05	7.90_{-1}	6.34_{-1}	5.30_{-1}	4.01_{-1}	2.95_{-1}	1.60_{-1}	1.11_{-1}	6.95_{-2}	5.11_{-2}	3.68_{-2}
-1	1s	2.26_{-3}	5.19_{-3}	7.33_{-3}	8.77_{-3}	9.67_{-3}	1.05_{-2}	1.06_{-2}	8.83_{-3}	7.22_{-3}	5.23_{-3}	4.11_{-3}	3.14_{-3}
-1	Total	1.05_{1}	8.01	6.35	5.26	4.50	3.51	2.66	1.51	1.08	6.97_{-1}	5.22_{-1}	3.82_{-1}
1	2p	4.82	3.39	2.59	2.10	1.78	1.38	1.04	5.92_{-1}	4.23_{-1}	2.74_{-1}	2.06_{-1}	1.51_{-1}
1	2s	1.69	1.14	8.38_{-1}	6.63_{-1}	5.49_{-1}	4.10_{-1}	2.99_{-1}	1.61_{-1}	1.11_{-1}	6.96_{-2}	5.11_{-2}	3.68_{-2}
1	1s	2.02_{-3}	7.13_{-3}	1.09_{-2}	1.31_{-2}	1.42_{-2}	1.46_{-2}	1.36_{-2}	9.95_{-3}	7.75_{-3}	5.41_{-3}	4.20_{-3}	3.18_{-3}
1	Total	1.30_{1}	9.07	6.87	5.56	4.69	3.60	2.71	1.53	1.08	6.99_{-1}	5.22_{-1}	3.83_{-1}
2	2p	3.26	2.81	2.29	3.79_{1}	1.67	1.32	1.01	5.84_{-1}	4.19_{-1}	2.73_{-1}	2.05_{-1}	1.51_{-1}
2	2s	1.08	9.30_{-1}	7.44_{-1}	1.09_{1}	5.17_{-1}	3.95_{-1}	2.92_{-1}	1.59_{-1}	1.10_{-1}	6.94_{-2}	5.10_{-2}	3.68_{-2}
2	1s	5.22_{-4}	3.74_{-3}	7.54_{-3}	1.60_{-4}	1.22_{-2}	1.36_{-2}	1.34_{-2}	1.01_{-2}	7.82_{-3}	5.43_{-3}	4.21_{-3}	3.19_{-3}
2	Total	8.69	7.48	6.09	9.77_1	4.39	3.45	2.63	1.51	1.08	6.96_{-1}	5.21_{-1}	3.82_{-1}
4	2p	1.57	1.80	1.65	1.49	1.35	1.13	9.04_{-1}	5.54_{-1}	4.05_{-1}	2.68_{-1}	2.02_{-1}	1.50_{-1}
4	2s	4.68_{-1}	5.87_{-1}	5.42_{-1}	4.82_{-1}	4.28_{-1}	3.47_{-1}	2.68_{-1}	1.53_{-1}	1.08_{-1}	6.85_{-2}	5.06_{-2}	3.65_{-2}
4	1s	1.98_{-5}	6.27_{-4}	2.29_{-3}	4.38_{-3}	6.30_{-3}	8.95_{-3}	1.05_{-2}	9.34_{-3}	7.54_{-3}	5.34_{-3}	4.17_{-3}	3.17_{-3}
4	Total	4.07	4.77	4.39	3.95	3.56	2.96	2.37	1.43	1.04	6.83_{-1}	5.14_{-1}	3.79_{-1}
6	2p	8.75_{-1}	1.23	1.22	1.15	1.08	9.43_{-1}	7.89_{-1}	5.14_{-1}	3.88_{-1}	2.64_{-1}	1.99_{-1}	1.47_{-1}
6	2s	2.25_{-1}	3.89_{-1}	4.01_{-1}	3.80_{-1}	3.52_{-1}	2.99_{-1}	2.41_{-1}	1.45_{-1}	1.04_{-1}	6.73_{-2}	5.00_{-2}	3.62_{-2}
6	1s	6.75_{-7}	9.66_{-5}	6.37_{-4}	1.67_{-3}	2.93_{-3}	5.24_{-3}	7.33_{-3}	8.03_{-3}	6.90_{-3}	5.11_{-3}	4.05_{-3}	3.11_{-3}
6	Total	2.20	3.23	3.24	3.07	2.87	2.50	2.08	1.33	9.97_{-1}	6.72_{-1}	5.06_{-1}	3.74_{-1}
8	2p	5.40_{-1}	8.91_{-1}	9.38_{-1}	9.19_{-1}	8.81_{-1}	7.98_{-1}	6.90_{-1}	4.73_{-1}	3.70_{-1}	2.55_{-1}	1.97_{-1}	1.45_{-1}
8	2s	1.15_{-1}	2.70_{-1}	3.05_{-1}	3.05_{-1}	2.92_{-1}	2.60_{-1}	2.17_{-1}	1.37_{-1}	1.00_{-1}	6.56_{-2}	4.91_{-2}	3.57_{-2}
8	1s	2.28_{-8}	1.51_{-5}	1.80_{-4}	6.46_{-4}	1.37_{-3}	3.06_{-3}	5.06_{-3}	6.70_{-3}	6.15_{-3}	4.79_{-3}	3.88_{-3}	3.02_{-3}
8	Total	1.31	2.32	2.49	2.45	2.35	2.12	1.82	1.23	9.51_{-1}	6.51_{-1}	4.99_{-1}	3.67_{-1}

TABLE III: Total ionization cross sections for multicharge bare ions on Nitrogen at different impact energies. Cross sections are in atomic units divided \mathbb{Z}_{P}^{2} , and projectile energies are in MeV/amu

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
-1	2p	2.21	1.87	1.56	1.33	1.16	9.23_{-1}	7.13_{-1}	4.17_{-1}	3.01_{-1}	1.97_{-1}	1.49_{-1}	1.10_{-1}
-1	2s	9.16_{-1}	6.97_{-1}	5.42_{-1}	4.42_{-1}	3.73_{-1}	2.85_{-1}	2.12_{-1}	1.16_{-1}	8.13_{-2}	5.13_{-2}	3.78_{-2}	2.73_{-2}
-1	1s	7.54_{-4}	2.00_{-3}	3.08_{-3}	3.92_{-3}	4.54_{-3}	5.29_{-3}	5.71_{-3}	5.28_{-3}	4.53_{-3}	3.41_{-3}	2.73_{-3}	2.11_{-3}
-1	Total	8.46	7.02	5.77	4.88	4.23	3.35	2.58	1.50	1.07	7.01_{-1}	5.27_{-1}	3.88_{-1}
1	2p	2.95	2.24	1.75	1.44	1.23	9.58_{-1}	7.29_{-1}	4.21_{-1}	3.02_{-1}	1.97_{-1}	1.49_{-1}	1.10_{-1}
1	2s	1.04	7.69_{-1}	5.82_{-1}	4.67_{-1}	3.90_{-1}	2.94_{-1}	2.16_{-1}	1.17_{-1}	8.16_{-2}	5.14_{-2}	3.79_{-2}	2.73_{-2}
1	1s	5.69_{-4}	2.52_{-3}	4.40_{-3}	5.76_{-3}	6.65_{-3}	7.48_{-3}	7.60_{-3}	6.14_{-3}	4.97_{-3}	3.57_{-3}	2.81_{-3}	2.15_{-3}
1	Total	1.09_{1}	8.26	6.42	5.26	4.48	3.48	2.64	1.51	1.08	7.02_{-1}	5.28_{-1}	3.88_{-1}
2	2p	1.89	1.82	1.53	1.31	1.14	9.13_{-1}	7.06_{-1}	4.15_{-1}	3.00_{-1}	1.97_{-1}	1.48_{-1}	1.09_{-1}
2	2s	6.11_{-1}	6.04_{-1}	5.04_{-1}	4.23_{-1}	3.63_{-1}	2.81_{-1}	2.10_{-1}	1.16_{-1}	8.11_{-2}	5.12_{-2}	3.78_{-2}	2.73_{-2}
2	1s	1.36_{-4}	1.24_{-3}	2.88_{-3}	4.39_{-3}	5.55_{-3}	6.90_{-3}	7.44_{-3}	6.25_{-3}	5.05_{-3}	3.61_{-3}	2.83_{-3}	2.16_{-3}
2	Total	6.88	6.66	5.62	4.79	4.17	3.31	2.55	1.49	1.07	6.99_{-1}	5.26_{-1}	3.87_{-1}
4	2p	8.22_{-1}	1.11	1.07	9.86_{-1}	9.04_{-1}	7.69_{-1}	6.26_{-1}	3.91_{-1}	2.89_{-1}	1.92_{-1}	1.46_{-1}	1.08_{-1}
4	2s	2.26_{-1}	3.51_{-1}	3.46_{-1}	3.18_{-1}	2.89_{-1}	2.40_{-1}	1.90_{-1}	1.11_{-1}	7.89_{-2}	5.05_{-2}	3.74_{-2}	2.71_{-2}
4	1s	4.08_{-6}	1.72_{-4}	7.54_{-4}	1.63_{-3}	2.59_{-3}	4.20_{-3}	5.55_{-3}	5.75_{-3}	4.87_{-3}	3.56_{-3}	2.81_{-3}	2.15_{-3}
4	Total	2.92	4.04	3.90	3.60	3.30	2.80	2.27	1.41	1.03	6.85_{-1}	5.19_{-1}	3.84_{-1}
6	2p	4.24_{-1}	7.35_{-1}	7.69_{-1}	7.46_{-1}	7.09_{-1}	6.33_{-1}	5.39_{-1}	3.60_{-1}	2.77_{-1}	1.89_{-1}	1.45_{-1}	1.07_{-1}
6	2s	9.41_{-2}	2.18_{-1}	2.44_{-1}	2.41_{-1}	2.29_{-1}	2.02_{-1}	1.67_{-1}	1.04_{-1}	7.57_{-2}	4.93_{-2}	3.71_{-2}	2.68_{-2}
6	1s	1.02_{-7}	2.09_{-5}	1.73_{-4}	5.31_{-4}	1.05_{-3}	2.23_{-3}	3.63_{-3}	4.84_{-3}	4.41_{-3}	3.39_{-3}	2.72_{-3}	2.11_{-3}
6	Total	1.46	2.64	2.80	2.72	2.59	2.31	1.96	1.30	9.92_{-1}	6.73_{-1}	5.15_{-1}	3.78_{-1}
8	2p	2.42_{-1}	5.21_{-1}	5.81_{-1}	5.84_{-1}	5.69_{-1}	5.27_{-1}	4.65_{-1}	3.29_{-1}	2.56_{-1}	1.81_{-1}	1.41_{-1}	1.05_{-1}
8	2s	4.16_{-2}	1.43_{-1}	1.79_{-1}	1.87_{-1}	1.85_{-1}	1.71_{-1}	1.47_{-1}	9.69_{-2}	7.21_{-2}	4.79_{-2}	3.63_{-2}	2.64_{-2}
8	1s	2.47_{-9}	2.52_{-6}	3.96_{-5}	1.73_{-4}	4.25_{-4}	1.17_{-3}	2.33_{-3}	3.92_{-3}	3.87_{-3}	3.16_{-3}	2.60_{-3}	2.05_{-3}
8	Total	8.10_{-1}	1.85	2.10	2.13	2.08	1.93	1.70	1.19	9.19_{-1}	6.46_{-1}	5.00_{-1}	3.70_{-1}

TABLE IV: Total ionization cross sections for multicharge bare ions on Oxigen at different impact energies. Cross sections are in atomic units divided \mathbb{Z}_P^2 , and projectile energies are in MeV/amu

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
-1	2p	1.61	1.41	1.19	1.02	8.99_{-1}	7.23_{-1}	5.63_{-1}	3.33_{-1}	2.41_{-1}	1.59_{-1}	1.20_{-1}	8.87_{-2}
-1	2s	5.68_{-1}	4.68_{-1}	3.77_{-1}	3.13_{-1}	2.67_{-1}	2.06_{-1}	1.55_{-1}	8.62_{-2}	6.06_{-2}	3.84_{-2}	2.84_{-2}	2.06_{-2}
-1	1s	2.74_{-4}	8.28_{-4}	1.38_{-3}	1.85_{-3}	2.23_{-3}	2.77_{-3}	3.19_{-3}	3.28_{-3}	2.93_{-3}	2.32_{-3}	1.89_{-3}	1.49_{-3}
-1	Total	7.58	6.56	5.51	4.73	4.13	3.31	2.57	1.51	1.09	7.16_{-1}	5.40_{-1}	3.99_{-1}
1	2p	2.15	1.71	1.36	1.13	9.65_{-1}	7.57_{-1}	5.79_{-1}	3.36_{-1}	2.43_{-1}	1.59_{-1}	1.20_{-1}	8.87_{-2}
1	2s	6.30_{-1}	5.22_{-1}	4.09_{-1}	3.34_{-1}	2.81_{-1}	2.14_{-1}	1.59_{-1}	8.71_{-2}	6.09_{-2}	3.85_{-2}	2.85_{-2}	2.06_{-2}
1	1s	1.75_{-4}	9.47_{-4}	1.85_{-3}	2.62_{-3}	3.21_{-3}	3.93_{-3}	4.32_{-3}	3.92_{-3}	3.30_{-3}	2.46_{-3}	1.96_{-3}	1.52_{-3}
1	Total	9.86	7.90	6.26	5.18	4.43	3.46	2.64	1.53	1.10	7.18_{-1}	5.41_{-1}	3.99_{-1}
2	2p	1.35	1.38	1.19	1.02	8.98_{-1}	7.21_{-1}	5.61_{-1}	3.32_{-1}	2.40_{-1}	1.58_{-1}	1.20_{-1}	8.85_{-2}
2	2s	3.41_{-1}	3.93_{-1}	3.45_{-1}	2.97_{-1}	2.58_{-1}	2.03_{-1}	1.54_{-1}	8.61_{-2}	6.05_{-2}	3.84_{-2}	2.84_{-2}	2.06_{-2}
2	1s	3.97_{-5}	4.45_{-4}	1.17_{-3}	1.93_{-3}	2.61_{-3}	3.55_{-3}	4.20_{-3}	4.01_{-3}	3.37_{-3}	2.50_{-3}	1.98_{-3}	1.53_{-3}
2	Total	6.08	6.31	5.45	4.70	4.11	3.30	2.56	1.51	1.09	7.15_{-1}	5.39_{-1}	3.98_{-1}
4	2p	5.67_{-1}	8.34_{-1}	8.22_{-1}	7.65_{-1}	7.06_{-1}	6.04_{-1}	4.95_{-1}	3.12_{-1}	2.31_{-1}	1.55_{-1}	1.18_{-1}	8.76_{-2}
4	2s	1.06_{-1}	2.10_{-1}	2.23_{-1}	2.13_{-1}	1.99_{-1}	1.70_{-1}	1.36_{-1}	8.17_{-2}	5.86_{-2}	3.78_{-2}	2.81_{-2}	2.04_{-2}
4	1s	1.00_{-6}	5.34_{-5}	2.69_{-4}	6.46_{-4}	1.11_{-3}	2.02_{-3}	2.99_{-3}	3.65_{-3}	3.25_{-3}	2.47_{-3}	1.97_{-3}	1.52_{-3}
4	Total	2.48	3.75	3.74	3.49	3.22	2.76	2.26	1.42	1.05	7.00_{-1}	5.31_{-1}	3.95_{-1}
6	2p	2.83_{-1}	5.47_{-1}	5.88_{-1}	5.76_{-1}	5.50_{-1}	4.95_{-1}	4.25_{-1}	2.87_{-1}	2.21_{-1}	1.51_{-1}	1.16_{-1}	8.62_{-2}
6	2s	3.69_{-2}	1.22_{-1}	1.50_{-1}	1.55_{-1}	1.52_{-1}	1.38_{-1}	1.18_{-1}	7.59_{-2}	5.59_{-2}	3.68_{-2}	2.78_{-2}	2.02_{-2}
6	1s	1.99_{-8}	5.35_{-6}	5.25_{-5}	1.83_{-4}	3.99_{-4}	9.80_{-4}	1.84_{-3}	2.98_{-3}	2.91_{-3}	2.35_{-3}	1.91_{-3}	1.50_{-3}
6	Total	1.20	2.43	2.65	2.61	2.51	2.26	1.94	1.31	1.00	6.84_{-1}	5.25_{-1}	3.88_{-1}
8	2p	1.56_{-1}	3.86_{-1}	4.43_{-1}	4.50_{-1}	4.41_{-1}	4.11_{-1}	3.65_{-1}	2.61_{-1}	2.04_{-1}	1.45_{-1}	1.12_{-1}	8.44_{-2}
8	2s	1.37_{-2}	7.50_{-2}	1.06_{-1}	1.17_{-1}	1.19_{-1}	1.14_{-1}	1.02_{-1}	7.00_{-2}	5.28_{-2}	3.56_{-2}	2.72_{-2}	1.99_{-2}
8	1s	0.37_{-9}	5.22_{-7}	1.01_{-5}	5.11_{-5}	1.42_{-4}	4.64_{-4}	1.09_{-3}	2.34_{-3}	2.51_{-3}	2.17_{-3}	1.82_{-3}	1.45_{-3}
8	Total	6.53_{-1}	1.69	1.98	2.03	2.00	1.87	1.66	1.19	9.27_{-1}	6.54_{-1}	5.05_{-1}	3.80_{-1}

TABLE V: Total ionization cross sections for multicharge bare ions on Phosphorous at different impact energies. Cross sections are in atomic units divided \mathbb{Z}_P^2 , and projectile energies are in MeV/amu

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
-1	3p	4.43	2.95	2.19	1.74	1.45	1.08	7.95_{-1}	4.36_{-1}	3.02_{-1}	1.87_1	1.39_1	9.88_{-2}
-1	3s	1.67	1.06	7.70_{-1}	6.03_{-1}	4.95_{-1}	3.65_{-1}	2.63_{-1}	1.38_{-1}	9.36_{-2}	5.74_{-2}	4.22_{-2}	2.95_{-2}
-1	2p	2.04_{-2}	3.20_{-2}	3.77_{-2}	4.03_{-2}	4.12_{-2}	4.04_{-2}	3.73_{-2}	2.87_{-2}	2.21_{-2}	1.53_{-2}	1.19_{-2}	9.05_{-3}
-1	2s	9.82_{-3}	2.01_{-2}	2.44_{-2}	2.55_{-2}	2.53_{-2}	2.35_{-2}	2.04_{-2}	1.40_{-2}	1.04_{-2}	7.01_{-3}	5.35_{-3}	3.99_{-3}
-1	1s	7.52_{-7}	4.44_{-6}	1.12_{-5}	2.03_{-5}	3.09_{-5}	5.44_{-5}	9.01_{-5}	2.05_{-4}	2.50_{-4}	2.68_{-4}	2.54_{-4}	2.25_{-4}
-1	Total	1.68_{1}	1.12_{1}	8.38	6.72	5.62	4.27	3.17	1.78	1.25	7.81_{-1}	5.84_{-1}	4.18_{-1}
1	3p	4.83	3.10	2.26	1.78	1.47	1.10	8.00_{-1}	4.36_{-1}	3.02_{-1}	1.87_{-1}	1.39_{-1}	9.88_{-2}
1	3s	1.72	1.09	7.85_{-1}	6.12_{-1}	5.02_{-1}	3.69_{-1}	2.65_{-1}	1.38_{-1}	9.36_{-2}	5.74_{-2}	4.22_{-2}	2.95_{-2}
1	2p	1.92_{-2}	4.22_{-2}	5.18_{-2}	5.44_{-2}	5.41_{-2}	5.01_{-2}	4.35_{-2}	2.87_{-2}	2.21_{-2}	1.53_{-2}	1.19_{-2}	9.05_{-3}
1	2s	8.78_{-3}	2.15_{-2}	2.70_{-2}	2.84_{-2}	2.80_{-2}	2.57_{-2}	2.19_{-2}	1.40_{-2}	1.04_{-2}	7.01_{-3}	5.35_{-3}	3.99_{-3}
1	1s	1.93_{-7}	2.65_{-6}	9.26_{-6}	1.99_{-5}	3.34_{-5}	6.51_{-5}	1.14_{-4}	2.05_{-4}	2.50_{-4}	2.68_{-4}	2.54_{-4}	2.25_{-4}
1	Total	1.81_1	1.181	8.70	6.94	5.79	4.38	3.23	1.78	1.25	7.81_{-1}	5.84_{-1}	4.18_{-1}
2	3p	3.27	2.60	2.03	1.65	1.39	1.06	7.82_{-1}	4.36_{-1}	3.02_{-1}	1.87_{-1}	1.39_{-1}	9.88_{-2}
2	3s	1.10	9.00_{-1}	7.00_{-1}	5.66_{-1}	4.74_{-1}	3.56_{-1}	2.59_{-1}	1.38_{-1}	9.36_{-2}	5.74_{-2}	4.22_{-2}	2.95_{-2}
2	2p	5.82_{-3}	2.42_{-2}	3.77_{-2}	4.45_{-2}	4.73_{-2}	4.68_{-2}	4.21_{-2}	2.87_{-2}	2.21_{-2}	1.53_{-2}	1.19_{-2}	9.05_{-3}
2	2s	2.52_{-3}	1.16_{-2}	1.84_{-2}	2.17_{-2}	2.30_{-2}	2.28_{-2}	2.04_{-2}	1.40_{-2}	1.04_{-2}	7.01_{-3}	5.35_{-3}	3.99_{-3}
2	1s	3.62_{-8}	1.04_{-6}	4.97_{-6}	1.27_{-5}	2.39_{-5}	5.32_{-5}	1.04_{-4}	2.05_{-4}	2.50_{-4}	2.68_{-4}	2.54_{-4}	2.25_{-4}
2	Total	1.20_1	9.76	7.75	6.39	5.45	4.21	3.16	1.78	1.25	7.81_{-1}	5.84_{-1}	4.18_{-1}
4	3p	1.58	1.72	1.53	1.33	1.18	9.42_{-1}	7.23_{-1}	4.10_{-1}	2.89_{-1}	1.83_{-1}	1.35_{-1}	9.88_{-2}
4	3s	4.70_{-1}	5.80_{-1}	5.20_{-1}	4.54_{-1}	3.99_{-1}	3.17_{-1}	2.41_{-1}	1.32_{-1}	9.15_{-2}	5.67_{-2}	4.12_{-2}	2.95_{-2}
4	2p	3.62_{-4}	5.66_{-3}	1.46_{-2}	2.23_{-2}	2.78_{-2}	3.29_{-2}	3.37_{-2}	2.66_{-2}	2.11_{-2}	1.50_{-2}	1.17_{-2}	9.05_{-3}
4	2s	1.45_{-4}	2.45_{-3}	6.33_{-3}	9.75_{-3}	1.22_{-2}	1.47_{-2}	1.53_{-2}	1.24_{-2}	9.76_{-3}	6.79_{-3}	5.24_{-3}	3.99_{-3}
4	1s	0.57_{-9}	8.05_{-8}	7.62_{-7}	2.91_{-6}	7.17_{-6}	2.26_{-5}	5.85_{-5}	1.90_{-4}	2.64_{-4}	2.99_{-4}	2.82_{-4}	2.25_{-4}
4	Total	5.68	6.35	5.72	5.06	4.52	3.69	2.88	1.68	1.20	7.68_{-1}	5.70_{-1}	4.18_{-1}

TABLE VI: Phosphorous Continuated

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
6	3p	8.79_{-1}	1.18	1.16	1.07	9.79_{-1}	8.23_{-1}	6.56_{-1}	3.91_{-1}	2.80_{-1}	1.80_{-1}	1.34_{-1}	9.88_{-2}
6	3s	2.26_{-1}	3.89_{-1}	3.92_{-1}	3.64_{-1}	3.33_{-1}	2.78_{-1}	2.20_{-1}	1.27_{-1}	8.91_{-2}	5.59_{-2}	4.09_{-2}	2.95_{-2}
6	2p	2.33_{-5}	1.37_{-3}	5.61_{-3}	1.09_{-2}	1.55_{-2}	2.16_{-2}	2.51_{-2}	2.31_{-2}	1.92_{-2}	1.42_{-2}	1.13_{-2}	9.05_{-3}
6	2s	8.24_{-6}	5.32_{-4}	2.21_{-3}	4.33_{-3}	6.26_{-3}	8.95_{-3}	1.08_{-2}	1.04_{-2}	8.77_{-3}	6.43_{-3}	5.06_{-3}	3.99_{-3}
6	1s	5.76**	4.38_{-9}	8.49_{-8}	4.93_{-7}	1.61_{-6}	7.29_{-6}	2.59_{-5}	1.30_{-4}	2.13_{-4}	2.74_{-4}	2.71_{-4}	2.25_{-4}
6	Total	3.09	4.34	4.29	4.01	3.71	3.17	2.58	1.59	1.15	7.50_{-1}	5.61_{-1}	4.18_{-1}
8	3p	5.40_{-1}	8.55_{-1}	8.99_{-1}	8.71_{-1}	8.22_{-1}	7.19_{-1}	5.94_{-1}	3.70_{-1}	2.69_{-1}	1.76_{-1}	1.31_{-1}	9.88_{-2}
8	3s	1.16_{-1}	2.72_{-1}	3.01_{-1}	2.95_{-1}	2.80_{-1}	2.44_{-1}	2.00_{-1}	1.21_{-1}	8.64_{-2}	5.49_{-2}	4.04_{-2}	2.95_{-2}
8	2p	1.63_{-6}	3.59_{-4}	2.31_{-3}	5.60_{-3}	9.07_{-3}	1.45_{-2}	1.87_{-2}	1.96_{-2}	1.72_{-2}	1.33_{-2}	1.08_{-2}	9.05_{-3}
8	2s	4.72_{-7}	1.21_{-4}	8.19_{-4}	2.04_{-3}	3.39_{-3}	5.65_{-3}	7.61_{-3}	8.63_{-3}	7.73_{-3}	5.98_{-3}	4.82_{-3}	3.99_{-3}
8	1s	4.72**	0.21_{-9}	8.39_{-9}	7.50_{-8}	3.27_{-7}	2.14_{-6}	1.05_{-5}	8.19_{-5}	1.60_{-4}	2.38_{-4}	2.50_{-4}	2.25_{-4}
8	Total	1.85	3.11	3.32	3.24	3.09	2.75	2.31	1.49	1.10	7.29_{-1}	5.50_{-1}	4.18_{-1}

TABLE VII: Total ionization cross sections for multicharge bare ions on Sulfur at different impact energies. Cross sections are in atomic units divided \mathbb{Z}_P^2 , and projectile energies are in MeV/amu

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
-1	3p	4.18	2.91	2.21	1.78	1.50	1.14	8.48_{-1}	4.67_{-1}	3.28_{-1}	2.08_{-1}	1.54_{-1}	1.12_{-1}
-1	3s	1.18	7.83_{-1}	5.76_{-1}	4.55_{-1}	3.76_{-1}	2.80_{-1}	2.03_{-1}	1.07_{-1}	7.31_{-2}	4.51_{-2}	3.28_{-2}	2.34_{-2}
-1	2p	1.16_{-2}	1.94_{-2}	2.38_{-2}	2.61_{-2}	2.72_{-2}	2.76_{-2}	2.62_{-2}	2.01_{-2}	1.59_{-2}	1.14_{-2}	8.92_{-3}	6.81_{-3}
-1	2s	5.45_{-3}	1.29_{-2}	1.66_{-2}	1.81_{-2}	1.84_{-2}	1.76_{-2}	1.57_{-2}	1.08_{-2}	8.23_{-3}	5.63_{-3}	4.32_{-3}	3.24_{-3}
-1	1s	3.78_{-7}	2.37_{-6}	6.21_{-6}	1.16_{-5}	1.81_{-5}	3.30_{-5}	5.68_{-5}	1.22_{-4}	1.59_{-4}	1.86_{-4}	1.86_{-4}	1.72_{-4}
-1	Total	1.50_1	1.04_{1}	7.96	6.46	5.45	4.19	3.14	1.76	1.24	7.95_{-1}	5.91_{-1}	4.31_{-1}
1	3p	4.47	3.04	2.27	1.82	1.52	1.15	8.53_{-1}	4.68_{-1}	3.28_{-1}	2.08_{-1}	1.54_{-1}	1.12_{-1}
1	3s	1.20	8.07_{-1}	5.89_{-1}	4.63_{-1}	3.82_{-1}	2.83_{-1}	2.05_{-1}	1.07_{-1}	7.33_{-2}	4.52_{-2}	3.28_{-2}	2.34_{-2}
1	2p	1.01_{-2}	2.49_{-2}	3.26_{-2}	3.57_{-2}	3.64_{-2}	3.50_{-2}	3.12_{-2}	2.17_{-2}	1.67_{-2}	1.16_{-2}	9.03_{-3}	6.86_{-3}
1	2s	4.87_{-3}	1.37_{-2}	1.84_{-2}	2.02_{-2}	2.05_{-2}	1.94_{-2}	1.70_{-2}	1.13_{-2}	8.48_{-3}	5.72_{-3}	4.37_{-3}	3.26_{-3}
1	1s	9.04_{-8}	1.34_{-6}	5.11_{-6}	1.09_{-5}	1.89_{-5}	3.86_{-5}	7.08_{-5}	1.55_{-4}	1.96_{-4}	2.17_{-4}	2.08_{-4}	1.87_{-4}
1	Total	1.59_{1}	1.09_{1}	8.23	6.64	5.59	4.27	3.19	1.77	1.25	7.97_{-1}	5.92_{-1}	4.31_{-1}
2	3р	2.86	2.47	2.00	1.66	1.42	1.10	8.29_{-1}	4.63_{-1}	3.26_{-1}	2.08_{-1}	1.54_{-1}	1.12_{-1}
2	3s	7.17_{-1}	6.47_{-1}	5.16_{-1}	4.23_{-1}	3.57_{-1}	2.72_{-1}	2.00_{-1}	1.06_{-1}	7.29_{-2}	4.50_{-2}	3.28_{-2}	2.34_{-2}
2	2p	2.89_{-3}	1.37_{-2}	2.31_{-2}	2.87_{-2}	3.14_{-2}	3.25_{-2}	3.03_{-2}	2.16_{-2}	1.67_{-2}	1.16_{-2}	9.02_{-3}	6.86_{-3}
2	2s	1.34_{-3}	7.20_{-3}	1.23_{-2}	1.52_{-2}	1.66_{-2}	1.71_{-2}	1.58_{-2}	1.11_{-2}	8.40_{-3}	5.70_{-3}	4.36_{-3}	3.26_{-3}
2	1s	1.68_{-8}	5.22_{-7}	2.62_{-6}	6.92_{-6}	1.34_{-5}	3.12_{-5}	6.37_{-5}	1.57_{-4}	2.04_{-4}	2.26_{-4}	2.17_{-4}	1.92_{-4}
2	Total	1.00_1	8.80	7.19	6.03	5.20	4.08	3.10	1.75	1.24	7.95_{-1}	5.91_{-1}	4.31_{-1}
4	3p	1.26	1.53	1.43	1.29	1.16	9.53_{-1}	7.51_{-1}	4.42_{-1}	3.17_{-1}	2.04_{-1}	1.52_{-1}	1.11_{-1}
4	3s	2.71_{-1}	3.94_{-1}	3.69_{-1}	3.29_{-1}	2.93_{-1}	2.37_{-1}	1.83_{-1}	1.03_{-1}	7.14_{-2}	4.45_{-2}	3.25_{-2}	2.33_{-2}
4	2p	1.49_{-4}	2.80_{-3}	8.10_{-3}	1.34_{-2}	1.75_{-2}	2.22_{-2}	2.39_{-2}	1.98_{-2}	1.58_{-2}	1.13_{-2}	8.87_{-3}	6.78_{-3}
4	2s	6.51_{-5}	1.37_{-3}	3.93_{-3}	6.46_{-3}	8.42_{-3}	1.07_{-2}	1.16_{-2}	9.83_{-3}	7.85_{-3}	5.52_{-3}	4.27_{-3}	3.22_{-3}
4	1s	0.26_{-9}	3.95_{-8}	3.93_{-7}	1.56_{-6}	3.94_{-6}	1.30_{-5}	3.54_{-5}	1.27_{-4}	1.87_{-4}	2.26_{-4}	2.21_{-4}	1.97_{-4}
4	Total	4.32	5.40	5.08	4.61	4.17	3.49	2.78	1.67	1.20	7.82_{-1}	5.84_{-1}	4.27_{-1}

TABLE VIII: Sulfur Continuated

Z_P	nl	0.1	0.2	0.3	0.4	0.5	0.7	1	2	3	5	7	10
6	3p	6.65_{-1}	1.01	1.04	9.93_{-1}	9.31_{-1}	8.07_{-1}	6.65_{-1}	4.15_{-1}	3.04_{-1}	1.99_{-1}	1.50_{-1}	1.10_{-1}
6	3s	1.17_{-1}	2.53_{-1}	2.69_{-1}	2.57_{-1}	2.39_{-1}	2.04_{-1}	1.64_{-1}	9.75_{-2}	6.91_{-2}	4.38_{-2}	3.22_{-2}	2.31_{-2}
6	2p	7.47_{-6}	5.73_{-4}	2.78_{-3}	6.00_{-3}	9.20_{-3}	1.40_{-2}	1.73_{-2}	1.70_{-2}	1.44_{-2}	1.07_{-2}	8.56_{-3}	6.62_{-3}
6	2s	3.06_{-6}	2.61_{-4}	1.26_{-3}	2.67_{-3}	4.09_{-3}	6.26_{-3}	7.94_{-3}	8.19_{-3}	7.02_{-3}	5.21_{-3}	4.12_{-3}	3.14_{-3}
6	1s	2.53**	2.08_{-9}	4.23_{-8}	2.56_{-7}	8.57_{-7}	4.07_{-6}	1.53_{-5}	8.51_{-5}	1.49_{-4}	2.06_{-4}	2.12_{-4}	1.95_{-4}
6	Total	2.23	3.53	3.67	3.53	3.33	2.93	2.44	1.56	1.15	7.61_{-1}	5.74_{-1}	4.22_{-1}
8	3p	3.94_{-1}	7.05_{-1}	7.81_{-1}	7.84_{-1}	7.59_{-1}	6.89_{-1}	5.88_{-1}	3.87_{-1}	2.89_{-1}	1.94_{-1}	1.47_{-1}	1.08_{-1}
8	3s	5.39_{-2}	1.69_{-1}	2.01_{-1}	2.04_{-1}	1.97_{-1}	1.76_{-1}	1.47_{-1}	9.22_{-2}	6.66_{-2}	4.29_{-2}	3.17_{-2}	2.29_{-2}
8	2p	3.98_{-7}	1.26_{-4}	1.02_{-3}	2.82_{-3}	5.02_{-3}	9.00_{-3}	1.26_{-2}	1.43_{-2}	1.28_{-2}	9.99_{-3}	8.15_{-3}	6.41_{-3}
8	2s	1.43_{-7}	5.19_{-5}	4.20_{-4}	1.17_{-3}	2.08_{-3}	3.79_{-3}	5.47_{-3}	6.69_{-3}	6.13_{-3}	4.82_{-3}	3.91_{-3}	3.04_{-3}
8	1s	1.97**	9.30**	3.99_{-9}	3.73_{-8}	1.67_{-7}	1.15_{-6}	5.96_{-6}	5.24_{-5}	1.10_{-4}	1.77_{-4}	1.94_{-4}	1.86_{-4}
8	Total	1.29	2.45	2.75	2.78	2.71	2.48	2.15	1.45	1.09	7.36_{-1}	5.60_{-1}	4.15_{-1}