

Supplementary material for:

Investigation of positron scattering from atomic fluorine and fluorine-containing molecules

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Table S1: Positron Scattering Cross-section of F atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	1.319	1.319	0	0	0	600	1.067	0.413	0.654	0.561	0
2	1.495	1.495	0	0	0	700	0.968	0.38	0.588	0.513	0
3	1.575	1.575	0	0	0	800	0.889	0.353	0.536	0.475	0
4	1.613	1.613	0	0	0	900	0.822	0.33	0.492	0.441	0
5	1.632	1.632	0	0	0	1000	0.766	0.31	0.456	0.413	0
6	1.639	1.639	0	0	0	1500	0.577	0.241	0.336	0.314	0
7	1.64	1.64	0	0	0	2000	0.467	0.199	0.268	0.255	0
8	1.637	1.637	0	0	0	2500	0.394	0.17	0.224	0.215	0
9	1.632	1.631	0.001	0	0	3000	0.342	0.15	0.192	0.186	0
10	1.625	1.624	0.001	0	0	3500	0.303	0.134	0.169	0.165	0
11	1.622	1.615	0.007	0	0.006	4000	0.273	0.121	0.152	0.149	0
12	1.683	1.6	0.083	0	0.082	4500	0.247	0.111	0.136	0.133	0
13	1.793	1.579	0.214	0	0.213	5000	0.227	0.102	0.125	0.123	0
14	1.925	1.554	0.371	0	0.37						
15	2.068	1.529	0.539	0	0.538						
16	2.209	1.504	0.705	0	0.704						
17	2.344	1.481	0.863	0	0.862						
18	2.473	1.461	1.012	0	1.007						
19	2.59	1.442	1.148	0.004	1.116						
20	2.698	1.426	1.272	0.015	1.193						
25	3.1	1.373	1.727	0.174	1.299						
30	3.322	1.343	1.979	0.404	1.204						
35	3.428	1.319	2.109	0.614	1.063						
40	3.464	1.296	2.168	0.779	0.924						
45	3.457	1.272	2.185	0.902	0.8						
50	3.424	1.246	2.178	0.989	0.695						
60	3.317	1.193	2.124	1.092	0.53						
70	3.187	1.139	2.048	1.136	0.412						
80	3.057	1.088	1.969	1.15	0.326						
90	2.93	1.04	1.89	1.147	0.261						
100	2.809	0.995	1.814	1.134	0.211						
200	2.004	0.708	1.296	0.938	0.037						
300	1.602	0.581	1.021	0.793	0.008						
400	1.361	0.507	0.854	0.693	0.002						
500	1.193	0.454	0.739	0.618	0.001						

Table S2: Positron Scattering Cross-section of F_2 atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	1.902	1.902	0	0	0	600	2.236	0.816	1.42	1.237	0
2	2.448	2.448	0	0	0	700	2.028	0.75	1.278	1.132	0
3	2.72	2.72	0	0	0	800	1.86	0.694	1.166	1.047	0
4	2.866	2.866	0	0	0	900	1.72	0.648	1.072	0.973	0
5	2.952	2.952	0	0	0	1000	1.6	0.608	0.992	0.909	0
6	3.002	3.002	0	0	0	1500	1.204	0.472	0.732	0.691	0
7	3.032	3.032	0	0	0	2000	0.976	0.39	0.586	0.561	0
8	3.046	3.046	0	0	0	2500	0.822	0.334	0.488	0.472	0
9	3.054	3.052	0.002	0	0	3000	0.714	0.294	0.42	0.409	0
10	3.214	3.04	0.174	0	0.172	3500	0.63	0.262	0.368	0.36	0
11	3.546	3.006	0.54	0	0.538	4000	0.568	0.238	0.33	0.324	0
12	3.944	2.958	0.986	0	0.984	4500	0.516	0.218	0.298	0.293	0
13	4.362	2.91	1.452	0	1.45	5000	0.472	0.2	0.272	0.268	0
14	4.77	2.866	1.904	0	1.902						
15	5.15	2.828	2.322	0	2.32						
16	5.5	2.798	2.702	0	2.698						
17	5.816	2.776	3.04	0.007	2.98						
18	6.096	2.758	3.338	0.032	3.166						
19	6.346	2.746	3.6	0.08	3.28						
20	6.57	2.74	3.83	0.149	3.34						
25	7.312	2.73	4.582	0.669	3.18						
30	7.652	2.728	4.924	1.225	2.766						
35	7.758	2.71	5.048	1.67	2.346						
40	7.738	2.678	5.06	1.993	1.986						
45	7.642	2.636	5.006	2.217	1.682						
50	7.51	2.584	4.926	2.37	1.436						
60	7.192	2.472	4.72	2.531	1.066						
70	6.856	2.356	4.5	2.583	0.81						
80	6.536	2.244	4.292	2.584	0.626						
90	6.24	2.14	4.1	2.557	0.494						
100	5.966	2.044	3.922	2.517	0.392						
200	4.216	1.432	2.784	2.063	0.058						
300	3.366	1.164	2.202	1.747	0.01						
400	2.856	1.008	1.848	1.529	0.002						
500	2.502	0.9	1.602	1.365	0						

Table S3: Positron Scattering Cross-section of HF atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	2.524	2.524	0	0	0	600	1.272	0.465	0.807	0.714	0
2	2.745	2.745	0	0	0	700	1.15	0.426	0.724	0.651	0
3	2.798	2.798	0	0	0	800	1.051	0.394	0.657	0.598	0
4	2.794	2.794	0	0	0	900	0.97	0.368	0.602	0.553	0
5	2.77	2.77	0	0	0	1000	0.9	0.345	0.555	0.514	0
6	2.739	2.739	0	0	0	1500	0.671	0.266	0.405	0.385	0
7	2.704	2.704	0	0	0	2000	0.539	0.219	0.32	0.309	0
8	2.669	2.669	0	0	0	2500	0.453	0.187	0.266	0.259	0
9	2.633	2.632	0.001	0	0	3000	0.391	0.164	0.227	0.222	0
10	2.663	2.592	0.071	0	0.07	3500	0.344	0.146	0.198	0.194	0
11	2.848	2.537	0.311	0	0.31	4000	0.308	0.132	0.176	0.173	0
12	3.098	2.474	0.624	0	0.623	4500	0.28	0.121	0.159	0.157	0
13	3.366	2.411	0.955	0	0.954	5000	0.255	0.111	0.144	0.142	0
14	3.623	2.351	1.272	0	1.271						
15	3.859	2.296	1.563	0	1.562						
16	4.07	2.247	1.823	0	1.822						
17	4.254	2.204	2.05	0.003	2.021						
18	4.415	2.167	2.248	0.018	2.14						
19	4.551	2.133	2.418	0.049	2.203						
20	4.666	2.103	2.563	0.096	2.223						
25	5.004	1.99	3.014	0.46	2.023						
30	5.091	1.904	3.187	0.837	1.692						
35	5.054	1.83	3.224	1.127	1.391						
40	4.955	1.76	3.195	1.328	1.146						
45	4.828	1.695	3.133	1.46	0.951						
50	4.691	1.634	3.057	1.545	0.796						
60	4.414	1.523	2.891	1.624	0.571						
70	4.158	1.426	2.732	1.639	0.422						
80	3.929	1.342	2.587	1.625	0.319						
90	3.724	1.268	2.456	1.597	0.244						
100	3.543	1.204	2.339	1.562	0.19						
200	2.455	0.829	1.626	1.244	0.021						
300	1.947	0.671	1.276	1.036	0.004						
400	1.64	0.578	1.062	0.897	0						
500	1.429	0.514	0.915	0.794	0						

Table S4: Positron Scattering Cross-section of CF_4 atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	6.441	6.441	0	0	0	600	5.541	2.13	3.411	2.571	0
2	7.854	7.854	0	0	0	700	5.012	1.948	3.064	2.319	0
3	8.492	8.492	0	0	0	800	4.585	1.796	2.789	2.109	0
4	8.801	8.801	0	0	0	900	4.232	1.671	2.561	1.942	0
5	8.962	8.962	0	0	0	1000	3.93	1.564	2.366	1.792	0
6	9.041	9.041	0	0	0	1500	2.939	1.202	1.737	1.31	0
7	9.073	9.073	0	0	0	2000	2.371	0.986	1.385	1.034	0
8	9.071	9.071	0	0	0	2500	1.992	0.841	1.151	0.856	0
9	9.057	9.051	0.006	0	0	3000	1.726	0.737	0.989	0.732	0
10	9.48	8.984	0.496	0	0.344	3500	1.519	0.655	0.864	0.631	0
11	10.38	8.858	1.522	0	1.076	4000	1.367	0.593	0.774	0.563	0
12	11.455	8.698	2.757	0	1.968	4500	1.24	0.542	0.698	0.505	0
13	12.572	8.539	4.033	0	2.9	5000	1.133	0.497	0.636	0.456	0
14	13.65	8.392	5.258	0	3.804						
15	14.644	8.262	6.382	0	4.64						
16	15.549	8.155	7.394	0	5.396						
17	16.355	8.068	8.287	0.033	5.96						
18	17.063	7.994	9.069	0.147	6.332						
19	17.686	7.936	9.75	0.354	6.56						
20	18.234	7.892	10.342	0.642	6.68						
25	19.975	7.74	12.235	2.681	6.36						
30	20.662	7.625	13.037	4.645	5.532						
35	20.764	7.487	13.277	6.071	4.692						
40	20.56	7.328	13.232	6.996	3.972						
45	20.183	7.155	13.028	7.549	3.364						
50	19.731	6.971	12.76	7.85	2.872						
60	18.735	6.609	12.126	7.997	2.132						
70	17.747	6.27	11.477	7.831	1.62						
80	16.836	5.96	10.876	7.553	1.252						
90	16.013	5.68	10.333	7.249	0.988						
100	15.266	5.427	9.839	6.948	0.784						
200	10.659	3.838	6.821	4.942	0.116						
300	8.456	3.105	5.351	3.948	0.02						
400	7.135	2.667	4.468	3.332	0.004						
500	6.222	2.363	3.859	2.896	0						

Table S5: Positron Scattering Cross-section of C_2F_6 atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	5.26	5.26	0	0	0	600	9.428	3.374	6.054	5.363	0
2	9.226	9.226	0	0	0	700	8.516	3.074	5.442	4.896	0
3	11.136	11.136	0	0	0	800	7.78	2.824	4.956	4.514	0
4	12.146	12.146	0	0	0	900	7.176	2.624	4.552	4.188	0
5	12.742	12.742	0	0	0	1000	6.662	2.454	4.208	3.903	0
6	13.118	13.118	0	0	0	1500	4.966	1.874	3.092	2.942	0
7	13.406	13.346	0.06	0	0.06	2000	4	1.536	2.464	2.376	0
8	15.314	13.364	1.95	0	1.95	2500	3.358	1.31	2.048	1.991	0
9	18.404	13.202	5.202	0	5.194	3000	2.904	1.146	1.758	1.718	0
10	21.724	13.008	8.716	0	8.708	3500	2.562	1.022	1.54	1.511	0
11	24.866	12.85	12.016	0	12.008	4000	2.296	0.922	1.374	1.352	0
12	27.692	12.764	14.928	0	14.92	4500	2.078	0.84	1.238	1.221	0
13	30.144	12.742	17.402	0	17.394	5000	1.902	0.776	1.126	1.112	0
14	32.24	12.77	19.47	0.002	19.422						
15	34.002	12.83	21.172	0.07	20.668						
16	35.472	12.912	22.56	0.288	21.242						
17	36.69	12.998	23.692	0.662	21.362						
18	37.69	13.088	24.602	1.168	21.154						
19	38.492	13.168	25.324	1.767	20.732						
20	39.142	13.242	25.9	2.429	20.17						
25	40.68	13.444	27.236	5.847	16.626						
30	40.596	13.386	27.21	8.537	13.332						
35	39.782	13.158	26.624	10.341	10.716						
40	38.656	12.84	25.816	11.47	8.704						
45	37.406	12.472	24.934	12.136	7.156						
50	36.144	12.092	24.052	12.505	5.944						
60	33.744	11.352	22.392	12.718	4.224						
70	31.598	10.68	20.918	12.58	3.096						
80	29.74	10.092	19.648	12.312	2.324						
90	28.11	9.57	18.54	11.996	1.77						
100	26.682	9.108	17.574	11.669	1.368						
200	18.346	6.308	12.038	9.166	0.152						
300	14.492	5.03	9.462	7.68	0.022						
400	12.192	4.276	7.916	6.682	0.006						
500	10.606	3.76	6.846	5.943	0						

Table S6: Positron Scattering Cross-section of C_6F_6 atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	8.418	8.418	0	0	0	600	16.458	5.268	11.19	10.292	0
2	16.11	16.11	0	0	0	700	14.802	4.752	10.05	9.353	0
3	19.512	19.512	0	0	0	800	13.476	4.338	9.138	8.582	0
4	38.562	20.34	18.222	0	18.222	900	12.39	3.996	8.394	7.941	0
5	64.614	21.288	43.326	0	43.326	1000	11.466	3.72	7.746	7.371	0
6	84.744	23.61	61.134	0	61.134	1500	8.478	2.796	5.682	5.505	0
7	98.586	26.436	72.15	0	72.15	2000	6.786	2.268	4.518	4.417	0
8	107.634	29.07	78.564	0	78.564	2500	5.676	1.92	3.756	3.691	0
9	113.28	31.23	82.05	0	82.038	3000	4.884	1.674	3.21	3.166	0
10	116.574	32.868	83.706	0.002	83.652	3500	4.29	1.488	2.802	2.77	0
11	118.254	34.038	84.216	0.272	82.536	4000	3.84	1.338	2.502	2.478	0
12	118.842	34.836	84.006	1.251	79.23	4500	3.468	1.218	2.25	2.231	0
13	118.668	35.334	83.334	2.886	74.844	5000	3.162	1.116	2.046	2.031	0
14	117.978	35.604	82.374	4.954	70.038						
15	116.922	35.694	81.228	7.234	65.184						
16	115.638	35.664	79.974	9.565	60.486						
17	114.174	35.52	78.654	11.828	56.058						
18	112.62	35.304	77.316	13.967	51.936						
19	111	35.034	75.966	15.931	48.144						
20	109.344	34.716	74.628	17.716	44.664						
25	101.124	32.76	68.364	24.065	31.302						
30	93.69	30.666	63.024	27.26	22.746						
35	87.228	28.68	58.548	28.68	17.064						
40	81.654	26.886	54.768	29.144	13.134						
45	76.836	25.296	51.54	29.097	10.32						
50	72.654	23.898	48.756	28.778	8.25						
60	65.748	21.588	44.16	27.797	5.454						
70	60.33	19.788	40.542	26.691	3.75						
80	55.98	18.348	37.632	25.654	2.628						
90	52.392	17.16	35.232	24.688	1.89						
100	49.368	16.164	33.204	23.811	1.374						
200	33.114	10.722	22.392	18.16	0.084						
300	25.872	8.298	17.574	15.059	0.006						
400	21.552	6.888	14.664	12.986	0						
500	18.612	5.946	12.666	11.467	0						

Table S7: Positron Scattering Cross-section of CHF_3 atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	4.83	4.83	0	0	0	600	4.879	1.76	3.119	2.763	0
2	6.557	6.557	0	0	0	700	4.402	1.603	2.799	2.518	0
3	7.337	7.337	0	0	0	800	4.018	1.474	2.544	2.317	0
4	7.723	7.723	0	0	0	900	3.7	1.366	2.334	2.147	0
5	7.927	7.927	0	0	0	1000	3.432	1.276	2.156	2	0
6	8.037	8.037	0	0	0	1500	2.552	0.973	1.579	1.503	0
7	8.092	8.092	0	0	0	2000	2.051	0.797	1.254	1.209	0
8	8.681	8.068	0.613	0	0.613	2500	1.72	0.679	1.041	1.012	0
9	10.051	7.941	2.11	0	2.106	3000	1.484	0.594	0.89	0.87	0
10	11.647	7.775	3.872	0	3.868	3500	1.305	0.529	0.776	0.761	0
11	13.216	7.624	5.592	0	5.588	4000	1.169	0.475	0.694	0.683	0
12	14.653	7.507	7.146	0	7.142	4500	1.06	0.436	0.624	0.615	0
13	15.911	7.423	8.488	0	8.484	5000	0.968	0.399	0.569	0.562	0
14	17	7.372	9.628	0	9.624						
15	17.919	7.342	10.577	0.021	10.396						
16	18.685	7.328	11.357	0.112	10.788						
17	19.325	7.324	12.001	0.287	10.915						
18	19.85	7.329	12.521	0.536	10.851						
19	20.276	7.333	12.943	0.841	10.664						
20	20.616	7.337	13.279	1.184	10.389						
25	21.422	7.313	14.109	3.007	8.565						
30	21.364	7.204	14.16	4.466	6.834						
35	20.913	7.031	13.882	5.444	5.461						
40	20.297	6.822	13.475	6.05	4.419						
45	19.628	6.604	13.024	6.407	3.62						
50	18.955	6.387	12.568	6.602	2.998						
60	17.678	5.975	11.703	6.711	2.116						
70	16.546	5.611	10.935	6.632	1.544						
80	15.565	5.295	10.27	6.485	1.152						
90	14.707	5.017	9.69	6.311	0.875						
100	13.954	4.771	9.183	6.134	0.672						
200	9.568	3.301	6.267	4.78	0.071						
300	7.541	2.631	4.91	3.987	0.01						
400	6.327	2.235	4.092	3.457	0						
500	5.496	1.965	3.531	3.065	0						

Table S8: Positron Scattering Cross-section of $C_2H_2F_2$ atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	6.256	6.256	0	0	0	600	5.853	1.905	3.948	3.63	0
2	8.547	8.547	0	0	0	700	5.252	1.718	3.534	3.288	0
3	9.493	9.493	0	0	0	800	4.772	1.567	3.205	3.01	0
4	11.303	9.828	1.475	0	1.475	900	4.383	1.445	2.938	2.779	0
5	18.018	9.617	8.401	0	8.401	1000	4.05	1.342	2.708	2.577	0
6	24.704	9.675	15.029	0	15.029	1500	2.977	1.006	1.971	1.91	0
7	29.912	10.072	19.84	0	19.84	2000	2.372	0.814	1.558	1.523	0
8	33.683	10.597	23.086	0	23.086	2500	1.98	0.689	1.291	1.269	0
9	36.299	11.128	25.171	0	25.167	3000	1.7	0.6	1.1	1.085	0
10	38.046	11.588	26.458	0	26.454	3500	1.488	0.532	0.956	0.945	0
11	39.155	11.953	27.202	0.02	26.997	4000	1.327	0.478	0.849	0.841	0
12	39.803	12.222	27.581	0.218	26.533	4500	1.195	0.434	0.761	0.755	0
13	40.117	12.405	27.712	0.66	25.468	5000	1.09	0.399	0.691	0.686	0
14	40.193	12.517	27.676	1.295	24.1						
15	40.094	12.572	27.522	2.051	22.604						
16	39.871	12.58	27.291	2.86	21.093						
17	39.557	12.551	27.006	3.676	19.624						
18	39.176	12.496	26.68	4.464	18.228						
19	38.75	12.416	26.334	5.205	16.927						
20	38.295	12.323	25.972	5.889	15.719						
25	35.831	11.701	24.13	8.4	11.019						
30	33.417	10.992	22.425	9.715	7.982						
35	31.239	10.302	20.937	10.32	5.976						
40	29.319	9.671	19.648	10.538	4.593						
45	27.639	9.106	18.533	10.549	3.608						
50	26.167	8.607	17.56	10.45	2.882						
60	23.724	7.783	15.941	10.106	1.908						
70	21.793	7.139	14.654	9.711	1.307						
80	20.232	6.622	13.61	9.327	0.919						
90	18.94	6.197	12.743	8.973	0.656						
100	17.847	5.838	12.009	8.644	0.481						
200	11.934	3.881	8.053	6.536	0.028						
300	9.286	3.006	6.28	5.381	0.002						
400	7.708	2.495	5.213	4.614	0.002						
500	6.635	2.154	4.481	4.056	0						

Table S9: Positron Scattering Cross-section of $C_2H_3F_3$ atom in units of \AA^2

E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}	E (eV)	Q_{total}	Q_{el}	Q_{inel}	Q_{ion}	Q_{ps}
1	6.53	6.53	0	0	0	600	6.472	2.305	4.167	3.757	0
2	9.278	9.278	0	0	0	700	5.805	2.088	3.717	3.398	0
3	10.467	10.467	0	0	0	800	5.298	1.916	3.382	3.126	0
4	11.035	11.035	0	0	0	900	4.866	1.772	3.094	2.884	0
5	11.333	11.333	0	0	0	1000	4.502	1.651	2.851	2.677	0
6	11.495	11.495	0	0	0	1500	3.323	1.25	2.073	1.99	0
7	11.942	11.552	0.39	0	0.39	2000	2.651	1.014	1.637	1.59	0
8	14.007	11.419	2.588	0	2.588	2500	2.213	0.86	1.353	1.323	0
9	16.683	11.186	5.497	0	5.492	3000	1.906	0.752	1.154	1.133	0
10	19.367	10.971	8.396	0	8.391	3500	1.671	0.667	1.004	0.989	0
11	21.803	10.805	10.998	0	10.993	4000	1.493	0.601	0.892	0.881	0
12	23.912	10.7	13.212	0	13.207	4500	1.349	0.547	0.802	0.793	0
13	25.691	10.644	15.047	0	15.042	5000	1.23	0.504	0.726	0.719	0
14	27.166	10.627	16.539	0.01	16.41						
15	28.372	10.629	17.743	0.11	17.099						
16	29.34	10.643	18.697	0.348	17.286						
17	30.115	10.659	19.456	0.713	17.145						
18	30.723	10.677	20.046	1.18	16.773						
19	31.188	10.687	20.501	1.714	16.264						
20	31.533	10.688	20.845	2.287	15.668						
25	32.066	10.59	21.476	5.1	12.417						
30	31.513	10.337	21.176	7.189	9.665						
35	30.515	9.997	20.518	8.512	7.593						
40	29.355	9.619	19.736	9.282	6.06						
45	28.177	9.24	18.937	9.695	4.915						
50	27.043	8.877	18.166	9.887	4.042						
60	24.975	8.218	16.757	9.903	2.828						
70	23.208	7.666	15.542	9.695	2.046						
80	21.708	7.198	14.51	9.413	1.52						
90	20.419	6.796	13.623	9.114	1.147						
100	19.306	6.449	12.857	8.821	0.877						
200	13.02	4.436	8.584	6.727	0.089						
300	10.171	3.51	6.661	5.545	0.011						
400	8.475	2.958	5.517	4.765	0						
500	7.322	2.582	4.74	4.194	0						