

Supplemental Material for:

Positron Scattering from Structurally Related Biomolecules

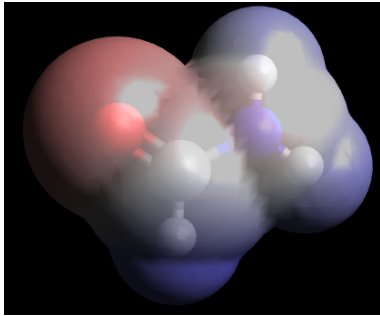
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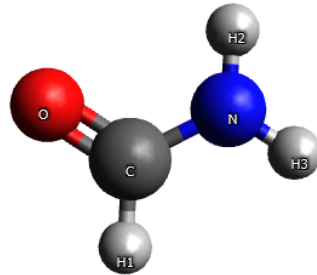
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Table S1: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from HCONH_2 , in units of \AA^2 .

$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	34.236	0	34.236	55.75683	90	16.789	7.701	5.808	2.43256
2	26.714	0	26.714	38.71197	100	15.778	7.406	5.459	2.14733
3	23.148	0	23.148	30.78365	120	14.167	6.893	4.908	1.73875
4	22.878	0	20.588	26.04567	140	12.931	6.464	4.491	1.44034
5	27.302	0	17.87	22.82853	160	11.938	6.099	4.158	1.21126
6	31.732	0	16.159	20.46533	180	11.126	5.782	3.884	1.04506
7	35.08	0	15.324	18.63542	200	10.437	5.504	3.653	0.91854
8	37.358	0	14.951	17.1619	250	9.091	4.933	3.199	0.70622
9	38.795	0	14.764	15.94243	300	8.095	4.485	2.862	0.57708
10	39.609	0	14.651	14.90936	350	7.32	4.12	2.598	0.49162
11	39.976	0.031	14.55	14.02047	400	6.695	3.815	2.387	0.42804
12	40.024	0.25	14.432	13.24324	450	6.18	3.557	2.211	0.37389
13	39.851	0.695	14.291	12.55599	500	5.742	3.331	2.062	0.33221
14	39.526	1.309	14.127	11.94298	600	5.047	2.964	1.824	0.27192
15	39.096	2.02	13.946	11.39163	700	4.514	2.673	1.642	0.23144
16	38.593	2.767	13.749	10.89201	800	4.093	2.436	1.499	0.20027
17	38.045	3.509	13.542	10.43644	900	3.746	2.239	1.379	0.17421
18	37.469	4.217	13.329	10.01883	1000	3.454	2.068	1.281	0.1529
19	36.88	4.875	13.115	9.63424	1500	2.521	1.515	0.957	0.08723
20	36.285	5.476	12.899	9.27866	2000	1.999	1.196	0.776	0.05848
30	30.793	8.684	10.902	6.77829	2500	1.664	0.989	0.658	0.04409
40	26.652	9.265	9.372	5.33534	3000	1.428	0.84	0.576	0.03589
50	23.591	9.104	8.241	4.40342	3500	1.252	0.729	0.515	0.03157
60	21.267	8.757	7.394	3.75897	4000	1.118	0.644	0.468	0.02718
70	19.451	8.382	6.744	3.25427	4500	1.014	0.577	0.432	0.02483
80	17.991	8.027	6.228	2.79833	5000	0.931	0.521	0.406	0.02655



(a) Electrostatic Potential Surface (EPS)



(b) Molecular geometry

Figure S1: Structures of HCONH_2

Table S2: Q_{ps} and Q_{exc} for positron scattering from HCONH₂, in units of Å².

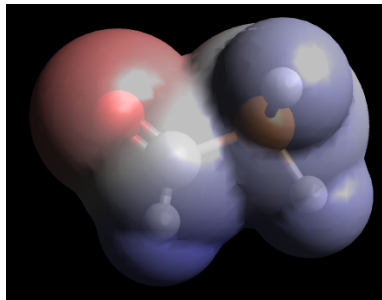
$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}
1	0	0	19	15.036	3.854	400	0	0.493
2	0	0	20	13.927	3.983	450	0	0.412
3	0	0	30	7.002	4.205	500	0	0.349
4	2.29	0	40	4.045	3.97	600	0	0.259
5	9.432	0	50	2.556	3.69	700	0	0.199
6	15.573	0	60	1.704	3.412	800	0	0.158
7	19.756	0	70	1.177	3.148	900	0	0.128
8	22.407	0	80	0.833	2.903	1000	0	0.105
9	24.028	0.003	90	0.6	2.68	1500	0	0.049
10	24.955	0.003	100	0.436	2.477	2000	0	0.027
11	25.156	0.239	120	0.237	2.129	2500	0	0.017
12	24.469	0.873	140	0.132	1.844	3000	0	0.012
13	23.292	1.573	160	0.072	1.609	3500	0	0.008
14	21.888	2.202	180	0.044	1.416	4000	0	0.006
15	20.411	2.719	200	0.025	1.255	4500	0	0.005
16	18.95	3.127	250	0.006	0.953	5000	0	0.004
17	17.552	3.442	300	0.001	0.747			
18	16.245	3.678	350	0.001	0.601			

Table S3: Q_{ps} and Q_{exc} for positron scattering from HCOPH₂, in units of Å².

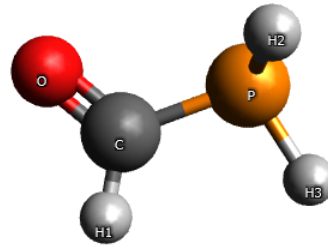
$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}
1	0	0	19	15.417	5.026	400	0	0.468
2	0	0	20	14.074	5.116	450	0	0.389
3	0.918	0	30	6.335	4.995	500	0	0.327
4	11.047	0	40	3.393	4.542	600	0	0.24
5	20.208	0	50	2.008	4.116	700	0	0.183
6	25.904	0	60	1.255	3.734	800	0	0.144
7	29.104	0	70	0.808	3.395	900	0	0.116
8	30.784	0	80	0.534	3.093	1000	0	0.095
9	31.558	0.003	90	0.357	2.826	1500	0	0.043
10	31.672	0.119	100	0.241	2.59	2000	0	0.023
11	30.616	0.878	120	0.112	2.194	2500	0	0.014
12	28.819	1.835	140	0.054	1.878	3000	0	0.01
13	26.705	2.711	160	0.025	1.624	3500	0	0.007
14	24.518	3.427	180	0.013	1.417	4000	0	0.005
15	22.393	3.978	200	0.004	1.247	4500	0	0.004
16	20.402	4.386	250	0.001	0.933	5000	0	0.003
17	18.574	4.68	300	0.001	0.722			
18	16.913	4.886	350	0	0.576			

Table S4: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from HCOPH₂, in units of Å².

$E(eV)$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(eV)$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	45.903	0	45.903	71.71248	90	20.259	9.599	7.477	2.73285
2	35.079	0	35.079	47.72947	100	19.12	9.217	7.072	2.51273
3	31.033	0	30.115	37.36029	120	17.28	8.561	6.413	2.15531
4	36.321	0	25.274	31.39367	140	15.84	8.017	5.891	1.85992
5	42.491	0	22.283	27.42519	160	14.67	7.554	5.467	1.61715
6	46.802	0	20.898	24.54335	180	13.697	7.154	5.113	1.43088
7	49.377	0	20.273	22.32571	200	12.865	6.804	4.81	1.28317
8	50.708	0	19.924	20.54638	250	11.238	6.084	4.22	1.01384
9	51.205	0	19.644	19.07608	300	10.029	5.52	3.786	0.83792
10	51.164	0.01	19.363	17.83172	350	9.09	5.065	3.449	0.7159
11	50.777	0.221	19.062	16.76091	400	8.333	4.684	3.181	0.62082
12	50.174	0.777	18.743	15.82472	450	7.711	4.364	2.958	0.54211
13	49.438	1.611	18.411	14.99684	500	7.186	4.086	2.773	0.48
14	48.638	2.607	18.086	13.96395	600	6.35	3.635	2.475	0.38847
15	47.796	3.665	17.76	12.91962	700	5.708	3.278	2.247	0.32439
16	46.931	4.714	17.429	12.01359	800	5.199	2.989	2.066	0.2778
17	46.059	5.708	17.097	11.22407	900	4.785	2.751	1.918	0.24176
18	45.19	6.624	16.767	10.53289	1000	4.434	2.546	1.793	0.21235
19	44.331	7.448	16.44	9.92486	1500	3.297	1.876	1.378	0.12012
20	43.49	8.18	16.12	9.38734	2000	2.651	1.49	1.138	0.07756
30	36.36	11.654	13.376	6.2449	2500	2.228	1.236	0.978	0.05556
40	31.397	11.98	11.482	4.85588	3000	1.927	1.053	0.864	0.04293
50	27.877	11.571	10.182	4.09088	3500	1.699	0.914	0.778	0.03612
60	25.263	11.031	9.243	3.6157	4000	1.525	0.809	0.711	0.03048
70	23.233	10.505	8.525	3.28504	4500	1.386	0.724	0.658	0.02745
80	21.604	10.026	7.951	2.99368	5000	1.275	0.654	0.618	0.02907



(a) Electrostatic Potential Surface (EPS)

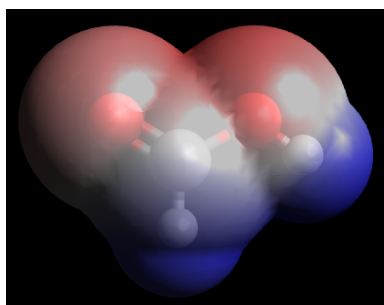


(b) Molecular geometry

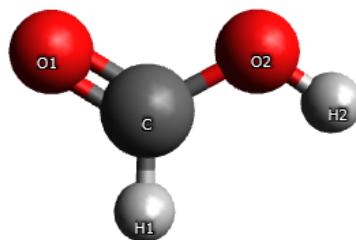
Figure S2: Structures of HCOPH₂

Table S5: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from HCOOH, in units of \AA^2 .

$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	29.439	0	29.439	48.64892	90	14.538	6.653	5.127	2.52983
2	23.194	0	23.194	34.41716	100	13.708	6.413	4.837	2.28036
3	20.153	0	20.153	27.60701	120	12.366	5.986	4.37	1.85237
4	18.284	0	18.284	23.47023	140	11.322	5.623	4.012	1.52407
5	17.45	0	16.914	20.63263	160	10.479	5.308	3.726	1.2735
6	19.193	0	15.401	18.53478	180	9.781	5.036	3.489	1.09207
7	21.579	0	14.063	16.90398	200	9.192	4.798	3.289	0.95475
8	23.736	0	13.082	15.58755	250	8.037	4.306	2.896	0.72699
9	25.458	0	12.413	14.49692	300	7.178	3.918	2.604	0.58988
10	26.749	0	11.959	13.57247	350	6.507	3.605	2.374	0.49934
11	27.672	0	11.642	12.77734	400	5.965	3.342	2.189	0.43211
12	28.297	0.01	11.406	12.08235	450	5.518	3.119	2.035	0.3756
13	28.688	0.123	11.217	11.46824	500	5.136	2.925	1.903	0.33217
14	28.901	0.389	11.055	10.92106	600	4.53	2.608	1.692	0.26943
15	28.972	0.785	10.906	10.42946	700	4.064	2.357	1.53	0.22727
16	28.94	1.268	10.766	9.9845	800	3.69	2.152	1.398	0.19857
17	28.827	1.799	10.628	9.5792	900	3.385	1.98	1.291	0.17723
18	28.651	2.346	10.491	9.20808	1000	3.126	1.831	1.201	0.15976
19	28.431	2.886	10.356	8.86671	1500	2.297	1.35	0.904	0.09267
20	28.177	3.404	10.221	8.5514	2000	1.829	1.07	0.735	0.06212
30	25.029	6.65	8.929	6.34283	2500	1.525	0.886	0.624	0.04673
40	22.165	7.549	7.861	5.06894	3000	1.316	0.757	0.549	0.03798
50	19.901	7.625	7.031	4.23762	3500	1.156	0.657	0.492	0.03324
60	18.116	7.441	6.388	3.653	4000	1.036	0.584	0.447	0.02852
70	16.684	7.18	5.88	3.21645	4500	0.942	0.524	0.414	0.02604
80	15.515	6.911	5.469	2.84215	5000	0.866	0.474	0.389	0.02761



(a) Electrostatic Potential Surface (EPS)



(b) Molecular geometry

Figure S3: Structures of HCOOH

Table S6: Q_{ps} and Q_{exc} for positron scattering from HCOOH, in units of \AA^2 .

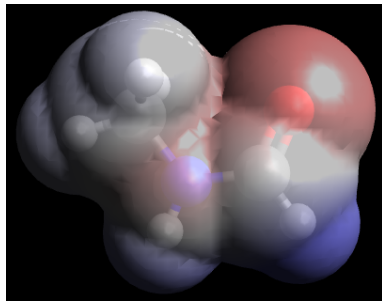
$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}
1	0	0	19	12.407	2.782	400	0	0.434
2	0	0	20	11.603	2.949	450	0.001	0.363
3	0	0	30	6.073	3.377	500	0	0.308
4	0	0	40	3.52	3.235	600	0	0.23
5	0.536	0	50	2.212	3.033	700	0	0.177
6	3.792	0	60	1.463	2.824	800	0	0.14
7	7.516	0	70	1.003	2.621	900	0	0.114
8	10.654	0	80	0.704	2.431	1000	0	0.094
9	13.042	0.003	90	0.503	2.255	1500	0	0.043
10	14.787	0.003	100	0.364	2.094	2000	0	0.024
11	16.027	0.003	120	0.198	1.812	2500	0	0.015
12	16.773	0.108	140	0.109	1.578	3000	0	0.01
13	16.823	0.525	160	0.061	1.384	3500	0	0.007
14	16.421	1.036	180	0.034	1.222	4000	0	0.005
15	15.758	1.523	200	0.019	1.086	4500	0	0.004
16	14.962	1.944	250	0.005	0.83	5000	0	0.003
17	14.11	2.29	300	0.002	0.654			
18	13.248	2.566	350	0	0.528			

Table S7: Q_{ps} and Q_{exc} for positron scattering from C_2H_5NO , in units of \AA^2 .

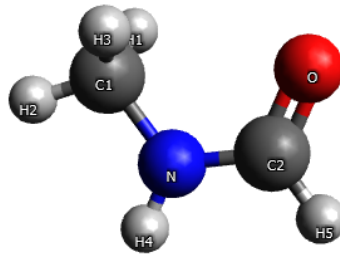
$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}	$E(eV)$	Q_{ps}	Q_{exc}
1	0	0	19	21.81	5.87	400	0	0.698
2	0	0	20	20.143	6.031	450	0	0.582
3	0	0	30	9.995	6.235	500	0	0.492
4	8.335	0	40	5.779	5.848	600	0	0.364
5	20.437	0	50	3.671	5.41	700	0	0.28
6	28.961	0	60	2.463	4.983	800	0	0.222
7	34.136	0	70	1.711	4.584	900	0	0.179
8	37.08	0	80	1.215	4.217	1000	0	0.147
9	38.629	0.004	90	0.878	3.884	1500	0	0.068
10	39.384	0.017	100	0.642	3.584	2000	0	0.038
11	38.83	0.663	120	0.352	3.069	2500	0	0.024
12	37.173	1.715	140	0.194	2.652	3000	0	0.016
13	34.973	2.759	160	0.109	2.31	3500	0	0.012
14	32.569	3.653	180	0.063	2.029	4000	0	0.009
15	30.153	4.369	200	0.036	1.795	4500	0	0.007
16	27.829	4.922	250	0.01	1.358	5000	0	0.005
17	25.654	5.337	300	0.002	1.062			
18	23.646	5.646	350	0.001	0.852			

Table S8: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from C_2H_5NO , in units of \AA^2 .

$E(eV)$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(eV)$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	53.208	0	53.208	84.74332	90	24.303	11.088	8.453	3.17997
2	40.654	0	40.654	56.99274	100	22.814	10.647	7.941	2.79673
3	34.963	0	34.963	44.7317	120	20.445	9.889	7.135	2.25423
4	38.298	0	29.963	37.59864	140	18.63	9.262	6.522	1.86927
5	46.321	0	25.884	32.82961	160	17.178	8.727	6.032	1.57899
6	52.905	0	23.944	29.359	180	15.984	8.264	5.628	1.36686
7	57.371	0	23.235	26.68683	200	14.975	7.858	5.286	1.20442
8	60.106	0	23.026	24.54282	250	13.004	7.025	4.611	0.93112
9	61.588	0	22.955	22.77191	300	11.548	6.373	4.111	0.76576
10	62.211	0	22.81	21.27348	350	10.419	5.844	3.722	0.65646
11	62.234	0.124	22.617	19.98449	400	9.508	5.401	3.409	0.57561
12	61.862	0.598	22.376	18.85741	450	8.761	5.029	3.15	0.50804
13	61.223	1.404	22.087	17.8604	500	8.13	4.704	2.934	0.45474
14	60.413	2.428	21.763	16.97043	600	7.129	4.176	2.589	0.36635
15	59.498	3.559	21.417	16.16923	700	6.362	3.758	2.324	0.30552
16	58.516	4.711	21.054	15.44249	800	5.756	3.419	2.115	0.25728
17	57.501	5.827	20.683	14.77912	900	5.263	3.139	1.945	0.22224
18	56.472	6.871	20.309	14.17036	1000	4.846	2.897	1.802	0.19422
19	55.441	7.827	19.934	13.60916	1500	3.518	2.111	1.339	0.11075
20	54.424	8.687	19.563	13.08971	2000	2.781	1.661	1.082	0.07442
30	45.541	13.041	16.27	9.24491	2500	2.307	1.369	0.914	0.05626
40	39.112	13.646	13.839	7.04626	3000	1.976	1.161	0.799	0.04589
50	34.454	13.282	12.091	5.71434	3500	1.729	1.004	0.713	0.04054
60	30.96	12.706	10.808	4.81094	4000	1.543	0.886	0.648	0.03505
70	28.252	12.119	9.838	4.15299	4500	1.393	0.789	0.597	0.03195
80	26.082	11.578	9.072	3.61718	5000	1.278	0.713	0.56	0.0344



(a) Electrostatic Potential Surface (EPS)

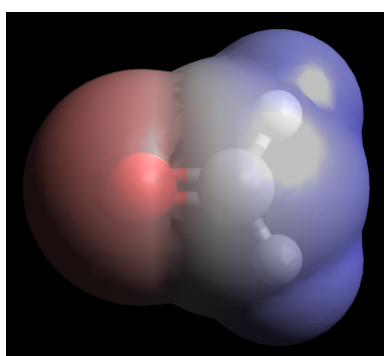


(b) Molecular geometry

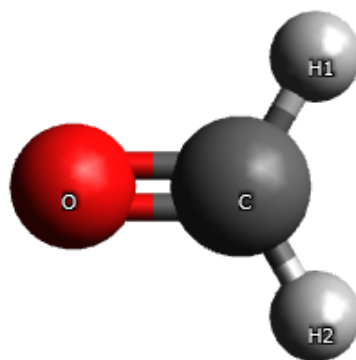
Figure S4: Structures of C_2H_5NO

Table S9: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from CH_2O , in units of \AA^2 .

$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	21.158	0	21.158	34.84578	90	10.831	4.929	3.834	1.57829
2	16.966	0	16.966	24.92176	100	10.193	4.739	3.614	1.41283
3	14.901	0	14.901	20.08386	120	9.165	4.409	3.262	1.17175
4	13.625	0	13.625	17.12211	140	8.369	4.129	2.991	0.98124
5	14.1	0	12.469	15.08007	160	7.73	3.89	2.774	0.82511
6	16.13	0	11.267	13.56339	180	7.199	3.684	2.593	0.71079
7	18.159	0	10.375	12.37879	200	6.752	3.503	2.439	0.62343
8	19.805	0	9.783	11.41814	250	5.877	3.132	2.137	0.47778
9	21.023	0	9.407	10.61841	300	5.228	2.842	1.912	0.39057
10	21.879	0	9.164	9.93748	350	4.725	2.607	1.736	0.33299
11	22.444	0	8.994	9.34902	400	4.319	2.41	1.595	0.29205
12	22.785	0.034	8.86	8.83251	450	3.984	2.246	1.477	0.25857
13	22.958	0.183	8.742	8.37423	500	3.701	2.102	1.378	0.22715
14	23.004	0.452	8.631	7.96425	600	3.252	1.868	1.22	0.18167
15	22.956	0.811	8.522	7.59453	700	2.907	1.683	1.098	0.15122
16	22.84	1.224	8.413	7.25872	800	2.633	1.533	1	0.13046
17	22.672	1.659	8.303	6.95192	900	2.411	1.408	0.922	0.11494
18	22.466	2.096	8.191	6.67019	1000	2.223	1.302	0.855	0.10177
19	22.232	2.517	8.078	6.41039	1500	1.62	0.951	0.638	0.0581
20	21.98	2.914	7.966	6.16988	2000	1.285	0.751	0.517	0.03886
30	19.217	5.255	6.881	4.477	2500	1.067	0.619	0.437	0.02923
40	16.852	5.799	5.992	3.51041	3000	0.917	0.527	0.383	0.02387
50	15.028	5.771	5.317	2.89764	3500	0.803	0.456	0.342	0.02092
60	13.616	5.584	4.807	2.4328	4000	0.718	0.403	0.311	0.01803
70	12.496	5.358	4.412	2.06294	4500	0.651	0.361	0.287	0.01658
80	11.587	5.136	4.095	1.78839	5000	0.597	0.326	0.269	0.01774



(a) Electrostatic Potential Surface (EPS)



(b) Molecular geometry

Figure S5: Structures of CH_2O

Table S10: Q_{ps} and Q_{exc} for positron scattering from CH_2O , in units of \AA^2 .

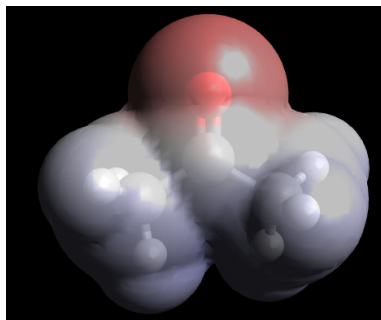
$E(\text{eV})$	Q_{ps}	Q_{exc}	$E(\text{eV})$	Q_{ps}	Q_{exc}	$E(\text{eV})$	Q_{ps}	Q_{exc}
1	0	0	19	9.393	2.244	400	0.001	0.313
2	0	0	20	8.743	2.357	450	0	0.261
3	0	0	30	4.462	2.619	500	0	0.221
4	0	0	40	2.576	2.485	600	0	0.164
5	1.631	0	50	1.627	2.313	700	0	0.126
6	4.863	0	60	1.084	2.141	800	0	0.1
7	7.784	0	70	0.748	1.978	900	0	0.081
8	10.022	0	80	0.529	1.827	1000	0	0.066
9	11.614	0.003	90	0.379	1.689	1500	0	0.031
10	12.713	0.002	100	0.277	1.563	2000	0	0.017
11	13.447	0.003	120	0.149	1.345	2500	0	0.011
12	13.677	0.214	140	0.082	1.167	3000	0	0.007
13	13.439	0.594	160	0.047	1.019	3500	0	0.005
14	12.925	0.996	180	0.025	0.897	4000	0	0.004
15	12.265	1.358	200	0.014	0.796	4500	0	0.003
16	11.542	1.661	250	0.004	0.604	5000	0	0.002
17	10.805	1.905	300	0	0.474			
18	10.083	2.096	350	0.001	0.381			

Table S11: Q_{ps} and Q_{exc} for positron scattering from CH_3COCH_3 , in units of \AA^2 .

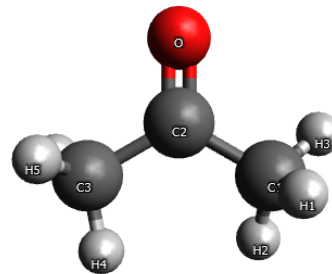
$E(\text{eV})$	Q_{ps}	Q_{exc}	$E(\text{eV})$	Q_{ps}	Q_{exc}	$E(\text{eV})$	Q_{ps}	Q_{exc}
1	0	0	19	22.849	6.288	400	0	0.725
2	0	0	20	21.077	6.451	450	0	0.604
3	0.127	0	30	10.391	6.643	500	0	0.51
4	11.396	0	40	6.005	6.219	600	0	0.377
5	24.343	0	50	3.831	5.74	700	0	0.289
6	32.841	0	60	2.583	5.275	800	0	0.228
7	37.765	0	70	1.804	4.842	900	0	0.185
8	40.426	0	80	1.288	4.448	1000	0	0.152
9	41.722	0.005	90	0.932	4.092	1500	0	0.07
10	42.291	0.054	100	0.681	3.772	2000	0	0.039
11	41.423	0.842	120	0.373	3.226	2500	0	0.024
12	39.478	1.984	140	0.209	2.782	3000	0	0.017
13	37.023	3.084	160	0.119	2.421	3500	0	0.012
14	34.393	4.014	180	0.071	2.123	4000	0	0.009
15	31.774	4.753	200	0.04	1.876	4500	0	0.007
16	29.277	5.32	250	0.009	1.417	5000	0	0.005
17	26.947	5.745	300	0.003	1.106			
18	24.803	6.059	350	0.002	0.885			

Table S12: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from CH_3COCH_3 , in units of \AA^2 .

$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	57.262	0	57.262	90.46728	90	25.795	11.654	9.117	3.00936
2	43.761	0	43.761	60.57685	100	24.207	11.181	8.573	2.68691
3	37.825	0	37.698	47.5089	120	21.687	10.375	7.713	2.1834
4	43.255	0	31.859	39.94965	140	19.751	9.705	7.055	1.8237
5	52.086	0	27.743	34.91063	160	18.201	9.135	6.526	1.54913
6	58.872	0	26.031	31.24799	180	16.921	8.641	6.086	1.34678
7	63.279	0	25.514	28.42805	200	15.841	8.212	5.713	1.19072
8	65.84	0	25.414	26.16404	250	13.728	7.33	4.972	0.92696
9	67.107	0	25.381	24.29168	300	12.168	6.639	4.42	0.76759
10	67.509	0.003	25.161	22.70501	350	10.954	6.074	3.993	0.65636
11	67.312	0.178	24.869	21.33751	400	9.988	5.612	3.651	0.572
12	66.732	0.742	24.528	20.13943	450	9.189	5.217	3.368	0.50746
13	65.908	1.652	24.149	19.07734	500	8.518	4.875	3.133	0.45519
14	64.931	2.78	23.744	18.12703	600	7.453	4.318	2.758	0.35688
15	63.861	4.008	23.326	17.26946	700	6.642	3.881	2.472	0.29107
16	62.743	5.246	22.9	16.48966	800	6	3.527	2.245	0.24485
17	61.597	6.435	22.47	15.77616	900	5.478	3.232	2.061	0.21138
18	60.45	7.544	22.044	15.11978	1000	5.042	2.981	1.909	0.1847
19	59.311	8.553	21.621	14.51325	1500	3.646	2.164	1.412	0.10517
20	58.189	9.457	21.204	13.95048	2000	2.872	1.698	1.135	0.07066
30	48.557	13.96	17.563	9.57473	2500	2.378	1.397	0.957	0.05352
40	41.633	14.512	14.897	7.06779	3000	2.033	1.182	0.834	0.04381
50	36.625	14.063	12.991	5.61613	3500	1.774	1.02	0.742	0.03886
60	32.887	13.415	11.614	4.646	4000	1.58	0.898	0.673	0.03371
70	29.995	12.769	10.58	3.94421	4500	1.426	0.799	0.62	0.03081
80	27.686	12.18	9.77	3.41643	5000	1.304	0.717	0.582	0.03341



(a) Electrostatic Potential Surface (EPS)



(b) Molecular geometry

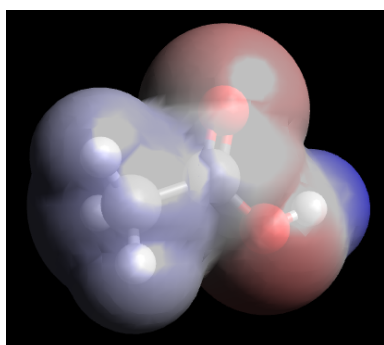
Figure S6: Structures of CH_3COCH_3

Table S13: Q_{total} , Q_{ion} , Q_{el} and Q_{mtcs} for positron scattering from HCOOCH_3 , in units of \AA^2 .

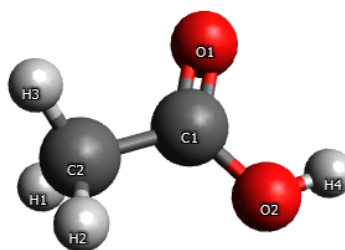
$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}	$E(\text{eV})$	Q_{total}	Q_{ion}	Q_{el}	Q_{mtcs}
1	47.558	0	47.558	76.540	90	21.823	9.884	7.773	3.234
2	36.594	0	36.594	52.210	100	20.538	9.507	7.327	2.923
3	31.538	0	31.538	41.262	120	18.475	8.85	6.613	2.362
4	28.632	0	28.508	34.831	140	16.88	8.297	6.064	1.948
5	31.046	0	25.468	30.507	160	15.596	7.822	5.625	1.638
6	35.62	0	22.754	27.349	180	14.535	7.415	5.259	1.412
7	39.719	0	20.971	24.912	200	13.637	7.056	4.947	1.240
8	42.834	0	19.917	22.954	250	11.879	6.319	4.333	0.953
9	45.025	0	19.3	21.336	300	10.576	5.741	3.876	0.779
10	46.469	0	18.857	19.966	350	9.562	5.272	3.52	0.659
11	47.335	0.003	18.525	18.787	400	8.743	4.878	3.233	0.568
12	47.772	0.126	18.25	17.756	450	8.071	4.548	2.995	0.500
13	47.898	0.508	18.001	16.844	500	7.5	4.259	2.794	0.446
14	47.794	1.128	17.758	16.030	600	6.591	3.786	2.473	0.357
15	47.525	1.91	17.518	15.297	700	5.895	3.414	2.225	0.297
16	47.139	2.781	17.277	14.631	800	5.343	3.112	2.029	0.256
17	46.667	3.679	17.033	14.024	900	4.892	2.861	1.867	0.225
18	46.135	4.563	16.787	13.467	1000	4.512	2.644	1.733	0.201
19	45.561	5.406	16.54	12.952	1500	3.291	1.935	1.294	0.116
20	44.964	6.19	16.295	12.476	2000	2.608	1.527	1.046	0.078
30	38.947	10.696	14.002	8.915	2500	2.172	1.263	0.887	0.059
40	34.05	11.697	12.174	6.862	3000	1.865	1.074	0.776	0.048
50	30.322	11.603	10.794	5.606	3500	1.636	0.931	0.694	0.042
60	27.447	11.207	9.751	4.742	4000	1.462	0.824	0.63	0.036
70	25.181	10.745	8.948	4.105	4500	1.325	0.737	0.582	0.033
80	23.346	10.298	8.304	3.618	5000	1.215	0.665	0.545	0.035

Table S14: Q_{ps} and Q_{exc} for positron scattering from HCOOCH_3 , in units of \AA^2 .

$E(\text{eV})$	Q_{ps}	Q_{exc}	$E(\text{eV})$	Q_{ps}	Q_{exc}	$E(\text{eV})$	Q_{ps}	Q_{exc}
1	0	0	19	18.983	4.632	400	0	0.632
2	0	0	20	17.644	4.835	450	0	0.528
3	0	0	30	8.968	5.281	500	0	0.447
4	0.124	0	40	5.166	5.013	600	0	0.332
5	5.578	0	50	3.258	4.667	700	0	0.256
6	12.866	0	60	2.169	4.32	800	0	0.202
7	18.748	0	70	1.498	3.99	900	0	0.164
8	22.917	0	80	1.06	3.684	1000	0	0.135
9	25.721	0.005	90	0.762	3.404	1500	0	0.062
10	27.608	0.004	100	0.554	3.15	2000	0	0.035
11	28.755	0.052	120	0.301	2.711	2500	0	0.022
12	28.766	0.63	140	0.167	2.352	3000	0	0.015
13	27.936	1.453	160	0.094	2.055	3500	0	0.011
14	26.641	2.267	180	0.052	1.809	4000	0	0.008
15	25.123	2.974	200	0.03	1.604	4500	0	0.006
16	23.529	3.552	250	0.007	1.22	5000	0	0.005
17	21.946	4.009	300	0.002	0.957			
18	20.422	4.363	350	0	0.77			



(a) Electrostatic Potential Surface (EPS)



(b) Molecular geometry

Figure S7: Structures of HCOOCH_3