

Improving polarization description in positron-molecule scattering: a model potential approach

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Incident positron momentum (a.u.)	s-wave eigenphase (rad)		
	H ₂	N ₂	CH ₄
0.008573132	0.01411269	0.03340589	0.13063085
0.019170107	0.03652013	0.07611124	0.29330678
0.027110625	0.05406132	0.10453511	0.39471020
0.060621201	0.11371377	0.19926181	0.62798867
0.085731324	0.14263317	0.23431420	0.68097297
0.121242402	0.17333215	0.25410801	0.68729384
0.148491010	0.18554381	0.25166616	0.66214361
0.171462649	0.19042626	0.23798514	0.63005327
0.191701069	0.19116275	0.22193283	0.59914581
0.209998000	0.18969175	0.20598375	0.57096193
0.226823764	0.18743980	0.18925334	0.54291593
0.242484804	0.18401944	0.17169634	0.51346372
0.257193973	0.17926157	0.15419835	0.48620551
0.271106252	0.17348814	0.13592294	0.45902773
0.284338636	0.16768931	0.11853010	0.43378212
0.296982020	0.15987559	0.10103990	0.40991292
0.309108686	0.15406447	0.08396869	0.38713826
0.320777244	0.14853989	0.06776179	0.36523596
0.332035992	0.14301263	0.05179953	0.34388346
0.342925298	0.13714682	0.03601836	0.32340909
0.353479306	0.13089376	0.02014428	0.30355441
0.363727205	0.12431535	0.00503020	0.28417029
0.373694180	0.11774518	-0.01028275	0.26554603
0.383402139	0.11105184	-0.02541386	0.24754969
0.392870284	0.10471918	-0.03950122	0.23017063
0.402115556	0.09822719	-0.05302265	0.21345369
0.411152989	0.09184499	-0.06614604	0.19716001
0.419996000	0.08613479	-0.07920945	0.18131395
0.428656622	0.08031205	-0.09189216	0.16596579
0.437145697	0.07445707	-0.10486336	0.15096256
0.445473029	0.06895290	-0.11678322	0.13633751
0.453647528	0.06334760	-0.12868665	0.12201189
0.461677312	0.05777664	-0.14065107	0.10805506
0.469569803	0.05222569	-0.15237581	0.09451364
0.477331813	0.04669777	-0.16373557	0.08089939
0.484969607	0.04122822	-0.17483022	0.06782491
0.492488964	0.03579676	-0.18614707	0.05489711

0.499895229	0.03041762	-0.19703658	0.04241586
0.507193356	0.02509071	-0.20824592	0.02998812
0.514387947	0.01981986	-0.21859087	0.01800779
0.521483288	0.01460521	-0.22936129	0.00611212
0.528483377	0.00946902	-0.23970258	-0.00544034
0.535391950	0.00435860	-0.24983387	-0.01675875
0.542212504	-0.00067671	-0.25985645	-0.02784970
0.548948322	-0.00566779	-0.26959595	-0.03872103
0.555602484	-0.01060377	-0.27932231	-0.04937989
0.562177890	-0.01535533	-0.28888153	-0.05983469
0.568677272	-0.02033630	-0.29839416	-0.07009781
0.575103208	-0.02513921	-0.30763578	-0.08016563
0.581458133	-0.02967827	-0.31680247	-0.09006366
0.587744349	-0.03435134	-0.32581068	-0.09982070
0.593964039	-0.03893616	-0.33464505	-0.10936934
0.600119271	-0.04392084	-0.34341360	-0.11877141
0.606212009	-0.04827460	-0.35203348	-0.12803110
0.612244118	-0.05248088	-0.36059214	-0.13718707
0.618217373	-0.05734147	-0.36901239	-0.14604522
0.624133463	-0.06186860	-0.37739469	-0.15487246
0.629994000	-0.06583572	-0.38569306	-0.16351244
0.635800519	-0.07081194	-0.39407586	-0.17206510
0.641554487	-0.07450154	-0.40185206	-0.18070153
0.647257306	-0.07901808	-0.40987132	-0.18912098
0.652910315	-0.08367150	-0.41808300	-0.19725378
0.658514799	-0.08697557	-0.42532069	-0.20558313
0.664071984	-0.09201495	-0.43371919	-0.21356707
0.669583049	-0.09563853	-0.44091662	-0.22138090
0.675049124	-0.10016615	-0.44839261	-0.22918483
0.680471293	-0.10363366	-0.45628440	-0.23688260
0.685850596	-0.10755263	-0.46331799	-0.24442493
0.691188035	-0.11132578	-0.47015434	-0.25197866
0.696484573	-0.11502076	-0.47779502	-0.25929620
0.701741135	-0.11827571	-0.48510585	-0.26669229
0.706958613	-0.12191722	-0.49188718	-0.27379189
0.712137866	-0.12546803	-0.49895889	-0.28083352
0.717279722	-0.12910405	-0.50597633	-0.28781488
0.722384980	-0.13271303	-0.51320175	-0.29469368
0.727454411	-0.13609680	-0.51904101	-0.30148685
0.732488758	-0.13926438	-0.52616429	-0.30815728
0.737488739	-0.14244282	-0.53293679	-0.31474655
0.742455049	-0.14579885	-0.53927590	-0.32124161
0.747388360	-0.14908080	-0.54550142	-0.32764250
0.752289319	-0.15242713	-0.55189327	-0.33394015
0.757158557	-0.15558870	-0.55844369	-0.34013761
0.761996680	-0.15874028	-0.56447091	-0.34631125
0.766804278	-0.16192569	-0.57076516	-0.35237003
0.771581920	-0.16506648	-0.57708430	-0.35834196
0.776330162	-0.16818988	-0.58311426	-0.36426281
0.781049537	-0.17130371	-0.58916846	-0.37006552

0.785740568	-0.17437503	-0.59484536	-0.37579838
0.790403758	-0.17748024	-0.60069377	-0.38145542
0.795039596	-0.18055812	-0.60641162	-0.38704410
0.799648560	-0.18358450	-0.61222513	-0.39255866
0.804231111	-0.18641146	-0.61793353	-0.39800591
0.808787698	-0.18937696	-0.62359070	-0.40338597
0.813318757	-0.19249237	-0.62912241	-0.40870122
0.817824712	-0.19569857	-0.63465721	-0.41395342
0.822305977	-0.19870784	-0.64013465	-0.41914479
0.826762953	-0.20164521	-0.64553526	-0.42427156
0.831196030	-0.20436387	-0.65090750	-0.42934887
0.835605589	-0.20739689	-0.65623357	-0.43436655
0.839992000	-0.21035071	-0.66150614	-0.43933029
0.844355624	-0.21331133	-0.66674318	-0.44424042
0.848696813	-0.21600194	-0.67193522	-0.44909846
0.853015908	-0.21878956	-0.67709095	-0.45390800
0.857313245	-0.22148394	-0.68222229	-0.45866770

Table S1: s-wave eigenphase for the elastic scattering of positrons from H₂, N₂ and CH₄ calculated in the S+V_{corr} approximation.

Scattering angle (degrees)	Differential scattering cross section ($\text{\AA}^2/\text{str}$)					
	1.0 eV	2.0 eV	3.0 eV	5.0 eV	6.0 eV	10.0 eV
0.0	56.685029	48.770821	43.488393	35.615840	32.728434	23.535681
2.5	56.567468	48.587024	43.267166	35.348738	32.443528	23.234309
5.0	56.216203	48.039596	42.609621	34.558359	31.602435	22.351493
7.5	55.635454	47.140292	41.533925	33.276817	30.245057	20.948902
10.0	54.832165	45.908282	40.069532	31.555494	28.434780	19.122197
12.5	53.815860	44.369527	38.255997	29.462002	26.254070	16.991330
15.0	52.598458	42.555941	36.141404	27.076256	23.798896	14.688817
17.5	51.194040	40.504396	33.780485	24.485964	21.172443	12.347431
20.0	49.618580	38.255575	31.232536	21.781837	18.478645	10.088791
22.5	47.889653	35.852747	28.559218	19.052883	15.816075	8.014113
25.0	46.026117	33.340507	25.822354	16.382071	13.272628	6.197952
27.5	44.047779	30.763515	23.081832	13.842641	10.921376	4.685375
30.0	41.975076	28.165307	20.393682	11.495259	8.817789	3.492452
32.5	39.828744	25.587179	17.808420	9.386138	6.998447	2.609579
35.0	37.629510	23.067218	15.369705	7.546165	5.481154	2.006870
37.5	35.397806	20.639482	13.113365	5.991000	4.266322	1.640651
40.0	33.153504	18.333360	11.066791	4.722062	3.339344	1.460172
42.5	30.915688	16.173110	9.248710	3.728225	2.673683	1.413724
45.0	28.702460	14.177600	7.669331	2.988054	2.234310	1.453579
47.5	26.530783	12.360223	6.330794	2.472376	1.981224	1.539439
50.0	24.416358	10.728993	5.227923	2.146973	1.872752	1.640321
52.5	22.373547	9.286802	4.349181	1.975226	1.868431	1.734992
55.0	20.415326	8.031810	3.677804	1.920527	1.931318	1.811243
57.5	18.553278	6.957956	3.193005	1.948350	2.029668	1.864372
60.0	16.797605	6.055555	2.871222	2.027892	2.137942	1.895226
62.5	15.157183	5.311964	2.687320	2.133225	2.237211	1.908153
65.0	13.639629	4.712277	2.615700	2.243961	2.315023	1.909128
67.5	12.251384	4.240045	2.631281	2.345444	2.364849	1.904234
70.0	10.997822	3.877979	2.710308	2.428529	2.385219	1.898577
72.5	9.883352	3.608629	2.830975	2.489004	2.378675	1.895676
75.0	8.911531	3.415023	2.973865	2.526751	2.350645	1.897253
77.5	8.085177	3.281240	3.122215	2.544740	2.308321	1.903373
80.0	7.406472	3.192928	3.262024	2.547918	2.259623	1.912811
82.5	6.877056	3.137736	3.382056	2.542134	2.212295	1.923551
85.0	6.498116	3.105685	3.473757	2.533114	2.173132	1.933329
87.5	6.270447	3.089444	3.531134	2.525609	2.147409	1.940124
90.0	6.194508	3.084532	3.550650	2.522746	2.138456	1.942552

Table S2: “Folded” differential cross sections for the elastic scattering of positrons from pyrazine calculated in the $S+V_{\text{corr}}$ approximation.

Incident positron energy (eV)	Integral cross section ($\text{\AA}^2$)
0.001	564.8967993
0.005	551.1507573
0.01	534.8500708
0.05	435.4649942
0.1	377.1866263
0.2	379.2401877
0.3	336.7276797
0.4	286.7141587
0.5	248.0873131
0.6	216.2143839
0.7	189.6147873
0.8	167.7455676
0.9	149.9519676
1.0	135.5387156
1.1	123.8730197
1.2	114.4086592
1.3	106.6798542
1.4	100.2884823
1.5	94.90303461
1.6	90.26703297
1.7	86.19232058
1.8	82.53750542
1.9	79.20859869
2.0	76.14059178
2.1	73.29161201
2.2	70.63300685
2.3	68.14374336
2.4	65.80861599
2.5	63.61304086
2.6	61.54530437
2.7	59.60243821
2.8	57.76932925
2.9	56.03718738
3.0	54.40777399
3.1	52.86663681
3.2	51.41127517
3.3	50.03456516
3.4	48.73109661
3.5	47.49743359
3.6	46.32660337
3.7	45.21704621
3.8	44.16267427
3.9	43.16118852
4.0	42.20737764
4.1	41.30087479
4.2	40.43560333
4.3	39.61126926
4.4	38.82357972
4.5	38.07052691

4.6	37.34994342
4.7	36.65998105
4.8	35.99798793
4.9	35.36284115
5.0	34.75319937
5.1	34.16609149
5.2	33.60126828
5.3	33.05712798
5.4	32.53277730
5.5	32.02671809
5.6	31.53703495
5.7	31.06615292
5.8	30.60985758
5.9	30.16630914
6.0	29.73856832
6.1	29.32041847
6.2	28.91889951
6.3	28.52861251
6.4	28.14746563
6.5	27.78026670
6.6	27.41782070
6.7	27.07030161
6.8	26.72829713
6.9	26.39759796
7.0	26.07391463
7.1	25.75601416
7.2	25.44754254
7.3	25.14759695
7.4	24.85202176
7.5	24.56394070
7.6	24.28244283
7.7	24.00717728
7.8	23.73870885
7.9	23.47531427
8.0	23.21700948
8.1	22.96468387
8.2	22.71729964
8.3	22.47554286
8.4	22.23825562
8.5	22.00569526
8.6	21.77780298
8.7	21.55463729
8.8	21.33562052
8.9	21.12096126
9.0	20.91063517
9.1	20.70419476
9.2	20.50187776
9.3	20.30340808
9.4	20.10932028
9.5	19.91844469

9.6	19.73084040
9.7	19.54775381
9.8	19.36781753
9.9	19.19152359
10.0	19.01838222

Table S3: Integral cross section for the elastic scattering of positrons from pyrazine in the $S+V_{\text{corr}}$ approximation.

Incident positron energy (eV)	s-wave eigenphase (rad)
0.001	3.032756
0.005	2.899333
0.01	2.800890
0.05	2.410031
0.1	2.150372
0.2	1.832590
0.3	1.622705
0.4	1.464641
0.5	1.337553
0.6	1.231292
0.7	1.140125
0.8	1.060504
0.9	0.990072
1.0	0.927181
1.1	0.870626
1.2	0.819489
1.3	0.773021
1.4	0.730608
1.5	0.691706
1.6	0.655861
1.7	0.622692
1.8	0.591864
1.9	0.563100
2.0	0.536167
2.1	0.510878
2.2	0.487075
2.3	0.464652
2.4	0.443487
2.5	0.423479
2.6	0.404582
2.7	0.386740
2.8	0.369901
2.9	0.354012
3.0	0.339047
3.1	0.324976
3.2	0.311770
3.3	0.299400
3.4	0.287845
3.5	0.277087
3.6	0.267107
3.7	0.257891
3.8	0.249414
3.9	0.241670
4.0	0.234633
4.1	0.228296
4.2	0.222649
4.3	0.217674
4.4	0.213358
4.5	0.209686

4.6	0.206651
4.7	0.204235
4.8	0.202430
4.9	0.201220
5.0	0.200596
5.1	0.200542
5.2	0.201053
5.3	0.202109
5.4	0.203691
5.5	0.205803
5.6	0.208412
5.7	0.211514
5.8	0.215088
5.9	0.219113
6.0	0.223579
6.1	0.228453
6.2	0.233719
6.3	0.239355
6.4	0.245336
6.5	0.251634
6.6	0.258221
6.7	0.265071
6.8	0.272142
6.9	0.279418
7.0	0.286857
7.1	0.294438
7.2	0.302119
7.3	0.309872
7.4	0.317663
7.5	0.325464
7.6	0.333254
7.7	0.340992
7.8	0.348666
7.9	0.356233
8.0	0.363688
8.1	0.371006
8.2	0.378168
8.3	0.385158
8.4	0.391962
8.5	0.398571
8.6	0.404974
8.7	0.411161
8.8	0.417128
8.9	0.422867
9.0	0.428384
9.1	0.433669
9.2	0.438725
9.3	0.443551
9.4	0.448152
9.5	0.460056

9.6	0.462388
9.7	0.460631
9.8	0.464353
9.9	0.467869
10.0	0.471184

Table S4: s-wave eigenphase for the elastic scattering of positrons from pyrazine in the $S+V_{\text{corr}}$ approximation.