

## Spectroscopic properties and spin-orbit coupling of electronic excited states of germanium dimer

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Fig S1. Potential energy curves of Ge<sub>2</sub> for (a)  $\Omega = 0^+$ , (b)  $\Omega = 0^-$ , (c)  $\Omega = 1$ , (d)  $\Omega = 2$  and (e)  $\Omega = 3$  and 4 states. In all cases, the ground state is shown for comparison.

Table SI. The raw data of PECs of the  $\Lambda$ -S states.

Table SII The raw data of PECs of the  $\Omega$  states.

Table SIII R-dependent transition dipole moments of the selected  $\Omega$  transitions for

$$F^3\Sigma_{u1}^+ - X^3\Sigma_{g1}^-, \quad F^3\Sigma_{u0}^+ - X^3\Sigma_{g1}^-, \quad H^3\Sigma_{u1}^- - X^3\Sigma_{g1}^-, \quad H^3\Sigma_{u1}^- - X^3\Sigma_{g0}^+, \\ H^3\Sigma_{u0}^- - X^3\Sigma_{g0}^+, \text{ and } H^3\Sigma_{u0}^- - X^3\Sigma_{g1}^-.$$

Table SIV Franck-Condon factors of the  $F^3\Sigma_{u1}^+ - X^3\Sigma_{g1}^-$ ,  $F^3\Sigma_{u0}^+ - X^3\Sigma_{g1}^-$ ,

$$H^3\Sigma_{u1}^- - X^3\Sigma_{g1}^-, \quad H^3\Sigma_{u1}^- - X^3\Sigma_{g0}^+, \quad H^3\Sigma_{u0}^- - X^3\Sigma_{g0}^+ \text{ and } H^3\Sigma_{u0}^- - X^3\Sigma_{g1}^-$$

transitions.

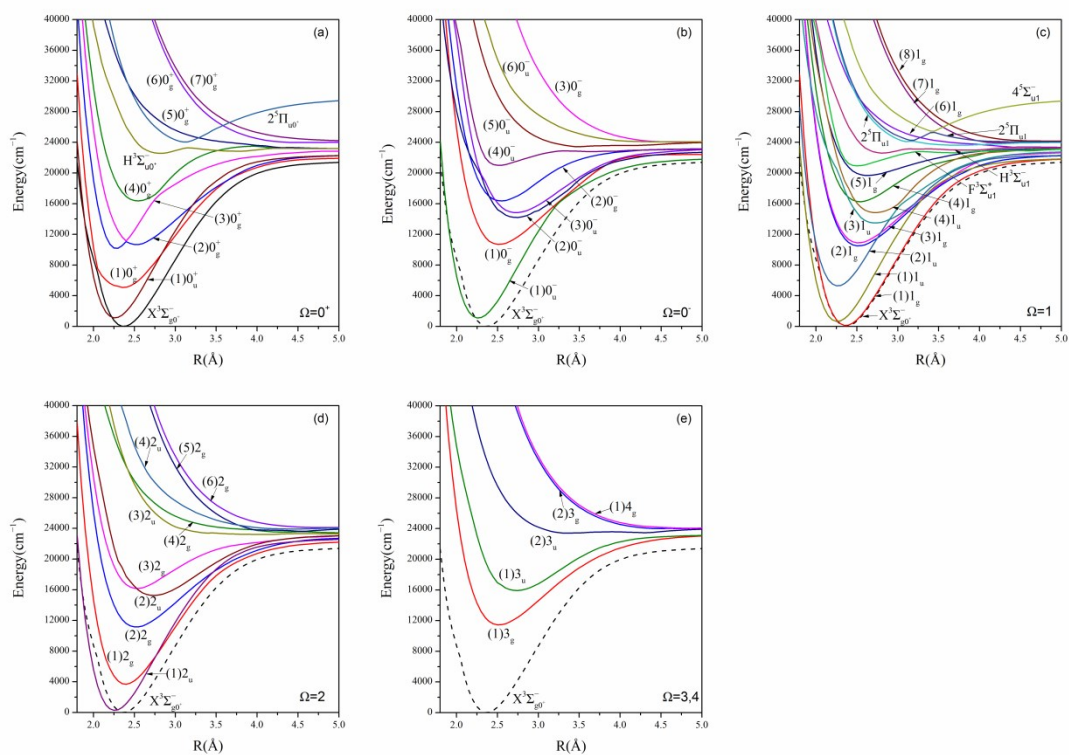


FIG. S1. Potential energy curves of  $\text{Ge}_2$  for (a)  $\Omega = 0^+$ , (b)  $\Omega = 0^-$ , (c)  $\Omega = 1$ , (d)  $\Omega = 2$ , and (e)  $\Omega = 3$  and 4 states. In all cases, the ground state is shown for comparison.

Table SI The raw data of PECs of the  $\Lambda$ -S states.

R	$\chi^2\Sigma_g^-$	$F^2\Sigma_u^-$	$H^2\Sigma_u^+$	$2^5\Pi_u$	$4^5\Sigma_u^-$
1.8	32721.19988	53455.34978	57821.99516	79594.53419	74928.4305
1.85	25052.54893	47895.15315	51495.55923	71073.39245	71188.68759
1.9	18925.97689	43800.5062	46399.06794	64065.2068	66555.88827
1.95	14007.49555	40893.94653	42294.79631	58195.13404	61942.50128
2	10085.5759	38834.70509	39003.12412	53254.20155	57871.43888
2.05	7004.914577	36469.65819	36355.26134	49070.56983	54235.74149
2.1	4633.037632	32698.73549	34228.57644	45505.42724	50996.51205
2.15	2857.726738	29332.92945	32489.18238	42445.71209	48113.19652
2.2	1583.119179	26556.44635	30990.86875	39794.74988	45618.72279
2.25	722.9452822	24339.66613	29602.63476	37490.79735	43351.32958
2.3	221.497381	22701.76569	28245.49755	35489.70971	41312.92335
2.35	14.2705	21641.66677	26963.63239	33742.86687	39487.48715
2.4	51.23580444	21070.39043	25831.21835	32219.02238	37844.19344
2.45	317.508411	20824.37425	24999.23142	30914.44084	36073.30978
2.5	746.1728161	20757.96496	24168.72432	29777.56549	34566.95203
2.55	1303.884397	20794.66375	23555.69068	28788.56923	33306.98672
2.6	1961.180883	20896.57866	23100.71358	27929.62006	32254.6632
2.65	2731.162141	21053.65026	22813.40193	27216.52031	31218.20176
2.7	3540.745775	21217.20522	22603.09824	26581.95444	30432.20018
2.75	4389.057779	21384.02609	22480.63033	26029.10265	29763.31325
2.8	5265.953645	21551.40944	22435.4575	25548.64977	29177.54116
2.85	6164.6678	21718.10541	22459.60186	25133.92995	28652.79433
2.9	7076.470789	21880.99616	22543.10282	24776.92998	28178.96342
2.95	7993.173165	22037.28516	22676.28439	24470.07451	27749.28436
3	8907.096671	22184.92232	22850.31895	24206.65757	27357.89095
3.05	9812.191232	22322.58011	23057.31426	23980.86604	27000.4474
3.1	10702.84179	22449.52901	23290.27944	23787.69352	26672.8555
3.15	11574.30966	22565.50604	23543.05654	23622.82999	26371.72547
3.2	12422.51577	22670.58981	23810.22879	23482.54143	26094.23977
3.25	13253.11266	22768.68976	24098.52175	23373.60225	25816.96715
3.3	14044.24793	22852.68542	24379.92047	23272.13179	25582.7281
3.35	14802.65092	22927.0743	24662.62016	23186.43951	25366.59305
3.4	15526.03107	22992.55278	24943.38207	23114.43267	25167.10564
3.45	16212.53206	23049.88392	25219.60581	23054.3797	24982.87535
3.5	16860.66534	23099.83305	25489.22265	23004.79587	24812.65341
3.55	17469.2755	23143.13049	25750.58656	22964.36858	24655.36192
3.6	18037.5168	23180.45327	26002.40615	22931.92176	24510.0749
3.65	18564.87375	23212.42544	26243.69931	22906.40399	24375.98225
3.7	19051.18496	23239.61681	26473.7634	22886.87787	24252.36369
3.75	19496.68082	23262.54465	26692.1392	22872.50775	24138.5591
3.8	19902.01184	23281.67404	26898.58733	22862.55355	24033.95775
3.85	20268.2815	23297.42585	27093.04837	22856.36085	23937.98445
3.9	20597.03724	23310.17931	27275.62731	22853.35169	23850.09598
3.95	20890.24955	23320.274	27446.55476	22853.0201	23769.77292
4	21150.24632	23328.01317	27606.16231	22854.91756	23696.51634
4.1	21581.17592	23337.50319	27893.13982	22863.89387	23569.31877
4.2	21911.98266	23340.53908	28140.46919	22877.7269	23464.92623
4.3	22164.23417	23338.66175	28352.48988	22894.49541	23380.06688
4.4	22356.68026	23333.13521	28533.57686	22912.78342	23311.78541
4.5	22504.37438	23324.98384	28687.89661	22931.56729	23257.44087
4.6	22618.79386	23315.03029	28819.26603	22950.12694	23214.70134
4.7	22708.43112	23303.92743	28931.09183	22967.97991	23181.53845
4.8	22779.4728	23292.17749	29026.34827	22984.81767	23156.20308
4.9	22836.41228	23280.15998	29107.60265	23000.46263	23137.20605
5	22882.52379	23268.15627	29177.04629	23014.83346	23123.29401
5.1	22920.21511	23256.37011	29236.53474	23027.91586	23113.42123
5.2	22951.27594	23244.93995	29287.63214	23039.74068	23106.72249
5.3	22977.05657	23233.96123	29331.65388	23050.36909	23102.49018
5.4	22998.58728	23223.49121	29369.69992	23059.87872	23100.14786
5.5	23016.66543	23213.56317	29402.69067	23068.35645	23099.23083
5.6	23031.92022	23204.1909	29431.40072	23075.89507	23099.37055
5.7	23044.84348	23195.37223	29456.47159	23082.58076	23100.26973
5.8	23055.83869	23187.09961	29478.44685	23088.50393	23101.70229
5.9	23065.22455	23179.35394	29497.7774	23093.7431	23103.48714
6	23073.26269	23172.11263	29514.85045	23098.37254	23105.48698
7	23113.20316	23122.17861	29615.22702	23123.48868	23124.48739
8	23125.00645	23098.71031	29655.78516	23131.56978	23134.0999
9	23129.06245	23087.72307	29654.58744	23134.61468	23137.85268
10	23130.68574	23083.08145	29648.84986	23135.93298	23139.42207



Table SIII R-dependent transition dipole moments of the selected  $\Omega$  transitions for

$$F^3\Sigma_{u1}^+ - X^3\Sigma_{g1}^-, \quad F^3\Sigma_{u0}^+ - X^3\Sigma_{g1}^-, \quad H^3\Sigma_{u1}^- - X^3\Sigma_{g1}^-, \quad H^3\Sigma_{u1}^- - X^3\Sigma_{g0}^+,$$

$$H^3\Sigma_{u0}^- - X^3\Sigma_{g0}^+, \text{ and } H^3\Sigma_{u0}^- - X^3\Sigma_{g1}^-.$$

R	$F^3\Sigma_{u1}^+ - X^3\Sigma_{g1}^-$	$F^3\Sigma_{u0}^+ - X^3\Sigma_{g1}^-$	$H^3\Sigma_{u1}^- - X^3\Sigma_{g1}^-$	$H^3\Sigma_{u1}^- - X^3\Sigma_{g0}^+$	$H^3\Sigma_{u0}^- - X^3\Sigma_{g0}^+$	$H^3\Sigma_{u0}^- - X^3\Sigma_{g1}^-$
2.1	0	0.9967	0.9936	0.9873	0.9989	0.1945
2.15	0	0.9964	0.9936	0.9916	0.9991	0.21635
2.2	0	0.9962	0.9965	0.9918	0.9994	0.25888
2.25	0	0.9958	0.9982	0.9902	0.9996	0.33831
2.3	0	0.9954	0.9988	0.9878	0.9997	0.46394
2.35	0	0.9951	0.999	0.9959	0.9997	0.62479
2.4	0	0.9946	0.9992	0.9954	0.9996	0.75697
2.45	0	0.9941	0.999	0.9949	0.9995	0.80449
2.5	0	0.9934	0.9988	0.9943	0.9993	0.81214
2.55	0.0076	0.993	0.9854	0.9939	0.9949	0.80436
2.6	0.0116	0.9922	0.9796	0.9932	0.9935	0.79296
2.65	0.0174	0.9913	0.9714	0.9924	0.9917	0.75744
2.7	0.0266	0.9902	0.9588	0.9914	0.9895	0.74036
2.75	0.0398	0.9888	0.9406	0.9902	0.9863	0.72682
2.8	0.0574	0.9873	0.9158	0.9887	0.9819	0.71449
2.85	0.076	0.9854	0.8858	0.987	0.9753	0.70123
2.9	0.0888	0.983	0.854	0.9849	0.9647	0.68655
2.95	0.0882	0.9802	0.8206	0.9824	0.9463	0.67032
3	0.0708	0.9768	0.775	0.9793	0.911	0.65252
3.05	0.0394	0.9726	0.6876	0.9755	0.8359	0.63311
3.1	0.0076	0.9671	0.5326	0.9707	0.6739	0.61211
3.15	0.0044	0.9602	0.3558	0.9647	0.4185	0.58951
3.2	0.0644	0.9514	0.2316	0.957	0.2128	0.56535
3.25	0.2104	0.9398	0.1564	0.947	0.1108	0.5322
3.3	0.3784	0.9246	0.106	0.9338	0.0643	0.50575
3.35	0.4194	0.9042	0.0692	0.9162	0.041	0.47831
3.4	0.3148	0.877	0.0414	0.8926	0.0282	0.45005
3.45	0.1892	0.8406	0.0234	0.8607	0.0204	0.42114
3.5	0.1144	0.7928	0.0142	0.8179	0.0154	0.39177
3.6	0.0552	0.6592	0.0066	0.6923	0.0096	0.33253
3.7	0.0364	0.4962	0.0038	0.5258	0.0064	0.27461
3.8	0.0312	0.3552	0.0024	0.3712	0.0044	0.22059
3.9	0.04	0.2606	0.0014	0.2641	0	0.17279
4	0.086	0.204	4E-4	0.1992	0	0.13263

Table SIV Franck-Condon factors of the  $F^3\Sigma_{u1}^+ - X^3\Sigma_{g1}^-$ ,  $F^3\Sigma_{u0}^+ - X^3\Sigma_{g1}^-$ ,  
 $H^3\Sigma_{u1}^- - X^3\Sigma_{g1}^-$ ,  $H^3\Sigma_{u1}^- - X^3\Sigma_{g0}^-$ ,  $H^3\Sigma_{u0}^- - X^3\Sigma_{g0}^-$  and  $H^3\Sigma_{u0}^- - X^3\Sigma_{g1}^-$   
transitions.

	$v''=0$	1	2	3	4	5	6	7	8	9
$F^3\Sigma_{u1}^+ - X^3\Sigma_{g1}^-$										
$v'=0$	0.05832	0.15901	0.22372	0.21183	0.15639	0.09726	0.05226	0.02450	0.01027	0.00402
1	0.13177	0.18082	0.07188	0.00011	0.04596	0.11910	0.14559	0.12382	0.08410	0.04914
2	0.15475	0.07922	0.00180	0.08318	0.09827	0.02726	0.00166	0.04520	0.09761	0.11795
3	0.14465	0.01411	0.05134	0.08475	0.07093	0.02727	0.08010	0.05756	0.00954	0.00454
4	0.12184	0.00027	0.08147	0.02289	0.07093	0.07318	0.02543	0.00279	0.04634	0.06793
5	0.09575	0.01280	0.06784	0.00010	0.06149	0.03045	0.00499	0.05412	0.04404	0.00346
6	0.07315	0.03085	0.03818	0.01761	0.05559	0.00008	0.04522	0.03893	0.00010	0.02873
7	0.05475	0.04454	0.01386	0.04050	0.02406	0.01687	0.04921	0.00192	0.02717	0.04464
8	0.04061	0.05156	0.00192	0.04937	0.00280	0.04123	0.01937	0.01161	0.04493	0.00893
9	0.02994	0.05273	0.00035	0.04370	0.00161	0.04468	0.00059	0.03658	0.02123	0.00376
$F^3\Sigma_{u0}^+ - X^3\Sigma_{g1}^-$										
$v'=0$	0.03873	0.12282	0.20036	0.21642	0.17740	0.11895	0.06750	0.03324	0.01470	0.00608
1	0.09983	0.17291	0.10355	0.00982	0.01817	0.09006	0.13885	0.13511	0.10080	0.06341
2	0.13478	0.10539	0.00254	0.04943	0.10214	0.05285	0.00171	0.02149	0.07596	0.11157
3	0.13888	0.03460	0.02365	0.08832	0.02646	0.00716	0.06514	0.07302	0.02570	$1.5 \times 10^{-6}$
4	0.12582	0.00283	0.06438	0.04446	0.00383	0.06353	0.04592	0.00060	0.02747	0.06599
5	0.10477	0.00282	0.07144	0.00461	0.04227	0.04851	0.00007	0.03808	0.05532	0.01418
6	0.08325	0.01663	0.05217	0.00395	0.05802	0.00711	0.02666	0.05014	0.00604	0.01423
7	0.06410	0.03143	0.02724	0.02323	0.03865	0.00348	0.04927	0.01219	0.01192	0.04604
8	0.04849	0.04161	0.00935	0.03898	0.01313	0.02455	0.03313	0.00140	0.04009	0.02127
9	0.03632	0.04615	0.00117	0.04259	0.00075	0.03874	0.00843	0.02089	0.03275	0.00005
$H^3\Sigma_{u1}^- - X^3\Sigma_{g1}^-$										
$v'=0$	$1.51 \times 10^{-10}$	$3.82 \times 10^{-9}$	$5.02 \times 10^{-8}$	$4.29 \times 10^{-7}$	$2.72 \times 10^{-6}$	$1.36 \times 10^{-5}$	$5.47 \times 10^{-5}$	$1.84 \times 10^{-4}$	$5.37 \times 10^{-4}$	$1.39 \times 10^{-3}$
1	$2.41 \times 10^{-9}$	$5.62 \times 10^{-8}$	$6.76 \times 10^{-7}$	$5.28 \times 10^{-6}$	$3.02 \times 10^{-5}$	$1.35 \times 10^{-4}$	$4.85 \times 10^{-4}$	$1.44 \times 10^{-3}$	$3.64 \times 10^{-3}$	$8.10 \times 10^{-3}$
2	$1.80 \times 10^{-8}$	$3.89 \times 10^{-7}$	$4.30 \times 10^{-6}$	$3.06 \times 10^{-5}$	$1.59 \times 10^{-4}$	$6.38 \times 10^{-4}$	$2.03 \times 10^{-3}$	$5.28 \times 10^{-3}$	$1.15 \times 10^{-2}$	$2.17 \times 10^{-2}$
3	$7.74 \times 10^{-8}$	$1.55 \times 10^{-6}$	$1.59 \times 10^{-5}$	$1.04 \times 10^{-4}$	$4.89 \times 10^{-4}$	$1.77 \times 10^{-3}$	$5.01 \times 10^{-3}$	$1.14 \times 10^{-2}$	$2.14 \times 10^{-2}$	$3.37 \times 10^{-2}$
$H^3\Sigma_{u1}^- - X^3\Sigma_{g0}^-$										
$v'=0$	$2.31 \times 10^{-10}$	$5.83 \times 10^{-9}$	$7.30 \times 10^{-8}$	$3.71 \times 10^{-6}$	$1.79 \times 10^{-5}$	$7.02 \times 10^{-5}$	$2.31 \times 10^{-4}$	$6.60 \times 10^{-4}$	$1.68 \times 10^{-3}$	$3.71 \times 10^{-6}$

1	$3.63 \times 10^{-9}$	$8.44 \times 10^{-8}$	$9.66 \times 10^{-7}$	$4.04 \times 10^{-5}$	$1.75 \times 10^{-4}$	$6.07 \times 10^{-4}$	$1.75 \times 10^{-3}$	$4.34 \times 10^{-3}$	$9.45 \times 10^{-3}$	$4.04 \times 10^{-5}$
2	$2.68 \times 10^{-8}$	$5.75 \times 10^{-7}$	$6.04 \times 10^{-6}$	$2.08 \times 10^{-4}$	$8.05 \times 10^{-4}$	$2.48 \times 10^{-3}$	$6.25 \times 10^{-3}$	$1.33 \times 10^{-2}$	$2.43 \times 10^{-2}$	$2.08 \times 10^{-4}$
3	$1.14 \times 10^{-7}$	$2.26 \times 10^{-6}$	$2.19 \times 10^{-5}$	$6.28 \times 10^{-4}$	$2.18 \times 10^{-3}$	$5.96 \times 10^{-3}$	$1.31 \times 10^{-2}$	$2.38 \times 10^{-2}$	$3.63 \times 10^{-2}$	$6.28 \times 10^{-4}$
$H^3 \Sigma_{u0+}^- - X^3 \Sigma_{g1}^-$										
$\nu'=0$	$1.17 \times 10^{-10}$	$2.99 \times 10^{-9}$	$3.98 \times 10^{-8}$	$3.45 \times 10^{-7}$	$2.21 \times 10^{-6}$	$1.12 \times 10^{-5}$	$4.56 \times 10^{-5}$	$1.56 \times 10^{-4}$	$4.61 \times 10^{-4}$	$1.21 \times 10^{-3}$
1	$2.13 \times 10^{-9}$	$5.02 \times 10^{-8}$	$6.10 \times 10^{-7}$	$4.81 \times 10^{-6}$	$2.79 \times 10^{-5}$	$1.26 \times 10^{-4}$	$4.56 \times 10^{-4}$	$1.36 \times 10^{-3}$	$3.49 \times 10^{-3}$	$7.86 \times 10^{-3}$
2	$1.93 \times 10^{-8}$	$4.19 \times 10^{-7}$	$4.65 \times 10^{-6}$	$3.33 \times 10^{-5}$	$1.73 \times 10^{-4}$	$6.97 \times 10^{-4}$	$2.23 \times 10^{-3}$	$5.79 \times 10^{-3}$	$1.27 \times 10^{-2}$	$2.38 \times 10^{-2}$
3	$1.10 \times 10^{-7}$	$2.20 \times 10^{-6}$	$2.24 \times 10^{-5}$	$1.45 \times 10^{-4}$	$6.80 \times 10^{-4}$	$2.43 \times 10^{-3}$	$6.78 \times 10^{-3}$	$1.52 \times 10^{-2}$	$2.79 \times 10^{-2}$	$4.28 \times 10^{-2}$
4	$3.97 \times 10^{-7}$	$7.34 \times 10^{-6}$	$6.86 \times 10^{-5}$	$4.06 \times 10^{-4}$	$1.71 \times 10^{-3}$	$5.44 \times 10^{-3}$	$1.33 \times 10^{-2}$	$2.55 \times 10^{-2}$	$3.89 \times 10^{-2}$	$4.72 \times 10^{-2}$
$H^3 \Sigma_{u0+}^- - X^3 \Sigma_{g0+}^-$										
$\nu'=0$	$1.79 \times 10^{-10}$	$4.58 \times 10^{-9}$	$5.81 \times 10^{-8}$	$4.86 \times 10^{-7}$	$3.02 \times 10^{-6}$	$1.48 \times 10^{-5}$	$5.87 \times 10^{-5}$	$1.96 \times 10^{-4}$	$5.68 \times 10^{-4}$	$1.47 \times 10^{-3}$
1	$3.22 \times 10^{-9}$	$7.55 \times 10^{-8}$	$8.74 \times 10^{-7}$	$6.64 \times 10^{-6}$	$3.72 \times 10^{-5}$	$1.63 \times 10^{-4}$	$5.71 \times 10^{-4}$	$1.67 \times 10^{-3}$	$4.17 \times 10^{-3}$	$9.18 \times 10^{-3}$
2	$2.88 \times 10^{-8}$	$6.20 \times 10^{-7}$	$6.54 \times 10^{-6}$	$4.50 \times 10^{-5}$	$2.27 \times 10^{-4}$	$8.80 \times 10^{-4}$	$2.72 \times 10^{-3}$	$6.85 \times 10^{-3}$	$1.46 \times 10^{-2}$	$2.67 \times 10^{-2}$
3	$1.63 \times 10^{-7}$	$3.22 \times 10^{-6}$	$3.11 \times 10^{-5}$	$1.94 \times 10^{-4}$	$8.74 \times 10^{-4}$	$3.01 \times 10^{-3}$	$8.09 \times 10^{-3}$	$1.75 \times 10^{-2}$	$3.11 \times 10^{-2}$	$4.59 \times 10^{-2}$
4	$6.41 \times 10^{-7}$	$1.17 \times 10^{-5}$	$1.03 \times 10^{-4}$	$5.84 \times 10^{-4}$	$2.36 \times 10^{-3}$	$7.19 \times 10^{-3}$	$1.68 \times 10^{-2}$	$3.08 \times 10^{-2}$	$4.48 \times 10^{-2}$	$5.15 \times 10^{-2}$