

## Supplementary material: Electronic structure, cold ion-atom elastic collisions proprieties and possibility of laser cooling of BeCs<sup>+</sup> molecular ion

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**S.Table 1.** The exponents and contraction coefficients of the primitive Gaussian orbitals for Beryllium and Cesium atoms.

Orbitals	Beryllium: Be		Cesium: Cs	
	Exponents	Contraction coefficients	Exponents	Contraction coefficients
s	4.930000	1	0.328926	0.411589
	1.280000	1	0.241529	0.682422
	0.423000	1	0.505020	1
	0.141000	1	0.029302	1
	0.028500	1	0.013282	1
	0.016250	1	0.005280	1
	0.000992	1	0.003000	1
p	5.230000	1	0.120000	1
	1.440000	1	0.065500	1
	0.494100	1	0.016200	1
	0.202400	1	0.004430	1
	0.092300	1		
	0.061150	1		
	0.032300	1		
	0.010910	1		
	0.007910	1		
d	1.280000	1	0.196894	0.189650
	0.410000	1	0.067471	0.227240
	0.180000	1	0.027948	1
	0.140000	1	0.010712	1
	0.110000	1	0.003000	1
	0.056900	1		
	0.020200	1		
	0.011160	1		
	0.022796	0.49521		

	0.008574	0.549272		
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**S. Table 2.** Avoided crossing's position  $R_c$  between electronic states of the molecular ion  $\text{BeCs}^+$ .

States	$R_c(\text{Bohr})$
$2^1\Sigma^+/3^1\Sigma^+$	22.50
$3^1\Sigma^+/4^1\Sigma^+$	30.21
$4^1\Sigma^+/5^1\Sigma^+$	10.94
$5^1\Sigma^+/6^1\Sigma^+$	5.78
	18.60
$6^1\Sigma^+/7^1\Sigma^+$	5.52
	14.72
$2^3\Pi/3^3\Pi$	6.68

**S. Table 3.** Interaction Energy ( $\text{cm}^{-1}$ ) as a function of internuclear distances  $R$  (Bohr) of 1- $7^1\Sigma^+$  electronic states of the molecular ion  $\text{BeCs}^+$ .

$R(\text{Bohr})$	$1^1\Sigma^+$	$2^1\Sigma^+$	$3^1\Sigma^+$	$4^1\Sigma^+$	$5^1\Sigma^+$	$6^1\Sigma^+$	$7^1\Sigma^+$
5	4227.7469	49746.642	57023.336	64366.75	77146.34	64104.395	82242.33
5.4545455	1370.6014	45809.975	55426.125	62138.301	73277.267	62359.287	79775.386
5.9090909	-341.66272	43155.11	54120.819	60056.68	68360.716	61082.351	70754.785
6.3636364	-1155.057	41575.129	53030.447	58362.932	66351.143	60122.812	68807.969
6.8181818	-1467.7491	40606.926	52032.594	57106.996	64700.771	58922.98	67322.814
7.2727273	-1500.391	39979.746	51101.96	56261.359	63327.596	57553.6	66132.764
7.7272727	-1394.999	39533.596	50267.062	55740.054	62151.022	56495.445	65122.209
8.1818182	-1237.9747	39189.819	49536.21	55432.59	61102.73	55696.631	64239.454
8.6363636	-1071.7163	38933.548	48902.721	55270.13	60153.927	55097.158	63467.197
9.0909091	-916.84684	38768.204	48346.472	55196.566	59296.359	54652.255	62798.234
9.5454545	-781.93456	38695.431	47846.324	55157.1	58540.24	54328.111	62224.675
10	-667.42348	38707.708	47387.506	55102.271	57905.845	54098.831	61736.342
10.454545	-572.3908	38797.773	46964.457	54982.777	57427.569	53944.656	61320.688
10.909091	-494.09143	38950.92	46573.826	54769.893	57117.025	53849.977	60966.245
11.363636	-429.39286	39151.706	46213.714	54477.506	56946.639	53802.005	60663.199
11.818182	-375.82626	39388.369	45884.702	54144.501	56870.627	53791.303	60402.814
12.272727	-331.23433	39648.897	45585.589	53808.094	56844.909	53809.873	60177.263
12.727273	-293.80719	39924.658	45316.3	53490.826	56842.738	53851.505	59980.624
13.181818	-262.26515	40207.64	45075.746	53203.608	56849.435	53910.529	59805.924
13.636364	-235.04347	40491.533	44861.448	52949.612	56857.137	53982.764	59645.782
14.090909	-211.91511	40770.036	44675.861	52736.399	56860.681	54064.634	59487.484
14.545455	-191.67368	41040.693	44512.194	52555.672	56858.368	54152.56	59306.028
15	-173.16577	41302.342	44364.677	52400.315	56849.731	54243.904	59079.817
15.454545	-158.87994	41532.91	44256.615	52310.61	56816.531	54336.271	58831.216
15.909091	-144.59412	41763.479	44148.553	52220.904	56783.33	54427.748	58587.497
16.363636	-130.79889	41987.313	44046.821	52142.475	56744.052	54516.677	58366.964
16.818182	-119.66999	42180.443	43971.673	52111.614	56676.942	54601.913	58179.155
17.272727	-110.22326	42342.504	43917.306	52119.54	56582.539	54682.621	58023.777
17.727273	-101.52226	42492.597	43870.351	52141.742	56478.502	54758.103	57899.629
18.181818	-92.821273	42642.689	43823.395	52163.945	56374.465	54828.194	57802.226
18.636364	-85.295966	42771.438	43788.285	52208.943	56259.723	54892.773	57726.808
19.090909	-78.647869	42878.067	43764.678	52275.798	56138.345	54951.908	57668.6
19.545455	-72.705607	42970.316	43748.33	52355.831	56018.46	55005.633	57623.341
20	-67.33262	43048.947	43738.099	52446.855	55903.112	55054.233	57587.288
20.454545	-62.445027	43116.022	43732.921	52546.492	55793.943	55097.996	57558.592
20.909091	-58.106719	43173.144	43731.887	52652.62	55691.719	55137.361	57535.081
21.363636	-55.800089	43193.477	43738.141	52746.812	55649.485	55172.544	57515.306
21.818182	-53.688182	43210.512	43744.967	52839.608	55612.894	55203.769	57498.445
22.272727	-51.576275	43227.548	43751.793	52932.403	55576.304	55231.714	57484.333
22.727273	-49.464368	43244.583	43758.619	53025.199	55539.713	55278.561	57472.803
23.181818	-47.35246	43261.618	43765.445	53117.994	55503.122	55297.934	57463.69

23.636364	-45.240553	43278.654	43772.27	53210.79	55466.531	55315.14	57456.827
24.090909	-43.128646	43295.689	43779.096	53303.586	55429.94	55330.501	57452.05
24.545455	-41.016739	43312.724	43785.922	53396.381	55393.349	55344.231	57449.192
25	-38.904832	43329.76	43792.748	53489.177	55356.758	55356.455	57448.088
25.454545	-36.792924	43346.795	43799.574	53581.972	55320.168	55367.17	57448.572
25.909091	-34.681017	43363.83	43806.399	53674.768	55283.577	55376.95	57450.478
26.363636	-32.56911	43380.865	43813.225	53767.563	55246.986	55385.604	57453.641
26.818182	-30.457203	43397.901	43820.051	53860.359	55210.395	55393.496	57457.894
27.272727	-28.345295	43414.936	43826.877	53953.155	55173.804	55400.573	57463.072
27.727273	-26.233388	43431.971	43833.702	54045.95	55137.213	55406.789	57469.01
28.181818	-24.121481	43449.007	43840.528	54138.746	55100.622	55412.488	57475.541
28.636364	-22.009574	43466.042	43847.354	54231.541	55064.032	55417.776	57482.499
29.090909	-19.897667	43483.077	43854.18	54324.337	55027.441	55422.503	57489.72
29.545455	-17.897189	43498.908	43860.722	54412.143	54995.257	55426.716	57497.037
30	-16.962282	43504.052	43864.305	54451.591	55004.354	55430.888	57504.847
30.454545	-16.107185	43508.897	43867.868	54487.647	55014.758	55434.41	57512.643
30.909091	-15.343298	43513.423	43871.137	54518.348	55027.27	55437.51	57520.376
31.363636	-14.437607	43517.605	43873.985	54544.189	55041.487	55440.648	57528.072
31.818182	-13.69923	43521.526	43876.728	54566.737	55056.624	55443.399	57535.457
32.272727	-13.022848	43525.326	43879.268	54586.042	55072.475	55445.958	57542.84
32.727273	-12.294121	43528.895	43881.601	54602.871	55088.349	55448.324	57549.813
33.181818	-11.555691	43532.075	43883.96	54617.358	55104.383	55450.346	57556.606
33.636364	-10.980401	43535.253	43885.982	54630.081	55120.142	55452.324	57562.978
34.090909	-10.481594	43538.014	43887.751	54641.228	55135.359	55454.179	57569.176
34.545455	-9.9647351	43540.764	43889.599	54651.02	55150.1	55455.916	57574.932
35	-9.437425	43543.414	43891.333	54659.913	55164.241	55457.372	57580.338
35.454545	-8.857859	43545.86	43892.788	54667.985	55177.758	55458.801	57585.667
35.909091	-8.5259212	43548.144	43894.223	54675.154	55190.632	55460.054	57590.551
36.363636	-8.0363321	43550.272	43895.692	54681.653	55202.853	55461.173	57594.966
36.818182	-7.7150744	43552.385	43896.841	54687.673	55214.435	55462.484	57599.431
37.272727	-7.2056208	43554.17	43898.098	54693.042	55225.226	55463.366	57603.34
37.727273	-6.803725	43556.031	43899.23	54698.297	55235.872	55464.397	57607.381
38.181818	-6.4685268	43557.858	43900.227	54702.951	55245.68	55465.161	57611.104
38.636364	-6.1802165	43559.432	43901.225	54707.281	55255.051	55465.998	57614.337
39.090909	-5.8670183	43561.077	43902.141	54711.418	55263.927	55466.719	57617.571
39.545455	-5.6458496	43562.518	43903.083	54715.185	55272.341	55467.481	57620.623
40	-5.2674	43563.843	43903.81	54718.723	55280.423	55467.791	57623.665
40.454545	-5.0831599	43565.229	43904.643	54722.051	55287.719	55468.631	57626.338
40.909091	-4.8709016	43566.609	43905.386	54725.235	55295.042	55469.309	57628.817
41.363636	-4.6442752	43567.806	43906.087	54728.021	55301.664	55469.734	57631.276
41.818182	-4.4140566	43568.957	43906.778	54730.706	55308.11	55470.089	57633.698
42.272727	-4.1838381	43570.108	43907.469	54733.392	55314.556	55470.517	57635.98
42.727273	-3.9616346	43571.115	43908.031	54735.741	55320.257	55470.972	57638.049
43.181818	-3.7399427	43572.112	43908.585	54738.069	55325.91	55471.371	57639.985
43.636364	-3.4916477	43573.11	43909.086	54740.197	55331.164	55471.713	57641.883
44.090909	-3.2614292	43574.061	43909.569	54742.231	55336.221	55472.013	57643.709

44.545455	-3.1079502	43574.829	43909.992	54743.919	55340.557	55472.277	57645.417
45	-2.9544712	43575.596	43910.414	54745.607	55344.893	55472.508	57647.019
45.454545	-2.8009921	43576.364	43910.836	54747.296	55349.229	55472.709	57648.538
45.909091	-2.6475131	43577.131	43911.258	54748.984	55353.565	55472.883	57649.993
46.363636	-2.4940341	43577.899	43911.68	54750.672	55357.9	55473.035	57651.407
46.818182	-2.3743205	43578.617	43912.059	54752.189	55361.871	55473.182	57652.798
47.272727	-2.291186	43579.282	43912.392	54753.519	55365.445	55473.368	57654.158
47.727273	-2.2080515	43579.947	43912.724	54754.849	55369.02	55473.601	57655.447
48.181818	-1.9998673	43580.638	43912.972	54756.036	55372.321	55473.747	57656.624
48.636364	-1.891923	43581.212	43913.33	54757.159	55375.415	55473.812	57657.674
49.090909	-1.7986881	43581.772	43913.703	54758.278	55378.492	55473.889	57658.678
49.545455	-1.7558	43582.293	43913.981	54759.321	55381.386	55473.994	57659.74
50	-1.7558	43582.782	43914.176	54760.299	55384.125		57660.842

**S. Table 4.** Interaction Energy ( $\text{cm}^{-1}$ ) as a function of internuclear distances  $R$  (Bohr) of  $(1-5)^3\Sigma^+$  electronic states of the molecular ion  $\text{BeCs}^+$ .

$R(\text{Bohr})$	$1^3\Sigma^+$	$2^3\Sigma^+$	$3^3\Sigma^+$	$4^3\Sigma^+$	$5^3\Sigma^+$
5	28211.317	55709.559	69942.951	75490.84	84198.072
5.4545455	24525.992	53602.918	67242.212	71926.047	80382.12
5.9090909	22127.27	52015.156	65059.533	69240.173	77363.182
6.3636364	20692.003	50758.542	63338.769	67183.093	75015.557
6.8181818	19917.476	49659.132	61952.126	65522.107	73102.214
7.2727273	19585.031	48613.194	60768.039	64104.956	71135.02
7.7272727	19532.497	47579.845	59671.761	62861.99	68679.493
8.1818182	19644.888	46566.59	58589.21	61801.327	66590.231
8.6363636	19847.863	45609.16	57512.945	60951.539	65020.526
9.0909091	20092.058	44746.623	56486.181	60296.008	63827.44
9.5454545	20345.816	44011.165	55553.478	59791.732	62889.374
10	20590.267	43411.277	54726.75	59387.74	62122.399
10.454545	20814.53	42951.816	54006.113	59048.651	61491.268
10.909091	21013.614	42620.522	53378.322	58742.989	60971.791
11.363636	21187.478	42398.54	52829.807	58449.524	60547.646
11.818182	21336.79	42270.035	52352.878	58156.754	60209.578
12.272727	21464.189	42215.943	51938.705	57861.119	59943.198
12.727273	21572.866	42220.545	51582.092	57565.07	59735.049
13.181818	21665.268	42269.062	51278.119	57272.6	59571.847
13.636364	21744.76	42348.311	51021.732	56987.838	59441.592
14.090909	21811.695	42450.203	50817.14	56716.211	59339.688
14.545455	21870.106	42563.266	50652.028	56456.832	59255.252
15	21922.699	42680.206	50517	56208.206	59181.653
15.454545	21962.683	42794.413	50456.026	55991.285	59128.66
15.909091	22002.668	42908.62	50395.052	55774.364	59075.667
16.363636	22040.872	43020.389	50346.093	55563.553	59024.919

16.818182	22071.619	43119.732	50347.931	55379.715	58983.204
17.272727	22096.783	43203.216	50386.294	55222.968	58944.498
17.727273	22120.261	43280.4	50437.675	55076.626	58906.619
18.181818	22143.738	43357.583	50489.056	54930.284	58868.74
18.636364	22164.212	43423.545	50558.82	54803.888	58830.944
19.090909	22181.547	43477.289	50645.191	54700.849	58791.793
19.545455	22197.293	43524.886	50737.621	54610.943	58751.287
20	22212.176	43568.583	50832.455	54530.597	58709.481
20.454545	22225.233	43604.93	50930.283	54468.922	58664.288
20.909091	22237.235	43636.795	51027.775	54420.523	58616.123
21.363636	22248.041	43664.528	51122.822	54385.506	58564.937
21.818182	22258.017	43689.034	51214.126	54362.95	58511.153
22.272727	22266.871	43709.966	51299.43	54354.046	58455.808
22.727273	22275.191	43728.745	51379.437	54354.419	58401.334
23.181818	22283.066	43745.898	51455.096	54361.85	58347.944
23.636364	22290.116	43760.905	51523.282	54379.367	58298.597
24.090909	22296.638	43773.915	51584.601	54404.658	58254.73
24.545455	22302.65	43785.779	51640.308	54435.343	58216.471
25	22308.268	43796.456	51689.886	54471.037	58185.322
25.454545	22313.414	43805.983	51733.969	54510.203	58160.885
25.909091	22318.228	43814.613	51773.374	54551.524	58143.347
26.363636	22322.755	43822.348	51808.385	54594.328	58132.438
26.818182	22326.807	43829.384	51839.334	54637.538	58128.087
27.272727	22330.686	43835.712	51866.968	54680.556	58129.36
27.727273	22334.331	43841.506	51891.568	54722.721	58135.839
28.181818	22337.673	43847.055	51913.581	54763.772	58147.254
28.636364	22340.819	43851.943	51933.252	54803.167	58162.671
29.090909	22343.812	43856.292	51950.93	54840.787	58181.546
29.545455	22346.585	43860.502	51967.031	54876.362	58203.383
30	22349.171	43864.305	51981.024	54909.353	58227.501
30.454545	22351.736	43867.868	51994.278	54941.277	58252.726
30.909091	22354.008	43871.137	52006.357	54970.926	58279.043
31.363636	22356.038	43873.985	52017.191	54998.337	58305.516
31.818182	22358.173	43876.728	52027.103	55024.038	58331.654
32.272727	22360.037	43879.268	52036.193	55047.957	58356.761
32.727273	22361.858	43881.598	52044.716	55070.098	58380.213
33.181818	22363.558	43883.817	52052.257	55090.938	58401.28
33.636364	22365.367	43885.982	52059.417	55110.027	58419.715
34.090909	22366.857	43887.751	52066.088	55127.89	58434.733
34.545455	22368.188	43889.599	52072.148	55144.699	58446.663
35	22369.667	43891.333	52077.829	55160.187	58455.785
35.454545	22370.929	43892.788	52082.965	55174.825	58462.366
35.909091	22372.251	43894.223	52087.865	55188.47	58467.041
36.363636	22373.315	43895.692	52092.524	55201.266	58470.266
36.818182	22374.464	43896.841	52096.752	55213.305	58472.515
37.272727	22375.416	43898.098	52100.626	55224.434	58473.786

37.727273	22376.414	43899.23	52104.482	55235.273	58474.724
38.181818	22377.412	43900.227	52107.97	55245.241	58475.059
38.636364	22378.409	43901.225	52111.251	55254.796	58475.163
39.090909	22379.266	43902.141	52114.253	55263.708	58475.163
39.545455	22380.047	43903.083	52117.237	55272.182	58475.103
40	22380.775	43903.81	52119.889	55280.234	58474.724
40.454545	22381.608	43904.643	52122.383	55287.719	58474.448
40.909091	22382.35	43905.386	52124.824	55295.042	58474.13
41.363636	22382.99	43906.087	52127.031	55301.664	58473.759
41.818182	22383.604	43906.778	52129.18	55308.11	58473.375
42.272727	22384.218	43907.469	52131.329	55314.556	58472.991
42.727273	22384.776	43908.031	52133.229	55320.257	58472.656
43.181818	22385.331	43908.585	52135.114	55325.91	58472.323
43.636364	22385.951	43909.086	52136.745	55331.164	58472.071
44.090909	22386.534	43909.569	52138.318	55336.221	58471.817
44.545455	22386.956	43909.992	52139.7	55340.557	58471.549
45	22387.378	43910.414	52141.081	55344.893	58471.28
45.454545	22387.8	43910.836	52142.462	55349.229	58471.012
45.909091	22388.223	43911.258	52143.843	55353.565	58470.743
46.363636	22388.645	43911.68	52145.225	55357.9	58470.475
46.818182	22389.064	43912.059	52146.462	55361.871	58470.255
47.272727	22389.48	43912.392	52147.542	55365.445	58470.089
47.727273	22389.895	43912.724	52148.623	55369.02	58469.923
48.181818	22390.156	43912.972	52149.576	55372.321	58469.701
48.636364	22390.514	43913.33	52150.508	55375.415	58469.593
49.090909	22390.887	43913.703	52151.44	55378.492	58469.5
49.545455	22391.217	43913.981	52152.344	55381.386	58469.404
50	22391.511	43914.176	52153.224	55384.125	58469.306

**S. Table 5.** Interaction Energy ( $\text{cm}^{-1}$ ) as a function of internuclear distances  $R$  (Bohr) of (1-4)  $^1\Pi$  and (1-3)  $^3\Pi$  electronic states of the molecular ion  $\text{BeCs}^+$ .

$R(\text{Bohr})$	$^1\Pi$	$2^1\Pi$	$3^1\Pi$	$4^1\Pi$	$1^3\Pi$	$2^3\Pi$	$3^3\Pi$
5	46037.656	61181.286	70745.617	79188.751	24416.819	64104.395	70311.011
5.4545455	44454.831	58753.391	68270.258	75348.633	23060.031	62359.287	67214.021
5.9090909	43457.712	56888.796	66459.405	72370.652	22277.917	61082.351	63638.665
6.3636364	42904.84	55523.302	65145.947	70036.255	21905.37	60122.812	61061.653
6.8181818	42660.838	54575.356	64163.955	68164.085	21783.16	58922.98	59719.426
7.2727273	42608.285	53955.303	63383.053	66625.056	21792.669	57553.6	59284.74
7.7272727	42660.148	53578.338	62716.404	65348.592	21859.661	56495.445	59084.282
8.1818182	42760.432	53372.934	62111.092	64300.433	21943.07	55696.631	59029.621
8.6363636	42876.271	53282.04	61542.331	63456.279	22023.112	55097.158	59075.553
9.0909091	42989.678	53262.981	61007.657	62785.482	22092.625	54652.255	59187.725
9.5454545	43092.553	53286.288	60517.467	62249.889	22149.827	54328.111	59338.526
10	43182.346	53332.886	60081.72	61813.378	22195.728	54098.831	59507.354
10.454545	43258.101	53392.057	59702.941	61448.837	22232.614	53944.656	59678.666

10.909091	43321.19	53458.421	59377.321	61137.38	22261.917	53849.977	59842.214
11.363636	43373.225	53529.841	59097.562	60867.126	22285.387	53802.005	59991.659
11.818182	43415.91	53605.725	58856.604	60629.799	22304.408	53791.303	60124.208
12.272727	43450.689	53686.04	58647.47	60419.518	22319.755	53809.873	60109.59
12.727273	43479.108	53770.886	58464.611	60232.379	22332.299	53851.505	59927.449
13.181818	43502.371	53859.884	58304.22	60065.269	22342.678	53910.529	59758.71
13.636364	43521.327	53952.58	58162.373	59915.388	22351.49	53982.764	59603.138
14.090909	43536.909	54047.67	58037.103	59781.013	22358.938	54064.634	59459.818
14.545455	43549.66	54144.738	57926.446	59659.759	22365.158	54152.56	59327.696
15	43559.859	54241.709	57829.248	59550.81	22370.427	54243.904	59206.454
15.454545	43568.55	54337.65	57743.837	59452.132	22375.131	54336.271	59095.103
15.909091	43575.474	54430.988	57669.784	59363.038	22379.289	54427.748	58994.078
16.363636	43581.168	54520.781	57606.229	59282.213	22382.574	54516.677	58902.651
16.818182	43585.869	54606.502	57552.23	59208.926	22385.712	54601.913	58820.851
17.272727	43589.799	54687.095	57507.222	59142.626	22388.446	54682.621	58748.408
17.727273	43593.114	54762.352	57470.758	59082.009	22390.624	54758.103	58685.61
18.181818	43595.786	54832.346	57442.032	59026.718	22392.595	54828.194	58632.567
18.636364	43597.83	54896.843	57420.296	58976.637	22394.521	54892.773	58588.522
19.090909	43599.838	54955.747	57404.747	58931.195	22395.986	54951.908	58551.799
19.545455	43601.382	55009.139	57394.963	58890.049	22397.19	55005.633	58526.174
20	43602.633	55057.274	57390.416	58852.762	22398.251	55054.233	58505.885
20.454545	43603.504	55100.982	57389.874	58818.967	22399.306	55097.996	58492.786
20.909091	43604.361	55139.821	57392.741	58788.515	22400.2	55137.361	58485.443
21.363636	43605.078	55174.735	57398.477	58761.149	22400.941	55172.544	58483.059
21.818182	43605.729	55205.744	57406.285	58736.65	22401.372	55203.769	58484.588
22.272727	43606.262	55233.358	57416	58714.563	22402.021	55231.714	58489.138
22.727273	43606.569	55257.881	57426.866	58694.434	22402.501	55256.526	58495.904
23.181818	43606.902	55279.589	57438.253	58676.42	22402.738	55278.561	58503.825
23.636364	43607.043	55298.81	57450.289	58660.204	22403.113	55297.934	58512.214
24.090909	43607.238	55315.965	57462.296	58645.513	22403.396	55315.14	58520.422
24.545455	43607.479	55331.165	57474.204	58632.282	22403.559	55330.501	58528.052
25	43607.488	55344.672	57485.729	58620.106	22403.835	55344.231	58534.396
25.454545	43607.488	55356.784	57497.106	58608.997	22403.977	55356.455	58539.425
25.909091	43607.488	55367.57	57507.85	58598.954	22404.233	55367.17	58543.162
26.363636	43607.488	55377.179	57517.888	58589.784	22404.199	55376.95	58545.313
26.818182	43607.488	55385.844	57527.547	58581.37	22404.436	55385.604	58546.406
27.272727	43607.488	55393.615	57536.775	58573.628	22404.445	55393.496	58546.181
27.727273	43607.488	55400.572	57545.237	58566.434	22404.443	55400.573	58545.215
28.181818	43607.488	55407.016	57553.232	58559.776	22404.666	55406.789	58543.233
28.636364	43607.252	55412.755	57560.683	58553.858	22404.666	55412.488	58541.17
29.090909	43607.268	55417.776	57567.718	58548.132	22404.666	55417.776	58538.425
29.545455	43607.223	55422.48	57574.22	58543.141	22404.666	55422.503	58535.44
30	43607.096	55427.135	57580.285	58538.293	22404.666	55426.716	58532.45
30.454545	43607.069	55430.914	57585.947	58533.982	22404.666	55430.888	58529.456
30.909091	43606.828	55434.408	57591.441	58529.74	22404.666	55434.41	58526.462
31.363636	43606.852	55437.703	57596.295	58526.026	22404.666	55437.51	58523.341

31.818182	43606.594	55440.654	57601.135	58522.56	22404.666	55440.648	58520.657
32.272727	43606.629	55443.4	57605.461	58519.283	22404.666	55443.399	58517.749
32.727273	43606.391	55445.957	57609.53	58516.222	22404.666	55445.958	58515.124
33.181818	43606.396	55448.322	57613.451	58513.491	22404.666	55448.324	58512.695
33.636364	43606.17	55450.348	57616.989	58510.738	22404.666	55450.346	58510.078
34.090909	43606.184	55452.325	57620.469	58508.505	22404.666	55452.324	58507.839
34.545455	43605.928	55454.179	57623.734	58506.109	22404.666	55454.179	58505.784
35	43605.959	55455.915	57626.864	58504.076	22404.666	55455.916	58503.67
35.454545	43605.721	55457.372	57629.72	58502.021	22404.666	55457.372	58501.818
35.909091	43605.724	55458.8	57632.322	58500.29	22404.665	55458.801	58500.07
36.363636	43605.497	55460.054	57634.956	58498.524	22404.681	55460.054	58498.29
36.818182	43605.512	55461.174	57637.385	58496.864	22404.467	55461.173	58496.844
37.272727	43605.431	55462.484	57639.64	58495.302	22404.458	55462.484	58495.29
37.727273	43605.293	55463.366	57641.717	58493.978	22404.447	55463.366	58493.978
38.181818	43605.123	55464.397	57643.719	58492.674	22404.447	55464.397	58492.674
38.636364	43605.072	55465.161	57645.692	58491.326	22404.447	55465.161	58491.326
39.090909	43605.024	55465.997	57647.514	58490.169	22404.446	55465.998	58490.169
39.545455	43604.866	55466.718	57649.346	58489.288	22404.395	55466.719	58489.288
40	43604.854	55467.477	57651.068	58488.106	22404.227	55467.481	58488.106
40.454545	43604.792	55467.792	57652.518	58487.648	22404.219	55467.791	58487.648
40.909091	43604.66	55468.631	57654.033	58486.389	22404.224	55468.631	58486.389
41.363636	43604.557	55469.308	57655.445	58485.312	22404.25	55469.309	58485.312
41.818182	43604.487	55469.734	57656.742	58484.58	22404.269	55469.734	58484.58
42.272727	43604.42	55470.089	57657.984	58483.979	22404.231	55470.089	58483.979
42.727273	43604.321	55470.517	57659.218	58483.331	22404.118	55470.517	58483.331
43.181818	43604.2	55470.972	57660.425	58482.652	22404.01	55470.972	58482.652
43.636364	43604.071	55471.371	57661.573	58482.004	22403.996	55471.371	58482.004
44.090909	43603.956	55471.713	57662.66	58481.416	22404.008	55471.713	58481.416
44.545455	43603.865	55472.013	57663.688	58480.895	22403.976	55472.013	58480.895
45	43603.792	55472.277	57664.662	58480.426	22403.915	55472.277	58480.426
45.454545	43603.729	55472.508	57665.586	58479.988	22403.845	55472.508	58479.988
45.909091	43603.665	55472.709	57666.464	58479.562	22403.79	55472.709	58479.562
46.363636	43603.587	55472.884	57667.297	58479.129	22403.773	55472.883	58479.129
46.818182	43603.485	55473.035	57668.091	58478.67	22403.818	55473.035	58478.67
47.272727	43603.383	55473.182	57668.85	58478.216	22403.872	55473.182	58478.216
47.727273	43603.32	55473.368	57669.576	58477.844	22403.816	55473.368	58477.844
48.181818	43603.32	55473.601	57670.275	58477.601	22403.591	55473.601	58477.601
48.636364	43603.249	55473.747	57670.95	58477.352	22403.492	55473.747	58477.352
49.090909	43603.136	55473.812	57671.597	58477.06	22403.536	55473.812	58477.06
49.545455	43603.081	55473.889	57672.214	58476.752	22403.595	55473.889	58476.752
50	43603.089	55473.994	57672.802	58476.454	22403.6	55473.994	58476.454

**S. Table 6.** Interaction Energy ( $\text{cm}^{-1}$ ) as a function of internuclear distances  $R$  (Bohr) of (1-2)  $^1\Delta$  and (1)  $^3\Delta$  electronic states of the molecular ion  $\text{BeCs}^+$ .

$R(\text{Bohr})$	$1\ ^1\Delta$	$2\ ^1\Delta$	$1\ ^3\Delta$
5	58776.09	69149.987	65934.899
5.4545455	58570.494	67389.544	64265.086
5.9090909	58367.485	65963.469	63068.864
6.3636364	58235.114	64832.387	62242.942
6.8181818	58167.228	63929.298	61666.996
7.2727273	58138.976	63195.046	61247.175
7.7272727	58129.851	62585.843	60923.256
8.1818182	58127.139	62071.712	60659.998
8.6363636	58125.146	61632.703	60438.586
9.0909091	58121.678	61255.238	60248.548
9.5454545	58116.29	60929.288	60083.268
10	58109.298	60647.307	59939.061
10.454545	58100.922	60402.771	59812.393
10.909091	58091.327	60190.61	59700.787
11.363636	58080.917	60006.3	59601.687
11.818182	58070.018	59845.714	59513.465
12.272727	58057.806	59705.863	59434.144
12.727273	58045.337	59583.652	59362.826
13.181818	58031.923	59476.674	59298.296
13.636364	58018.772	59383.181	59239.162
14.090909	58004.886	59300.88	59185.635
14.545455	57991.006	59228.407	59136.347
15	57977.174	59164.315	59091.23
15.454545	57963.473	59107.595	59049.802
15.909091	57950.093	59057.027	59011.516
16.363636	57937.082	59011.97	58976.236
16.818182	57924.599	58971.723	58943.892
17.272727	57911.995	58935.775	58913.499
17.727273	57900.688	58903.165	58885.789
18.181818	57889.896	58873.69	58860.47
18.636364	57879.104	58847.082	58836.866
19.090909	57869.34	58822.82	58815.165
19.545455	57859.906	58800.731	58794.709
20	57851.022	58780.515	58775.749
20.454545	57842.734	58761.823	58758.241
20.909091	57834.747	58744.681	58742.146
21.363636	57827.335	58728.952	58727.007
21.818182	57820.504	58714.477	58712.91
22.272727	57814.031	58701.084	58699.861
22.727273	57807.693	58688.607	58687.651
23.181818	57801.545	58676.958	58676.18
23.636364	57795.822	58666.109	58665.534
24.090909	57790.772	58656.031	58655.617

24.545455	57786.429	58646.679	58646.422
25	57782.364	58637.979	58637.754
25.454545	57778.144	58629.849	58629.709
25.909091	57773.874	58622.218	58621.991
26.363636	57769.914	58615.027	58614.929
26.818182	57766.35	58608.266	58608.247
27.272727	57763.177	58601.937	58601.926
27.727273	57760.383	58596.041	58596.035
28.181818	57757.746	58590.541	58590.488
28.636364	57754.77	58585.343	58585.234
29.090909	57751.611	58580.389	58580.387
29.545455	57749.246	58575.683	58575.691
30	57747.351	58571.242	58571.041
30.454545	57745.222	58567.084	58567.084
30.909091	57742.418	58563.205	58563.102
31.363636	57739.832	58559.505	58559.387
31.818182	57737.928	58555.942	58555.92
32.272727	57736.447	58552.549	58552.635
32.727273	57735.102	58549.364	58549.365
33.181818	57733.652	58546.406	58546.402
33.636364	57732.046	58543.623	58543.66
34.090909	57730.284	58540.944	58540.903
34.545455	57728.624	58538.361	58538.387
35	57727.68	58535.944	58535.946
35.454545	57726.907	58533.558	58533.495
35.909091	57725.739	58531.185	58531.445
36.363636	57724.311	58528.991	58529.15
36.818182	57722.762	58527.141	58527.167
37.272727	57721.35	58525.518	58525.509
37.727273	57720.367	58523.641	58523.547
38.181818	57719.667	58521.726	58521.66
38.636364	57719.074	58520	58520.191
39.090909	57718.308	58518.45	58518.448
39.545455	57717.215	58516.963	58517.015
40	57716.122	58515.516	58515.516
40.454545	57714.736	58514.103	58514.096
40.909091	57710.738	58512.739	58512.738
41.363636	57701.471	58511.443	58511.446
41.818182	57684.276	58510.212	58510.214
42.272727	57656.497	58509.031	58509.032
42.727273	57615.474	58507.894	58507.893
43.181818	57558.552	58506.81	58506.81
43.636364	57483.071	58505.792	58505.792
44.090909	57386.375	58504.82	58504.82
44.545455	57265.805	58503.875	58503.875
45	57118.704	58502.957	58502.957

45.454545	56942.415	58502.067	58502.067
45.909091	56734.279	58501.207	58501.207
46.363636	56491.638	58500.38	58500.38
46.818182	56211.837	58499.588	58499.588
47.272727	55892.215	58498.83	58498.83
47.727273	55530.117	58498.103	58498.103
48.181818	55122.884	58497.403	58497.403
48.636364	54667.858	58496.725	58496.725
49.090909	54162.382	58496.078	58496.078
49.545455	53603.798	58495.473	58495.473
50	52989.449	58494.893	58494.893

**S. Table 7.** Permanent electric dipole moments data of (1-7)  $^1\Sigma^+$  electronic states of the BeCs<sup>+</sup> molecular ion.

<i>R</i> (Bohr)	$1^1\Sigma^+$	$2^1\Sigma^+$	$3^1\Sigma^+$	$4^1\Sigma^+$	$5^1\Sigma^+$	$7^1\Sigma^+$	$8^1\Sigma^+$
5	-0.320414	-0.91276	-3.491588	-2.994222	0.001755	-0.988639	-0.227337
5.2525253	-0.33987467	-0.96038834	-3.792387	-2.8003744	-0.48787573	-0.89906817	-0.048811535
5.5050505	-0.34907152	-1.0122883	-4.1078895	-2.5213308	-0.84669952	-0.94659786	0.11491252
5.7575758	-0.348201	-1.0675266	-4.4300528	-2.1797828	-1.0729415	-1.2749354	-3.5714112
6.010101	-0.33891432	-1.1250741	-4.7442078	-1.8201245	-1.2270343	0.047629848	-3.9190594
6.2626263	-0.32192204	-1.1852489	-5.0280949	-1.4889087	-1.378222	-0.22586477	-4.3077552
6.5151515	-0.29861545	-1.2492168	-5.2588473	-1.227314	-1.5830302	-0.29797385	-4.6629935
6.7676768	-0.26978846	-1.3193045	-5.4166167	-1.0657493	-1.8729901	-0.29618004	-4.9423658
7.020202	-0.23654336	-1.3979532	-5.5007511	-1.0064839	-2.2538844	-0.23919119	-5.1337849
7.2727273	-0.19972245	-1.4876376	-5.5232927	-1.0347148	-2.7224354	-0.117932	-5.2383819
7.5252525	-0.16011497	-1.5905242	-5.5037842	-1.1258707	-5.2631906	0.089149815	-3.2702107
7.7777778	-0.11862956	-1.7064466	-5.4626688	-1.2532513	-5.2243804	0.38725789	-3.8781251
8.030303	-0.075901788	-1.8354058	-5.412542	-1.4015062	-5.1329825	0.68606509	-4.5287557
8.2828283	-0.032586182	-1.9755231	-5.3617242	-1.5612402	-5.0046662	0.66994167	-5.1978344
8.5353535	0.010774737	-2.1247162	-5.3147686	-1.730134	-4.8525621	0.32356678	-5.8610059
8.7878788	0.053744515	-2.2803072	-5.2737542	-1.9102982	-4.6867897	-2.7594665	-6.4982142
9.040404	0.09594901	-2.4400726	-5.2399611	-2.1087838	-4.5102051	-2.39777	-7.0938318
9.2929293	0.13716772	-2.6018121	-5.2134801	-4.1676302	-2.4859421	-2.1745368	-7.6430128
9.5454545	0.17713539	-2.7638452	-5.1950353	-4.1010254	-2.6024962	-2.0448009	-8.1420302
9.7979798	0.21583173	-2.9248461	-5.1841978	-3.8424619	-2.9240593	-1.973291	-8.5983947
10.050505	0.25324974	-3.0839512	-5.1808846	-3.5329673	-3.306677	-1.9433819	-9.0192251
10.30303	0.28929144	-3.2402928	-5.1858486	-3.1653382	-3.7550198	-1.9476091	-9.4090018
10.555556	0.32395748	-3.3932205	-5.1995379	-2.7553338	-4.2499852	-1.9785526	-9.7748077
10.808081	0.35738401	-3.5425864	-5.2216235	-4.1856852	-2.9059277	-2.0288967	-10.124359
11.060606	0.38964273	-3.6881849	-5.2521997	-5.2193972	-1.957826	-2.0939358	-10.462912
11.313131	0.42077378	-3.8297577	-5.2915946	-5.6264609	-1.6340509	-2.1698975	-10.79472
11.565657	0.45086201	-3.9672295	-5.3397805	-5.9654901	-1.3747486	-2.2528984	-11.123831
11.818182	0.47996374	-4.1004109	-5.3969864	-6.2427826	-1.1725882	-2.3395814	-11.453692

12.070707	0.50820873	-4.22948	-5.4626671	-6.4738905	-1.0117353	-2.4269976	-11.786812
12.323232	0.53563399	-4.3541698	-5.5371546	-6.6688566	-0.8816868	-2.5126706	-12.125337
12.575758	0.56230893	-4.4743863	-5.620379	-6.8371814	-0.77301118	-2.5945103	-12.470311
12.828283	0.58833144	-4.5902202	-5.7118651	-6.9865714	-0.67861215	-2.671058	-12.821002
13.080808	0.61369682	-4.7010685	-5.812376	-7.1201948	-0.59554906	-2.7402851	-13.174474
13.333333	0.63847758	-4.8068	-5.9217034	-7.2420473	-0.52097308	-2.8010782	-13.519583
13.585859	0.66273586	-4.9072888	-6.0396372	-7.3547519	-0.45361755	-2.8527717	-13.831447
13.838384	0.68651698	-5.002254	-6.1661944	-7.4600309	-0.39333905	-2.8947863	-14.053579
14.090909	0.70967476	-5.0880987	-6.3059066	-7.5568653	-0.34596056	-2.9218048	-13.794619
14.343434	0.73239078	-5.1665619	-6.4558279	-7.6481882	-0.3099899	-2.9373321	-12.967915
14.59596	0.75510679	-5.2450251	-6.6057491	-7.7395111	-0.27401924	-2.9528594	-12.14121
14.848485	0.7774317	-5.315222	-6.7663632	-7.8264692	-0.25366329	-2.9573102	-10.776339
15.10101	0.79905026	-5.3646112	-6.9518122	-7.9065723	-0.28571801	-2.9421181	-10.127382
15.353535	0.82020092	-5.3965293	-7.1571628	-7.9827329	-0.36820554	-2.9145082	-10.977154
15.606061	0.84135158	-5.4284473	-7.3625134	-8.0588936	-0.45069306	-2.8868984	-11.826927
15.858586	0.86250223	-5.4603653	-7.5678639	-8.1350543	-0.53318059	-2.8592885	-12.676699
16.111111	0.88365289	-5.4922834	-7.7732145	-8.2112149	-0.61566811	-2.8316787	-13.526471
16.363636	0.90450794	-5.5083989	-7.9955882	-8.2854439	-0.7502158	-2.7983299	-14.264647
16.616162	0.92487374	-5.4954187	-8.2488869	-8.3567579	-0.98008542	-2.7570423	-14.819524
16.868687	0.94506357	-5.4675872	-8.517407	-8.427428	-1.2545085	-2.7153131	-15.320552
17.121212	0.96489652	-5.3986953	-8.8271539	-8.4973991	-1.5992845	-2.6775807	-15.748217
17.373737	0.98448509	-5.2986605	-9.1679912	-8.5670515	-1.9839188	-2.6439196	-16.133635
17.626263	1.0040737	-5.1986258	-9.5088286	-8.6367038	-2.368553	-2.6102586	-16.519052
17.878788	1.0236622	-5.098591	-9.8496659	-8.7063561	-2.7531873	-2.5765975	-16.904469
18.131313	1.0432508	-4.9985563	-10.190503	-8.7760084	-3.1378216	-2.5429364	-17.289887
18.383838	1.0627493	-4.8838088	-10.545876	-8.8456363	-3.5245002	-2.5119129	-17.663797
18.636364	1.0818682	-4.7053762	-10.964108	-8.9151626	-3.9132867	-2.4925192	-17.990556
18.888889	1.1008856	-4.5064535	-11.402435	-8.9846508	-4.2894546	-2.4772968	-18.307434
19.141414	1.1082424	-4.3031456	-11.855184	-9.0615716	-4.6421706	-2.4784916	-18.610167
19.393939	0.96506086	-4.3600194	-12.185386	-9.2368243	-4.9143032	-2.6273965	-18.867454
19.646465	1.1572328	-3.761158	-12.862515	-9.1918272	-5.3067451	-2.4638904	-19.195905
19.89899	1.1758198	-3.4731543	-13.387662	-9.2600278	-5.6132507	-2.4690874	-19.476292
20.151515	1.1943021	-3.1679448	-13.929355	-9.3273637	-5.9036752	-2.479621	-19.749043
20.40404	1.2126956	-2.8513561	-14.481819	-9.3936284	-6.1812537	-2.4948978	-20.015445
20.656566	1.2310118	-2.5283924	-15.040116	-9.458697	-6.4488089	-2.5142712	-20.276621
20.909091	1.2492416	-2.2032059	-15.600013	-9.5220241	-6.7065102	-2.5382409	-20.532188
21.161616	1.2673946	-1.8814881	-16.155858	-9.5832944	-6.9566842	-2.5663607	-20.782936
21.414141	1.2854665	-1.5693434	-16.701514	-9.6418125	-7.2005928	-2.5987223	-21.02897
21.666667	1.3034626	-1.2711507	-17.23262	-9.697137	-7.439832	-2.63503	-21.27074
21.919192	1.3214043	-0.98829342	-17.747958	-9.7492192	-7.6775348	-2.6739801	-21.509787
22.171717	1.3392617	-0.72914199	-18.238919	-9.7962893	-7.9128624	-2.7170146	-21.744626
22.424242	1.3571192	-0.46999057	-18.72988	-9.8433593	-8.1481901	-2.7600491	-21.979465
22.676768	1.3748382	-0.26149306	-19.169063	-9.8777571	-8.3863325	-2.8087829	-22.208715
22.929293	1.3925479	-0.05636671	-19.604799	-9.9113115	-8.6246623	-2.8578959	-22.437593
23.181818	1.4102242	0.13562038	-20.027122	-9.9404344	-8.8654572	-2.9080225	-22.665492
23.434343	1.4278297	0.29984375	-20.421101	-9.9601532	-9.1115064	-2.9602812	-22.891331

23.686869	1.4453754	0.4420165	-20.792553	-9.969701	-9.3647811	-3.0135933	-23.116112
23.939394	1.4628774	0.56823654	-21.14769	-9.9700201	-9.6252207	-3.0672888	-23.340392
24.191919	1.480326	0.6772081	-21.485156	-9.957561	-9.8962184	-3.1208624	-23.564543
24.444444	1.497743	0.77665873	-21.812851	-9.9362273	-10.174848	-3.1740197	-23.788858
24.69697	1.5151167	0.86369448	-22.127786	-9.901217	-10.465499	-3.2262363	-24.013648
24.949495	1.53245	0.94044071	-22.432115	-9.8514648	-10.769453	-3.2770371	-24.239235
25.20202	1.5497388	1.0075074	-22.726432	-9.7833797	-11.090284	-3.3256804	-24.466055
25.454545	1.5669949	1.0679164	-23.013835	-9.6990096	-11.426313	-3.3721738	-24.694094
25.707071	1.5842163	1.1221433	-23.294796	-9.5956913	-11.780183	-3.4159789	-24.923629
25.959596	1.6014036	1.1710833	-23.57022	-9.4717215	-12.153652	-3.4567044	-25.154864
26.212121	1.6185528	1.214937	-23.840287	-9.3217185	-12.551984	-3.4933766	-25.388138
26.464646	1.6356769	1.2556948	-24.107073	-9.1518666	-12.969353	-3.5270799	-25.622975
26.717172	1.6527688	1.2929993	-24.370175	-8.9544865	-13.413209	-3.5560437	-25.859871
26.969697	1.6698287	1.327462	-24.630217	-8.7276699	-13.88547	-3.5803404	-26.098862
27.222222	1.6868636	1.3599676	-24.888131	-8.4759071	-14.38184	-3.600529	-26.339526
27.474747	1.7038685	1.3903497	-25.143722	-8.19274	-14.908587	-3.6154212	-26.582154
27.727273	1.72085	1.4192786	-25.3977	-7.8827739	-15.461266	-3.6256715	-26.826333
27.979798	1.7378044	1.4467949	-25.650093	-7.5424652	-16.043318	-3.6305027	-27.072155
28.232323	1.7547341	1.4731891	-25.901205	-7.1744438	-16.652091	-3.6298188	-27.319327
28.484848	1.7716413	1.4986345	-26.15122	-6.7807358	-17.285634	-3.6237547	-27.567682
28.737374	1.7885244	1.5232586	-26.400269	-6.3636772	-17.941569	-3.6119235	-27.817012
28.989899	1.805386	1.547198	-26.648498	-5.9275567	-18.615623	-3.5945178	-28.067086
29.242424	1.822227	1.5705785	-26.896044	-5.4775713	-19.302665	-3.5715933	-28.317652
29.494949	1.8390482	1.5934743	-27.142987	-5.0184087	-19.998017	-3.5431434	-28.568515
29.747475	1.8558488	1.6159039	-27.389341	-4.5552406	-20.696427	-3.5084789	-28.81947
30	1.872617	1.6377266	-27.634895	-4.1027617	-21.382664	-3.4635036	-29.069992

**S. Table 8.** Permanent electric dipole moments data of  $(1-5)^3\Sigma^+$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$1^3\Sigma^+$	$2^3\Sigma^+$	$3^3\Sigma^+$	$4^3\Sigma^+$	$5^3\Sigma^+$
5	0.021526	-4.104878	-6.735462	1.421406	-0.468714
5.2525253	0.030498879	-4.3141942	-6.7199727	1.0315517	-0.26893791
5.5050505	0.027627848	-4.5242968	-6.6047099	0.55610929	-0.20390731
5.7575758	0.016642545	-4.7319519	-6.4037614	-0.0014241818	-0.22010403
6.010101	0.001231899	-4.9337924	-6.1413462	-0.62618151	-0.28724837
6.2626263	-0.016335	-5.1255469	-5.8290443	-1.3139373	-0.41824262
6.5151515	-0.034056333	-5.3036078	-5.4792154	-2.0570673	-0.66577403
6.7676768	-0.050396677	-5.4636547	-5.1013499	-2.8514114	-1.1892099
7.020202	-0.064186848	-5.6032604	-4.7119899	-3.6834568	-2.3418328
7.2727273	-0.074475182	-5.7209678	-4.3346423	-4.5298281	-4.0445783
7.5252525	-0.080402438	-5.8169472	-4.0070266	-5.3447606	-4.5392713
7.7777778	-0.081742778	-5.8953194	-3.7692802	-6.0688374	-4.3980282
8.030303	-0.077972212	-5.9602525	-3.669368	-6.6270957	-4.2883371
8.2828283	-0.069095485	-6.0180657	-3.7250328	-6.9777074	-4.29798
8.5353535	-0.055065778	-6.0750836	-3.9237357	-7.1170418	-4.423006

8.7878788	-0.036235818	-6.1368774	-4.2199188	-7.0894518	-4.6436087
9.040404	-0.012827111	-6.2082685	-4.5676645	-6.9421269	-4.9456356
9.2929293	0.014524232	-6.2918959	-4.9280636	-6.7220566	-5.3122187
9.5454545	0.045499841	-6.390679	-5.2766889	-6.4531466	-5.738481
9.7979798	0.079245692	-6.5043924	-5.6021203	-6.1526168	-6.2153464
10.050505	0.11511357	-6.6326172	-5.900303	-5.8268804	-6.7386794
10.30303	0.15264365	-6.7759308	-6.1679037	-5.4768638	-7.3092118
10.555556	0.19122086	-6.9337615	-6.4051377	-5.1055511	-7.9229692
10.808081	0.23025521	-7.1042574	-6.6156595	-4.7206844	-8.5690861
11.060606	0.26931212	-7.286426	-6.8015682	-4.332985	-9.2351536
11.313131	0.30802413	-7.4797341	-6.9640847	-3.9575431	-9.9052331
11.565657	0.34609102	-7.6833453	-7.1051146	-3.6121525	-10.560375
11.818182	0.38326615	-7.8968824	-7.2256493	-3.315332	-11.181662
12.070707	0.41945799	-8.1193152	-7.3280576	-3.0759536	-11.758843
12.323232	0.45453338	-8.3506525	-7.4126328	-2.9025878	-12.283507
12.575758	0.48845277	-8.5905674	-7.4803738	-2.7949813	-12.755516
12.828283	0.52127059	-8.8383961	-7.5329206	-2.7456516	-13.181405
13.080808	0.55290026	-9.0946614	-7.5696206	-2.7528666	-13.563865
13.333333	0.5834245	-9.3589353	-7.5916195	-2.806674	-13.912241
13.585859	0.61292199	-9.6307574	-7.5999867	-2.8983808	-14.234684
13.838384	0.64146309	-9.9098072	-7.595462	-3.0212503	-14.537558
14.090909	0.6687296	-10.198776	-7.5732882	-3.1790584	-14.821978
14.343434	0.69509515	-10.494887	-7.538347	-3.3593178	-15.09602
14.59596	0.7214607	-10.790998	-7.5034059	-3.5395772	-15.370063
14.848485	0.74702884	-11.093428	-7.456837	-3.7372695	-15.637913
15.10101	0.77118048	-11.406094	-7.3892549	-3.963032	-15.897553
15.353535	0.7944067	-11.724682	-7.3078545	-4.2056369	-16.153131
15.606061	0.81763291	-12.04327	-7.2264542	-4.4482418	-16.408709
15.858586	0.84085912	-12.361858	-7.1450538	-4.6908467	-16.664286
16.111111	0.86408533	-12.680446	-7.0636535	-4.9334516	-16.919864
16.363636	0.88674972	-13.001297	-6.9739686	-5.1860552	-17.172169
16.616162	0.90849032	-13.324934	-6.8708474	-5.4552037	-17.417966
16.868687	0.92992721	-13.648147	-6.763307	-5.7304071	-17.65946
17.121212	0.95074888	-13.967647	-6.646804	-6.0196178	-17.884287
17.373737	0.97116946	-14.283832	-6.5241498	-6.3189362	-18.095145
17.626263	0.99159003	-14.600018	-6.4014956	-6.6182545	-18.306004
17.878788	1.0120106	-14.916203	-6.2788414	-6.9175729	-18.516862
18.131313	1.0324312	-15.232388	-6.1561872	-7.2168912	-18.727721
18.383838	1.0527111	-15.546683	-6.0309694	-7.5207203	-18.929448
18.636364	1.0724045	-15.852709	-5.8946282	-7.8441347	-19.089095
18.888889	1.0919517	-16.155904	-5.7545971	-8.1740427	-19.229353
19.141414	1.0997644	-16.452697	-5.6269736	-8.5077276	-19.346544
19.393939	0.95673687	-16.710573	-5.7216361	-8.7855072	-19.52011
19.646465	1.1496005	-17.044056	-5.3038769	-9.2162048	-19.446978
19.89899	1.1685541	-17.333834	-5.14365	-9.5802507	-19.436866
20.151515	1.1873643	-17.620235	-4.977458	-9.9541021	-19.365313

20.40404	1.2060617	-17.90369	-4.8057951	-10.336942	-19.228989
20.656566	1.2246601	-18.184631	-4.6293237	-10.727745	-19.029144
20.909091	1.243151	-18.462803	-4.4474927	-11.127587	-18.750185
21.161616	1.2615411	-18.738512	-4.2609999	-11.535595	-18.394605
21.414141	1.2798407	-19.011726	-4.0700633	-11.951872	-17.960626
21.666667	1.2980433	-19.282619	-3.875429	-12.375631	-17.456863
21.919192	1.316181	-19.551933	-3.6791914	-12.80389	-16.920477
22.171717	1.3342185	-19.818806	-3.4804754	-13.239107	-16.333661
22.424242	1.352256	-20.085678	-3.2817594	-13.674324	-15.746845
22.676768	1.3701307	-20.348782	-3.0840084	-14.116576	-15.1584
22.929293	1.3879947	-20.611635	-2.8863216	-14.559296	-14.569847
23.181818	1.4058203	-20.87363	-2.6903034	-15.002403	-13.998033
23.434343	1.4235649	-21.133813	-2.4978448	-15.446299	-13.461839
23.686869	1.4412395	-21.392582	-2.310463	-15.888776	-12.970132
23.939394	1.4588655	-21.650304	-2.1280115	-16.329125	-12.516363
24.191919	1.4764318	-21.906845	-1.9524902	-16.765771	-12.108853
24.444444	1.4939613	-22.162698	-1.7816936	-17.199588	-11.729236
24.69697	1.5114426	-22.417615	-1.6179789	-17.628865	-11.387887
24.949495	1.5288818	-22.671694	-1.4614685	-18.053182	-11.08098
25.20202	1.5462656	-22.924909	-1.3132066	-18.471443	-10.809164
25.454545	1.5636171	-23.177473	-1.1716503	-18.884535	-10.56343
25.707071	1.5809283	-23.429377	-1.0372493	-19.291884	-10.343692
25.959596	1.5982067	-23.680659	-0.90990322	-19.693335	-10.148149
26.212121	1.6154383	-23.931272	-0.79046323	-20.087833	-9.9785341
26.464646	1.6326435	-24.181433	-0.67646008	-20.477375	-9.8264532
26.717172	1.6498139	-24.431033	-0.56927148	-20.860433	-9.696283
26.969697	1.6669506	-24.680106	-0.46852756	-21.237038	-9.5873245
27.222222	1.6840605	-24.928771	-0.37277377	-21.608406	-9.4954536
27.474747	1.701136	-25.176961	-0.28273916	-21.973495	-9.424214
27.727273	1.7181866	-25.424772	-0.19720794	-22.333376	-9.370849
27.979798	1.7352087	-25.672172	-0.11647625	-22.687424	-9.3382965
28.232323	1.7522049	-25.919199	-0.039950014	-23.036069	-9.3264157
28.484848	1.7691755	-26.165876	0.032716515	-23.379493	-9.336226
28.737374	1.7861215	-26.412211	0.10174229	-23.71771	-9.3700163
28.989899	1.8030446	-26.658228	0.16749586	-24.051	-9.4292125
29.242424	1.8199455	-26.903954	0.23038545	-24.379757	-9.5148271
29.494949	1.836825	-27.149403	0.29063424	-24.704137	-9.6293868
29.747475	1.8536833	-27.394558	0.34818555	-25.023822	-9.7799936
30	1.8705064	-27.639263	0.40190486	-25.336343	-10.00282

**S. Table 9.** Permanent electric dipole moments data of (1-5)  $^1\Pi$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$1^1\Pi$	$2^1\Pi$	$3^1\Pi$	$4^1\Pi$	$5^1\Pi$
5	-0.873706	-0.786032	-5.202501	-3.058997	-0.527494
5.2525253	-0.88178331	-0.81883411	-5.4563898	-3.0412595	-0.51808511
5.5050505	-0.87985503	-0.89698306	-5.6901177	-3.0498227	-0.50013551
5.7575758	-0.86949367	-1.0091985	-5.9043659	-3.0654003	-0.47419655
6.010101	-0.85291946	-1.1415581	-6.102398	-3.0872111	-0.44193512
6.2626263	-0.83112979	-1.2856242	-6.2838694	-3.122529	-0.4041989
6.5151515	-0.80523667	-1.434622	-6.4472424	-3.1805152	-0.36228655
6.7676768	-0.77569216	-1.5849984	-6.5863722	-3.2735297	-0.3170938
7.020202	-0.74299742	-1.7349482	-6.6933173	-3.4130667	-0.26968313
7.2727273	-0.70740864	-1.8840543	-6.7567471	-3.6120165	-0.220893
7.5252525	-0.66908514	-2.0327556	-6.7614564	-3.8853109	-0.17151409
7.7777778	-0.62838611	-2.1819936	-6.6986192	-4.2385664	-0.12222322
8.030303	-0.5854217	-2.3330485	-6.5563281	-4.6807112	-0.073579364
8.2828283	-0.54046832	-2.4872337	-6.3364217	-5.2057558	-0.025983949
8.5353535	-0.49374423	-2.6460077	-6.0503777	-5.7982899	0.020219303
8.7878788	-0.44556476	-2.8104724	-5.7239507	-6.4290721	0.064878364
9.040404	-0.39617567	-2.9819346	-5.3863262	-7.0658431	0.10781913
9.2929293	-0.34592195	-3.1608738	-5.0633476	-7.6808983	0.14908431
9.5454545	-0.29506853	-3.348386	-4.7739411	-8.2532864	0.18856769
9.7979798	-0.24395159	-3.5440655	-4.5223151	-8.778749	0.22644536
10.050505	-0.1928366	-3.7475612	-4.3069575	-9.2590093	0.26284003
10.30303	-0.14198296	-3.9590892	-4.1265971	-9.6950649	0.29774239
10.555556	-0.091665016	-4.1782253	-3.976191	-10.092557	0.3312349
10.808081	-0.042055764	-4.4038465	-3.8488487	-10.459826	0.36350821
11.060606	0.0066770606	-4.6352585	-3.7403167	-10.802117	0.39466097
11.313131	0.054365434	-4.8719697	-3.6476568	-11.123144	0.42476083
11.565657	0.10089942	-5.113333	-3.5679278	-11.426817	0.45390507
11.818182	0.14615551	-5.3589394	-3.4990426	-11.715909	0.48215128
12.070707	0.19015376	-5.6081714	-3.4386174	-11.993622	0.50962795
12.323232	0.23280643	-5.8609197	-3.3854307	-12.261524	0.53637079
12.575758	0.27410771	-6.1170186	-3.3380741	-12.521345	0.56244734
12.828283	0.31413423	-6.3762494	-3.2950977	-12.77481	0.58793902
13.080808	0.3527869	-6.6389487	-3.2557342	-13.022545	0.61284844
13.333333	0.39013583	-6.9051523	-3.2187452	-13.26577	0.6372365
13.585859	0.4262595	-7.1749159	-3.1830864	-13.505435	0.66116176
13.838384	0.46121575	-7.4483977	-3.1478611	-13.742257	0.68465452
14.090909	0.49456354	-7.7278449	-3.1114456	-13.976122	0.70758968
14.343434	0.52674559	-8.0120195	-3.0733834	-14.208221	0.7301249
14.59596	0.55892764	-8.2961942	-3.0353212	-14.44032	0.75266011
14.848485	0.59003801	-8.5853746	-2.9945433	-14.671305	0.77483104

15.10101	0.61916559	-8.8854749	-2.9458324	-14.901305	0.7963543
15.353535	0.64695705	-9.1938846	-2.8901034	-15.131259	0.81743506
15.606061	0.67474852	-9.5022943	-2.8343743	-15.361212	0.83851582
15.858586	0.70253998	-9.810704	-2.7786453	-15.591166	0.85959658
16.111111	0.73033144	-10.119114	-2.7229163	-15.82112	0.88067733
16.363636	0.75727343	-10.433561	-2.6612577	-16.051617	0.90147589
16.616162	0.78281391	-10.758223	-2.5891991	-16.28331	0.92180528
16.868687	0.807862	-11.086748	-2.5126743	-16.515862	0.94196502
17.121212	0.83194632	-11.422368	-2.4267959	-16.751034	0.96177495
17.373737	0.85538239	-11.762549	-2.334529	-16.988243	0.98134777
17.626263	0.87881846	-12.10273	-2.2422622	-17.225451	1.0009206
17.878788	0.90225453	-12.442911	-2.1499953	-17.46266	1.0204934
18.131313	0.92569061	-12.783092	-2.0577285	-17.699868	1.0400662
18.383838	0.94889922	-13.124451	-1.9633277	-17.938077	1.0595517
18.636364	0.97115677	-13.470364	-1.8601993	-18.180641	1.0786663
18.888889	0.99317675	-13.816586	-1.7553267	-18.424657	1.0976803
19.141414	1.0032474	-14.15771	-1.6642516	-18.670085	1.1050434
19.393939	0.86103802	-14.433802	-1.7748512	-18.910821	0.96186252
19.646465	1.057621	-14.851921	-1.432642	-19.167893	1.1540428
19.89899	1.078671	-15.194403	-1.3242103	-19.418945	1.1726429
20.151515	1.0994986	-15.534556	-1.2161303	-19.671759	1.1911348
20.40404	1.1201379	-15.872164	-1.1088266	-19.926065	1.209544
20.656566	1.140617	-16.207228	-1.002535	-20.181592	1.2278775
20.909091	1.1609184	-16.539041	-0.89779156	-20.438364	1.2461491
21.161616	1.181066	-16.867531	-0.79486198	-20.696109	1.2643095
21.414141	1.2010493	-17.192216	-0.6942279	-20.954651	1.2824039
21.666667	1.2208823	-17.513021	-0.596117	-21.213747	1.300421
21.919192	1.2406082	-17.830788	-0.50020981	-21.472915	1.3183867
22.171717	1.2601686	-18.143859	-0.40770919	-21.732193	1.336273
22.424242	1.2797289	-18.456929	-0.31520856	-21.991471	1.3541594
22.676768	1.2990214	-18.761644	-0.22953524	-22.24965	1.3718985
22.929293	1.318296	-19.065803	-0.1443163	-22.507756	1.3896277
23.181818	1.337506	-19.367866	-0.060989595	-22.765278	1.4073256
23.434343	1.3565791	-19.665499	0.018333192	-23.021557	1.4249572
23.686869	1.3755406	-19.959477	0.094101141	-23.276378	1.4425311
23.939394	1.394416	-20.250684	0.16705204	-23.529885	1.4600617
24.191919	1.4131898	-20.538702	0.23661907	-23.781634	1.477541
24.444444	1.4319057	-20.824846	0.30411956	-24.032225	1.4949905
24.69697	1.4505387	-21.108422	0.36871601	-24.281112	1.5123955
24.949495	1.4690956	-21.389687	0.43059858	-24.528306	1.529771
25.20202	1.4875691	-21.668569	0.48957632	-24.773594	1.5470803
25.454545	1.50598	-21.945661	0.546302	-25.01735	1.5643665
25.707071	1.5243265	-22.220953	0.60070889	-25.259485	1.5816233
25.959596	1.5426082	-22.49456	0.65289118	-25.500033	1.5988391
26.212121	1.5608183	-22.766372	0.70263943	-25.73881	1.6160259
26.464646	1.578982	-23.036987	0.75073171	-25.976375	1.6331831

26.717172	1.5970837	-23.306141	0.79677299	-26.21243	1.6503175
26.969697	1.6151263	-23.573943	0.84088548	-26.447065	1.6674094
27.222222	1.6331216	-23.84071	0.8835113	-26.680609	1.6844995
27.474747	1.6510604	-24.1063	0.92442752	-26.912915	1.7015163
27.727273	1.6689553	-24.370963	0.96398905	-27.144254	1.7185258
27.979798	1.6868004	-24.634633	1.0021067	-27.37458	1.7355121
28.232323	1.7045989	-24.897426	1.0389522	-27.604035	1.7524821
28.484848	1.7223508	-25.159402	1.0746114	-27.832707	1.7694206
28.737374	1.7400615	-25.420593	1.1091501	-28.060663	1.7863423
28.989899	1.7577301	-25.681063	1.1426681	-28.287996	1.8032408
29.242424	1.7753605	-25.940887	1.175287	-28.514804	1.8201149
29.494949	1.7929538	-26.200099	1.207068	-28.741152	1.8369734
29.747475	1.8105074	-26.458665	1.2379869	-28.967053	1.8538114
30	1.8279989	-26.716265	1.267664	-29.192393	1.8706177

**S. Table10.** Permanent electric dipole moments data of (1-2)  $^3\Pi$  electronic states of the  $\text{BeCs}^+$  molecular ion.

<b>R(Bohr)</b>	$1^3\Pi$	$2^3\Pi$
5	-0.409897	-5.32116
5.2525253	-0.33325923	-5.5512843
5.5050505	-0.28394929	-2.5837197
5.7575758	-0.26558539	-2.7467505
6.010101	-0.29216752	-2.8702999
6.2626263	-2.8631707	-0.45392232
6.5151515	-2.2290418	-1.2465568
6.7676768	-3.0831741	-0.55450117
7.020202	-3.6100778	-0.19252064
7.2727273	-3.8256306	-0.14391345
7.5252525	-3.9969711	-0.14048137
7.7777778	-4.1586712	-0.146521
8.030303	-4.3177327	-0.15386864
8.2828283	-4.4765381	-0.15917364
8.5353535	-4.6360161	-0.16058858
8.7878788	-4.7965488	-0.15724664
9.040404	-4.9584125	-0.1483794
9.2929293	-5.1216943	-0.13401736
9.5454545	-5.2866383	-0.11381041
9.7979798	-5.4532552	-0.088447856
10.050505	-5.6216134	-0.05851804
10.30303	-5.7919795	-11.85477
10.555556	-5.9645756	-12.113834
10.808081	-6.1394467	-12.365746
11.060606	-6.3167746	-12.609906

11.313131	-6.4968548	-12.844847
11.565657	-6.6799233	-13.066926
11.818182	-6.8663523	-13.221758
12.070707	-7.0562232	-13.172509
12.323232	-7.2499826	-13.631457
12.575758	-7.4479255	-13.873348
12.828283	-7.6501075	-14.058777
13.080808	-7.8572212	-14.222964
13.333333	-8.0694418	-14.370269
13.585859	-8.2868634	-14.501132
13.838384	-8.5096571	-14.615056
14.090909	-8.7407893	-14.702328
14.343434	-8.9783957	-14.768751
14.59596	-9.2160022	-14.835175
14.848485	-9.4602148	-14.880267
15.10101	-9.7182469	-14.882544
15.353535	-9.9864966	-14.854414
15.606061	-10.254746	-14.826284
15.858586	-10.522996	-14.798154
16.111111	-10.791246	-14.770024
16.363636	-11.066725	-14.723302
16.616162	-11.354402	-14.647416
16.868687	-11.646691	-14.564017
17.121212	-11.947914	-14.476186
17.373737	-12.255062	-14.388585
17.626263	-12.56221	-14.300984
17.878788	-12.869358	-14.213384
18.131313	-13.176506	-14.125783
18.383838	-13.485491	-14.042117
18.636364	-13.80192	-13.977501
18.888889	-14.119689	-13.923316
19.141414	-14.434935	-13.89658
19.393939	-14.701805	-14.040616
19.646465	-15.078219	-13.861451
19.89899	-15.397879	-13.877417
20.151515	-15.716868	-13.917553
20.40404	-16.034847	-13.981811
20.656566	-16.351651	-14.068924
20.909091	-16.666788	-14.184407
21.161616	-16.980076	-14.32856
21.414141	-17.291085	-14.505799
21.666667	-17.599684	-14.717182
21.919192	-17.906262	-14.956575
22.171717	-18.209717	-15.239264
22.424242	-18.513171	-15.521954
22.676768	-18.810695	-15.887069

22.929293	-19.107824	-16.25767
23.181818	-19.403389	-16.649838
23.434343	-19.695646	-17.087596
23.686869	-19.985082	-17.562674
23.939394	-20.272336	-18.06489
24.191919	-20.557034	-18.595556
24.444444	-20.840206	-19.140769
24.69697	-21.121265	-19.703141
24.949495	-21.400391	-20.276159
25.20202	-21.677497	-20.853783
25.454545	-21.953064	-21.429757
25.707071	-22.227065	-21.999198
25.959596	-22.499587	-22.557373
26.212121	-22.770512	-23.097411
26.464646	-23.040364	-23.622062
26.717172	-23.308891	-24.124281
26.969697	-23.57618	-24.602251
27.222222	-23.842516	-25.059982
27.474747	-24.107757	-25.493077
27.727273	-24.372127	-25.905989
27.979798	-24.635565	-26.296935
28.232323	-24.898165	-26.66845
28.484848	-25.159985	-27.022195
28.737374	-25.421052	-27.359407
28.989899	-25.681422	-27.682077
29.242424	-25.941166	-27.992368
29.494949	-26.200312	-28.29161
29.747475	-26.45883	-28.58001
30	-26.716396	-28.854134

**S. Table. 11.** Permanent electric dipole moments data of (1-2)  $1,3\Delta$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$1^1\Delta$	$2^1\Delta$	$1^3\Delta$
5	-1.239037	-3.801576	-4.005049
5.2525253	-1.3001242	-3.9423704	-4.2400871
5.5050505	-1.3630846	-4.0780335	-4.4704746
5.7575758	-1.4220167	-4.2139999	-4.697504
6.010101	-1.4733922	-4.3541485	-4.923091
6.2626263	-1.5149642	-4.5011134	-5.1482107
6.5151515	-1.5466192	-4.655786	-5.3739613
6.7676768	-1.5684729	-4.8188057	-5.6010223

7.020202	-1.5817959	-4.9901615	-5.8299577
7.2727273	-1.5873355	-5.1690613	-6.061165
7.5252525	-1.5861601	-5.3560449	-6.2951372
7.7777778	-1.5792054	-5.5498872	-6.5310914
8.030303	-1.5670959	-5.7511556	-6.7700053
8.2828283	-1.5501069	-5.9599429	-7.0115797
8.5353535	-1.5282413	-6.1750273	-7.2555834
8.7878788	-1.5020254	-6.3976358	-7.5021999
9.040404	-1.4709083	-6.6275835	-7.7514474
9.2929293	-1.4351228	-6.864213	-8.0026594
9.5454545	-1.3941415	-7.1083715	-8.25617
9.7979798	-1.3485274	-7.3599223	-8.5116263
10.050505	-1.2978597	-7.6176943	-8.768532
10.30303	-1.2421995	-7.8827988	-9.0268966
10.555556	-1.1815502	-8.1546034	-9.2867404
10.808081	-1.1160707	-8.4317592	-9.5474744
11.060606	-1.0465536	-8.7149789	-9.8090205
11.313131	-0.97272378	-9.0034248	-10.071041
11.565657	-0.89865161	-9.2964384	-10.333431
11.818182	-0.81426563	-9.5940734	-10.596253
12.070707	-0.73138037	-9.8941354	-10.858431
12.323232	-0.64608458	-10.197317	-11.120392
12.575758	-0.559342	-10.502313	-11.382131
12.828283	-0.47258728	-10.808573	-11.643126
13.080808	-0.38444021	-11.115438	-11.903539
13.333333	-0.29832129	-11.421913	-12.163058
13.585859	-0.21142835	-11.727731	-12.421735
13.838384	-0.12604371	-12.032567	-12.679433
14.090909	-0.04388051	-12.334485	-12.935501
14.343434	0.03553474	-12.633936	-13.190611
14.59596	0.11494999	-12.933387	-13.445721
14.848485	0.19139167	-13.230132	-13.699649
15.10101	0.26125026	-13.519727	-13.951288
15.353535	0.32566092	-13.804035	-14.201231
15.606061	0.39007158	-14.088344	-14.451175
15.858586	0.45448223	-14.372653	-14.701119
16.111111	0.51889289	-14.656962	-14.951063
16.363636	0.57952155	-14.937274	-15.199928
16.616162	0.63362939	-15.210704	-15.446812
16.868687	0.68348069	-15.481212	-15.692868
17.121212	0.72958102	-15.746264	-15.937563
17.373737	0.77125815	-16.007404	-16.181184
17.626263	0.81293528	-16.268545	-16.424805
17.878788	0.85461241	-16.529685	-16.668426
18.131313	0.89628954	-16.790825	-16.912047
18.383838	0.93432723	-17.050472	-17.155327

18.636364	0.96562018	-17.304216	-17.397059
18.888889	1.0025432	-17.556565	-17.638319
19.141414	1.0323229	-17.805693	-17.878706
19.393939	1.0617885	-18.054454	-18.118946
19.646465	1.0912542	-18.303214	-18.359186
19.89899	1.1196524	-18.550633	-18.599426
20.151515	1.1458226	-18.796089	-18.83889
20.40404	1.1705594	-19.040559	-19.078006
20.656566	1.1948676	-19.284297	-19.316952
20.909091	1.2189552	-19.527074	-19.55564
21.161616	1.2396857	-19.767158	-19.793799
21.414141	1.2597956	-20.006768	-20.032236
21.666667	1.2799056	-20.246377	-20.27027
21.919192	1.3000155	-20.485987	-20.508203
22.171717	1.3201254	-20.725597	-20.745981
22.424242	1.3402354	-20.965207	-20.983759
22.676768	1.3603453	-21.204816	-21.221173
22.929293	1.3804552	-21.444426	-21.458562
23.181818	1.4005651	-21.684036	-21.695903
23.434343	1.4206751	-21.923645	-21.933138
23.686869	1.440785	-22.163255	-22.170286
23.939394	1.4552713	-22.402198	-22.407355
24.191919	1.4769245	-22.639902	-22.64435
24.444444	1.4999715	-22.877514	-22.881334
24.69697	1.5167407	-23.114954	-23.118271
24.949495	1.5341841	-23.352272	-23.355167
25.20202	1.5507696	-23.589486	-23.591907
25.454545	1.5690949	-23.8266	-23.828682
25.707071	1.5776386	-24.063637	-24.065434
25.959596	1.6042908	-24.300607	-24.302143
26.212121	1.6185741	-24.537505	-24.538822
26.464646	1.6301068	-24.774374	-24.775484
26.717172	1.655289	-25.010925	-25.012101
26.969697	1.6664121	-25.247916	-25.248726
27.222222	1.690323	-25.484637	-25.485263
27.474747	1.706868	-25.721323	-25.721799
27.727273	1.7235114	-25.95801	-25.958336
27.979798	1.7415096	-26.194614	-26.194872
28.232323	1.7573319	-26.431206	-26.431408
28.484848	1.7730589	-26.667798	-26.667945
28.737374	1.7922027	-26.904364	-26.904481
28.989899	1.8089196	-27.140911	-27.141018
29.242424	1.8259037	-27.37743	-27.377554
29.494949	1.8429613	-27.613966	-27.61409
29.747475	1.850647	-27.850474	-27.850618
30	1.86894	-28.086966	-28.087091

**S. Table 12.** Transition electric dipole moments between low-lying  $1,3\Sigma^+$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$2^1\Sigma^+ - 1^1\Sigma^+$	$R(\text{Bohr})$	$3^1\Sigma^+ - 1^1\Sigma^+$	$R(\text{Bohr})$	$4^1\Sigma^+ - 1^1\Sigma^+$	$R(\text{Bohr})$	$5^1\Sigma^+ - 1^1\Sigma^+$
4.5	1.867665	4.5	0.189702	4.5	0.198056	4.5	0.050878
4.6	1.852071	4.6	0.227301	4.6	0.190988	4.6	0.051612
4.7	1.839879	4.7	0.245557	4.7	0.179982	4.7	0.051315
4.8	1.830605	4.8	0.254219	4.8	0.166443	4.8	0.050239
4.9	1.823847	4.9	0.257429	4.9	0.151502	4.9	0.0486
5	1.81927	5	0.257264	5	0.545194	5	0.046591
5.1	1.816585	5.1	0.254889	5.1	0.54528	5.1	0.044383
5.2	1.81554	5.2	0.251011	5.2	0.544835	5.2	0.042124
5.3	1.815914	5.3	0.246092	5.3	0.543766	5.3	0.039932
5.4	1.817512	5.4	0.240454	5.4	0.542028	5.4	0.037898
5.5	1.820162	5.5	0.234343	5.5	0.5396	5.5	0.036083
5.6	1.823712	5.6	0.227958	5.6	0.536475	5.6	0.034519
5.7	1.828029	5.7	0.221476	5.7	0.532649	5.7	0.033211
5.8	1.83299	5.8	0.215064	5.8	0.528115	5.8	0.032143
5.9	1.838483	5.9	0.208891	5.9	0.52287	5.9	0.03128
6	1.844404	6	0.203133	6	0.516907	6	0.030571
6.1	1.850653	6.1	0.197979	6.1	0.510221	6.1	0.029961
6.2	1.857135	6.2	0.193628	6.2	0.502814	6.2	0.029391
6.3	1.863754	6.3	0.190296	6.3	0.494691	6.3	0.028801
6.4	1.870415	6.4	0.188201	6.4	0.48587	6.4	0.028139
6.5	1.877023	6.5	0.187564	6.5	0.476379	6.5	0.027356
6.6	1.883481	6.6	0.188592	6.6	0.466258	6.6	0.026411
6.7	1.889696	6.7	0.191469	6.7	0.45556	6.7	0.02527
6.8	1.895572	6.8	0.196346	6.8	0.444346	7.7	0.015026
6.9	1.901018	6.9	0.203328	6.9	0.432681	7.8	0.019458
7	1.905946	7	0.212469	7	0.420636	7.9	0.024434
7.1	1.910274	7.1	0.223775	7.1	0.408276	8	0.029938
7.25	1.915478	7.25	0.244672	7.25	0.389277	8.1	0.035947
7.3	1.916836	7.3	0.252639	7.3	0.382849	8.2	0.042432
7.45	1.91969	7.45	0.279297	7.45	0.363351	8.3	0.049359
7.5	1.920215	7.5	0.289031	7.5	0.356796	8.4	0.056689
7.65	1.920462	7.65	0.320452	7.65	0.337012	8.5	0.064376
7.7	1.920093	7.7	0.331581	7.7	0.330387	8.6	0.072371
7.8	1.918672	7.8	0.354671	7.8	0.317104	8.7	0.080621
7.9	1.916341	7.9	0.378702	7.9	0.303787	8.8	0.08907
8	1.913113	8	0.403478	8	0.290447	8.9	0.097656
8.1	1.909009	8.1	0.428815	8.1	0.277093	9	0.10632
8.2	1.90406	8.2	0.45454	8.2	0.26373	9.1	0.114995
8.3	1.898303	8.3	0.480496	8.3	0.250363	9.2	0.123618
8.4	1.891781	8.4	0.506541	8.4	0.236993	9.3	0.115809
8.5	1.884543	8.5	0.532549	8.5	0.223623	9.43	0.097813
8.6	1.876639	8.6	0.558412	8.6	0.210251	9.5	0.088009

8.7	1.868123	8.7	0.584036	8.7	0.196871	9.66	0.065237
8.8	1.85905	8.8	0.609339	8.8	0.183477	9.7	0.059455
8.9	1.849474	8.9	0.634255	8.9	0.170059	9.87	0.034433
9	1.839449	9	0.658729	9	0.156603	9.93	0.025419
9.1	1.829029	9.1	0.682717	9.1	0.14309	10	0.014781
9.2	1.818265	9.2	0.706184	9.2	0.129501	10.1	0.000637
9.3	1.807206	9.3	0.729101	9.3	-0.132119	10.25	0.024192
9.43	1.792468	9.43	0.758041	9.43	-0.142874	10.3	0.032135
9.5	1.784394	9.5	0.773215	9.5	-0.148476	10.43	0.0529
9.66	1.765668	9.66	0.806804	9.66	-0.160614	10.52	0.06729
9.7	1.760942	9.7	0.814961	9.7	-0.163476	10.66	0.089488
9.87	1.740739	9.87	0.848558	9.87	-0.174689	10.7	0.095751
9.93	1.733585	10.52	0.96131	10.52	-0.197495	10.85	0.194342
10	1.725237	10.66	0.982461	10.66	-0.197335	11	0.190057
10.1	1.713328	10.7	0.988309	10.7	-0.196959	11.1	0.186454
10.25	1.695557	10.85	1.009482	10.85	-0.118737	11.25	0.180216
10.3	1.689672	11	1.029488	11	0.140672	11.3	0.17797
10.43	1.674487	11.1	1.042194	11.1	0.154571	11.4	0.173304
10.52	1.664093	11.25	1.060334	11.25	0.174199	11.56	0.165542
10.66	1.648156	11.3	1.066141	11.3	0.180402	11.6	0.163574
10.7	1.64366	11.4	1.077402	11.4	0.192289	11.75	0.156197
10.85	1.627052	11.56	1.094466	11.56	0.209892	11.8	0.153757
11	1.610876	11.6	1.098553	11.6	0.214028	11.99	0.144674
11.1	1.600353	11.75	1.113257	11.75	0.22864	12.1	0.139599
11.25	1.584987	11.8	1.117944	11.8	0.233209	12.21	0.134684
11.3	1.579981	11.99	1.134805	11.99	0.249298	12.3	0.130788
11.4	1.570149	12.1	1.143899	12.1	0.257759	12.46	0.124153
11.56	1.554935	12.21	1.152517	12.21	0.26565	12.5	0.122553
11.6	1.551232	12.3	1.159224	12.3	0.271712	12.64	0.117135
11.75	1.537721	12.46	1.1704	12.46	0.281679	12.7	0.114899
11.8	1.533349	12.5	1.173048	12.5	0.284019	12.82	0.110576
11.99	1.517351	12.64	1.181869	12.64	0.291766	12.9	0.107801
12.1	1.50854	12.7	1.185439	12.7	0.294885	13	0.10445
12.21	1.500064	12.82	1.192212	12.82	0.300782	13.1	0.101223
12.3	1.49338	12.9	1.19646	12.9	0.304475	13.26	0.096307
12.46	1.482059	13	1.201476	13	0.308835	13.3	0.095122
12.5	1.479341	13.1	1.206171	13.1	0.312924	13.46	0.090554
12.64	1.470187	13.26	1.213035	13.26	0.318937	13.5	0.089453
12.7	1.466433	13.3	1.214629	13.3	0.320342	13.64	0.08572
12.82	1.459232	13.46	1.220529	13.46	0.325593	13.7	0.084175
12.9	1.454657	13.5	1.221887	13.5	0.326816	13.85	0.08045
13	1.449193	13.64	1.22628	13.64	0.330825	13.92	0.078775
13.1	1.444011	13.7	1.227994	13.7	0.332418	14	0.076908
13.26	1.436304	13.85	1.231848	13.85	0.336082	14.69	0.062648
13.3	1.43449	13.92	1.233439	13.92	0.337642	14.82	0.060289
13.46	1.427675	14	1.235098	14	0.33931	15	0.057178

13.5	1.426082	14.69	1.242714	14.69	0.349004	16.25	0.040524
13.64	1.420854	14.82	1.242864	14.82	0.349954	16.42	0.038999
13.7	1.418777	15	1.242425	15	0.350845	16.67	0.037134
13.85	1.414013	16.25	1.219149	16.25	0.34497	16.83	0.036189
13.92	1.411997	16.42	1.213225	16.42	0.342765	17	0.035405
14	1.409854	16.67	1.203256	16.67	0.339017	18.33	0.036729
14.69	1.398302	16.83	1.196069	16.83	0.336325	18.53	0.037824
14.82	1.397479	17	1.187721	17	0.333237	18.79	0.039449
15	1.397027	18.33	1.094208	18.33	0.303017	18.93	0.040394
16.25	1.414802	18.53	1.07532	18.53	0.297854	19.13	0.041801
16.42	1.419906	18.79	1.048685	18.79	0.291016	19.35	0.041801
16.67	1.428523	18.93	1.033347	18.93	0.287291	19.55	0.044859
16.83	1.434721	19.76	0.927965	19.76	0.265004	19.76	0.046386
17	1.441882	19.92	0.904902	19.92	0.260733	19.92	0.04753
18.33	1.517203	20.11	0.876465	20.11	0.255694	20.11	0.048853
18.53	1.531237	20.33	0.842231	20.33	0.24992	20.33	0.050325
18.79	1.550374	20.58	0.801851	20.58	0.243454	20.58	0.051902
18.93	1.561059	20.74	0.775323	20.74	0.239376	20.74	0.05285
19.13	1.576726	20.95	0.739886	20.95	0.234104	20.95	0.054017
19.55	1.610842	21.12	0.710831	21.12	0.229907	21.12	0.054894
19.76	1.628297	21.36	0.669529	21.36	0.224099	21.36	0.056024
19.92	1.64167	21.82	0.590745	21.82	0.213372	21.82	0.057828
20.11	1.65754	22.44	0.489166	22.44	0.199808	22.44	0.059501
20.33	1.675768	23.1	0.391785	23.1	0.186536	23.1	0.060354
20.58	1.696085	23.43	0.34832	23.43	0.180349	23.43	0.060438
20.74	1.708759	23.65	0.321406	23.65	0.176389	23.65	0.060374
20.95	1.724885	23.85	0.298377	23.85	0.172902	23.85	0.060233
21.12	1.737438	24	0.281996	24	0.170355	24	0.060078
21.36	1.754278	24.56	0.227356	24.33	0.164957	24.33	0.059589
21.82	1.783249	24.74	0.211871	24.56	0.161359	24.56	0.05913
22.44	1.814806	24.95	0.195002	24.74	0.158634	24.74	0.058706
23.1	1.839254	25.13	0.181519	24.95	0.155555	24.95	0.058139
23.43	1.848405	25.35	0.1662	25.13	0.152999	25.13	0.057592
23.65	1.85354	25.55	0.153319	25.35	0.149979	25.35	0.056848
23.85	1.857615	25.75	0.141376	25.55	0.14733	25.55	0.0561
24	1.860336	25.95	0.130311	25.75	0.14477	25.75	0.055286
24.33	1.865435	26.13	0.121058	25.95	0.142298	25.95	0.054405
24.56	1.868363	26.39	0.10879	26.13	0.140147	26.13	0.053556
24.74	1.870347	26.52	0.103112	26.39	0.13716	26.39	0.052235
24.95	1.872364	26.73	0.094535	26.52	0.135719	26.52	0.051534
25.13	1.873869	26.92	0.087374	26.73	0.133461	26.73	0.050343
25.35	1.875464	27.19	0.078035	26.92	0.131491	26.92	0.049205
25.55	1.876712	27.36	0.072704	27.19	0.128809	27.19	0.047491
25.75	1.877794	27.55	0.067165	27.36	0.127187	27.36	0.046354
25.95	1.878732	27.74	0.062041	27.55	0.125433	27.55	0.045034
26.13	1.87947	27.99	0.055878	27.74	0.123739	27.74	0.043662

26.39	1.880383	28.19	0.051386	27.99	0.121594	27.99	0.041782
26.52	1.880781	28.3	0.04907	28.19	0.119943	28.19	0.040223
26.73	1.881354	28.5	0.045121	28.3	0.119058	28.3	0.039346
26.92	1.881806	28.7	0.041488	28.5	0.117488	28.5	0.037718
27.19	1.882359	28.9	0.038148	28.7	0.115966	28.7	0.036057
27.36	1.882659	29.1	0.035076	28.9	0.114483	28.9	0.034362
27.55	1.882957	29.3	0.032254	29.1	0.113037	29.1	0.032648
27.74	1.883223	29.5	0.02966	29.3	0.111625	29.3	0.03092
27.99	1.883529	29.7	0.027277	29.5	0.11024	29.5	0.029188
28.19	1.883743	29.8	0.02616	29.7	0.108878	29.7	0.027461
28.3	1.883851	30.5	0.01954	29.8	0.108205	29.8	0.026602
28.5	1.884031	30.9	0.016558	30.5	0.103601	30.5	0.020798
28.7	1.884193	31.1	0.015249	30.9	0.101031	30.9	0.017739
28.9	1.884341	31.25	0.014339	31.1	0.099759	31.1	0.016303
29.1	1.884474	31.53	0.012788	31.25	0.098812	31.25	0.015272
29.3	1.884595	31.76	0.011647	31.53	0.097057	31.53	0.013455
29.5	1.884707	31.96	0.010743	31.76	0.09563	31.76	0.012074
29.7	1.884809	32.14	0.009993	31.96	0.094402	31.96	0.010955
29.8	1.884857	32.34	0.009226	32.14	0.093307	32.14	0.010012
30.5	1.885151	32.56	0.008453	32.34	0.092103	32.34	0.009037
30.9	1.885291	32.73	0.007905	32.56	0.090796	32.56	0.008048
31.1	1.885355	34.42	0.004154	32.73	0.089798	32.73	0.007343
31.25	1.885402	37	0.001706	32.91	0.088755	32.91	0.006649
31.53	1.885483	39.99	0.000689		0.087442	33.14	0.00584
31.76	1.885546	40.06	0.000676	33.26	0.086766	33.26	0.005449
31.96	1.885598	41	0.000519	33.52	0.085323	33.52	0.004674
32.14	1.885644	42.3	0.000366	33.64	0.084668	33.64	0.004348
32.34	1.885692	43.2	0.00029	33.93	0.083111	33.93	0.003633
32.56	1.885743	44	0.000237	34.04	0.082531	34.04	0.003388
32.73	1.88578	46.6	0.00013	34.25	0.081439	34.25	0.002955
32.91	1.885819	47.8	0.000101	34.42	0.08057	34.42	0.002638
33.14	1.885867	48.23	9.3e-05	34.63	0.079514	34.63	0.002283
33.26	1.885891	49.3	7.6e-05	34.87	0.078332	34.87	0.001922
33.52	1.885941	50.32	6.3e-05	35.04	0.077511	35.04	0.001693
33.64	1.885963	51.64	4.9e-05	35.32	0.076185	35.32	0.00136
33.93	1.886015			35.53	0.075213	35.53	0.001141
34.04	1.886034			35.76	0.074169	35.76	0.00093
34.25	1.88607			35.88	0.073633	35.88	0.00083
34.42	1.886098			36.26	0.071974	36.26	0.000554
34.63	1.886131			36.53	0.070828	36.53	0.000392
34.87	1.886167			36.87	0.069424	36.87	0.000221
35.04	1.886192			37	0.068898	37	0.000164
35.32	1.886231			37.7	0.066165	37.7	7.7e-05
35.53	1.88626			37.8	0.065787	37.8	0.000104
35.76	1.886289			38.3	0.063947	38.3	0.000217
35.88	1.886305			38.7	0.062528	38.7	0.000285

36.26	1.88635	38.9	0.061836	38.9	0.000313
36.53	1.886381	39.04	0.061358	39.04	0.00033
36.87	1.886417	39.23	0.060718	39.23	0.000352
37	1.88643	39.46	0.059956	39.46	0.000375
37.7	1.886497	39.77	0.058951	39.77	0.0004
37.8	1.886506	39.99	0.058253	39.99	0.000415
38.3	1.886548	40.06	0.058033	40.06	0.00042
38.7	1.886578	41	0.055196	41	0.00046
38.9	1.886593	42.3	0.051595	42.3	0.000476
39.04	1.886603	43.2	0.049302	43.2	0.000469
39.23	1.886616	44	0.04739	44	0.000455
39.46	1.886631	46.6	0.041899	46.6	0.000375
39.77	1.88665	47.8	0.039692	47.8	0.000328
39.99	1.886663	48.23	0.038946	48.23	0.000312
40.06	1.886668	49.3	0.037182	49.3	0.00027
41	1.886717	50.32	0.035617	50.32	0.000232

**S. Table 13.** Transition electric dipole moments between low-lying  $1,3\Sigma^+$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$3^1\Sigma^+ - 2^1\Sigma^+$	$R(\text{Bohr})$	$4^1\Sigma^+ - 2^1\Sigma^+$	$R(\text{Bohr})$	$4^1\Sigma^+ - 3^1\Sigma^+$	$R(\text{Bohr})$	$5^1\Sigma^+ - 4^1\Sigma^+$
4.5	0.74955	4.5	1.218567	4.5	0.33999	4.5	1.881608
4.6	0.83106	4.6	1.168314	4.6	0.35523	4.6	2.11736
4.7	0.893213	4.7	1.119582	4.7	0.386248	4.7	2.336072
4.8	0.94638	4.8	1.075197	4.8	0.427909	4.8	2.535635
4.9	0.994811	4.9	1.0366	4.9	0.478458	4.9	2.715467
5	1.040554	5	0.693238	5	1.419745	5	1.773994
5.1	1.084704	5.1	0.646111	5.1	1.446641	5.1	1.90358
5.2	1.127887	5.2	0.596187	5.2	1.46689	5.2	2.013423
5.3	1.170475	5.3	0.543737	5.3	1.479198	5.3	2.101873
5.4	1.212689	5.4	0.488969	5.4	1.482315	5.4	2.168464
5.5	1.254659	5.5	0.432048	5.5	1.475043	5.5	2.21384
5.6	1.296452	5.6	0.373119	5.6	1.456258	5.6	2.239633
5.7	1.338089	5.7	0.31231	5.7	1.424956	5.7	2.248266
5.8	1.379564	5.8	0.249747	5.8	1.380298	5.8	2.242702
5.9	1.420844	5.9	0.185557	5.9	1.321684	5.9	2.226175
6	1.461886	6	0.119893	6	1.248813	6	2.201907
6.1	1.502644	6.1	0.052943	6.1	1.161762	6.1	2.172862
6.2	1.543075	6.2	-0.015056	6.2	1.061051	6.2	2.141581
6.3	1.583163	6.3	-0.083798	6.3	0.947685	6.3	2.110081
6.4	1.622922	6.4	-0.152913	6.4	0.82317	6.4	2.079848
6.5	1.662411	6.5	-0.221962	6.5	0.689474	6.5	2.051871
6.6	1.701741	6.6	-0.290449	6.6	0.548937	6.6	2.026724
6.7	1.741071	6.7	-0.357845	6.7	0.404135	6.7	2.004659
6.8	1.780605	6.8	-0.423607	6.8	0.257712	6.8	1.985696
6.9	1.820574	6.9	-0.48721	6.9	0.112202	6.9	1.969694

7	1.861216	7	-0.54817	7.1	0.1674	7	1.956416
7.1	1.902761	7.1	-0.606062	7.25	0.360822	7.1	1.945565
7.25	1.967191	7.25	-0.686404	7.3	0.42152	7.25	1.933112
7.3	1.989304	7.3	-0.711323	7.45	0.591572	7.3	1.929805
7.45	2.057692	7.45	-0.7802	7.5	0.644232	7.45	1.169252
7.5	2.081182	7.5	-0.80116	7.65	0.79063	7.5	1.089435
7.65	2.153677	7.65	-0.857999	7.7	0.83578	7.65	0.854841
7.7	2.178484	7.7	-0.874944	7.8	0.9211	7.7	0.778396
7.8	2.228974	7.8	-0.905892	7.9	1.000416	7.8	0.62829
7.9	2.280513	7.9	-0.933014	8	1.074549	7.9	0.481972
8	2.332935	8	-0.956459	8.1	1.144345	8	0.339462
8.1	2.386066	8.1	-0.976403	8.2	1.210656	8.3	-0.065772
8.2	2.439727	8.2	-0.993042	8.3	1.274309	8.4	-0.19377
8.3	2.493745	8.3	-1.006585	8.4	1.336104	8.5	-0.318447
8.4	2.547956	8.4	-1.017249	8.5	1.396801	8.6	-0.439948
8.5	2.602207	8.5	-1.025258	8.6	1.457124	8.7	-0.558409
8.6	2.656365	8.6	-1.030829	8.7	1.517753	8.8	-0.673961
8.7	2.710315	8.7	-1.034177	8.8	1.579334	8.9	-0.786705
8.8	2.76396	8.8	-1.035507	8.9	1.642474	9	-0.896721
8.9	2.817221	8.9	-1.035013	9	1.707748	9.1	-1.004023
9	2.870038	9	-1.032871	9.1	1.775698	9.2	-1.108561
9.1	2.922367	9.1	-1.029243	10.85	3.555874	9.3	-1.210197
9.2	2.974181	9.2	-1.024271	11	3.707369	9.43	-1.337548
9.3	3.025464	9.3	-0.278725	11.1	3.800093	9.5	-1.403593
9.43	3.091335	9.43	-0.225809	11.25	3.926132	9.66	-1.546555
9.5	3.126436	9.5	-0.19755	11.3	3.964681	9.7	-1.58026
9.66	3.205735	9.66	-0.133546	11.4	4.036749	9.87	-1.712076
9.7	3.225365	9.7	-0.117667	11.56	4.13892	9.93	-1.753378
9.87	3.307989	9.87	-0.050705	11.6	4.162114	10	-1.797442
9.93	3.336858	9.93	-0.027283	11.75	4.241534	10.1	-1.851638
10	3.370362	10	-0.000111	11.8	4.265556	10.25	-1.910275
10.1	3.417915	10.1	0.038365	11.99	4.347024	10.3	-1.922971
10.25	3.488636	10.25	0.095089	12.1	4.38792	10.43	-1.938179
10.3	3.512066	10.3	0.11365	12.21	4.424848	10.52	-1.932801
10.43	3.572692	10.43	0.160812	12.3	4.452419	10.66	-1.897859
10.52	3.61445	10.52	0.192309	12.46	4.496241	10.7	-1.882026
10.66	3.679125	10.66	0.238893	12.5	4.506255	10.85	-1.801043
10.7	3.697552	10.7	0.251576	12.64	4.538636	11	-1.690171
10.85	3.766503	10.85	0.794075	12.7	4.551334	11.1	-1.603103
11	3.835299	11	0.762933	12.82	4.574793	11.25	-1.458448
11.1	3.881129	11.1	0.742385	12.9	4.589093	11.3	-1.40758
11.25	3.949902	11.25	0.712434	13	4.605574	11.4	-1.303355
11.3	3.972848	11.3	0.702775	13.1	4.620605	11.56	-1.133242
11.4	4.018794	11.4	0.684052	13.26	4.641861	11.6	-1.090615
11.56	4.092516	11.56	0.655955	13.3	4.646668	11.75	-0.932111
11.6	4.110997	11.6	0.649314	13.46	4.664003	11.8	-0.880056

11.75	4.180522	11.75	0.625827	13.5	4.66788	11.99	-0.687204
11.8	4.203786	11.8	0.618491	13.64	4.680087	12.1	-0.579668
11.99	4.292649	11.99	0.592809	13.7	4.684689	12.21	-0.475318
12.1	4.344474	12.1	0.579444	13.85	4.694612	12.3	-0.392297
12.21	4.396607	12.21	0.567094	13.92	4.698492	12.46	-0.249703
12.3	4.439508	12.3	0.557688	14	4.702361	12.5	-0.214995
12.46	4.516361	12.46	0.542369	14.69	4.712271	12.64	-0.096255
12.5	4.535698	12.5	0.538796	14.82	4.709711	12.7	-0.046573
12.64	4.603781	12.64	0.527007	15	4.703979	12.82	0.050863
12.7	4.633159	12.7	0.522266	16.25	4.599726	12.9	0.114535
12.82	4.692286	12.82	0.513283	16.42	4.577657	13	0.192864
12.9	4.731984	12.9	0.507624	16.67	4.542176	13.1	0.269992
13	4.781931	13	0.500873	16.83	4.51767	13.26	0.391408
13.1	4.832243	13.1	0.494434	17	4.490179	13.3	0.421464
13.26	4.913513	13.26	0.484665	20.33	0.594296	13.46	0.540852
13.3	4.933982	13.3	0.482307	20.58	0.667244	13.5	0.570553
13.46	5.016455	13.46	0.473143	20.74	0.713751	13.64	0.674318
13.5	5.037224	13.5	0.470905	20.95	0.774186	13.7	0.718787
13.64	5.110388	13.64	0.463189	21.12	0.822334	13.85	0.830275
13.7	5.141967	13.7	0.459922	21.36	0.888663	13.92	0.882584
13.85	5.221497	13.85	0.451801	21.82	1.008528	14	0.942687
13.92	5.25889	13.92	0.448012	22.44	1.150676	14.69	1.487315
14	5.301837	14	0.443666	23.1	1.274416	14.82	1.597629
14.69	5.680802	14.69	0.403652	23.43	1.32593	15	1.755695
14.82	5.753658	14.82	0.39526	23.65	1.356786	16.25	3.061165
15	5.855101	15	0.383013	23.85	1.382621	16.42	3.266018
16.25	6.562208	16.25	0.27074	24	1.400718	16.67	3.574735
16.42	6.655893	16.42	0.250924	24.33	1.437074	16.83	3.775042
16.67	6.790907	16.67	0.219465	24.56	1.45995	17	3.988304
16.83	6.87513	16.83	0.19782	24.74	1.476644	18.33	5.49421
17	6.96231	17	0.173479	24.95	1.49496	18.53	5.679387
18.33	7.505349	18.33	0.068568	25.13	1.509809	18.79	5.903308
18.53	7.554638	18.53	0.113187	25.35	1.527067	18.93	6.016588
18.79	7.600626	18.79	0.174344	25.55	1.54206	19.76	6.6045
18.93	7.615959	18.93	0.208702	25.75	1.556534	19.92	6.705214
19.13	7.625242	19.13	0.259425	25.95	1.570614	20.11	6.821047
19.35	7.625242	19.55	0.371632	26.13	1.583048	20.33	6.950918
19.55	7.590807	19.76	0.43017	26.39	1.600763	20.58	7.094108
19.76	7.543373	19.92	3.849817	26.52	1.609568	20.74	7.183834
19.92	7.492694	20.11	3.800309	26.73	1.623787	20.95	7.299882
20.11	7.415605	20.33	3.742153	26.92	1.636701	21.12	7.392743
20.33	7.302922	20.58	3.675112	27.19	1.655292	21.36	7.522721
20.58	7.144272	20.74	3.631754	27.36	1.667081	21.82	7.770188
20.74	7.025945	20.95	3.574429	27.55	1.680409	22.44	8.104938
20.95	6.85159	21.12	3.527772	27.74	1.693901	23.1	8.467531
21.12	6.695484	21.36	3.461709	27.99	1.711886	23.43	8.651921

21.36	6.454402	21.82	3.335422	28.19	1.726444	23.65	8.775941
21.82	5.9368	22.44	3.169008	28.3	1.734495	23.85	8.88934
22.44	5.168541	23.1	3.001037	28.5	1.749182	24	8.97472
23.1	4.336276	23.43	2.921583	28.7	1.76388	24.33	9.163166
23.43	3.936631	23.65	2.870384	28.9	1.77851	24.56	9.294579
23.65	3.680705	23.85	2.825049	29.1	1.792993	24.74	9.397145
23.85	3.456618	24	2.791777	29.3	1.807238	24.95	9.516131
24	3.294348	24.33	2.720636	29.5	1.821149	25.13	9.617199
24.33	2.955924	24.56	2.672559	29.7	1.834636	25.35	9.739045
24.56	2.735634	24.74	2.635681	29.8	1.841191	25.55	9.847629
24.74	2.57228	24.95	2.593357	30.5	1.882663	25.75	9.953478
24.95	2.391703	25.13	2.557568	30.9	1.902274	25.95	10.055871
25.13	2.24535	25.35	2.514282	31.1	1.910865	26.13	10.144395
25.35	2.076803	25.55	2.47521	31.25	1.916775	26.39	10.264783
25.55	1.933148	25.75	2.436241	31.53	1.926606	26.52	10.321046
25.75	1.798278	25.95	2.397214	31.76	1.933555	26.73	10.405383
25.95	1.671844	26.13	2.361902	31.96	1.938817	26.92	10.473673
26.13	1.564939	26.39	2.310326	32.14	1.942971	27.19	10.555277
26.39	1.421473	26.52	2.284187	32.34	1.946983	27.36	10.59593
26.52	1.354363	26.73	2.241313	32.56	1.950723	27.55	10.630166
26.73	1.252091	26.92	2.201697	32.73	1.953172	27.74	10.651243
26.92	1.165816	27.19	2.143728	32.91	1.955382	27.99	10.656551
27.19	1.051918	27.36	2.10615	33.14	1.957693	28.19	10.640492
27.36	0.986259	27.55	2.063004	33.26	1.958692	28.3	10.623324
27.55	0.917457	27.74	2.018546	33.52	1.960424	28.5	10.575985
27.74	0.853225	27.99	1.957918	33.64	1.961045	28.7	10.506683
27.99	0.775207	28.19	1.907579	33.93	1.962142	28.9	10.414297
28.19	0.71775	28.3	1.879183	34.04	1.962426	29.1	10.297955
28.3	0.687919	28.5	1.826254	34.25	1.962793	29.3	10.157165
28.5	0.636706	28.7	1.771664	34.42	1.962941	29.5	9.991849
28.7	0.589188	28.9	1.715474	34.63	1.962965	29.7	9.802373
28.9	0.545114	29.1	1.657781	34.87	1.962811	29.8	9.698823
29.1	0.504245	29.3	1.598728	35.04	1.962601	30.5	8.826606
29.3	0.466373	29.5	1.538501	35.32	1.962109	30.9	8.236041
29.5	0.43129	29.7	1.477323	35.53	1.96164	31.1	7.924154
29.7	0.398791	29.8	1.446458	35.76	1.961048	31.25	7.685304
29.8	0.383459	30.5	1.228643	35.88	1.960712	31.53	7.232582
30.5	0.291237	30.9	1.106216	36.26	1.959554	31.76	6.85831
30.9	0.248788	31.1	1.046548	36.53	1.958666	31.96	6.534235
31.1	0.229931	31.25	1.002694	36.87	1.957497	32.14	6.24555
31.25	0.216738	31.53	0.923262	37	1.95704	32.34	5.929891
31.53	0.19409	31.76	0.860699	39.04	1.949855	32.56	5.590703
31.76	0.177264	31.96	0.808465	40.06	1.946556	32.73	5.335481
31.96	0.163825	34.04	0.396529	44	1.93639	32.91	5.072625
35.04	0.048463	36.87	0.138945	46.6	1.931509	40.06	0.500858
44	0.002678	40.06	0.041986	47.8	1.929619	46.6	0.064243

48.23	0.003001	41	0.02967	48.23	1.928989	48.23	0.039657
49.3	0.002731	49.3	0.001779	49.3	1.927519	49.3	0.028952
50.32	0.002435	50.32	0.001294	50.32	1.926237	50.32	0.021464

**S. Table 14.** Transition electric dipole moments between low-lying  $^3\Sigma^+$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$2^3\Sigma^+ - 1^3\Sigma^+$	$R(\text{Bohr})$	$3^3\Sigma^+ - 1^3\Sigma^+$	$R(\text{Bohr})$	$3^3\Sigma^+ - 2^3\Sigma^+$	$R(\text{Bohr})$	$4^3\Sigma^+ - 3^3\Sigma^+$
4.5	0.078289	4.5	1.439056	4.5	1.820208	4.5	-1.235296
4.6	0.0466	4.6	1.383705	4.6	1.826987	4.6	-1.373886
4.7	0.012518	4.7	1.329827	4.7	1.840553	4.7	-1.522922
4.8	0.023367	4.8	1.277486	4.8	1.860267	4.8	-1.681006
4.9	0.0606	4.9	1.226699	4.9	1.885474	4.9	-1.846437
5	0.098846	5	1.177436	5	1.915514	5	-2.01729
5.1	0.137858	5.1	1.129634	5.1	1.94973	5.1	-2.191475
5.2	0.177455	5.2	1.0832	5.2	1.987479	5.2	-2.366825
5.3	0.217505	5.3	1.038027	5.3	2.028139	5.3	-2.541188
5.4	0.257911	5.4	0.993993	5.4	2.071118	5.4	-2.712506
5.5	0.298594	5.5	0.950973	5.5	2.115866	5.5	-2.878901
5.6	0.339495	5.6	0.908829	5.6	2.161885	5.6	-3.038721
5.7	0.380562	5.7	0.867417	5.7	2.208736	5.7	-3.190568
5.8	0.421751	5.8	0.826577	5.8	2.256045	5.8	-3.333292
5.9	0.463019	5.9	0.786149	5.9	2.3035	5.9	-3.465954
6	0.504328	6	0.745952	6	2.350853	6	-3.587768
6.1	0.545641	6.1	0.705799	6.1	2.397912	6.1	-3.698028
6.2	0.586912	6.2	0.665509	6.2	2.444533	6.2	-3.796048
6.3	0.628099	6.3	0.624898	6.3	2.490619	6.3	-3.881093
6.4	0.669152	6.4	0.583789	6.4	2.536112	6.4	-3.952338
6.5	0.710024	6.5	0.542001	6.5	2.580988	6.5	-4.008837
6.6	0.750651	6.6	0.499388	6.6	2.625254	6.6	-4.049519
6.7	0.790973	6.7	0.455799	6.7	2.668943	6.7	-4.073195
6.8	0.830921	6.8	0.411111	6.8	2.712115	6.8	-4.078574
6.9	0.87042	6.9	0.365195	6.9	2.754842	6.9	-4.06431
7	0.909389	7	0.317981	7	2.797206	7	-4.029036
7.1	0.947748	7.1	0.269406	7.1	2.839281	7.1	-3.97144
7.25	1.003943	7.25	0.193971	7.25	2.90197	7.25	-3.840697
7.3	1.022268	7.3	0.168169	7.3	2.922759	7.3	-3.784851
7.45	1.075876	7.45	0.088973	7.45	2.984729	7.45	-3.579837
7.5	1.093245	7.5	0.06208	7.5	3.005205	7.5	-3.499084
7.65	1.143696	7.65	0.01957	7.65	3.065769	7.65	-3.221235
7.7	1.15992	7.7	0.046942	7.7	3.085561	7.7	-3.117504
7.8	1.191413	7.8	0.101551	7.8	3.124327	7.8	-2.89534
7.9	1.221566	7.9	0.155517	7.9	3.161716	7.9	-2.656477
8	1.250295	8	0.208264	8	3.197383	8	-2.405038
8.1	1.277531	8.1	0.25917	8.1	3.231017	8.1	-2.145649
8.2	1.303208	8.2	0.3077	8.2	3.262351	8.2	-1.88307
8.3	1.327276	8.3	0.353369	8.3	3.291212	8.3	-1.621859

8.4	1.349687	8.4	0.395812	8.4	3.317513	8.4	-1.366036
8.5	1.370409	8.5	0.434793	8.5	3.341262	8.5	-1.118845
8.6	1.389414	8.6	0.470209	8.6	3.362549	8.6	-0.882633
8.7	1.406693	8.7	0.502081	8.7	3.381527	8.7	-0.658843
8.8	1.422241	8.8	0.530532	8.8	3.398393	8.8	-0.448089
8.9	1.436058	8.9	0.555752	8.9	3.413371	8.9	-0.250331
9	1.448161	9	0.578006	9	3.426693	9	-0.064974
9.1	1.458567	9.1	0.597573	9.1	3.438588	9.1	0.108904
9.2	1.467303	9.2	0.614753	9.2	3.449278	9.2	0.272453
9.3	1.474402	9.3	0.629839	9.3	3.458965	9.3	0.426926
9.43	1.481241	9.43	0.64678	9.43	3.470367	9.43	0.616262
9.5	1.483834	9.5	0.654835	9.5	3.476064	9.5	0.713694
9.66	1.486998	9.66	0.670954	9.66	3.488252	9.66	0.927026
9.7	1.487205	9.7	0.674561	9.7	3.491165	9.7	0.978687
9.87	1.485591	9.87	0.688409	9.87	3.50319	9.87	1.192797
9.93	1.484091	9.93	0.692819	9.93	3.507358	9.93	1.266741
10	1.48175	10	0.697716	10	3.512212	10	1.352233
10.1	1.477341	10.1	0.70432	10.1	3.519176	10.1	1.47331
10.25	1.46849	10.25	0.713563	10.25	3.529815	10.25	1.65352
10.3	1.464972	10.3	0.71651	10.3	3.533441	10.3	1.713401
10.43	1.45457	10.43	0.723953	10.43	3.543109	10.43	1.869001
10.52	1.446358	10.52	0.72897	10.52	3.550039	10.52	1.976804
10.66	1.432051	10.66	0.736639	10.66	3.561255	10.66	2.144799
10.7	1.427639	10.7	0.738812	10.7	3.564563	10.7	2.192869
10.85	1.4099	10.85	0.746931	10.85	3.577401	10.85	2.373312
11	1.390414	11	0.755053	11	3.590934	11	2.553676
11.1	1.376543	11.1	0.760493	11.1	3.600342	11.1	2.673536
11.25	1.354544	11.25	0.768708	11.25	3.615016	11.25	2.852094
11.3	1.346918	11.3	0.771462	11.3	3.620051	11.3	2.911135
11.4	1.331263	11.4	0.776997	11.4	3.630329	11.4	3.028267
11.56	1.305197	11.56	0.785918	11.56	3.647301	11.56	3.212348
11.6	1.298502	11.6	0.78816	11.6	3.651638	11.6	3.257603
11.75	1.272831	11.75	0.796597	11.75	3.668193	11.75	3.424091
11.8	1.264092	11.8	0.799418	11.8	3.673803	11.8	3.478351
11.99	1.230167	11.99	0.810157	11.99	3.695458	11.99	3.678227
12.1	1.210076	12.1	0.816374	12.1	3.708178	12.1	3.789028
12.21	1.189713	12.21	0.822575	12.21	3.720977	12.21	3.896008
12.3	1.172875	12.3	0.827632	12.3	3.731475	12.3	3.980622
12.46	1.142627	12.46	0.836561	12.46	3.75011	12.46	4.124496
12.5	1.135013	12.5	0.838778	12.5	3.754748	12.5	4.159158
12.64	1.108233	12.64	0.846476	12.64	3.77086	12.64	4.276397
12.7	1.096707	12.7	0.849743	12.7	3.777688	12.7	4.324736
12.82	1.073593	12.82	0.856209	12.82	3.791159	12.82	4.418081
12.9	1.058151	12.9	0.860465	12.9	3.799973	12.9	4.477911
13	1.038839	13	0.865728	13	3.810771	13	4.550103
13.1	1.019517	13.1	0.87088	13.1	3.821266	13.1	4.619521

13.26	0.988655	13.26	0.878955	13.26	3.837352	13.26	4.725144
13.3	0.980954	13.3	0.880934	13.3	3.841219	13.3	4.750555
13.46	0.950246	13.46	0.888683	13.46	3.855979	13.46	4.848468
13.5	0.942597	13.5	0.890576	13.5	3.859478	13.5	4.872054
13.64	0.915931	13.64	0.897057	13.64	3.871063	13.64	4.951972
13.7	0.90456	13.7	0.899763	13.7	3.875691	13.7	4.985024
13.85	0.876304	13.85	0.90633	13.85	3.886296	13.85	5.064725
13.92	0.86321	13.92	0.909295	13.92	3.890743	13.92	5.100561
14	0.848323	14	0.912605	14	3.895407	14	5.140521
14.69	0.724066	14.69	0.937418	14.69	3.914248	14.69	5.447334
14.82	0.701615	14.82	0.941313	14.82	3.912937	14.82	5.498676
15	0.671092	15	0.946296	15	3.908295	15	5.566896
16.25	0.479434	16.25	0.968215	16.25	3.778292	16.25	5.965392
16.42	0.456346	16.42	0.969658	16.42	3.747223	16.42	6.011012
16.67	0.42375	16.67	0.971227	16.67	3.696015	16.67	6.074854
16.83	0.403748	16.83	0.971916	16.83	3.659933	16.83	6.11375
17	0.383234	17	0.972401	17	3.618906	17	6.153435
18.33	0.248439	18.33	0.970556	18.33	3.219515	18.33	6.405868
18.53	0.231942	18.53	0.969851	18.53	3.15032	18.53	6.43429
18.79	0.211861	18.79	0.968931	18.79	3.057948	18.79	6.466943
18.93	0.201668	18.93	0.968457	18.93	3.007242	18.93	6.482371
19.76	0.14947	19.13	0.967822	19.76	2.696989	19.13	6.501595
19.92	0.140902	19.35	0.967822	19.92	2.635961	19.35	6.501595
20.11	0.131295	19.55	0.966764	20.11	2.563236	19.55	6.530093
20.33	0.12091	19.76	0.966415	20.33	2.478831	19.76	6.537631
20.58	0.110014	19.92	0.966241	20.58	2.382865	19.92	6.540057
20.74	0.103516	20.11	0.966146	20.74	2.321522	20.11	6.538951
20.95	0.095521	20.33	0.966192	20.95	2.241214	20.33	6.531885
21.12	0.08947	20.58	0.966454	21.12	2.176444	20.58	6.515755
21.36	0.081526	20.74	0.966737	21.36	2.085541	20.74	6.500615
21.82	0.068098	20.95	0.96724	21.82	1.913609	20.95	6.474704
22.44	0.053251	21.12	0.967751	22.44	1.688634	21.12	6.448502
23.1	0.040823	21.36	0.968623	23.1	1.460907	21.36	6.403142
23.43	0.035697	21.82	0.970704	23.43	1.352706	21.82	6.287692
23.65	0.032628	22.44	0.974096	23.65	1.282954	22.44	6.070658
23.85	0.030055	23.1	0.97796	23.85	1.221301	23.1	5.763806
24	0.028254	23.43	0.979831	24	1.176208	23.43	5.583683
24.33	0.02465	23.65	0.981016	24.33	1.080594	23.65	5.454892
24.56	0.022404	23.85	0.982036	24.56	1.016973	23.85	5.332402
24.74	0.020782	24	0.982765	24.74	0.968958	24	5.237483
24.95	0.019035	24.33	0.984225	24.95	0.914934	24.33	5.020719
25.13	0.01765	24.56	0.985126	25.13	0.870357	24.56	4.864296
25.35	0.016089	24.74	0.98576	25.35	0.818041	24.74	4.739447
25.55	0.014787	24.95	0.986415	25.55	0.772548	24.95	4.591751
25.75	0.013584	25.13	0.986917	25.75	0.72901	25.13	4.463879
25.95	0.012473	25.35	0.98744	25.95	0.687409	25.35	4.306592

26.13	0.011557	25.55	0.987835	26.13	0.651592	25.55	4.163207
26.39	0.010342	25.75	0.988159	26.39	0.602531	25.75	4.019959
26.52	0.009781	25.95	0.988409	26.52	0.579159	25.95	3.877302
26.73	0.008937	26.13	0.988583	26.73	0.542994	26.13	3.749784
26.92	0.008235	26.39	0.988744	26.92	0.511925	26.39	3.567626
27.19	0.007329	26.52	0.988787	27.19	0.470377	26.52	3.477665
27.36	0.006807	26.73	0.988809	27.36	0.44573	26.73	3.334204
27.55	0.006268	26.92	0.988782	27.55	0.419514	26.92	3.206617
27.74	0.00577	27.19	0.988676	27.74	0.394654	27.19	3.029378
27.99	0.005173	27.36	0.988571	27.99	0.363921	27.36	2.920431
28.19	0.004738	27.55	0.988422	28.19	0.34088	27.55	2.801254
28.3	0.004516	27.74	0.988244	28.3	0.328769	27.74	2.684935
28.5	0.004134	27.99	0.987971	28.5	0.307731	27.99	2.536415
28.7	0.003785	28.19	0.987724	28.7	0.287909	28.19	2.421425
28.9	0.003464	28.3	0.987578	28.9	0.269246	28.3	2.359659
29.1	0.00317	28.5	0.987299	29.1	0.251685	28.5	2.250084
29.3	0.0029	28.7	0.987002	29.3	0.23517	28.7	2.144063
29.5	0.002653	28.9	0.98669	29.5	0.219648	28.9	2.041611
29.7	0.002426	29.1	0.986366	29.7	0.205068	29.1	1.94274
29.8	0.002321	29.3	0.986032	29.8	0.198115	29.3	1.847436
30.5	0.001693	29.5	0.98569	30.5	0.155191	29.5	1.755682
30.9	0.001411	29.7	0.985341	30.9	0.134694	29.7	1.667443
31.1	0.001289	29.8	0.985165	31.1	0.125413	29.8	1.624625
31.25	0.001205	30.5	0.983907	31.25	0.118846	30.5	1.348629
31.53	0.001061	30.9	0.983176	31.53	0.107433	30.9	1.208796
31.76	0.000954	31.1	0.982825	31.76	0.098829	31.1	1.143513
31.96	0.000869	31.25	0.982559	31.96	0.091872	31.25	1.096504
32.14	0.000802	31.53	0.982062	32.14	0.086005	31.53	1.013109
32.34	0.000732	31.76	0.981661	32.34	0.079896	31.76	0.948698
32.56	0.00066	31.96	0.981315	32.56	0.073646	31.96	0.895575
32.73	0.00061	32.14	0.981007	32.73	0.069132	32.14	0.849979
32.91	0.000564	32.34	0.980668	32.91	0.064635	32.34	0.801698
33.14	0.000507	32.56	0.980301	33.14	0.059289	32.56	0.751373
33.26	0.000482	32.73	0.98002	33.26	0.056667	32.73	0.714412
33.52	0.000428	32.91	0.979729	33.52	0.051353	32.91	0.677037
33.64	0.000406	33.14	0.979361	33.64	0.049063	33.14	0.631814
33.93	0.000356	33.26	0.979173	33.93	0.043918	33.26	0.609308
34.04	0.000336	33.52	0.978771	34.04	0.042103	33.52	0.562996
34.25	0.00031	33.64	0.978587	34.25	0.038833	33.64	0.542712
34.42	0.000288	33.93	0.978153	34.42	0.036362	33.93	0.4964
34.63	0.000262	34.04	0.977979	34.63	0.033517	34.04	0.479772
34.87	0.000205	34.25	0.977687	34.87	0.030514	34.25	0.449499
35.04	0.000219	34.42	0.977443	35.04	0.028554	34.42	0.42628
35.32	0.000197	34.63	0.977153	35.32	0.025582	34.63	0.399101
35.53	0.000183	34.87	0.97673	35.53	0.023546	34.87	0.370054
35.76	0.000154	35.04	0.976594	35.76	0.021491	35.04	0.350647

35.88	0.000145	35.32	0.976226	35.88	0.020494	35.32	0.320739
36.26	0.000145	37	0.974216	40.06	0.003804	41	0.049658
36.53	0.000108	40.06	0.971308	46.6	0.000469	47.8	0.005986
36.87	0.00011	48.23	0.96663	48.23	0.000335	48.23	0.005285
37	0.000106	49.3	0.966229	49.3	0.000273	49.3	0.003875
50.32	6.00E-06	50.32	0.96588	50.32	0.000226	50.32	0.002892

**S. Table 15.** Transition electric dipole moments between low-lying  $^1\Pi$  electronic states of the  $\text{BeCs}^+$  molecular ion.

$R(\text{Bohr})$	$2\ ^1\Pi - 1^1\Pi$	$R(\text{Bohr})$	$3\ ^1\Pi - 1^1\Pi$	$R(\text{Bohr})$	$4\ ^1\Pi - 1^1\Pi$	$R(\text{Bohr})$	$3\ ^1\Pi - 2^1\Pi$
4.5	0.304799	4.5	0.791449	4.5	1.010185	4.5	0.894308
4.6	0.265443	4.6	0.705768	4.6	1.153076	4.6	0.887784
4.7	0.225367	4.7	0.623281	4.7	1.273522	4.7	0.868789
4.8	0.185085	4.8	0.544587	4.8	1.367801	4.8	0.838836
4.9	0.145049	4.9	0.470112	4.9	1.438551	4.9	0.7995
5	0.105634	5	0.400113	5	1.490492	5	0.752378
5.1	0.067144	5.1	0.334692	5.1	1.52811	5.1	0.699041
5.2	0.029817	5.2	0.27382	5.2	1.555048	5.2	0.640979
5.3	0.006166	5.3	0.217352	5.3	1.574119	5.3	0.579561
5.4	0.04068	5.4	0.165055	5.4	1.58747	5.4	0.515997
5.5	0.07364	5.5	0.116636	5.5	1.59674	5.5	0.451323
5.6	0.105008	5.6	0.07175	5.6	1.60318	5.6	0.386388
5.7	0.134785	5.7	0.030027	5.7	1.607742	5.7	0.321855
5.8	0.163006	5.8	0.008914	5.8	1.611144	5.8	0.258211
5.9	0.189738	5.9	0.045459	5.9	1.613914	5.9	0.195782
6	0.215073	6	0.079982	6	1.616429	6	0.134757
6.1	0.239122	6.1	0.112845	6.1	1.618941	6.1	0.075198
6.2	0.262011	6.2	0.144393	6.2	1.621602	6.2	0.017079
6.3	0.283877	6.3	0.174946	6.3	1.62448	6.3	0.039715
6.4	0.304857	6.4	0.204805	6.4	1.627572	6.4	0.095357
6.5	0.325093	6.5	0.23425	6.5	1.630819	6.5	0.150068
6.6	0.344721	6.6	0.263537	6.6	1.634118	6.6	0.204102
6.7	0.363871	6.7	0.2929	6.7	1.637326	6.7	0.25774
6.8	0.382664	6.8	0.322554	6.8	1.640276	6.8	0.311276
6.9	0.401212	6.9	0.35269	6.9	1.642776	6.9	0.365012
7	0.419615	7	0.383478	7	1.644619	7	0.419249
7.1	0.437961	7.1	0.415065	7.1	1.64559	7.1	0.474288
7.25	0.465534	7.25	0.464201	7.25	1.644926	7.25	0.558967
7.3	0.47477	7.3	0.481092	7.3	1.644027	7.3	0.587891
7.45	0.502698	7.45	0.533399	7.45	1.638917	7.45	0.677175
7.5	0.512094	7.5	0.551386	7.5	1.636321	7.5	0.707857
7.65	0.54059	7.65	0.606956	7.65	1.625512	7.65	0.802948
7.7	0.550196	7.7	0.625987	7.7	1.620827	7.7	0.835705
7.8	0.569571	7.8	0.664724	7.8	1.609716	7.8	0.902856
7.9	0.589161	7.9	0.704222	7.9	1.596179	7.9	0.972183
8	0.608951	8	0.744268	8	1.580122	8	1.043617

8.1	0.62892	8.1	0.784591	8.1	1.561497	8.1	1.117016
8.2	0.649041	8.2	0.824876	8.2	1.540309	8.2	1.192164
8.3	0.669277	8.3	0.864763	8.3	1.516621	8.3	1.268773
8.4	0.689587	8.4	0.903867	8.4	1.490553	8.4	1.3465
8.5	0.709927	8.5	0.941786	8.5	1.462287	8.5	1.424955
8.6	0.730245	8.6	0.978123	8.6	1.432059	8.6	1.503723
8.7	0.750489	8.7	1.012499	8.7	1.400149	8.7	1.582385
8.8	0.770604	8.8	1.044575	8.8	1.366873	8.8	1.660535
8.9	0.790531	8.9	1.074064	8.9	1.332562	8.9	1.737802
9	0.810213	9	1.100736	9	1.297559	9	1.81386
9.1	0.829592	9.1	1.124428	9.1	1.262189	9.1	1.888444
9.2	0.848609	9.2	1.14504	9.2	1.226759	9.2	1.961346
9.3	0.867207	9.3	1.162535	9.3	1.191547	9.3	2.032419
9.43	0.890668	9.43	1.180651	9.43	1.146485	9.43	2.121934
9.5	0.902929	9.5	1.188285	9.5	1.122693	9.5	2.168758
9.66	0.929863	9.66	1.200394	9.66	1.069888	9.66	2.27217
9.7	0.936343	9.7	1.202309	9.7	1.057071	9.7	2.297249
9.87	0.962657	9.87	1.205815	9.87	1.004491	9.87	2.400504
9.93	0.971445	9.93	1.205365	9.93	0.986694	9.93	2.435701
10	0.981355	10	1.203803	10	0.966447	10	2.475979
10.1	0.994848	10.1	1.199747	10.1	0.93849	10.1	2.532103
10.25	1.013571	10.25	1.189974	10.25	0.89868	10.25	2.613327
10.3	1.019396	10.3	1.185814	10.3	0.885967	10.3	2.639651
10.43	1.033545	10.43	1.173091	10.43	0.854186	10.43	2.706438
10.52	1.042486	10.52	1.162803	10.52	0.833229	10.52	2.751338
10.66	1.054987	10.66	1.144662	10.66	0.802251	10.66	2.819139
10.7	1.058243	10.7	1.139045	10.7	0.793751	10.7	2.838075
10.85	1.0692	10.85	1.116456	10.85	0.76319	10.85	2.907448
11	1.078188	11	1.091748	11	0.734599	11	2.974377
11.1	1.0831	11.1	1.074274	11.1	0.71656	11.1	3.017721
11.25	1.088875	11.25	1.046797	11.25	0.690935	11.25	3.080938
11.3	1.090383	11.3	1.037344	11.3	0.682753	11.3	3.101543
11.4	1.092786	11.4	1.018052	11.4	0.666906	11.4	3.142117
11.56	1.094972	11.56	0.986282	11.56	0.642896	11.56	3.205271
11.6	1.095208	11.6	0.978191	11.6	0.637139	11.6	3.220736
11.75	1.095024	11.75	0.947429	11.75	0.616367	11.75	3.277629
11.8	1.094597	11.8	0.937049	11.8	0.609717	11.8	3.296218
11.99	1.09138	11.99	0.897176	11.99	0.585615	11.99	3.36523
12.1	1.088415	12.1	0.87387	12.1	0.572452	12.1	3.404052
12.21	1.084683	12.21	0.85047	12.21	0.559826	12.21	3.442079
12.3	1.081085	12.3	0.831287	12.3	0.549874	12.3	3.47262
12.46	1.073544	12.46	0.797183	12.46	0.532968	12.46	3.525682
12.5	1.07144	12.5	0.788667	12.5	0.52889	12.5	3.538706
12.64	1.063424	12.64	0.758937	12.64	0.515059	12.64	3.583553
12.7	1.059691	12.7	0.746243	12.7	0.509334	12.7	3.602426
12.82	1.051721	12.82	0.720963	12.82	0.498223	12.82	3.639556

12.9	1.046051	12.9	0.704205	12.9	0.491058	12.9	3.663859
13	1.038585	13	0.683383	13	0.482359	13	3.693735
13.1	1.030721	13.1	0.662714	13.1	0.473932	13.1	3.723055
13.26	1.017373	13.26	0.630004	13.26	0.46098	13.26	3.768813
13.3	1.013898	13.3	0.6219	13.3	0.457839	13.3	3.780029
13.46	0.99949	13.46	0.589808	13.46	0.445639	13.46	3.824
13.5	0.995767	13.5	0.58187	13.5	0.442675	13.5	3.834768
13.64	0.982391	13.64	0.554361	13.64	0.432563	13.64	3.871731
13.7	0.976502	13.7	0.542709	13.7	0.428348	13.7	3.887224
13.85	0.961407	13.85	0.513954	13.85	0.418101	13.85	3.925025
13.92	0.954194	13.92	0.500723	13.92	0.413455	13.92	3.942201
14	0.945829	14	0.485755	14	0.408247	14	3.961459
14.69	0.869579	14.69	0.363705	14.69	0.367218	14.69	4.109887
14.82	0.854626	14.82	0.342188	14.82	0.360164	14.82	4.133983
15	0.833735	15	0.313195	15	0.350698	15	4.16511
16.25	0.68722	16.25	0.137872	16.25	0.292742	16.25	4.297823
16.42	0.667597	16.42	0.117544	16.42	0.285711	16.42	4.303003
16.67	0.639043	16.67	0.089157	16.67	0.275671	16.67	4.304363
16.83	0.620986	16.83	0.071921	16.83	0.269422	16.83	4.301219
17	0.602012	18.33	0.056016	17	0.262927	17	4.294354
18.33	0.462676	18.53	0.068772	18.33	0.216491	18.33	4.111642
18.53	0.443332	18.79	0.083973	18.53	0.210099	18.53	4.064541
18.79	0.41888	18.93	0.091534	18.79	0.20199	18.79	3.996062
18.93	0.406046	19.76	0.128061	18.93	0.197715	18.93	3.955923
19.76	0.334929	19.92	0.1336	19.76	0.173603	19.76	3.675494
19.92	0.32222	20.11	0.139608	19.92	0.169183	19.92	3.614085
20.11	0.307556	20.33	0.145828	20.11	0.164026	20.11	3.538564
20.33	0.291157	20.58	0.151999	20.33	0.158176	20.33	3.447952
20.58	0.273279	20.74	0.155479	20.58	0.151683	20.58	3.341398
20.74	0.26226	20.95	0.159528	20.74	0.147612	20.74	3.271499
20.95	0.248297	21.12	0.162403	20.95	0.142369	20.95	3.178081
21.12	0.237402	21.36	0.165888	21.12	0.138206	21.12	3.10131
21.36	0.222643	21.82	0.1709	21.36	0.132452	21.36	2.991617
21.82	0.196348	22.44	0.174788	21.82	0.121828	21.82	2.778977
22.44	0.164898	23.1	0.176192	22.44	0.108343	22.44	2.492962
23.1	0.136126	23.43	0.176114	23.1	0.095049	23.1	2.197178
23.43	0.123426	23.65	0.175838	23.43	0.088817	23.43	2.054953
23.65	0.115543	23.85	0.175456	23.65	0.084818	23.65	1.962734
23.85	0.108765	24	0.175099	23.85	0.08129	23.85	1.880873
24	0.103914	24.33	0.174134	24	0.07871	24	1.820778
24.33	0.093914	24.56	0.173341	24.33	0.07324	24.33	1.692695
24.56	0.087464	24.74	0.172666	24.56	0.069591	24.56	1.606914
24.74	0.082702	24.95	0.171831	24.74	0.066829	24.74	1.541839
24.95	0.077444	25.13	0.17108	24.95	0.063712	24.95	1.468243
25.13	0.073182	25.35	0.170128	25.13	0.061127	25.13	1.407171
25.35	0.068266	25.55	0.169239	25.35	0.058077	25.35	1.335063

25.55	0.064061	25.75	0.168338	25.55	0.055408	25.55	1.271927
25.75	0.060104	25.95	0.167425	25.75	0.052836	25.75	1.211092
25.95	0.056374	26.13	0.1666	25.95	0.050359	25.95	1.152528
26.13	0.053203	26.39	0.16541	26.13	0.048211	26.13	1.101754
26.39	0.048918	26.52	0.164815	26.39	0.045238	26.39	1.031591
26.52	0.0469	26.73	0.163863	26.52	0.043809	26.52	0.997893
26.73	0.043803	26.92	0.163012	26.73	0.041578	26.73	0.945372
26.92	0.041173	27.19	0.16182	26.92	0.039645	26.92	0.899846
27.19	0.037689	27.36	0.161083	27.19	0.037027	27.19	0.838334
27.36	0.035645	27.55	0.160272	27.36	0.035455	27.36	0.80147
27.55	0.033484	27.74	0.159476	27.55	0.033766	27.55	0.761918
27.74	0.031444	27.99	0.158455	27.74	0.032147	27.74	0.724058
27.99	0.028953	28.19	0.157657	27.99	0.030119	27.99	0.676754
28.19	0.027091	28.3	0.157226	28.19	0.028579	28.19	0.640888
28.3	0.02612	28.5	0.156458	28.3	0.027761	28.3	0.621885
28.5	0.024437	28.7	0.15571	28.5	0.026329	28.5	0.588609
28.7	0.02286	28.9	0.154981	28.7	0.024962	28.7	0.556936
28.9	0.021382	29.1	0.154272	28.9	0.023659	28.9	0.526798
29.1	0.019994	29.3	0.153582	29.1	0.022417	29.1	0.498146
29.3	0.018694	29.5	0.15291	29.3	0.021236	29.3	0.470906
29.5	0.017482	29.7	0.152256	29.5	0.020111	29.5	0.445035
29.7	0.016344	29.8	0.151937	29.7	0.019041	29.7	0.420471
29.8	0.015801	30.5	0.149824	29.8	0.018525	29.8	0.408661
30.5	0.01247	30.9	0.148708	30.5	0.015263	30.5	0.334192
30.9	0.010885	31.1	0.148175	30.9	0.013647	30.9	0.297527
31.1	0.01017	31.25	0.147784	31.1	0.012902	31.1	0.280641
31.25	0.009659	31.53	0.147078	31.25	0.012369	31.25	0.268571
31.53	0.008778	31.76	0.146521	31.53	0.011425	31.53	0.247342
31.76	0.008114	31.96	0.146049	31.76	0.010704	31.76	0.2311
31.96	0.007577	32.14	0.145636	31.96	0.010111	31.96	0.217804
32.14	0.007122	32.34	0.145189	32.14	0.009605	32.14	0.206461
32.34	0.006654	32.56	0.144714	32.34	0.00907	32.34	0.194523
32.56	0.006163	32.73	0.144355	32.56	0.008516	32.56	0.182145
32.73	0.00581	32.91	0.143985	32.73	0.008111	32.73	0.173103
32.91	0.005459	33.14	0.143527	32.91	0.007701	32.91	0.163995
33.14	0.005044	33.26	0.143292	33.14	0.007206	33.14	0.15302
33.26	0.004835	33.52	0.142796	33.26	0.006962	33.26	0.147587
33.52	0.004422	33.64	0.142577	33.52	0.006456	33.52	0.136431
33.64	0.004233	33.93	0.142056	33.64	0.006236	33.64	0.13156
33.93	0.003824	34.04	0.141862	33.93	0.005734	33.93	0.120487
34.04	0.003681	34.25	0.141502	34.04	0.005554	34.04	0.11651
34.25	0.003419	34.42	0.141219	34.25	0.005227	34.25	0.109289
34.42	0.003218	34.63	0.140877	34.42	0.004973	34.42	0.103765
34.63	0.002989	34.87	0.140499	34.63	0.004678	34.63	0.09731
34.87	0.002742	35.04	0.140239	34.87	0.004361	34.87	0.090407
35.04	0.00258	35.32	0.139819	35.04	0.004156	35.04	0.08581

35.32	0.002338	35.53	0.139515	35.32	0.003824	35.32	0.07873
35.53	0.002166	35.76	0.139192	35.53	0.003595	35.53	0.073788
35.76	0.001993	35.88	0.139026	35.76	0.003362	35.76	0.06873
35.88	0.001906	36.26	0.138521	35.88	0.003252	35.88	0.066227
36.26	0.001663	36.53	0.138177	36.26	0.002904	36.26	0.058864
36.53	0.001505	36.87	0.137757	36.53	0.002682	36.53	0.05412
36.87	0.00133	37	0.137605	36.87	0.002429	36.87	0.048678
37	0.001264	37.7	0.136811	37	0.002337	37	0.046745
37.7	0.000977	37.8	0.136705	37.7	0.001901	37.7	0.03754
37.8	0.000936	38.3	0.136181	37.8	0.001847	37.8	0.036381
38.3	0.000772	38.7	0.135789	38.3	0.001593	38.3	0.031081
38.7	0.000664	38.9	0.135598	38.7	0.001415	38.7	0.027382
38.9	0.00061	39.04	0.135467	38.9	0.001334	38.9	0.02569
39.04	0.000584	39.23	0.135293	39.04	0.001279	39.04	0.024583
39.23	0.000539	39.46	0.135087	39.23	0.001209	39.23	0.023143
39.46	0.000495	39.77	0.134819	39.46	0.001131	39.46	0.021507
39.77	0.000431	39.99	0.134635	39.77	0.001029	39.77	0.01948
39.99	0.00039	40.06	0.134576	39.99	0.000966	39.99	0.018162
40.06	0.000385	41	0.133843	40.06	0.000944	40.06	0.017753
41	0.000256	42.3	0.132946	41	0.000712	41	0.013118
42.3	0.000148	43.2	0.132395	42.3	0.00048	42.3	0.008585
43.2	9.8e-05	44	0.131948	43.2	0.000363	43.2	0.006385
44	7.2e-05	46.6	0.130723	44	0.000283	44	0.004899
46.6	1.7e-05	47.8	0.130258	46.6	0.000124	46.6	0.002037
47.8	8.00E-06	48.23	0.130102	47.8	8.3e-05	47.8	0.001354
48.23	2.00E-06	49.3	0.129744	48.23	7.2e-05	48.23	0.001162
49.3	1.00E-06	50.32	0.129434	49.3	5.1e-05	49.3	0.000801
50.32	2.00E-06			50.32	3.6e-05	50.32	0.000559