Table S1. The rovibrational constants for the different vibrational levels of different electronic states of the spin-free CdBr molecule.

$(2)^2\Sigma^+$					
v	**E_v (cm^{-1})**	**$B_v\times10^{-2}$ (cm^{-1})**	**$D_v\times10^{-9}$ (cm^{-1})**	**R_{min} (Å)**	**R_{max} (Å)**
0	58.82	3.0704	8.4027	3.332	3.488
1	293.31	3.0726	8.6200	3.238	3.587
2	410.06	3.0734	8.7227	3.207	3.621
3	526.48	3.0740	8.8249	3.181	3.651
4	642.58	3.0743	8.9281	3.158	3.677
5	758.34	3.0744	9.0259	3.136	3.702
6	873.76	3.0743	9.1255	3.117	3.725
7	988.85	3.0740	9.2247	3.098	3.747
8	1103.59	3.0735	9.3192	3.081	3.768
9	1217.99	3.0729	9.4146	3.065	3.788
10	1332.05	3.0721	9.5092	3.050	3.807
11	1445.75	3.0711	9.6056	3.035	3.826
12	1559.10	3.0699	9.6952	3.021	3.844
13	1672.09	3.0686	9.7948	3.008	3.862
14	1784.73	3.0670	9.8702	2.996	3.879
15	1897.01	3.0654	9.9593	2.983	3.896
16	2008.93	3.0636	10.030	2.971	3.913
17	2231.69	3.0595	10.186	2.949	3.945
18	2342.54	3.0572	10.270	2.938	3.960
19	2453.02	3.0548	10.345	2.928	3.977
20	2563.14	3.0522	10.425	2.917	3.992
21	2672.90	3.0496	10.483	2.908	4.007
22	2782.31	3.0468	10.538	2.898	4.022
23	2891.35	3.0439	10.586	2.889	4.037
24	3000.05	3.0409	10.622	2.880	4.052
25	3108.40	3.0379	10.679	2.871	4.067
26	3216.41	3.0348	10.739	2.862	4.081
27	3324.07	3.0314	10.931	2.854	4.096
28	3431.36	3.0274	11.178	2.845	4.110
29	3538.21	3.0230	11.353	2.837	4.125
30	3644.61	3.0185	11.196	2.829	4.139
31	3750.61	3.0148	10.762	2.822	4.153
32	3856.33	3.0119	10.620	2.814	4.167
33	3961.81	3.0086	11.163	2.807	4.181
34	4066.93	3.0036	11.868	2.799	4.195
35	4171.55	2.9981	11.579	2.792	4.209
36	4275.76	2.9941	10.747	2.785	4.223
37	4379.72	2.9909	11.052	2.779	4.236
38	4483.38	2.9859	12.067	2.772	4.250
39	4586.56	2.9800	11.754	2.765	4.264
40	4689.33	2.9758	10.825	2.759	4.278
41	4791.85	2.9720	11.579	2.752	4.291
42	4894.01	2.9660	12.279	2.746	4.305
43	4995.70	2.9606	11.264	2.740	4.318

44	5097.08	2.9567	11.329	2.734	4.332
45	5198.15	2.9511	12.329	2.728	4.346
46	5298.76	2.9451	11.612	2.722	4.359
47	5399.03	2.9407	11.401	2.717	4.373
48	5498.99	2.9351	12.331	2.712	4.386
49	5598.52	2.9290	11.728	2.705	4.400
50	5697.71	2.9243	11.617	2.700	4.413
51	5796.56	2.9184	12.349	2.695	4.426
52	5894.99	2.9124	11.731	2.690	4.440
53	5993.09	2.9072	11.919	2.684	4.453
54	6090.84	2.9010	12.281	2.679	4.467
55	6188.19	2.8952	11.763	2.674	4.480
56	6285.20	2.8896	12.215	2.667	4.494
57	6381.84	2.8832	12.120	2.664	4.507
58	6574.03	2.8713	12.318	2.654	4.534
59	6669.57	2.8652	12.023	2.650	4.547
60	6764.76	2.8591	12.278	2.645	4.561
61	6859.58	2.8527	12.199	2.640	4.574
62	6954.04	2.8466	12.194	2.636	4.588
63	7048.14	2.8402	12.333	2.631	4.601
64	7141.87	2.8339	12.187	2.627	4.615
65	7235.25	2.8274	12.382	2.623	4.628
66	7328.27	2.8210	12.240	2.618	4.642
67	7420.92	2.8145	12.365	2.614	4.655
68	7513.22	2.8079	12.341	2.610	4.669
69	7605.16	2.8014	12.358	2.606	4.682
70	7696.73	2.7947	12.394	2.602	4.696
71	7787.95	2.7882	12.370	2.598	4.709
72	7878.81	2.7814	12.423	2.594	4.723
73	7969.31	2.7747	12.400	2.590	4.736
74	8059.46	2.7680	12.466	2.586	4.750
75	8149.25	2.7612	12.413	2.582	4.763
$(2)^2\Pi$					
v	**E_v (cm^{-1})**	**$B_v \times 10^{-2}$ (cm^{-1})**	**$D_v \times 10^{-8}$ (cm^{-1})**	**R_{min} (Å)**	**R_{max} (Å)**
0	132.72	5.8230	1.1371	2.422	2.527
1	394.93	5.7862	1.1219	2.389	2.572
2	655.36	5.7487	1.0491	2.370	2.605
3	915.85	5.7044	0.9149	2.357	2.633
4	1178.25	5.6542	0.8382	2.347	2.659
5	1442.30	5.6065	0.9168	2.337	2.683
6	1705.24	5.5687	1.0672	2.330	2.706
7	1964.51	5.5372	1.0882	2.322	2.727
8	2220.24	5.5023	0.9788	2.315	2.748
9	2473.89	5.4635	0.9604	2.308	2.768
10	2725.52	5.4277	1.0613	2.302	2.788
11	2974.23	5.3961	1.1362	2.296	2.807
12	3219.62	5.3653	1.1425	2.291	2.826
13	3461.87	5.3339	1.1361	2.285	2.844
14	3701.17	5.3023	1.1458	2.280	2.862

15	3937.56	5.2707	1.1732	2.276	2.880
16	4171.02	5.2400	1.2264	2.271	2.898
$(1)^4\Sigma^+$					
v	**E_v (cm^{-1})**	**$B_v \times 10^{-2}$ (cm^{-1})**	**$D_v \times 10^{-9}$ (cm^{-1})**	**R_{min} (Å)**	**R_{max} (Å)**
0	41.95	3.9668	3.6249	2.890	3.075
1	124.14	3.9168	3.7641	2.836	3.160
2	203.97	3.8661	3.9153	2.802	3.225
3	281.42	3.8146	4.0589	2.777	3.284
4	356.56	3.7624	4.2113	2.756	3.339
5	429.41	3.7098	4.3769	2.738	3.391
6	499.99	3.6567	4.5265	2.723	3.442
7	568.35	3.6030	4.6871	2.710	3.492
8	634.53	3.5488	4.8723	2.698	3.542
9	698.54	3.4944	5.0482	2.687	3.592
10	760.43	3.4393	5.2154	2.678	3.642
11	820.22	3.3835	5.4139	2.669	3.692
$(3)^4\Pi$					
v	**E_v (cm^{-1})**	**$B_v \times 10^{-2}$ (cm^{-1})**	**$D_v \times 10^{-8}$ (cm^{-1})**	**R_{min} (Å)**	**R_{max} (Å)**
0	64.05	4.2665	1.9158	2.833	2.983
1	190.80	4.2381	1.9564	2.785	3.047
2	315.64	4.2094	1.9982	2.755	3.095
3	438.59	4.1804	2.0382	2.731	3.136
4	559.65	4.1511	2.0833	2.711	3.174
5	678.83	4.1214	2.1259	2.694	3.209
6	796.13	4.0915	2.1734	2.679	3.242
7	911.54	4.0611	2.2156	2.666	3.275
8	1025.07	4.0304	2.2677	2.653	3.306
9	1136.72	3.9993	2.3123	2.642	3.337
10	1246.50	3.9678	2.3674	2.632	3.367
11	1354.38	3.9360	2.4157	2.622	3.397
12	1564.51	3.8710	2.5287	2.604	3.457
13	1666.74	3.8377	2.5867	2.596	3.486
14	1767.07	3.8041	2.6509	2.589	3.516
15	1865.50	3.7700	2.7098	2.581	3.545
16	1962.03	3.7353	2.7817	2.575	3.575
17	2056.64	3.7001	2.8513	2.568	3.605
18	2149.32	3.6644	2.9239	2.562	3.636
19	2240.08	3.6281	2.9999	2.556	3.666

Table S2. The rovibrational constants for the different vibrational levels of different electronic states of the pin-orbit coupling of CdBr molecule.

$(1)^2\Pi_{3/2}$					
v	**E_v (cm^{-1})**	**$B_v \times 10^{-2}$ (cm^{-1})**	**$D_v \times 10^{-8}$ (cm^{-1})**	**R_{min} (Å)**	**R_{max} (Å)**
0	131.77	5.8804	1.2056	2.424	2.530
1	390.12	5.8415	1.1801	2.391	2.575
2	647.14	5.8025	1.1306	2.371	2.608
3	903.47	5.7595	1.0347	2.357	2.637
4	1160.29	5.7128	0.97329	2.346	2.663
5	1417.37	5.6666	0.99212	2.337	2.688
6	1673.49	5.6256	1.1044	2.328	2.711
7	1926.72	5.5911	1.1762	2.320	2.733
8	2176.42	5.5564	1.1274	2.313	2.754
9	2423.39	5.5196	1.1356	2.306	2.775
10	2667.61	5.4850	1.2004	2.299	2.795
11	2908.64	5.4515	1.1980	2.293	2.814
12	3146.67	5.4166	1.1796	2.287	2.833
13	3381.90	5.3812	1.1768	2.282	2.852
14	3614.33	5.3449	1.1486	2.278	2.871
$(1)^4\Sigma^+_{1/2}$					
v	**E_v (cm^{-1})**	**$B_v \times 10^{-2}$ (cm^{-1})**	**$D_v \times 10^{-8}$ (cm^{-1})**	**R_{min} (Å)**	**R_{max} (Å)**
0	36.64	3.9247	4.6335	2.931	3.130
1	107.96	3.8623	4.9069	2.875	3.225
2	176.49	3.7986	5.1760	2.840	3.300
3	242.32	3.7350	5.3094	2.814	3.368
4	305.88	3.6771	5.0427	2.794	3.431
5	368.07	3.6292	4.8461	2.776	3.484
6	429.20	3.5748	6.0728	2.760	3.539
7	487.63	3.4962	7.4407	2.747	3.599
8	542.37	3.4182	7.2067	2.735	3.662
9	594.21	3.3419	7.9102	2.725	3.727
10	643.21	3.2699	7.2047	2.716	3.795