Electronic Supplementary Material for PCCP

Supplementary material for the article:

Pure rotational spectra of PbSe and PbTe: potential function, Born-Oppenheimer breakdown, field shift effect and magnetic shielding

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Content:

TABLE SI: Rotational transitions $J' \leftarrow J$ of PbSe isotopologues. (A–B) are the mass number of the component atoms, v is the vibrational quantum number. Note: Line frequencies above 30 GHz are from Refs. [12,14].

Line no.	(A–B)	v	J	Frequency (MHz)
1	208–80	0	1	6059.94768
2	208–80	0	2	9089.90978
3	208–80	0	3	12119.85692
4	208–80	0	4	15149.78509
5	208–80	0	5	18179.68895
6	208–80	0	6	21209.56417
7	208–80	0	23	72708.35700
8	208–80	0	34	106014.78300
9	208–80	0	35	109041.72900
10	208–80	1	1	6044.34574
11	208–80	1	2	9066.50662
12	208–80	1	3	12088.65283
13	208–80	1	4	15110.77990
14	208–80	1	5	18132.88267
15	208–80	1	6	21154.95661
16	208–80	1	23	72521.10900
17	208–80	1	34	105741.66700
18	208–80	1	35	108760.81400
19	208–80	2	1	6028.71575
20	208–80	2	2	9043.06159
21	208–80	2	3	12057.39279
22	208–80	2	4	15071.70471
23	208–80	2	5	18085.99241
24	208–80	2	6	21100.25103
25	208–80	2	23	72333.52600
26	208–80	2	34	105468.08400
27	208–80	2	35	108479.38800
28	208–80	3	1	6013.05707
29	208–80	3	2	9019.57354
30	208–80	3	3	12026.07576
31	208–80	3	4	15032.55887

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TABLE SI: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
32	208–80	3	5	18039.01680
33	208–80	3	6	21045.44606
34	208–80	3	23	72145.60600
35	208–80	3	34	105193.98900
36	208–80	3	35	108197.46800
37	208–80	4	1	5997.37008
38	208–80	4	2	8996.04305
39	208–80	4	3	11994.70073
40	208–80	4	4	14993.34050
41	208–80	4	5	17991.95396
42	208–80	4	6	20990.53921
43	208–80	4	23	71957.32100
44	208–80	4	34	104919.38500
45	208–80	4	35	107915.00700
46	208–80	5	3	11963.26652
47	208–80	5	4	14954.04764
48	208–80	5	5	17944.80276
49	208–80	5	23	71768.70800
50	208–80	5	34	104644.26800
51	208–80	5	35	107632.04000
52	208–80	6	3	11931.77277
53	208–80	6	4	14914.68012
54	208–80	6	5	17897.56075
55	208–80	6	23	71579.72300
56	208–80	6	34	104368.62300
57	208–80	6	35	107348.50300
58	208–80	7	3	11900.21676
59	208–80	7	23	71390.36900
60	208–80	7	34	104092.46700
61	208–80	7	35	107064.44400
62	208–80	8	3	11868.60012
63	208–80	8	23	71200.63300
64	208–80	8	35	106779.79000
65	208–80	9	3	11836.92005

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TABLE SI: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
66	208–80	9	35	106494.58900
67	208–80	10	3	11805.17487
68	208–80	10	35	106208.79200
69	208–80	11	3	11773.36601
70	208–80	11	35	105922.43200
71	208–80	12	3	11741.49138
72	208–80	13	3	11709.54665
73	208–78	0	1	6172.19737
74	208–78	0	2	9258.28375
75	208–78	0	3	12344.35505
76	208–78	0	4	15430.40639
77	208–78	0	5	18516.43271
78	208–78	0	6	21602.42899
79	208–78	0	34	107977.85900
80	208–78	1	1	6156.15935
81	208–78	1	2	9234.22652
82	208–78	1	3	12312.27878
83	208–78	1	4	15390.31104
84	208–78	1	5	18468.31789
85	208–78	1	6	21546.29521
86	208–78	1	34	107697.13300
87	208–78	2	1	6140.09166
88	208–78	2	2	9210.12606
89	208–78	2	3	12280.14341
90	208–78	2	4	15350.14287
91	208–78	2	5	18420.11640
92	208–78	2	6	21490.05963
93	208–78	2	34	107415.87600
94	208–78	4	34	106851.86000
95	206–80	0	1	6076.28697
96	206–80	0	2	9114.41843
97	206–80	0	3	12152.53502
98	206–80	0	4	15190.63333
99	206–80	0	5	18228.70572

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TABLE SI: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
100	206–80	0	6	21266.75004
101	206–80	0	34	106300.53700
102	206–80	1	1	6060.62153
103	206–80	1	2	9090.92107
104	206–80	1	3	12121.20444
105	206–80	1	4	15151.46989
106	206–80	1	5	18181.70983
107	206–80	1	6	21211.92078
108	206–80	1	34	106026.31900
109	206–80	2	1	6044.92918
110	206–80	2	2	9067.38108
111	206–80	2	3	12089.81676
112	206–80	2	4	15112.23706
113	206–80	2	5	18134.62962
114	206–80	2	6	21156.99445
115	206–80	3	34	105476.44600
116	206–80	4	34	105200.69500
117	206–80	5	34	104924.45300
118	207–80	0	1	6068.07469
119	207–80	0	2	9102.10022
120	207–80	0	3	12136.11099
121	207–80	0	4	15170.10356
122	207–80	0	5	18204.06993
123	207–80	0	6	21238.00841
124	207–80	0	35	109187.90600
125	207–80	1	1	6052.44151
126	207–80	1	2	9078.65015
127	207–80	1	3	12104.84394
128	207–80	1	4	15131.01971
129	207–80	1	5	18157.16894
130	207–80	1	6	21183.29116
131	207–80	1	35	108906.43500
132	207–80	3	35	108341.99600
133	207–80	4	35	108058.92900

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TABLE SI: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
134	207–80	5	35	107775.37900
135	206–78	0	1	6188.53639
136	206–78	0	2	9282.79154
137	206–78	0	3	12377.03174
138	206–78	0	4	15471.25325
139	206–78	0	5	18565.44874
140	206–78	0	6	21659.61368
141	206–78	0	34	108263.61000
142	206–78	1	34	107981.75300
143	206–78	2	34	107699.39000
144	206–78	3	34	107416.50800
145	207–78	0	1	6180.32382
146	207–78	0	2	9270.47330
147	207–78	0	3	12360.60830
148	207–78	0	4	15450.72372
149	207–78	0	5	18540.81374
150	207–78	0	6	21630.87277
151	207–78	0	33	105032.81000
152	207–78	0	34	108119.99500
153	207–78	1	33	104759.56100
154	207–78	1	34	107838.70200
155	207–78	2	33	104485.80700
156	207–78	2	34	107556.90000
157	207–78	3	33	104211.56000
158	207–78	3	34	107274.57100
159	207–78	4	33	103936.78900
160	207–78	4	34	106991.71900
161	208–82	0	1	5953.12562
162	208–82	0	2	8929.67543
163	208–82	0	3	11906.21280
164	208–82	0	4	14882.73083
165	208–82	0	5	17859.22536
166	208–82	0	6	20835.69263
167	208–82	0	35	107120.22000

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TABLE SI: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
168	208–82	1	35	106846.70700
169	208–82	2	35	106572.73100
170	208–82	3	35	106298.23000
171	208–76	0	1	6290.28911
172	208–76	0	2	9435.42097
173	208–76	0	3	12580.53573
174	208–76	0	4	15725.63220
175	208–76	0	5	18870.70191
176	208–76	0	6	22015.73970
177	208–76	0	33	106901.02300
178	208–76	1	33	106620.45000
179	208–76	2	33	106339.36300
180	208–76	3	33	106057.72400
181	208–76	4	33	105775.59100
182	208–77	0	1	6230.37916
183	208–77	0	2	9345.55569
184	208–77	0	3	12460.71728
185	208–77	0	4	15575.85835
186	208–77	0	5	18690.97422
187	208–77	0	6	21806.05918
188	206–82	0	1	5969.46429
189	206–82	0	2	8954.18581
190	206–82	0	3	11938.89155
191	206–82	0	4	14923.57905
192	206–82	0	5	17908.24315
193	206–82	0	6	20892.87962
194	206–82	0	35	107414.12700
195	206–82	1	35	107139.49600
196	206–82	2	35	106864.38600
197	207–82	0	1	5961.25231
198	207–82	0	2	8941.86736
199	207–82	0	3	11922.46683
200	207–82	0	4	14903.04867
201	207–82	0	5	17883.60677

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TABLE SI: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
202	207–82	0	6	20864.13737
203	206–76	0	1	6306.62672
204	206–76	0	2	9459.92743
205	206–76	0	3	12613.21225
206	206–76	0	4	15766.47806
207	206–76	0	5	18919.71643
208	206–76	0	6	22072.92354
209	206–76	0	33	107178.62100
210	206–76	1	33	106896.93700
211	206–76	2	33	106614.75300
212	207–76	0	1	6298.41457
213	207–76	0	2	9447.60954
214	207–76	0	3	12596.78994
215	207–76	0	4	15745.94886
216	207–76	0	5	18895.08132
217	207–76	0	6	22044.18246
218	207–77	0	1	6238.50582
219	207–77	0	2	9357.74599
220	207–77	0	3	12476.97087
221	207–77	0	4	15596.17535
222	207–77	0	5	18715.35435
223	207–77	0	6	21834.50276
224	206–77	0	1	6246.71727
225	206–77	0	2	9370.06369
226	206–77	0	3	12493.39447
227	206–77	0	4	15616.70455
228	206–77	0	5	18739.98925
229	206–77	0	6	21863.24283
230	204–80	0	34	106591.77100
231	204–80	0	35	109635.19200
232	204–80	1	35	109351.97500

TABLE SII: Rotational transitions $J' \leftarrow J$ of PbTe isotopologues. (A–B) are the mass number of the component atoms, v is the vibrational quantum number. Note: Line frequencies above 30 GHz are from Refs. [12,14].

Line no.	(A–B)	v	J	Frequency (MHz)
1	208–130	0	1	3750.27988
2	208–130	0	2	5625.41511
3	208–130	0	3	7500.54504
4	208–130	0	4	9375.66647
5	208–130	0	5	11250.77755
6	208–130	0	6	13125.87843
7	208–130	0	7	15000.96493
8	208–130	0	8	16876.03570
9	208–130	0	9	18751.08875
10	208–130	0	10	20626.12216
11	208–130	0	11	22501.13412
12	208–130	0	12	24376.12224
13	208–130	0	13	26251.08582
14	208–130	0	22	43124.28500
15	208–130	0	37	71237.46400
16	208–130	0	46	88097.77500
17	208–130	0	47	89970.68300
18	208–130	0	48	91843.52300
19	208–130	0	49	93716.27100
20	208–130	0	57	108694.51200
21	208–130	1	3	7484.34905
22	208–130	1	5	11226.48236
23	208–130	1	6	13097.53319
24	208–130	1	7	14968.57264
25	208–130	1	8	16839.59321
26	208–130	1	9	18710.59573
27	208–130	1	10	20581.58116
28	208–130	1	11	22452.54292
29	208–130	1	12	24323.48324
30	208–130	1	37	71083.56200
31	208–130	1	46	87907.37800

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
32	208–130	1	47	89776.27000
33	208–130	1	48	91645.04300
34	208–130	1	49	93513.73900
35	208–130	1	57	108459.53100
36	208–130	2	4	9335.13889
37	208–130	2	5	11202.14494
38	208–130	2	6	13069.13950
39	208–130	2	7	14936.11939
40	208–130	2	8	16803.08487
41	208–130	2	37	70929.39100
42	208–130	2	46	87716.67800
43	208–130	2	47	89581.48400
44	208–130	2	48	91446.20400
45	208–130	2	49	93310.82700
46	208–130	2	57	108224.13600
47	208–130	3	4	9314.81854
48	208–130	3	5	11177.76220
49	208–130	3	8	16766.50890
50	208–130	3	37	70774.92600
51	208–130	3	46	87525.60500
52	208–130	3	47	89386.35100
53	208–130	3	48	91247.01600
54	208–130	3	49	93107.58100
55	208–130	3	57	107988.30800
56	208–130	4	5	11153.33333
57	208–130	4	37	70620.17800
58	208–130	4	46	87334.13900
59	208–130	4	47	89190.83600
60	208–130	4	48	91047.41100
61	208–130	4	49	92903.89700
62	208–130	4	57	107752.03100
63	208–130	5	5	11128.85819
64	208–130	5	46	87142.39100
65	208–130	5	37	70465.13300

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
66	208–130	5	47	88994.99000
67	208–130	5	48	90847.48600
68	208–130	5	49	92699.86900
69	208–130	5	57	107515.32600
70	208–130	6	5	11104.33931
71	208–130	6	37	70309.81400
72	208–130	6	46	86950.23800
73	208–130	6	47	88798.73100
74	208–130	6	48	90647.16300
75	208–130	6	49	92495.47200
76	208–130	6	57	107278.17600
77	208–130	7	5	11079.77051
78	208–130	7	46	86757.73300
79	208–130	7	48	90446.44900
80	208–130	7	47	88602.15800
81	208–130	7	57	107040.56000
82	208–130	8	5	11055.15814
83	208–130	8	47	88405.16200
84	208–130	8	48	90245.34100
85	208–130	8	57	106802.46000
86	208–130	9	5	11030.49660
87	208–130	9	48	90043.83300
88	208–130	9	57	106563.93800
89	208–130	10	5	11005.78376
90	208–130	10	48	89841.99100
91	208–130	10	57	106324.90200
92	208–130	11	5	10981.02170
93	208–130	11	57	106085.37600
94	208–130	12	5	10956.21025
95	208–130	12	57	105845.40400
96	208–130	13	5	10931.35009
97	208–128	0	1	3786.38741
98	208–128	0	2	5679.57695
99	208–128	0	3	7572.75962

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
100	208–128	0	4	9465.93496
101	208–128	0	5	11359.09960
102	208–128	0	6	13252.25260
103	208–128	0	7	15145.39227
104	208–128	0	8	17038.51421
105	208–128	0	9	18931.61940
106	208–128	0	10	20824.70443
107	208–128	0	11	22717.76734
108	208–128	0	12	24610.80762
109	208–128	0	13	26503.81990
110	208–128	0	37	71923.16600
111	208–128	0	46	88945.63900
112	208–128	0	47	90836.57900
113	208–128	0	48	92727.41800
114	208–128	0	49	94618.16400
115	208–128	0	56	107850.50100
116	208–128	1	3	7556.32843
117	208–128	1	4	9445.39507
118	208–128	1	5	11334.45299
119	208–128	1	6	13223.49859
120	208–128	1	7	15112.52889
121	208–128	1	8	17001.54337
122	208–128	1	9	18890.54028
123	208–128	1	10	20779.51967
124	208–128	1	11	22668.47324
125	208–128	1	12	24557.40297
126	208–128	1	37	71767.03500
127	208–128	1	46	88752.50000
128	208–128	1	47	90639.33200
129	208–128	1	48	92526.05500
130	208–128	1	49	94412.70600
131	208–128	1	56	107616.23800
132	208–128	2	4	9424.81868
133	208–128	2	5	11309.76046

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
134	208–128	2	6	13194.69134
135	208–128	2	7	15079.60598
136	208–128	2	8	16964.50592
137	208–128	2	37	71610.61600
138	208–128	2	46	88559.05200
139	208–128	2	47	90441.70500
140	208–128	2	48	92324.33900
141	208–128	2	49	94206.85800
142	208–128	2	56	107381.54900
143	208–128	3	4	9404.20529
144	208–128	3	5	11285.02300
145	208–128	3	7	15046.62303
146	208–128	3	8	16927.39965
147	208–128	3	37	71453.90900
148	208–128	3	46	88365.18500
149	208–128	3	47	90243.75700
150	208–128	3	48	92122.24100
151	208–128	3	49	94000.62600
152	208–128	3	56	107146.41600
153	208–128	4	46	88170.98000
154	208–128	4	47	90045.40400
155	208–128	4	48	91919.77200
156	208–128	4	49	93794.00800
157	208–128	4	56	106910.85300
158	208–128	5	46	87976.38500
159	208–128	5	47	89846.71100
160	208–128	5	48	91716.91900
161	208–128	5	49	93586.99700
162	208–128	6	46	87781.45400
163	208–128	6	47	89647.60800
164	208–128	6	48	91513.66200
165	208–128	6	49	93379.62100
166	208–128	7	46	87586.15900
167	208–128	7	47	89448.15300

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
168	208–128	7	49	93171.89600
169	208–128	8	46	87390.46300
170	208–128	8	47	89248.30600
171	208–128	8	48	91106.04200
172	208–128	8	49	92963.66400
173	208–128	9	49	92755.07600
174	208–128	9	47	89048.01700
175	208–126	0	1	3823.63183
176	208–126	0	2	5735.44238
177	208–126	0	3	7647.24677
178	208–126	0	4	9559.04300
179	208–126	0	5	11470.82967
180	208–126	0	6	13382.60377
181	208–126	0	7	15294.36354
182	208–126	0	8	17206.10788
183	208–126	0	9	19117.83185
184	208–126	0	10	21029.53782
185	208–126	0	11	22941.21935
186	208–126	0	12	24852.87738
187	208–126	0	37	72630.43100
188	208–126	0	46	89820.17300
189	208–126	0	47	91729.69300
190	208–126	0	55	107002.15500
191	208–126	0	57	110819.18400
192	208–126	1	3	7630.57121
193	208–126	1	4	9538.19982
194	208–126	1	5	11445.81857
195	208–126	1	6	13353.42283
196	208–126	1	7	15261.01381
197	208–126	1	8	17168.58828
198	208–126	1	9	19076.14345
199	208–126	1	10	20983.68094
200	208–126	1	11	22891.19418
201	208–126	1	37	72471.99400

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
202	208–126	1	55	106768.59600
203	208–126	1	57	110577.26900
204	208–126	2	4	9517.31932
205	208–126	2	5	11420.75977
206	208–126	2	6	13324.18967
207	208–126	2	7	15227.60380
208	208–126	2	8	17131.00148
209	208–126	2	37	72313.23800
210	208–126	2	55	106534.61400
211	208–126	2	57	110334.92800
212	208–126	3	5	11395.65623
213	208–126	3	6	13294.90117
214	208–126	3	7	15194.13096
215	208–126	3	8	17093.34644
216	208–126	3	37	72154.23800
217	208–126	3	55	106300.18700
218	208–126	3	57	110092.10800
219	208–126	4	55	106065.32800
220	208–126	4	57	109848.86100
221	208–126	5	57	109605.13600
222	208–124	0	1	3862.06488
223	208–124	0	2	5793.09294
224	208–124	0	3	7724.11363
225	208–124	0	4	9655.12684
226	208–124	0	5	11586.12930
227	208–124	0	6	13517.11959
228	208–124	0	7	15448.09515
229	208–124	0	8	17379.05378
230	208–124	0	9	19309.99406
231	208–124	0	11	23171.81058
232	208–124	0	12	25102.68218
233	208–124	0	36	71430.73900
234	208–124	0	46	90722.63000
235	208–124	0	51	100365.09300

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
236	208–124	0	55	108077.09700
237	208–124	1	55	107839.99400
238	208–124	2	55	107602.46800
239	208–124	3	55	107364.49800
240	208–124	4	55	107126.08300
241	208–122	0	1	3901.74608
242	208–122	0	2	5852.61263
243	208–122	0	3	7803.47433
244	208–122	0	4	9754.32697
245	208–122	0	5	11705.16854
246	208–122	0	6	13655.99859
247	208–122	0	7	15606.81197
248	208–122	0	8	17557.61040
249	208–122	0	9	19508.38856
250	208–122	0	35	70214.98100
251	208–122	0	45	89705.81500
252	208–122	0	46	91654.38900
253	208–122	0	54	107239.30300
254	208–122	1	54	107002.83400
255	208–122	3	54	106528.56500
256	206–130	0	1	3764.28758
257	206–130	0	2	5646.42698
258	206–130	0	3	7528.55915
259	206–130	0	4	9410.68419
260	206–130	0	5	11292.79920
261	206–130	0	6	13174.90304
262	206–130	0	7	15056.99283
263	206–130	0	8	16939.06640
264	206–130	0	9	18821.12213
265	206–130	0	10	20703.15837
266	206–130	0	11	22585.17242
267	206–130	0	12	24467.16301
268	206–130	0	13	26349.12912
269	206–130	0	46	88426.68200

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
270	206–130	0	47	90306.59600
271	206–130	0	53	101584.06200
272	206–130	0	57	109100.25500
273	206–130	1	3	7512.27216
274	206–130	1	4	9390.32524
275	206–130	1	5	11268.36925
276	206–130	1	6	13146.39879
277	206–130	1	7	15024.41684
278	206–130	1	8	16902.41810
279	206–130	1	9	18780.40176
280	206–130	1	10	20658.36641
281	206–130	1	11	22536.30977
282	206–130	1	57	108863.94400
283	206–130	2	5	11243.89233
284	206–130	2	6	13117.84482
285	206–130	2	7	14991.78421
286	206–130	2	57	108627.22200
287	206–130	3	6	13089.23856
288	206–130	3	7	14959.09043
289	206–130	3	57	108390.06300
290	206–130	4	57	108152.47400
291	206–130	5	57	107914.42900
292	206–128	0	1	3800.39508
293	206–128	0	2	5700.58798
294	206–128	0	3	7600.77338
295	206–128	0	4	9500.95175
296	206–128	0	5	11401.11998
297	206–128	0	6	13301.27604
298	206–128	0	7	15201.41826
299	206–128	0	8	17101.54459
300	206–128	0	9	19001.65142
301	206–128	0	10	20901.73970
302	206–128	0	11	22801.80544
303	206–128	0	12	24701.84778

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
304	206–128	0	37	72189.16300
305	206–128	0	46	89274.54400
306	206–128	0	47	91172.46100
307	206–128	0	53	102557.93600
308	206–128	0	55	106352.26300
309	206–128	1	3	7584.25150
310	206–128	1	4	9480.29816
311	206–128	1	5	11376.33658
312	206–128	1	6	13272.36131
313	206–128	1	7	15168.37303
314	206–128	1	8	17064.36805
315	206–128	1	9	18960.34511
316	206–128	1	10	20856.30149
317	206–128	1	11	22752.23657
318	206–128	1	37	72032.15600
319	206–128	1	55	106120.81100
320	206–128	2	5	11351.50777
321	206–128	2	37	71874.87400
322	206–128	2	55	105888.97000
323	206–128	3	5	11326.63249
324	206–128	3	6	13214.37120
325	206–128	3	37	71717.30200
326	206–128	3	55	105656.68500
327	206–128	4	55	105423.97400
328	206–126	0	1	3837.63803
329	206–126	0	2	5756.45210
330	206–126	0	3	7675.26064
331	206–126	0	4	9594.06054
332	206–126	0	5	11512.84957
333	206–126	0	6	13431.62738
334	206–126	0	7	15350.39047
335	206–126	0	8	17269.13637
336	206–126	0	9	19187.86461
337	206–126	0	10	21106.57184

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
338	206–126	0	11	23025.25733
339	206–126	0	12	24943.91625
340	206–126	0	46	90149.08500
341	206–126	0	55	107393.92000
342	206–126	1	5	11487.70052
343	206–126	1	6	13402.28585
344	206–126	1	7	15316.85648
345	206–126	1	8	17231.41135
346	206–126	1	9	19145.94729
347	206–126	1	10	21060.46383
348	206–126	1	55	107159.08100
349	206–126	2	6	13372.88847
350	206–126	2	55	106923.79100
351	206–126	3	6	13343.44200
352	206–126	3	55	106688.07700
353	206–126	4	55	106451.91800
354	206–124	0	1	3876.07165
355	206–124	0	2	5814.10284
356	206–124	0	3	7752.12653
357	206–124	0	4	9690.14247
358	206–124	0	5	11628.14884
359	206–124	0	6	13566.14234
360	206–124	0	7	15504.12085
361	206–124	0	8	17442.08186
362	206–124	0	9	19380.02553
363	206–122	0	1	3915.75217
364	206–122	0	2	5873.62271
365	206–122	0	3	7831.48708
366	206–122	0	4	9789.34277
367	206–122	0	5	11747.18803
368	206–122	0	6	13705.02040
369	206–122	0	7	15662.83767
370	206–122	0	8	17620.63824
371	206–122	0	9	19578.41929

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
372	204–130	0	1	3778.56411
373	204–130	0	2	5667.84076
374	204–130	0	3	7557.11177
375	204–130	0	4	9446.37508
376	204–130	0	5	11335.62867
377	204–130	0	6	13224.87048
378	204–130	0	7	15114.09468
379	204–130	0	8	17003.30936
380	204–130	0	9	18892.50250
381	204–128	0	1	3814.67101
382	204–128	0	2	5722.00221
383	204–128	0	3	7629.32648
384	204–128	0	4	9536.64230
385	204–128	0	5	11443.94901
386	204–128	0	6	13351.24309
387	204–128	0	7	15258.52244
388	204–128	0	8	17165.78692
389	204–128	0	9	19073.03193
390	204–126	0	2	5777.86723
391	204–126	0	3	7703.81252
392	204–126	0	4	9629.75040
393	204–126	0	5	11555.67822
394	204–126	0	6	13481.59388
395	204–126	0	7	15407.49372
396	204–126	0	8	17333.37862
397	204–126	0	9	19259.24450
398	204–124	0	4	9725.83322
399	204–124	0	5	11670.97751
400	204–125	0	4	9677.34120
401	204–125	0	5	11612.78740
402	204–125	0	6	13548.22160
403	206–123	0	2	5843.58030
404	206–123	0	3	7791.43080
405	206–123	0	4	9739.27290

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
406	206–123	0	5	11687.10470
407	206–123	0	6	13634.92400
408	206–125	0	1	3856.67470
409	206–125	0	2	5785.00700
410	206–125	0	3	7713.33300
411	206–125	0	4	9641.65080
412	206–125	0	5	11569.95830
413	206–125	0	6	13498.25340
414	206–125	0	7	15426.53410
415	206–125	0	8	17354.79830
416	206–125	0	9	19283.04390
417	206–125	0	10	21211.26890
418	206–125	0	11	23139.47130
419	207–122	0	2	5863.06350
420	207–122	0	3	7817.40800
421	207–122	0	4	9771.74410
422	207–122	0	5	11726.06950
423	207–122	0	6	13680.38220
424	207–122	0	7	15634.68000
425	207–122	0	8	17588.96080
426	207–122	0	9	19543.22240
427	207–124	0	2	5803.54330
428	207–124	0	3	7738.04800
429	207–124	0	4	9672.54430
430	207–124	0	5	11607.03020
431	207–124	0	6	13541.50360
432	207–124	0	7	15475.96250
433	207–124	0	8	17410.40460
434	207–124	0	9	19344.82790
435	207–126	0	1	3830.59870
436	207–126	0	2	5745.89300
437	207–126	0	3	7661.18110
438	207–126	0	4	9576.46100
439	207–126	0	5	11491.73070

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TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
440	207–126	0	6	13406.98820
441	207–126	0	7	15322.23130
442	207–126	0	8	17237.45810
443	207–126	0	9	19152.66640
444	207–126	0	10	21067.85440
445	207–126	0	11	22983.01980
446	207–126	0	12	24898.16070
447	207–126	1	5	11466.65000
448	207–126	1	6	13377.72730
449	207–126	1	7	15288.79030
450	207–126	1	9	19110.86520
451	207–128	0	1	3793.35490
452	207–128	0	2	5690.02740
453	207–128	0	3	7586.69380
454	207–128	0	4	9483.35230
455	207–128	0	5	11380.00070
456	207–128	0	6	13276.63710
457	207–128	0	7	15173.25950
458	207–128	0	8	17069.86580
459	207–128	0	9	18966.45410
460	207–128	0	10	20863.02240
461	207–128	0	11	22759.56870
462	207–128	0	12	24656.09090
463	207–128	0	37	72055.47100
464	207–128	0	47	91003.65400
465	207–128	0	55	106155.36900
466	207–128	1	5	11355.28680
467	207–128	1	6	13247.80390
468	207–128	1	7	15140.30670
469	207–128	1	8	17032.79340
470	207–128	1	9	18925.26170
471	207–128	1	10	20817.70980
472	207–128	1	37	71898.90800
473	207–128	1	55	105924.57400

continued on the next page

TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
474	207–128	2	37	71742.06400
475	207–128	3	37	71584.92400
476	207–130	0	1	3757.24760
477	207–130	0	2	5635.86640
478	207–130	0	3	7514.47940
479	207–130	0	4	9393.08460
480	207–130	0	5	11271.67990
481	207–130	0	6	13150.26340
482	207–130	0	7	15028.83320
483	207–130	0	8	16907.38730
484	207–130	0	9	18785.92360
485	207–130	0	10	20664.44040
486	207–130	0	11	22542.93560
487	207–130	0	12	24421.40720
488	207–130	0	13	26299.85320
489	207–130	0	56	107020.94200
490	207–130	0	57	108896.32300
491	207–130	1	5	11247.31770
492	207–130	1	6	13121.84060
493	207–130	1	7	14996.34960
494	207–130	1	8	16870.84270
495	207–130	1	9	18745.31790
496	207–130	1	56	106789.38500
497	207–130	1	57	108660.69500
498	207–130	2	56	106557.40400
499	207–130	2	57	108424.62100
500	207–130	3	56	106324.97100
501	207–130	3	57	108188.14500
502	207–130	4	56	106092.16000
503	207–130	4	57	107951.21600
504	207–130	5	57	107713.84700
505	207–130	6	57	107476.02800
506	208–123	0	2	5822.57080
507	208–123	0	3	7763.41800

continued on the next page

TABLE SII: *continued*

Line no.	(A–B)	v	J	Frequency (MHz)
508	208–123	0	4	9704.25690
509	208–123	0	5	11645.08530
510	208–123	0	6	13585.90120
511	208–123	0	7	15526.70250
512	208–123	0	9	19408.25290
513	208–125	0	1	3842.66800
514	208–125	0	2	5763.99690
515	208–125	0	3	7685.31970
516	208–125	0	4	9606.63430
517	208–125	0	5	11527.93880
518	208–125	0	6	13449.23090
519	208–125	0	7	15370.50880
520	208–125	0	8	17291.77030
521	208–125	0	9	19213.01350
522	208–125	0	10	21134.23620
523	208–125	0	11	23055.43650
524	207–123	0	4	9721.67360
525	207–123	0	5	11665.98530
526	207–123	0	9	19443.08610
527	207–125	0	2	5774.44770
528	207–125	0	3	7699.25410
529	207–125	0	4	9624.05220
530	207–125	0	5	11548.84010
531	207–125	0	6	13473.61570
532	207–125	0	7	15398.37690
533	207–125	0	9	19247.84810

TABLE SIII: Dunham constants, spectroscopic parameters, mass-independent U_{lm} constants, and BOB-correction terms for 16 isotopologues of PbSe obtained using method A (see text)[a].

Isotopologue	x^b / %	Y_{01} / MHz B_e	Y_{11} / MHz $-\alpha_e$	Y_{21} / kHz γ_e	Y_{31} / Hz ϵ_e	Y_{02} / kHz $-D_e$	Y_{12} / Hz $-\beta_e$
$^{208}Pb^{80}Se$	26.00	1516.936172(10)	−3.8936033(99)	−3.4051(23)	−21.11(14)	−0.200430(20)	−0.4214(48)
$^{208}Pb^{78}Se$	12.46	1545.053073(11)	−4.002359(10)	−3.5325(24)	−22.10(14)	−0.207929(21)	−0.4412(51)
$^{206}Pb^{80}Se$	11.96	1521.028876(12)	−3.909373(10)	−3.4235(23)	−21.25(14)	−0.201513(20)	−0.4243(49)
$^{207}Pb^{80}Se$	10.96	1518.971937(10)	−3.9014449(99)	−3.4143(23)	−21.18(14)	−0.200969(20)	−0.4229(48)
$^{206}Pb^{78}Se$	5.73	1549.145766(12)	−4.018274(10)	−3.5512(24)	−22.25(14)	−0.209032(21)	−0.4442(51)
$^{207}Pb^{78}Se$	5.25	1547.088832(10)	−4.010273(10)	−3.5418(24)	−22.18(14)	−0.208478(21)	−0.4427(51)
$^{208}Pb^{76}Se$	4.91	1574.633831(13)	−4.117850(10)	−3.6691(25)	−23.18(15)	−0.215967(22)	−0.4627(53)
$^{208}Pb^{82}Se$	4.57	1490.179075(12)	−3.7910388(97)	−3.2860(23)	−20.19(13)	−0.193422(19)	−0.4031(46)
$^{208}Pb^{77}Se$	4.00	1559.626887(11)	−4.059122(10)	−3.5995(25)	−22.63(14)	−0.211870(21)	−0.4517(52)
$^{206}Pb^{76}Se$	2.26	1578.726513(14)	−4.133917(11)	−3.6882(25)	−23.33(15)	−0.217092(22)	−0.4657(54)
$^{206}Pb^{82}Se$	2.10	1494.271789(13)	−3.8066693(97)	−3.3041(23)	−20.33(13)	−0.194486(19)	−0.4059(47)
$^{207}Pb^{76}Se$	2.07	1576.669585(13)	−4.125840(11)	−3.6786(25)	−23.25(15)	−0.216526(22)	−0.4642(53)
$^{207}Pb^{82}Se$	1.93	1492.214845(12)	−3.7988109(97)	−3.2950(23)	−20.26(13)	−0.193951(19)	−0.4045(46)
$^{206}Pb^{77}Se$	1.84	1563.719574(13)	−4.075112(10)	−3.6184(25)	−22.78(15)	−0.212984(21)	−0.4547(52)
$^{207}Pb^{77}Se$	1.69	1561.662643(11)	−4.067073(10)	−3.6089(25)	−22.70(15)	−0.212424(21)	−0.4532(52)
$^{204}Pb^{80}Se$	0.69	1525.200313(19)	−3.925469(10)	−3.4423(24)	−21.40(14)	−0.202620(20)	−0.4272(49)
		U_{01}/uMHz	$U_{11}/u^{3/2}$MHz	U_{21}/u^2MHz	$U_{31}/u^{5/2}$MHz	U_{02}/u^2MHz	$U_{12}/u^{5/2}$MHz
PbSe		87580.535(56)	−1707.9744(43)	−11.3493(77)	−0.5346(35)	−0.668040(67)	−0.01067(12)
			$\delta_{01}^{Pb} = 51.71(96)^c$ kHz	$\delta_{01}^{Se} = 19.94(17)^c$ kHz			
			$\Delta_{01}^{Pb} = -12.92(24)$	$\Delta_{01}^{Se} = -1.915(16)$			

[a]Numbers in parentheses give one standard deviation in units of the last quoted digit.

[b]Natural abundance (%) of the isotopologue.

[c]Adopting $^{208}Pb^{80}Se$ as the reference isotopologue.

TABLE SIV: Dunham constants, spectroscopic parameters, mass-independent U_{lm} constants, and BOB-correction terms for 26 isotopologues of PbTe obtained using method A (see text)[a].

Isotopologue	x^b / %	Y_{01} / MHz B_e	Y_{11} / MHz $-\alpha_e$	Y_{21} / kHz γ_e	Y_{31} / Hz ϵ_e	Y_{02} / kHz $-D_e$	Y_{12} / Hz $-\beta_e$
$^{208}Pb^{130}Te$	17.86	938.5816677(65)	−2.0209726(66)	−1.7838(18)	−8.79(11)	−0.0815125(52)	−0.1687(12)
$^{208}Pb^{128}Te$	16.63	947.6231916(63)	−2.0502458(67)	−1.8184(19)	−9.01(12)	−0.0830905(53)	−0.1728(12)
$^{208}Pb^{126}Te$	9.87	956.9493571(65)	−2.0805872(68)	−1.8543(19)	−9.23(12)	−0.0847341(54)	−0.1771(12)
$^{206}Pb^{130}Te$	8.21	942.0891264(67)	−2.0323126(66)	−1.7972(18)	−8.88(11)	−0.0821229(52)	−0.1703(12)
$^{206}Pb^{128}Te$	7.65	951.1306471(66)	−2.0616401(67)	−1.8318(19)	−9.09(12)	−0.0837068(53)	−0.1744(12)
$^{207}Pb^{130}Te$	7.53	940.3263237(64)	−2.0266106(66)	−1.7905(18)	−8.84(11)	−0.0818158(52)	−0.1695(12)
$^{207}Pb^{128}Te$	7.01	949.3678460(62)	−2.0559108(67)	−1.8251(19)	−9.05(12)	−0.0833968(53)	−0.1736(12)
$^{206}Pb^{126}Te$	4.54	960.4568094(68)	−2.0920374(68)	−1.8679(19)	−9.32(12)	−0.0853564(54)	−0.1787(13)
$^{207}Pb^{126}Te$	4.16	958.6940099(64)	−2.0862800(68)	−1.8611(19)	−9.27(12)	−0.0850434(54)	−0.1779(12)
$^{208}Pb^{125}Te$	3.70	961.7163389(68)	−2.0961532(68)	−1.8729(19)	−9.35(12)	−0.0855804(54)	−0.1793(13)
$^{208}Pb^{124}Te$	2.48	966.5734981(72)	−2.1120534(69)	−1.8918(19)	−9.47(12)	−0.0864470(55)	−0.1815(13)
$^{206}Pb^{125}Te$	1.70	965.2237900(72)	−2.1076318(69)	−1.8865(19)	−9.43(12)	−0.0862058(55)	−0.1809(13)
$^{207}Pb^{125}Te$	1.56	963.4609910(67)	−2.1018602(69)	−1.8797(19)	−9.39(12)	−0.0858912(54)	−0.1801(13)
$^{208}Pb^{122}Te$	1.34	976.5098600(84)	−2.1447052(70)	−1.9309(20)	−9.71(13)	−0.0882336(56)	−0.1862(13)
$^{206}Pb^{124}Te$	1.14	970.0809470(76)	−2.1235609(69)	−1.9056(20)	−9.55(12)	−0.0870756(55)	−0.1832(13)
$^{207}Pb^{124}Te$	1.05	968.3181490(72)	−2.1177748(69)	−1.8987(19)	−9.51(12)	−0.0867594(55)	−0.1824(13)
$^{206}Pb^{122}Te$	0.61	980.0173050(87)	−2.1562716(70)	−1.9448(20)	−9.80(13)	−0.0888686(56)	−0.1879(13)
$^{207}Pb^{122}Te$	0.56	978.2545090(83)	−2.1504559(70)	−1.9378(20)	−9.75(13)	−0.0885491(56)	−0.1871(13)
$^{204}Pb^{130}Te$	0.48	945.6640590(87)	−2.0438924(67)	−1.8109(19)	−8.96(12)	−0.0827474(52)	−0.1719(12)
$^{208}Pb^{123}Te$	0.47	971.4946340(78)	−2.1282038(69)	−1.9111(20)	−9.59(12)	−0.0873296(55)	−0.1839(13)
$^{204}Pb^{128}Te$	0.44	954.7055770(86)	−2.0732753(68)	−1.8456(19)	−9.18(12)	−0.0843373(53)	−0.1760(12)
$^{204}Pb^{126}Te$	0.26	964.0317360(89)	−2.1037294(69)	−1.8819(19)	−9.40(12)	−0.0859931(55)	−0.1803(13)
$^{206}Pb^{123}Te$	0.21	975.0020810(81)	−2.1397405(70)	−1.9249(20)	−9.67(12)	−0.0879613(56)	−0.1855(13)
$^{207}Pb^{123}Te$	0.20	973.2392840(77)	−2.1339397(70)	−1.9180(20)	−9.63(12)	−0.0876435(56)	−0.1847(13)
$^{204}Pb^{125}Te$	0.10	968.7987150(92)	−2.1193527(69)	−1.9005(19)	−9.52(12)	−0.0868456(55)	−0.1826(13)
$^{204}Pb^{124}Te$	0.07	973.6558700(96)	−2.1353112(70)	−1.9196(20)	−9.64(12)	−0.0877186(56)	−0.1849(13)
		U_{01}/uMHz	$U_{11}/u^{3/2}$MHz	U_{21}/u^2MHz	$U_{31}/u^{5/2}$MHz	U_{02}/u^2MHz	$U_{12}/u^{5/2}$MHz
PbTe		75052.812(31)	−1445.0336(47)	−11.405(12)	−0.5026(63)	−0.521172(33)	−0.009645(69)
			$\delta_{01}^{Pb} = 28.63(37)^c$ kHz	$\delta_{01}^{Te} = 7.17(11)^c$ kHz			
			$\Delta_{01}^{Pb} = -11.56(15)$	$\Delta_{01}^{Te} = -1.809(28)$			

[a]Numbers in parentheses give one standard deviation in units of the last quoted digit.

[b]Natural abundance (%) of the isotopologue.

[c]Adopting $^{208}Pb^{130}Te$ as the reference isotopologue.