

SUPPORTING INFORMATION

On the efficiency of treating singularities in triatomic variational vibrational computations. The vibrational states of H_3^+ up to dissociation

Tamás Szidarovszky, Attila G. Császár, and Gábor Czako^{*}

Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös University,
P. O. Box 32, H-1518 Budapest 112, Hungary

^{*} Corresponding author's e-mail: czako@chem.elte.hu. Current address: Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, Atlanta, GA 30322

Table S1. Even and odd-parity vibrational band origins of H_3^+ and relative energies with respect to most converged results (given in Table S2) in this study, calculated in Jacobi coordinates employing *primitive* exact Spherical-DVR with $\alpha = 0$, using basis set size (85 80 30) and $R_j^{\text{max}} = 17.65$ bohr ($j = 1$ or 2). Deviations and band origins are all given in cm^{-1} .^a

	even	ΔE	odd	ΔE		even	ΔE	odd	ΔE
1	0.00 ^b	0.00	2520.86	0.00	345	28701.47	-15.23	30114.12	-24.43
2	2520.87	0.00	4996.97	0.00	346	28718.19	-12.61	30136.04	-40.15
3	3178.79	-0.01	5554.11	0.00	347	28735.78	-29.07	30194.38	-39.04
4	4777.04	0.01	7004.18	-0.01	348	28741.63	-18.76	30213.54	-20.52
5	4996.96	0.00	7491.58	-0.01	349	28764.00	-40.32	30228.48	-16.00
6	5554.06	0.05	7869.51	-0.04	350	28811.46	-3.26	30267.64	-16.60
7	6263.08	-0.04	8488.21	0.00	351	28856.38	-17.87	30288.31	-33.97
8	7004.20	-0.03	9110.43	-0.01	352	28868.40	8.86	30301.28	-37.37
9	7283.72	0.01	9651.80	-0.02	353	28883.48	16.16	30339.05	-15.07
10	7768.73	-0.04	9996.00	-0.01	354	28901.92	31.20	30379.19	-24.17
11	7869.56	-0.09	10209.05	0.01	355	28962.98	-6.53	30400.43	-32.64
12	8487.91	0.30	10644.83	-0.22	356	28971.79	4.10	30419.62	-19.04
13	8999.01	0.00	10859.18	0.00	357	28996.44	-9.57	30454.49	-24.89
14	9110.40	0.01	11323.43	-0.06	358	29020.55	-25.07	30460.90	-18.08
15	9253.09	0.05	11526.44	-0.02	359	29041.49	-18.68	30477.41	-10.98
16	9651.92	-0.14	11655.62	0.02	360	29082.85	-18.87	30491.28	-2.96
17	9967.17	0.09	12076.91	-0.08	361	29093.09	-12.71	30518.75	-11.85
18	9996.05	-0.05	12299.14	0.05	362	29144.65	-27.95	30584.35	-18.43
19	10593.46	-0.70	12472.46	-0.07	363	29175.15	-16.44	30618.37	-42.34
20	10645.27	-0.65	12695.73	0.07	364	29180.78	6.08	30634.98	-29.59
21	10859.20	-0.01	12830.48	0.23	365	29207.00	-8.76	30639.95	-21.23
22	10919.83	-0.01	13317.22	-0.40	366	29244.42	-24.31	30659.02	-23.17
23	11323.46	-0.09	13389.44	-0.05	367	29263.04	-21.95	30668.60	-8.89
24	11655.54	0.11	13585.88	0.04	368	29269.44	-13.80	30688.57	-25.16
25	11812.38	0.16	13690.44	-0.02	369	29282.95	-7.59	30723.41	-47.72
26	12077.16	-0.33	13753.30	-0.22	370	29333.37	-18.16	30750.40	-18.07
27	12147.20	0.67	14055.16	-0.28	371	29358.01	-8.43	30761.56	-20.73
28	12299.17	0.02	14215.17	0.19	372	29371.92	-15.36	30769.93	-21.02
29	12374.28	0.04	14472.21	-0.23	373	29422.92	-46.44	30811.04	-53.70
30	12472.22	0.16	14564.18	-0.31	374	29445.64	-18.36	30819.72	-26.31
31	12588.21	0.21	14878.20	-0.10	375	29464.46	-14.94	30865.10	-51.88
32	12694.93	0.87	14890.15	-1.21	376	29491.83	-10.41	30871.30	-18.35
33	13288.85	-1.51	15114.06	0.00	377	29507.75	-6.29	30911.47	-47.14
34	13317.69	-0.87	15185.59	-0.07	378	29550.63	-25.05	30928.41	-11.29
35	13389.58	-0.19	15210.67	0.09	379	29555.58	-21.05	30961.82	-37.82
36	13397.29	-0.26	15328.83	-0.28	380	29570.45	-27.55	30992.21	-23.61
37	13585.90	0.02	15371.40	0.27	381	29579.35	-27.71	31008.97	-26.52
38	13690.50	-0.09	15770.14	-0.25	382	29596.86	-12.27	31021.49	-4.08
39	13716.02	-0.12	15886.16	-0.01	383	29607.45	-21.98	31036.83	-16.55
40	14059.02	-4.14	15963.91	-1.17	384	29618.07	-1.36	31051.15	-26.71

41	14189.41	0.01	16007.27	0.17	385	29637.72	-19.12	31068.87	-12.82
42	14215.63	-0.28	16246.51	-0.49	386	29659.40	-11.92	31109.17	-27.04
43	14473.11	-1.13	16450.05	-0.05	387	29701.58	-10.90	31143.39	-30.63
44	14664.43	-0.23	16559.23	-2.48	388	29709.49	-15.57	31175.68	-28.46
45	14877.90	0.19	16591.58	-2.85	389	29730.30	-15.46	31180.71	-30.18
46	14887.71	0.64	16673.35	-0.86	390	29787.91	-1.98	31217.82	-22.11
47	14888.95	0.00	16718.93	-0.62	391	29798.32	-4.74	31230.89	-23.18
48	14939.09	2.12	16861.56	-0.88	392	29811.36	-14.85	31236.25	-16.76
49	15068.52	-0.01	16911.27	-0.59	393	29822.15	-12.98	31251.28	-30.53
50	15113.76	0.29	17083.01	-1.35	394	29850.03	-9.62	31259.87	-36.73
51	15164.74	-0.92	17217.19	-3.22	395	29867.23	-21.57	31274.33	-12.91
52	15208.11	2.67	17384.22	-2.92	396	29888.42	-20.87	31294.53	-12.25
53	15327.26	1.31	17447.50	-1.46	397	29900.89	-8.51	31330.41	-31.08
54	15769.52	0.38	17606.80	-0.64	398	29920.33	-14.92	31344.12	-32.31
55	15868.27	0.24	17686.74	-0.01	399	29939.14	-31.04	31359.22	-27.37
56	15882.01	4.13	17698.80	-0.47	400	29966.76	-15.28	31384.38	-43.54
57	15908.17	0.53	17813.43	-4.13	401	30008.56	-36.79	31406.21	-21.75
58	16007.27	0.18	17852.63	-2.14	402	30031.97	-14.25	31453.24	-38.25
59	16193.17	-0.74	17867.70	-10.97	403	30046.65	-15.21	31469.62	-26.59
60	16246.58	-0.56	17969.11	-1.31	404	30053.76	-6.76	31486.43	-32.02
61	16451.59	-1.61	18196.10	-1.30	405	30064.74	-5.09	31499.40	-31.82
62	16453.65	-0.67	18333.08	-4.75	406	30090.94	-10.91	31520.60	-36.40
63	16557.13	-0.35	18352.40	0.62	407	30106.88	-22.16	31559.56	-39.88
64	16681.68	-9.19	18435.56	-0.43	408	30135.95	-46.15	31573.21	-31.19
65	16703.06	-0.19	18577.08	-1.49	409	30146.91	-3.77	31601.72	-26.87
66	16719.60	-1.30	18709.31	-1.59	410	30193.72	-38.49	31616.53	-33.23
67	16865.46	-4.78	18796.86	-1.15	411	30214.54	-3.70	31638.50	-17.44
68	16912.40	-1.71	18868.82	-2.90	412	30250.08	-37.79	31674.06	-40.65
69	17057.39	-0.60	18926.35	-1.46	413	30254.53	-3.29	31682.84	-27.58
70	17213.30	0.67	19045.53	-1.82	414	30275.02	-19.76	31709.74	-45.21
71	17263.63	-0.07	19087.03	-4.94	415	30298.26	-3.58	31726.41	-57.14
72	17382.16	-0.87	19182.05	-3.31	416	30321.34	2.31	31740.83	-26.13
73	17439.79	-3.71	19221.16	-8.05	417	30355.15	-18.89	31757.50	-36.80
74	17446.25	-0.23	19274.22	-1.84	418	30394.86	-39.95	31767.62	-39.39
75	17589.37	2.53	19284.99	-10.86	419	30399.01	-25.39	31785.85	-35.90
76	17605.26	0.91	19302.18	-1.46	420	30432.46	-31.69	31791.57	-16.33
77	17686.44	-3.19	19430.99	-3.58	421	30446.00	-16.95	31805.41	-14.53
78	17698.34	-0.03	19499.27	-3.47	422	30470.38	-18.99	31843.18	-45.24
79	17744.35	0.03	19714.52	-3.57	423	30486.20	-19.56	31866.23	-9.03
80	17856.27	0.43	19746.40	-5.47	424	30505.22	-16.77	31894.94	-29.69
81	17967.87	-0.02	19840.83	-3.10	425	30515.73	-9.32	31922.47	-9.33
82	18187.81	6.98	19872.62	-2.02	426	30568.25	-12.70	31945.02	-28.14
83	18213.10	1.17	20052.18	-3.21	427	30584.33	-18.07	31951.15	-20.78
84	18337.64	15.37	20075.20	-1.52	428	30594.91	-18.65	31966.42	-14.07
85	18362.97	1.47	20103.73	-3.36	429	30611.10	-6.99	31985.39	-14.18
86	18435.36	-0.22	20211.78	-5.14	430	30628.67	-23.28	32015.52	-21.89

87	18450.07	1.63	20250.27	-6.33	431	30655.92	-37.37	32073.97	-28.58
88	18575.61	-0.06	20285.82	-9.90	432	30662.98	-3.33	32093.48	-31.91
89	18588.63	0.22	20381.79	-10.51	433	30677.66	-2.37	32101.97	-28.28
90	18706.66	1.06	20425.62	-1.65	434	30740.49	-8.05	32110.02	-30.85
91	18797.23	-1.50	20502.75	-3.24	435	30754.91	-13.70	32129.75	-14.78
92	18808.46	0.10	20599.51	0.17	436	30764.98	-23.16	32174.89	-39.78
93	18924.50	0.42	20774.04	-4.99	437	30805.14	-47.80	32179.81	-36.38
94	19051.17	-7.53	20782.90	-5.81	438	30814.61	-22.29	32183.98	-21.94
95	19083.66	-1.53	20801.78	-4.96	439	30833.62	-40.11	32212.40	-31.02
96	19102.98	0.94	20850.61	-2.51	440	30874.69	-21.76	32253.91	-18.96
97	19214.94	-1.84	20944.85	-9.50	441	30879.92	-22.80	32266.42	-15.02
98	19238.32	1.98	20992.31	-5.41	442	30900.45	-36.05	32295.94	-15.43
99	19273.49	-1.09	21105.32	-4.18	443	30912.77	-9.45	32308.07	-21.91
100	19311.01	-10.25	21151.87	0.19	444	30946.88	-29.67	32318.66	-31.48
101	19421.10	-0.91	21181.23	-1.89	445	30974.95	-42.89	32368.32	-44.36
102	19427.31	0.08	21284.84	-3.86	446	30993.28	-24.87	32381.48	-41.40
103	19495.57	0.25	21321.70	-4.38	447	31015.06	-32.41	32397.00	-17.12
104	19745.03	-4.12	21342.10	-7.82	448	31027.67	-22.56	32404.44	-22.74
105	19777.50	-5.48	21440.00	-3.48	449	31050.16	-29.66	32416.97	-20.11
106	19806.69	-15.28	21546.51	-9.57	450	31055.16	-30.80	32439.93	-29.45
107	19846.27	-8.52	21598.28	-10.32	451	31084.45	-27.99	32451.21	-38.65
108	19871.27	-0.61	21613.43	-5.93	452	31103.20	-29.80	32482.54	-28.14
109	20052.01	-3.03	21666.02	-1.68	453	31138.18	-25.13	32507.88	-50.31
110	20077.46	0.42	21681.42	-6.38	454	31153.89	-39.06	32539.84	-63.83
111	20101.24	-0.90	21760.05	-4.16	455	31164.15	-31.85	32547.26	-19.87
112	20179.52	-2.42	21888.93	-1.67	456	31202.10	-54.69	32574.97	-34.70
113	20207.22	-0.65	21891.90	-2.68	457	31209.47	-20.36	32600.21	-39.61
114	20214.84	-3.42	21898.53	-8.83	458	31222.13	-26.61	32615.78	-35.08
115	20244.18	-0.18	22108.29	-2.39	459	31241.95	-34.37	32627.33	-41.08
116	20317.13	-1.63	22168.83	-4.24	460	31249.68	-29.33	32644.34	-28.15
117	20430.06	-6.15	22169.82	0.26	461	31277.91	-34.15	32668.99	-34.53
118	20494.00	5.55	22206.86	-4.77	462	31290.12	-31.12	32686.00	-37.42
119	20508.51	0.68	22311.33	-5.29	463	31300.34	-39.17	32693.79	-28.16
120	20590.57	8.96	22337.80	-6.28	464	31305.83	-23.82	32712.35	-31.21
121	20617.66	-2.14	22388.09	-7.06	465	31324.83	-25.81	32736.68	-47.28
122	20758.61	10.31	22432.83	-8.51	466	31343.53	-31.59	32743.98	-32.68
123	20771.56	5.52	22516.67	-8.46	467	31368.30	-39.90	32756.16	-33.53
124	20833.60	3.44	22531.98	-13.44	468	31389.82	-49.00	32782.67	-54.81
125	20849.18	-1.05	22565.86	-14.12	469	31398.05	-39.00	32789.36	-52.00
126	20910.58	7.36	22605.66	-10.59	470	31418.32	-34.04	32814.00	-36.88
127	20978.79	8.04	22632.33	-5.41	471	31431.24	-16.20	32824.40	-29.54
128	21033.49	-0.53	22720.70	-4.19	472	31465.97	-11.22	32832.68	-28.17
129	21108.97	-7.83	22807.37	-10.05	473	31486.09	-19.71	32856.33	-50.80
130	21153.54	-1.54	22883.27	-10.93	474	31525.86	-41.80	32875.98	-43.59
131	21201.29	0.85	22917.68	1.28	475	31549.37	-29.75	32885.30	-28.87
132	21217.68	6.46	22964.49	-7.30	476	31558.02	-17.14	32916.08	-56.98

133	21272.10	8.87	23013.55	-8.30	477	31566.81	-24.92	32922.73	-48.23
134	21322.49	-5.17	23027.02	-3.37	478	31598.30	-30.15	32952.55	-36.33
135	21433.34	3.23	23042.59	-5.68	479	31616.74	-32.98	32985.95	-24.67
136	21457.60	5.49	23088.00	-6.58	480	31620.14	-31.17	33017.16	-40.06
137	21546.49	-9.66	23171.74	-6.95	481	31639.80	-18.67	33031.03	-25.31
138	21604.34	3.23	23250.27	-4.68	482	31655.59	-22.77	33056.38	-44.70
139	21628.00	-1.61	23367.51	1.67	483	31684.92	-29.48	33069.57	-29.28
140	21666.57	-2.26	23400.03	-1.89	484	31687.47	-18.24	33079.73	-33.93
141	21674.71	0.28	23431.56	-5.88	485	31718.00	-21.48	33106.17	-28.17
142	21742.80	-2.06	23476.76	3.80	486	31735.71	-21.13	33126.59	-28.56
143	21759.66	-3.93	23499.47	-14.10	487	31746.94	-19.34	33128.42	-28.47
144	21889.56	-2.31	23528.70	-13.65	488	31769.74	-26.55	33163.44	-41.57
145	21891.01	-1.69	23594.08	-14.09	489	31800.72	-25.52	33184.56	-37.27
146	22018.62	-26.52	23661.77	-9.13	490	31803.15	-25.95	33196.65	-33.72
147	22075.94	-0.52	23699.28	-6.82	491	31837.16	-39.76	33202.53	-28.43
148	22111.04	-5.17	23735.30	-7.56	492	31868.78	-47.05	33230.54	-39.17
149	22161.27	-0.64	23821.82	-9.89	493	31904.58	-47.74	33234.52	-34.04
150	22173.58	-3.43	23917.48	-12.50	494	31911.61	-46.59	33277.40	-51.43
151	22207.56	-5.45	23954.38	-5.54	495	31928.91	-53.30	33294.42	-48.36
152	22287.21	2.49	23967.99	-18.26	496	31948.13	-35.13	33306.88	-31.93
153	22305.10	0.93	23982.89	-8.06	497	31969.69	-45.29	33320.05	-35.33
154	22381.73	-0.57	24027.55	-5.00	498	31979.11	-27.20	33355.79	-26.93
155	22421.15	-8.13	24040.51	-2.53	499	31990.48	-19.44	33394.28	-42.32
156	22471.00	0.11	24078.20	-3.15	500	32021.05	-49.49	33397.99	-27.62
157	22505.37	3.00	24162.60	-5.04	501	32039.86	-46.33	33441.32	-56.02
158	22524.09	-5.72	24174.14	-12.41	502	32055.08	-9.83	33445.58	-23.21
159	22606.63	-11.65	24233.53	-11.84	503	32080.34	-18.99	33460.94	-25.99
160	22621.49	-2.89	24318.97	-6.25	504	32084.78	-14.80	33471.96	-31.92
161	22655.22	-28.33	24372.21	-3.81	505	32101.44	-22.26	33477.73	-26.89
162	22694.48	-1.34	24405.94	-6.46	506	32108.44	-14.61	33500.63	-47.30
163	22718.45	-1.87	24424.23	-2.83	507	32131.59	-16.50	33524.75	-45.07
164	22787.34	9.85	24462.74	-5.22	508	32149.48	-7.74	33529.91	-37.24
165	22857.76	-11.68	24489.51	-3.20	509	32165.14	-10.25	33543.48	-37.05
166	22912.72	6.07	24553.48	-6.93	510	32230.13	-48.86	33576.89	-56.86
167	23017.53	6.15	24586.20	-6.77	511	32243.52	-8.69	33593.86	-45.49
168	23037.42	-1.55	24661.06	-18.68	512	32257.11	-6.01	33609.13	-31.50
169	23043.22	-6.30	24698.34	-9.55	513	32269.49	-9.98	33624.18	-38.60
170	23089.10	-7.64	24726.58	-9.14	514	32290.23	-9.27	33639.39	-48.69
171	23141.32	0.26	24751.93	-14.99	515	32308.77	-21.37	33650.19	-40.06
172	23171.43	-6.73	24776.77	-17.76	516	32322.86	-24.54	33676.56	-33.12
173	23211.98	-4.75	24804.06	-2.29	517	32346.72	-6.99	33694.94	-38.37
174	23244.04	1.46	24914.47	-7.77	518	32383.88	-39.45	33709.94	-51.82
175	23295.83	11.64	24924.39	-16.39	519	32385.92	-4.47	33725.55	-38.68
176	23366.93	2.14	24969.92	-5.07	520	32419.83	-22.88	33738.54	-26.57
177	23387.52	8.81	24994.10	-13.25	521	32422.04	-15.97	33781.04	-42.85
178	23401.45	-3.36	25062.66	-9.56	522	32436.85	-26.09	33793.40	-27.13

179	23491.19	-5.75	25091.23	-4.45	523	32475.80	-21.74	33809.22	-35.16
180	23514.96	0.08	25147.08	-9.33	524	32499.90	-38.39	33820.73	-29.08
181	23542.19	-3.63	25157.44	-8.99	525	32506.02	-29.83	33835.27	-26.76
182	23587.26	-7.40	25190.87	-38.37	526	32510.97	-17.41	33861.68	-44.05
183	23603.70	6.61	25230.46	-7.85	527	32526.95	-6.37	33874.76	-43.57
184	23667.11	-14.49	25306.84	-4.45	528	32545.06	-16.91	33888.03	-34.25
185	23746.02	-18.24	25347.18	2.93	529	32554.97	-20.35	33913.12	-47.84
186	23794.19	17.76	25372.19	-1.56	530	32590.56	-50.86	33932.18	-42.71
187	23898.57	-6.90	25429.42	-15.12	531	32608.71	-27.94	33944.67	-31.64
188	23905.96	-0.97	25434.31	-5.36	532	32627.68	-41.66	33951.13	-37.85
189	23916.20	7.98	25458.52	-7.04	533	32633.74	-18.00	33958.44	-28.00
190	23946.04	3.79	25528.00	-21.25	534	32653.63	-31.10	33994.85	-40.43
191	23974.76	-0.33	25611.78	-16.15	535	32669.26	-35.03	34002.23	-41.50
192	24010.89	-1.13	25621.39	-18.59	536	32697.91	-36.03	34035.99	-20.46
193	24037.35	0.53	25689.30	-9.95	537	32706.39	-41.33	34051.25	-22.11
194	24049.80	1.53	25715.13	-8.48	538	32714.12	-27.65	34068.55	-30.52
195	24068.34	6.73	25750.59	-8.84	539	32740.03	-50.14	34084.00	-42.19
196	24158.24	-0.64	25838.10	-15.63	540	32754.42	-43.44	34095.14	-37.26
197	24162.05	4.15	25875.15	-14.60	541	32760.61	-37.90	34104.33	-38.83
198	24222.58	-0.90	25912.68	-9.37	542	32770.70	-43.26	34110.03	-32.61
199	24314.11	-1.37	25931.04	-12.75	543	32793.21	-55.72	34126.22	-47.59
200	24334.28	-8.39	25937.35	-12.65	544	32804.80	-40.21	34127.26	-45.98
201	24358.22	10.07	25960.93	-4.20	545	32826.87	-49.63	34139.98	-37.05
202	24373.85	-1.95	25984.59	-8.34	546	32840.23	-45.60	34162.78	-42.10
203	24408.04	-25.68	26019.61	-15.86	547	32862.95	-58.45	34200.03	-71.39
204	24418.56	3.01	26037.80	-10.60	548	32870.33	-37.96	34209.16	-52.50
205	24486.95	-0.48	26100.57	-11.00	549	32889.89	-51.33	34219.56	-43.04
206	24561.90	-15.38	26112.56	-5.35	550	32907.13	-50.68	34248.86	-59.33
207	24581.25	-2.02	26144.36	-17.92	551	32917.71	-58.61	34260.74	-59.70
208	24592.71	-2.66	26156.83	-5.37	552	32943.59	-67.81	34279.55	-52.22
209	24685.18	3.36	26217.87	-11.02	553	32950.83	-35.83	34295.00	-55.53
210	24707.10	-6.91	26271.98	-7.78	554	32968.30	-52.31	34310.28	-36.06
211	24748.92	-12.09	26303.06	-7.32	555	32990.96	-30.15	34325.96	-31.70
212	24762.22	-3.14	26311.60	-9.69	556	33002.55	-40.80	34353.41	-53.00
213	24809.37	-7.53	26356.26	-21.74	557	33029.45	-51.96	34365.24	-44.13
214	24848.26	-7.64	26386.92	-8.51	558	33033.16	-28.05	34386.58	-60.52
215	24882.66	-9.82	26452.91	-11.96	559	33064.16	-42.12	34414.50	-58.23
216	24910.09	-2.09	26467.47	-6.07	560	33085.94	-40.25	34427.29	-50.75
217	24972.59	-7.57	26489.57	-12.90	561	33096.28	-47.79	34434.59	-51.73
218	24990.52	-9.81	26499.96	-4.94	562	33137.69	-59.79	34462.73	-50.95
219	25002.79	-5.43	26592.22	-11.72	563	33158.02	-63.89	34470.54	-45.74
220	25075.63	-22.55	26615.20	-31.70	564	33168.54	-68.15	34497.23	-56.11
221	25084.93	1.94	26653.61	-7.93	565	33185.67	-49.82	34499.67	-27.23
222	25155.33	-8.07	26699.93	-18.95	566	33198.06	-35.68	34520.64	-47.74
223	25166.53	-17.92	26740.92	-12.44	567	33229.39	-54.93	34526.67	-47.31
224	25198.67	-7.60	26765.75	-20.18	568	33240.00	-53.68	34536.16	-49.49

225	25231.22	-8.70	26773.17	-10.62	569	33253.75	-62.19	34547.24	-33.30
226	25326.01	-8.60	26834.20	-31.27	570	33270.21	-44.58	34555.23	-25.91
227	25353.45	-3.46	26863.81	-10.40	571	33296.76	-62.95	34578.05	-42.04
228	25369.24	0.81	26878.72	-9.04	572	33316.54	-41.55	34588.45	-51.50
229	25404.58	-34.04	26897.27	-26.72	573	33326.92	-42.64	34617.76	-58.30
230	25414.89	-0.46	26967.74	-7.82	574	33335.78	-20.55	34621.90	-26.84
231	25456.01	-4.39	26989.07	-8.41	575	33357.11	-27.97	34633.30	-36.03
232	25503.74	2.89	27003.95	-21.84	576	33364.28	-17.48	34641.38	-35.03
233	25535.28	-6.98	27026.17	2.17	577	33369.37	-17.54	34676.14	-43.22
234	25539.97	28.06	27055.37	-17.23	578	33393.88	-33.54	34698.95	-53.13
235	25605.90	-10.45	27106.97	-2.74	579	33399.52	-29.20	34711.43	-43.99
236	25660.50	3.04	27126.43	-18.92	580	33410.88	-25.50	34722.53	-45.02
237	25688.67	-9.17	27161.28	-19.57	581	33456.56	-48.85	34724.17	-30.85
238	25714.48	-11.17	27189.14	-25.83	582	33471.00	-36.07	34741.62	-31.25
239	25731.65	-24.97	27194.87	-6.65	583	33489.24	-38.13	34764.36	-47.84
240	25734.26	-2.66	27297.03	-12.22	584	33491.31	-37.88	34773.15	-47.00
241	25751.68	-10.08	27300.22	-8.96	585	33519.30	-54.48	34786.44	-42.70
242	25815.07	7.43	27356.70	-17.89	586	33525.67	-45.06	34788.06	-37.96
243	25895.15	4.06	27414.18	-14.20	587	33548.97	-42.38	34800.50	-36.59
244	25907.47	-4.15	27431.81	-26.79	588	33554.81	-42.81	34814.65	-24.08
245	25925.70	-7.13	27456.09	-21.75	589	33565.66	-45.71	34830.40	-35.91
246	25967.05	-10.34	27485.73	-15.11	590	33586.89	-50.81	34832.35	-24.01
247	26004.17	-0.43	27533.06	-21.49	591	33599.34	-50.71	34842.67	-30.98
248	26021.96	5.39	27583.08	-10.22	592	33617.81	-32.17	34852.60	-28.76
249	26067.72	0.79	27587.51	-7.89	593	33629.46	-33.69	34855.95	-21.73
250	26100.56	6.64	27644.91	-12.10	594	33629.99	-19.76	34867.18	-31.64
251	26120.55	5.69	27670.60	-3.19	595	33647.92	-4.81	34880.46	-22.73
252	26128.89	6.81	27700.61	-31.35	596	33678.69	-35.26	34888.32	-23.41
253	26163.59	-12.14	27704.51	-9.52	597	33688.28	-29.90	34906.45	-24.50
254	26193.24	-7.73	27725.79	-1.79	598	33715.14	-46.52	34922.45	-26.09
255	26214.06	-7.18	27771.29	-16.32	599	33733.76	-46.92	34934.24	-35.28
256	26266.88	-35.48	27785.63	-27.13	600	33751.96	-40.13		
257	26275.82	-11.74	27797.91	-13.69	601	33766.74	-49.09		
258	26294.49	1.29	27836.46	-10.57	602	33789.79	-51.60		
259	26341.19	-13.25	27849.56	-23.03	603	33814.84	-49.17		
260	26372.07	3.43	27875.43	-11.80	604	33820.58	-29.60		
261	26406.18	-27.77	27877.35	-8.74	605	33844.93	-44.93		
262	26437.89	3.01	27913.96	-20.57	606	33851.05	-43.06		
263	26464.33	-2.76	27974.34	-23.39	607	33866.85	-35.62		
264	26500.20	-5.04	28010.52	-11.44	608	33881.07	-48.40		
265	26522.86	-8.05	28035.20	-9.11	609	33889.39	-36.32		
266	26533.78	-3.39	28047.86	-21.09	610	33903.82	-43.24		
267	26577.72	2.79	28100.96	-11.56	611	33918.87	-54.13		
268	26653.36	-7.40	28124.72	-15.45	612	33936.58	-44.17		
269	26660.39	-4.70	28158.61	-29.77	613	33952.88	-39.88		
270	26687.19	-6.21	28160.14	-22.80	614	33958.38	-27.74		

271	26725.67	2.67	28210.56	-11.52	615	33988.00	-31.96
272	26767.73	-5.12	28234.67	-19.01	616	34011.58	-50.60
273	26793.62	-15.33	28254.49	-20.48	617	34022.69	-30.92
274	26804.70	-1.68	28319.32	-18.46	618	34035.76	-26.89
275	26819.79	6.37	28333.39	-19.55	619	34053.39	-37.78
276	26878.92	-25.66	28402.52	-29.01	620	34058.94	-30.62
277	26883.98	-13.55	28413.49	-19.38	621	34071.04	-37.85
278	26960.09	-4.18	28436.85	-18.44	622	34074.05	-32.03
279	26963.35	-3.41	28441.37	-16.09	623	34087.83	-22.33
280	26989.60	-9.04	28444.90	-16.74	624	34106.11	-29.22
281	27034.17	-3.80	28503.84	-16.30	625	34130.69	-51.94
282	27052.91	-14.71	28509.80	-17.37	626	34143.03	-40.30
283	27067.78	-1.71	28531.50	-22.75	627	34158.01	-37.64
284	27098.30	6.35	28562.38	-15.60	628	34173.00	-46.86
285	27140.50	0.99	28584.34	-33.31	629	34180.93	-33.43
286	27147.59	-5.66	28617.62	-20.02	630	34201.54	-44.02
287	27163.32	-0.07	28653.88	-22.44	631	34208.69	-50.05
288	27181.28	6.65	28667.81	-22.93	632	34216.09	-44.79
289	27192.40	5.31	28698.57	-11.64	633	34237.52	-61.55
290	27218.72	-8.06	28716.51	-9.72	634	34256.57	-55.16
291	27283.34	1.48	28742.60	-19.06	635	34263.72	-36.99
292	27349.02	-10.07	28762.35	-25.79	636	34280.35	-41.08
293	27404.01	-24.00	28828.36	-20.47	637	34297.15	-34.81
294	27410.64	-9.78	28848.72	-27.26	638	34328.68	-54.52
295	27441.95	-7.54	28871.06	-32.42	639	34341.85	-41.73
296	27449.76	11.72	28912.64	-13.15	640	34353.35	-40.13
297	27492.97	-22.65	28926.95	-19.47	641	34370.28	-49.69
298	27520.63	-9.21	28962.04	-29.05	642	34379.22	-45.45
299	27566.25	-3.53	28981.37	-25.01	643	34389.68	-33.37
300	27589.08	-9.64	29001.33	-14.31	644	34411.97	-41.42
301	27613.88	-26.23	29040.06	-17.11	645	34438.34	-55.92
302	27642.62	-9.70	29098.90	-18.62	646	34461.44	-49.71
303	27665.24	-2.24	29126.76	-10.15	647	34474.93	-50.05
304	27681.66	-12.76	29151.63	-28.53	648	34482.56	-41.72
305	27705.34	-10.35	29186.49	-27.80	649	34500.49	-42.93
306	27726.64	-2.77	29206.98	-13.61	650	34516.52	-43.80
307	27739.29	-12.74	29233.08	-34.59	651	34522.68	-35.43
308	27756.47	2.19	29235.59	-15.86	652	34537.46	-29.39
309	27787.02	-21.46	29281.90	-26.18	653	34547.21	-33.25
310	27807.76	-23.55	29285.97	-13.34	654	34556.69	-27.14
311	27815.42	-17.66	29309.97	-34.71	655	34571.35	-41.27
312	27839.08	-12.25	29335.83	-22.89	656	34583.59	-47.48
313	27869.18	-13.10	29368.30	-18.71	657	34593.65	-34.22
314	27876.90	-8.98	29394.34	-18.00	658	34609.87	-31.61
315	27923.08	-29.56	29448.55	-20.01	659	34625.28	-29.99
316	27960.60	-9.53	29460.40	-10.72	660	34631.37	-24.74

317	27985.12	-2.19	29487.56	-30.12	661	34636.99	-19.13
318	28018.82	-19.61	29491.02	-9.92	662	34676.31	-43.23
319	28032.72	-6.38	29534.53	-8.93	663	34683.97	-38.52
320	28060.44	-4.35	29554.61	-11.65	664	34686.93	-19.80
321	28116.07	-9.68	29559.55	-7.82	665	34724.88	-57.01
322	28135.87	-26.58	29576.39	-22.24	666	34725.40	-48.02
323	28151.10	-22.27	29594.31	-9.25	667	34745.89	-61.41
324	28183.23	-5.92	29613.55	-3.31	668	34751.47	-35.24
325	28215.03	-15.87	29637.76	-19.21	669	34756.90	-30.34
326	28244.53	-10.42	29682.82	-35.26	670	34779.38	-35.36
327	28302.32	-11.36	29710.09	-19.18	671	34781.39	-36.21
328	28304.28	-3.44	29731.79	-16.61	672	34791.13	-40.90
329	28331.54	-17.67	29745.93	-19.45	673	34795.77	-33.73
330	28360.38	-11.21	29770.55	-26.58	674	34811.82	-42.72
331	28381.99	-8.30	29800.19	-13.99	675	34827.26	-36.99
332	28388.04	6.07	29816.28	-22.75	676	34835.25	-40.58
333	28409.88	6.37	29852.41	-12.04	677	34852.91	-41.69
334	28430.50	-5.38	29876.10	-30.40	678	34861.05	-37.79
335	28438.21	-10.03	29910.99	-34.74	679	34868.29	-43.70
336	28469.91	-22.64	29931.75	-39.65	680	34879.32	-43.58
337	28488.57	-0.93	29935.70	-30.07	681	34884.54	-33.08
338	28498.64	-6.09	29965.09	-14.14	682	34887.10	-29.92
339	28508.39	-15.57	30010.82	-38.82	683	34895.86	-30.97
340	28553.11	-2.09	30037.02	-35.35	684	34899.41	-17.06
341	28605.88	-8.29	30058.32	-26.64	685	34909.44	-19.61
342	28627.42	-15.04	30062.31	-23.77	686	34913.05	-16.00
343	28659.43	-27.77	30098.04	-50.98	687	34921.76	-22.72
344	28684.58	-10.34	30101.32	-20.89	688	34938.67	-27.71

^a Calculations were performed with $m(\text{H}) = 1.007825 \text{ u}$, the PES was taken from [J. J. Munro, J. Ramanlal, J. Tennyson, and H. Y. Mussa, *Mol. Phys.*, 2006, **104**, 115].

^b The ZPVE is 4361.60 cm^{-1} .

Table S2. Even and odd-parity vibrational band origins of H_3^+ calculated in Jacobi coordinates employing PO(relaxed) exact Bessel-DVR with basis set size (120 120 51) and $R_j^{\text{max}} = 22.00$ bohr ($j = 1$ or 2). Band origins are all given in cm^{-1} .^a

	even	odd		even	odd		even	odd		even	odd
1	0.00 ^b	2520.86	173	23207.23	24801.78	345	28686.24	30089.69	517	32339.73	33656.57
2	2520.86	4996.96	174	23245.50	24906.69	346	28705.58	30095.89	518	32344.43	33658.12
3	3178.78	5554.11	175	23307.47	24908.00	347	28706.71	30155.33	519	32381.45	33686.88
4	4777.05	7004.17	176	23369.07	24964.85	348	28722.87	30193.02	520	32396.95	33711.97
5	4996.96	7491.57	177	23396.32	24980.85	349	28723.68	30212.48	521	32406.07	33738.19
6	5554.11	7869.47	178	23398.09	25053.10	350	28808.20	30251.04	522	32410.77	33766.27
7	6263.05	8488.21	179	23485.45	25086.78	351	28838.51	30254.35	523	32454.06	33774.06
8	7004.17	9110.42	180	23515.05	25137.74	352	28877.26	30263.91	524	32461.50	33791.65
9	7283.73	9651.78	181	23538.56	25148.45	353	28899.64	30323.98	525	32476.19	33808.51
10	7768.70	9995.99	182	23579.86	25152.51	354	28933.11	30355.02	526	32493.56	33817.62
11	7869.47	10209.06	183	23610.31	25222.61	355	28956.46	30367.78	527	32520.58	33831.20
12	8488.21	10644.61	184	23652.62	25302.39	356	28975.90	30400.58	528	32528.15	33853.79
13	8999.02	10859.19	185	23727.78	25350.11	357	28986.87	30429.60	529	32534.62	33865.28
14	9110.42	11323.37	186	23811.95	25370.62	358	28995.48	30442.82	530	32539.70	33889.47
15	9253.14	11526.43	187	23891.67	25414.30	359	29022.81	30466.43	531	32580.77	33913.04
16	9651.78	11655.65	188	23904.99	25428.94	360	29063.98	30488.33	532	32586.02	33913.29
17	9967.25	12076.83	189	23924.19	25451.49	361	29080.38	30506.90	533	32615.74	33930.44
18	9995.99	12299.19	190	23949.82	25506.75	362	29116.71	30565.92	534	32622.53	33954.42
19	10592.76	12472.39	191	23974.42	25595.63	363	29158.70	30576.03	535	32634.23	33960.73
20	10644.61	12695.80	192	24009.75	25602.80	364	29186.86	30605.38	536	32661.88	34015.53
21	10859.18	12830.71	193	24037.88	25679.35	365	29198.23	30618.72	537	32665.07	34029.14
22	10919.82	13316.83	194	24051.33	25706.65	366	29220.11	30635.84	538	32686.47	34038.03
23	11323.37	13389.39	195	24075.07	25741.75	367	29241.08	30659.71	539	32689.89	34041.81
24	11655.65	13585.91	196	24157.59	25822.47	368	29255.64	30663.42	540	32710.97	34057.88
25	11812.54	13690.42	197	24166.20	25860.54	369	29275.36	30675.69	541	32722.70	34065.50
26	12076.84	13753.08	198	24221.68	25903.31	370	29315.21	30732.33	542	32727.43	34077.42
27	12147.87	14054.88	199	24312.74	25918.29	371	29349.58	30740.83	543	32737.50	34078.63
28	12299.18	14215.36	200	24325.89	25924.70	372	29356.56	30748.91	544	32764.60	34081.28
29	12374.32	14471.98	201	24368.28	25956.73	373	29376.47	30757.34	545	32777.24	34102.93
30	12472.38	14563.87	202	24371.90	25976.26	374	29427.28	30793.42	546	32794.63	34120.69
31	12588.41	14878.10	203	24382.36	26003.76	375	29449.52	30813.22	547	32804.51	34128.64
32	12695.80	14888.95	204	24421.57	26027.20	376	29481.42	30852.95	548	32832.37	34156.66
33	13287.34	15114.05	205	24486.47	26089.57	377	29501.46	30864.34	549	32838.56	34176.52
34	13316.82	15185.53	206	24546.53	26107.21	378	29525.58	30917.13	550	32856.45	34189.54
35	13389.39	15210.76	207	24579.23	26126.44	379	29534.53	30924.00	551	32859.10	34201.04
36	13397.03	15328.54	208	24590.05	26151.46	380	29542.90	30968.59	552	32875.78	34227.33
37	13585.92	15371.68	209	24688.54	26206.85	381	29551.63	30982.45	553	32915.00	34239.47
38	13690.41	15769.89	210	24700.19	26264.20	382	29584.58	31017.41	554	32915.99	34274.22
39	13715.89	15886.15	211	24736.84	26295.74	383	29585.47	31020.28	555	32960.81	34294.26
40	14054.88	15962.74	212	24759.08	26301.91	384	29616.71	31024.44	556	32961.75	34300.42
41	14189.41	16007.45	213	24801.84	26334.52	385	29618.60	31056.05	557	32977.49	34321.11

42	14215.35	16246.02	214	24840.61	26378.41	386	29647.48	31082.13	558	33005.11	34326.06
43	14471.99	16450.00	215	24872.85	26440.96	387	29690.68	31112.76	559	33022.04	34356.27
44	14664.20	16556.75	216	24907.99	26461.40	388	29693.93	31147.22	560	33045.69	34376.54
45	14878.09	16588.73	217	24965.03	26476.66	389	29714.85	31150.53	561	33048.49	34382.86
46	14888.35	16672.49	218	24980.71	26495.02	390	29785.94	31195.71	562	33077.90	34411.78
47	14888.96	16718.31	219	24997.36	26580.49	391	29793.58	31207.71	563	33094.13	34424.80
48	14941.21	16860.68	220	25053.08	26583.50	392	29796.51	31219.49	564	33100.39	34441.12
49	15068.52	16910.67	221	25086.87	26645.68	393	29809.17	31220.75	565	33135.85	34472.43
50	15114.05	17081.67	222	25147.25	26680.98	394	29840.42	31223.14	566	33162.39	34472.90
51	15163.82	17213.97	223	25148.61	26728.47	395	29845.66	31261.41	567	33174.47	34479.36
52	15210.78	17381.30	224	25191.07	26745.56	396	29867.55	31282.28	568	33186.32	34486.67
53	15328.57	17446.05	225	25222.52	26762.55	397	29892.38	31299.33	569	33191.56	34513.95
54	15769.90	17606.16	226	25317.41	26802.93	398	29905.41	31311.81	570	33225.63	34529.32
55	15868.51	17686.73	227	25349.99	26853.41	399	29908.10	31331.85	571	33233.80	34536.02
56	15886.14	17698.33	228	25370.04	26869.68	400	29951.48	31340.84	572	33274.99	34536.95
57	15908.70	17809.30	229	25370.54	26870.55	401	29971.78	31384.46	573	33284.28	34559.46
58	16007.45	17850.49	230	25414.43	26959.92	402	30017.72	31414.99	574	33315.23	34595.06
59	16192.43	17856.73	231	25451.62	26980.65	403	30031.44	31443.02	575	33329.14	34597.27
60	16246.03	17967.80	232	25506.63	26982.11	404	30047.00	31454.42	576	33346.80	34606.35
61	16449.98	18194.80	233	25528.30	27028.34	405	30059.65	31467.57	577	33351.83	34632.92
62	16452.98	18328.33	234	25568.04	27038.14	406	30080.02	31484.19	578	33360.35	34645.81
63	16556.78	18353.02	235	25595.45	27104.23	407	30084.72	31519.68	579	33370.32	34667.44
64	16672.49	18435.13	236	25663.53	27107.51	408	30089.80	31542.02	580	33385.37	34677.51
65	16702.87	18575.59	237	25679.50	27141.71	409	30143.13	31574.85	581	33407.71	34693.32
66	16718.30	18707.72	238	25703.31	27163.31	410	30155.23	31583.30	582	33434.93	34710.37
67	16860.68	18795.71	239	25706.68	27188.22	411	30210.85	31621.07	583	33451.11	34716.52
68	16910.69	18865.93	240	25731.60	27284.81	412	30212.29	31633.40	584	33453.43	34726.15
69	17056.78	18924.90	241	25741.60	27291.26	413	30251.23	31655.27	585	33464.82	34743.74
70	17213.97	19043.71	242	25822.50	27338.81	414	30255.26	31664.53	586	33480.61	34750.10
71	17263.56	19082.10	243	25899.21	27399.97	415	30294.68	31669.27	587	33506.59	34763.91
72	17381.30	19178.75	244	25903.33	27405.03	416	30323.64	31714.70	588	33512.00	34790.57
73	17436.08	19213.11	245	25918.56	27434.34	417	30336.26	31720.70	589	33519.95	34794.49
74	17446.02	19272.38	246	25956.71	27470.63	418	30354.90	31728.22	590	33536.08	34808.34
75	17591.90	19274.14	247	26003.74	27511.57	419	30373.63	31749.95	591	33548.63	34811.69
76	17606.17	19300.72	248	26027.35	27572.86	420	30400.77	31775.23	592	33585.63	34823.84
77	17683.24	19427.42	249	26068.51	27579.62	421	30429.05	31790.88	593	33595.77	34834.22
78	17698.31	19495.80	250	26107.21	27632.81	422	30451.39	31797.94	594	33610.23	34835.54
79	17744.37	19710.95	251	26126.24	27667.41	423	30466.64	31857.20	595	33643.10	34857.73
80	17856.70	19740.93	252	26135.70	27669.26	424	30488.44	31865.25	596	33643.44	34864.91
81	17967.84	19837.73	253	26151.46	27694.99	425	30506.41	31913.14	597	33658.38	34881.94
82	18194.79	19870.60	254	26185.51	27724.00	426	30555.54	31916.88	598	33668.62	34896.36
83	18214.27	20048.97	255	26206.88	27754.97	427	30566.25	31930.38	599	33686.83	34898.97
84	18353.01	20073.67	256	26231.40	27758.51	428	30576.26	31952.35	600	33711.84	
85	18364.44	20100.37	257	26264.08	27784.22	429	30604.11	31971.21	601	33717.65	
86	18435.13	20206.64	258	26295.78	27825.89	430	30605.39	31993.63	602	33738.19	
87	18451.71	20243.94	259	26327.94	27826.54	431	30618.55	32045.39	603	33765.67	

88	18575.55	20275.92	260	26375.50	27863.63	432	30659.65	32061.57	604	33790.98
89	18588.84	20371.29	261	26378.40	27868.60	433	30675.29	32073.69	605	33800.00
90	18707.72	20423.97	262	26440.90	27893.39	434	30732.44	32079.17	606	33807.98
91	18795.73	20499.50	263	26461.57	27950.95	435	30741.21	32114.97	607	33831.22
92	18808.56	20599.69	264	26495.16	27999.07	436	30741.82	32135.11	608	33832.68
93	18924.92	20769.05	265	26514.81	28026.09	437	30757.33	32143.42	609	33853.07
94	19043.64	20777.09	266	26530.39	28026.77	438	30792.32	32162.05	610	33860.57
95	19082.13	20796.81	267	26580.51	28089.40	439	30793.51	32181.38	611	33864.74
96	19103.92	20848.11	268	26645.95	28109.27	440	30852.94	32234.95	612	33892.41
97	19213.10	20935.35	269	26655.69	28128.84	441	30857.12	32251.40	613	33913.01
98	19240.30	20986.89	270	26680.98	28137.34	442	30864.40	32280.51	614	33930.64
99	19272.39	21101.14	271	26728.34	28199.04	443	30903.32	32286.16	615	33956.04
100	19300.76	21152.06	272	26762.60	28215.66	444	30917.22	32287.18	616	33960.98
101	19420.19	21179.34	273	26778.29	28234.01	445	30932.06	32323.95	617	33991.77
102	19427.39	21280.98	274	26803.02	28300.86	446	30968.41	32340.08	618	34008.87
103	19495.82	21317.33	275	26826.16	28313.84	447	30982.65	32379.87	619	34015.61
104	19740.91	21334.28	276	26853.26	28373.51	448	31005.11	32381.71	620	34028.32
105	19772.02	21436.51	277	26870.43	28394.10	449	31020.50	32396.86	621	34033.19
106	19791.41	21536.94	278	26955.91	28418.41	450	31024.36	32410.48	622	34042.02
107	19837.75	21587.96	279	26959.95	28425.28	451	31056.46	32412.56	623	34065.50
108	19870.65	21607.49	280	26980.56	28428.16	452	31073.40	32454.40	624	34076.88
109	20048.98	21664.34	281	27030.36	28487.54	453	31113.05	32457.57	625	34078.75
110	20077.88	21675.05	282	27038.20	28492.43	454	31114.83	32476.01	626	34102.73
111	20100.33	21755.88	283	27066.07	28508.75	455	31132.29	32527.39	627	34120.37
112	20177.11	21887.26	284	27104.66	28546.78	456	31147.40	32540.28	628	34126.14
113	20206.57	21889.22	285	27141.49	28551.02	457	31189.11	32560.60	629	34147.51
114	20211.42	21889.69	286	27141.93	28597.60	458	31195.52	32580.70	630	34157.52
115	20244.00	22105.90	287	27163.25	28631.44	459	31207.58	32586.25	631	34158.64
116	20315.50	22164.59	288	27187.93	28644.88	460	31220.35	32616.19	632	34171.30
117	20423.91	22170.08	289	27197.70	28686.94	461	31243.76	32634.47	633	34175.98
118	20499.55	22202.09	290	27210.66	28706.79	462	31259.00	32648.58	634	34201.41
119	20509.18	22306.04	291	27284.82	28723.54	463	31261.17	32665.63	635	34226.74
120	20599.53	22331.52	292	27338.95	28736.56	464	31282.01	32681.13	636	34239.27
121	20615.52	22381.04	293	27380.01	28807.89	465	31299.02	32689.40	637	34262.34
122	20768.92	22424.32	294	27400.86	28821.46	466	31311.93	32711.30	638	34274.16
123	20777.07	22508.20	295	27434.41	28838.65	467	31328.40	32722.63	639	34300.12
124	20837.03	22518.54	296	27461.48	28899.49	468	31340.83	32727.86	640	34313.22
125	20848.13	22551.74	297	27470.31	28907.48	469	31359.05	32737.36	641	34320.59
126	20917.93	22595.06	298	27511.42	28932.99	470	31384.28	32777.12	642	34333.76
127	20986.83	22626.92	299	27562.72	28956.36	471	31415.04	32794.86	643	34356.31
128	21032.96	22716.51	300	27579.45	28987.02	472	31454.75	32804.51	644	34370.55
129	21101.15	22797.31	301	27587.65	29022.96	473	31466.38	32805.52	645	34382.42
130	21152.00	22872.33	302	27632.92	29080.28	474	31484.07	32832.39	646	34411.73
131	21202.14	22918.96	303	27663.00	29116.60	475	31519.62	32856.43	647	34424.88
132	21224.14	22957.19	304	27668.90	29123.09	476	31540.87	32859.10	648	34440.85
133	21280.96	23005.26	305	27695.00	29158.69	477	31541.89	32874.50	649	34457.56

134	21317.32	23023.65	306	27723.87	29193.36	478	31568.14	32916.22	650	34472.72
135	21436.58	23036.91	307	27726.54	29198.49	479	31583.76	32961.28	651	34487.25
136	21463.09	23081.43	308	27758.66	29219.73	480	31588.97	32977.10	652	34508.07
137	21536.83	23164.79	309	27765.56	29255.73	481	31621.12	33005.72	653	34513.97
138	21607.57	23245.59	310	27784.22	29272.64	482	31632.82	33011.68	654	34529.56
139	21626.39	23369.18	311	27797.76	29275.26	483	31655.44	33040.29	655	34530.08
140	21664.32	23398.14	312	27826.83	29312.95	484	31669.23	33045.79	656	34536.11
141	21674.98	23425.68	313	27856.08	29349.59	485	31696.52	33078.00	657	34559.43
142	21740.74	23480.57	314	27867.92	29376.34	486	31714.57	33098.03	658	34578.26
143	21755.73	23485.37	315	27893.51	29428.53	487	31727.60	33099.95	659	34595.29
144	21887.24	23515.05	316	27951.07	29449.67	488	31743.20	33121.87	660	34606.63
145	21889.32	23579.99	317	27982.93	29457.44	489	31775.20	33147.29	661	34617.86
146	21992.09	23652.64	318	27999.21	29481.10	490	31777.20	33162.93	662	34633.07
147	22075.42	23692.46	319	28026.34	29525.60	491	31797.40	33174.09	663	34645.45
148	22105.87	23727.74	320	28056.09	29542.95	492	31821.73	33191.37	664	34667.13
149	22160.63	23811.93	321	28106.39	29551.73	493	31856.84	33200.48	665	34667.87
150	22170.15	23904.98	322	28109.30	29554.15	494	31865.03	33225.97	666	34677.38
151	22202.11	23948.84	323	28128.83	29585.06	495	31875.61	33246.06	667	34684.48
152	22289.70	23949.73	324	28177.31	29610.24	496	31913.00	33274.95	668	34716.23
153	22306.03	23974.82	325	28199.16	29618.55	497	31924.40	33284.72	669	34726.56
154	22381.16	24022.55	326	28234.11	29647.56	498	31951.91	33328.86	670	34744.02
155	22413.02	24037.97	327	28290.96	29690.92	499	31971.04	33351.95	671	34745.18
156	22471.10	24075.05	328	28300.84	29715.18	500	31971.56	33370.37	672	34750.23
157	22508.38	24157.56	329	28313.87	29726.48	501	31993.54	33385.30	673	34762.04
158	22518.38	24161.73	330	28349.17	29743.97	502	32045.26	33422.38	674	34769.10
159	22594.98	24221.68	331	28373.69	29786.20	503	32061.35	33434.95	675	34790.27
160	22618.60	24312.72	332	28394.11	29793.53	504	32069.98	33440.04	676	34794.67
161	22626.89	24368.41	333	28416.25	29840.36	505	32079.19	33450.84	677	34811.22
162	22693.15	24399.48	334	28425.13	29845.70	506	32093.83	33453.33	678	34823.26
163	22716.58	24421.41	335	28428.18	29876.26	507	32115.09	33479.68	679	34824.59
164	22797.19	24457.52	336	28447.27	29892.09	508	32141.74	33492.67	680	34835.74
165	22846.07	24486.30	337	28487.64	29905.63	509	32154.89	33506.43	681	34851.46
166	22918.79	24546.54	338	28492.55	29950.95	510	32181.28	33520.03	682	34857.18
167	23023.68	24579.43	339	28492.82	29972.01	511	32234.83	33548.37	683	34864.89
168	23035.87	24642.38	340	28551.02	30001.67	512	32251.09	33577.63	684	34882.35
169	23036.92	24688.79	341	28597.59	30031.68	513	32259.52	33585.58	685	34889.83
170	23081.46	24717.43	342	28612.37	30038.54	514	32280.96	33590.69	686	34897.06
171	23141.58	24736.94	343	28631.67	30047.06	515	32287.40	33610.13	687	34899.05
172	23164.70	24759.01	344	28674.24	30080.43	516	32298.32	33643.44	688	34910.96

^a Calculations were performed with $m(\text{H}) = 1.007825 u$, the PES was taken from [J. J. Munro, J. Ramanlal, J. Tennyson, and H. Y. Mussa, *Mol. Phys.*, 2006, **104**, 115]. During the PO-DVR 600 primitive Bessel-DVR basis functions were used for both stretching type coordinates.

^b The ZPVE is 4361.60 cm^{-1} .