Accurate prediction of H_3O^+ and D_3O^+ sensitivity coefficients to probe a variable proton-to-electron mass ratio

Supplementary Material

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Table 1: Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{16}O^+$ in the ground vibrational state.

J	K	ν_{calc}/GHz	A/s^{-1}	T	J	K	ν_{calc}/GHz	A/s^{-1}	T
1	1	1655.8577	0.859E-1	-1.940	9	4	1299.1987	0.156E-1	-1.851
2	1	1632.1427	0.275E-1	-1.935	9	5	1361.3791	0.277E-1	-1.867
2	2	1657.2795	0.115E+0	-1.940	9	6	1440.7479	0.465E-1	-1.887
3	1	1597.1617	0.130E-1	-1.927	9	7	1539.6082	0.758E-1	-1.909
3	2	1621.8135	0.540E-1	-1.932	9	8	1660.8177	0.122E+0	-1.933
3	3	1663.6273	0.130E+0	-1.941	9	9	1807.9346	0.194E+0	-1.960
4	1	1551.6036	0.718E-2	-1.917	10	1	1116.0095	0.517E-3	-1.794
4	2	1575.6236	0.299E-1	-1.922	10	2	1133.9754	0.218E-2	-1.800
4	3	1616.3635	0.722E-1	-1.931	10	3	1164.3403	0.528E-2	-1.810
4	4	1674.9135	0.141E+0	-1.942	10	4	1207.1102	0.104E-1	-1.823
5	1	1496.3542	0.433E-2	-1.904	10	5	1265.3697	0.185E-1	-1.840
5	2	1519.6085	0.181E-1	-1.909	10	6	1339.7326	0.311E-1	-1.861
5	3	1559.1102	0.436E-1	-1.918	10	7	1432.3974	0.508E-1	-1.884
5	4	1615.7120	0.854E-1	-1.930	10	8	1546.0712	0.818E-1	-1.909
5	5	1691.1924	0.151E+0	-1.944	10	9	1684.1080	0.131E+0	-1.936
6	1	1432.4704	0.274E-2	-1.888	10	10	1850.6608	0.208E+0	-1.964
6	2	1454.8402	0.114E-1	-1.894	11	1	1028.6003	0.341E-3	-1.762
6	3	1492.7651	0.276E-1	-1.902	11	2	1045.3255	0.144E-2	-1.768
6	4	1547.2271	0.541E-1	-1.914	11	3	1067.9266	0.344E-2	-1.754
6	5	1619.8437	0.958E-1	-1.929	11	4	1112.7743	0.689E-2	-1.791
6	6	1712.5291	0.160E+0	-1.947	11	5	1166.9778	0.123E-1	-1.809
7	1	1361.1517	0.178E-2	-1.869	11	6	1236.1629	0.207E-1	-1.831
7	2	1382.5344	0.745E-2	-1.875	11	7	1322.4210	0.339E-1	-1.855
7	3	1419.9413	0.177E-1	-1.873	11	8	1428.3078	0.547E-1	-1.881
7	4	1470.7199	0.353E-1	-1.896	11	9	1556.9798	0.876E-1	-1.909
7	5	1540.1308	0.625E-1	-1.912	11	10	1712.3208	0.140E+0	-1.939
7	6	1628.7283	0.105E+0	-1.930	11	11	1899.1299	0.224E+0	-1.969
7	7	1739.0173	0.170E+0	-1.951	12	1	940.6819	0.222E-3	-1.725
8	1	1283.7070	0.118E-2	-1.848	12	2	956.1391	0.943E-3	-1.733
8	2	1304.0163	0.492E-2	-1.853	12	3	982.2569	0.231E-2	-1.744
8	3	1338.4028	0.119E-1	-1.863	12	4	1017.6294	0.454E-2	-1.755
8	4	1387.5621	0.234E-1	-1.875	12	5	1067.6920	0.810E-2	-1.774
8	5	1453.4769	0.414E-1	-1.891	12	6	1131.5933	0.137E-1	-1.797
8	6	1537.6131	0.696E-1	-1.910	12	7	1211.3128	0.225E-1	-1.822
8	7	1642.3757	0.113E+0	-1.931	12	8	1309.2553	0.364E-1	-1.850
8	8	1770.7731	0.181E+0	-1.955	12	9	1428.3843	0.585E-1	-1.879
9	1	1201.5193	0.780E-3	-1.822	12	10	1572.3335	0.937E-1	-1.910
9	2	1220.6846	0.327E-2	-1.829	12	11	1745.5500	0.151E+0	-1.942
9	3	1247.2272	0.736E-2	-1.769	12	12	1953.5372	0.243E+0	-1.974

Table 2: Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{18}O^+$ in the ground vibrational state.

J	K	ν_{calc}/GHz	A/s^{-1}	T	J	K	ν_{calc}/GHz	A/s^{-1}	T
1	1	1608.7744	0.788E-1	-1.956	9	4	1249.7781	0.139E-1	-1.863
2	1	1584.8777	0.252E-2	-1.951	9	5	1311.5302	0.248E-1	-1.881
2	2	1610.0266	0.105E+0	-1.956	9	6	1390.4774	0.419E-1	-1.901
3	1	1549.6465	0.119E-1	-1.943	9	7	1488.9820	0.687E-1	-1.924
3	2	1574.2941	0.495E-1	-1.948	9	8	1609.9871	0.111E+0	-1.949
3	3	1616.1228	0.120E+0	-1.957	9	9	1757.1626	0.178E+0	-1.976
4	1	1503.7957	0.655E-2	-1.933	10	1	1067.7086	0.455E-3	-1.804
4	2	1527.7903	0.273E-1	-1.938	10	2	1085.4457	0.191E-2	-1.811
4	3	1568.5089	0.661E-1	-1.946	10	3	1115.4586	0.466E-2	-1.821
4	4	1627.0739	0.130E+0	-1.958	10	4	1157.7924	0.919E-2	-1.834
5	1	1448.2441	0.393E-2	-1.919	10	5	1215.5004	0.164E-1	-1.852
5	2	1471.4472	0.164E-1	-1.925	10	6	1289.2850	0.278E-1	-1.874
5	3	1510.9033	0.397E-1	-1.933	10	7	1381.3957	0.457E-1	-1.897
5	4	1567.4392	0.781E-1	-1.946	10	8	1494.6172	0.740E-1	-1.924
5	5	1642.9342	0.139E+0	-1.961	10	9	1632.4068	0.119E+0	-1.952
6	1	1384.0878	0.248E-2	-1.903	10	10	1799.0512	0.191E+0	-1.981
6	2	1406.3764	0.104E-1	-1.908	11	1	980.8269	0.297E-3	-1.770
6	3	1444.1869	0.250E-1	-1.917	11	2	997.2851	0.125E-2	-1.778
6	4	1498.5317	0.493E-1	-1.930	11	3	1020.2468	0.302E-2	-1.769
6	5	1571.0658	0.875E-1	-1.945	11	4	1063.8066	0.605E-2	-1.801
6	6	1663.7686	0.147E+0	-1.964	11	5	1117.3373	0.108E-1	-1.820
7	1	1312.5691	0.160E-2	-1.883	11	6	1185.7894	0.184E-1	-1.842
7	2	1333.8368	0.670E-2	-1.889	11	7	1271.2962	0.303E-1	-1.867
7	3	1372.3392	0.152E-1	-1.849	11	8	1376.4827	0.491E-1	-1.895
7	4	1421.6592	0.319E-1	-1.911	11	9	1504.5995	0.793E-1	-1.924
7	5	1490.8797	0.568E-1	-1.927	11	10	1659.6530	0.128E+0	-1.954
7	6	1579.3572	0.957E-1	-1.946	11	11	1846.6000	0.206E+0	-1.986
7	7	1689.6703	0.156E+0	-1.967	12	1	893.7115	0.191E-3	-1.732
8	1	1235.0417	0.105E-2	-1.860	12	2	908.8659	0.813E-3	-1.740
8	2	1255.1996	0.440E-2	-1.866	12	3	934.5041	0.200E-2	-1.752
8	3	1289.3581	0.107E-1	-1.876	12	4	969.2948	0.394E-2	-1.763
8	4	1338.2431	0.210E-1	-1.889	12	5	1018.5693	0.707E-2	-1.783
8	5	1403.8511	0.374E-1	-1.906	12	6	1081.5894	0.120E-1	-1.807
8	6	1487.7198	0.631E-1	-1.925	12	7	1160.3673	0.199E-1	-1.833
8	7	1592.3211	0.103E+0	-1.947	12	8	1257.3680	0.323E-1	-1.862
8	8	1720.7555	0.167E+0	-1.971	12	9	1375.6386	0.524E-1	-1.893
9	1	1152.9337	0.692E-3	-1.834	12	10	1518.9249	0.847E-1	-1.925
9	2	1171.9093	0.290E-2	-1.841	12	11	1691.8180	0.137E+0	-1.958
9	3	1200.2604	0.685E-2	-1.819	12	12	1900.0058	0.223E+0	-1.991

Table 3: The rotation-inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{16}O^+$ in the ground vibrational state[a].

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	ν_{exp}/MHz	A/s^{-1}	T^b	T^c
E'	0^-	1	1	E''	0^+	2	1	308483.172	307192.410[d]	0.556E-3	-5.992	-6.017
E'	0^+	3	2	E''	0^-	2	2	362865.643	364797.427[d,e]	0.432E-3	3.227	3.210
E''	0^+	3	1	E'	0^-	2	1	386507.906	388458.641	0.838E-3	2.891	2.876
A_2'	0^+	3	0	A_2''	0^-	2	0	394315.581	396272.412[f]	0.100E-2	2.788	2.775
A_2''	0^-	0	0	A_2'	0^+	1	0	985361.418	984711.888	0.362E-1	-2.575	-2.577
A_2''	0^+	4	3	A_2'	0^-	3	3	1028722.980	1031293.719	0.803E-2	0.492	0.491
E'	0^+	4	2	E''	0^-	3	2	1067224.066	1069826.484	0.155E-1	0.392	0.391
E''	0^+	4	1	E'	0^-	3	1	1089903.366	1092523.071	0.207E-1	0.336	0.335
A_2''	0^+	5	3	A_2'	0^-	4	3	1741874.136	1745127.371	0.589E-1	-0.154	-0.153
E'	0^+	5	2	E''	0^-	4	2	1778525.083	1781805.268	0.829E-1	-0.198	-0.197
E''	0^+	5	1	E'	0^-	4	1	1800111.519	1803407.189	0.986E-1	-0.223	-0.222
A_2'	0^+	5	0	A_2''	0^-	4	0	1807154.483	1810454.545	0.104E+0	-0.231	-0.230
E''	0^+	7	5	E'	0^-	6	5	3073339.801	3077891.800	0.255E+0	-0.521	-0.520
A_2''	0^-	2	0	A_2'	0^+	1	0	2970878.114	2972100[g]	0.399E+0	-1.515	-1.515
E'	0^-	2	1	E''	0^+	1	1	2979517.263	2980725[g]	0.301E+0	-1.518	-1.517
E''	0^-	3	2	E'	0^+	2	2	3641958.615	3643830[h]	0.437E+0	-1.422	-1.421
E'	0^-	3	1	E''	0^+	2	1	3615812.275	3617711[h]	0.687E+0	-1.416	-1.415
A_2'	0^-	4	3	A_2''	0^+	3	3	4308712.151	4311203[h]	0.591E+0	-1.356	-1.355
E''	0^-	4	2	E'	0^+	3	2	4264661.127	4267265[h]	0.990E+0	-1.347	-1.346
E'	0^-	4	1	E''	0^+	3	1	4238668.671	4241306[h]	0.122E+1	-1.341	-1.341
A_2''	0^-	4	0	A_2'	0^+	3	0	4230078.747	4232743[h]	0.130E+1	-1.340	-1.339
E''	0^-	5	4	E'	0^+	4	4	4979729.095	4982921[h]	0.768E+0	-1.309	-1.308

[a] If not stated otherwise, the experimental frequencies have been taken from Ref. [1]. [b] Calculated using theoretical frequencies. [c] Calculated using experimental frequencies. [d] Also observed astronomically in Ref. [2] [e] Also observed astronomically in Ref. [3] [f] Also observed astronomically in Ref. [4] [g] Astronomical observation from Ref. [5]. [h] Astronomical observation from Ref. [6].

Table 4: The rotation-inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{18}O^+$ in the ground vibrational state.

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	A/s^{-1}	T
A_2''	0^-	0	0	A_2'	0^+	1	0	939604	0.314E-1	-2.633
E'	0^-	2	1	E''	0^+	1	1	2929768	0.287E+0	-1.520
A_2''	0^-	2	0	A_2'	0^+	1	0	2921121	0.379E+0	-1.518
E'	0^-	1	1	E''	0^+	2	1	263884	0.349E-3	-6.765
E''	0^-	3	2	E'	0^+	2	2	3590704	0.419E+0	-1.423
E'	0^-	3	1	E''	0^+	2	1	3564536	0.659E+0	-1.416
E'	0^+	3	2	E''	0^-	2	2	406384	0.607E-3	2.728
E''	0^+	3	1	E'	0^-	2	1	430012	0.116E-2	2.452
A_2'	0^+	3	0	A_2''	0^-	2	0	437812	0.137E-2	2.367
A_2'	0^-	4	3	A_2''	0^+	3	3	4255872	0.570E+0	-1.356
E''	0^-	4	2	E'	0^+	3	2	4211784	0.955E+0	-1.347
E'	0^-	4	1	E''	0^+	3	1	4185782	0.118E+1	-1.341
A_2''	0^-	4	0	A_2'	0^+	3	0	4177192	0.125E+1	-1.339
A_2''	0^+	4	3	A_2'	0^-	3	3	1071240	0.908E-2	0.414
E'	0^+	4	2	E''	0^-	3	2	1109700	0.174E-1	0.320
E''	0^+	4	1	E'	0^-	3	1	1132340	0.233E-1	0.268
E''	0^-	5	4	E'	0^+	4	4	4925223	0.744E+0	-1.309
A_2'	0^+	5	0	A_2''	0^+	4	3	4703383	0.813E-3	-1.020
A_2'	0^-	5	3	A_2''	0^+	4	3	4862806	0.128E+1	-1.296
E'	0^+	5	4	E''	0^-	4	4	1730710	0.322E-1	-0.121
E''	0^-	5	2	E'	0^+	4	2	4819190	0.165E+1	-1.288
E'	0^-	5	1	E''	0^+	4	1	4793510	0.187E+1	-1.283
A_2''	0^+	5	3	A_2'	0^-	4	3	1783394	0.633E-1	-0.185
E''	0^+	5	2	E'	0^-	4	2	1819952	0.889E-1	-0.228
E''	0^+	5	1	E'	0^-	4	1	1841471	0.106E+0	-0.252
A_2'	0^+	5	0	A_2''	0^-	4	0	1848471	0.111E+0	-0.260
A_2'	0^-	5	3	A_2''	0^-	4	0	2007895	0.113E-3	-0.990

Table 5: The frequencies (ν), Einstein coefficients (A), and sensitivities (T) of the strongest 'forbidden' rotation-inversion transitions in the ground vibrational state of $H_3{}^{16}O^+$.

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	A/s^{-1}	T
A_2'	0^+	7	0	A_2''	0^+	6	3	6013041	0.532E-1	-1.012
A_2'	0^-	7	3	A_2''	0^-	6	0	3320905	0.115E-1	-0.982
A_2''	0^+	8	3	A_2'	0^+	7	0	3986710	0.132E-1	-0.985
A_2''	0^-	8	0	A_2'	0^-	7	3	6509745	0.713E-1	-0.980
A_2'	0^+	9	0	A_2''	0^+	8	3	7288334	0.473E+0	-1.011
E'	0^-	9	1	E''	0^-	8	4	7989021	0.354E-2	-0.974
A_2'	0^-	9	3	A_2''	0^-	8	0	4609322	0.133E+0	-0.962
E''	0^+	10	1	E'	0^+	9	2	7028329	0.327E-2	-0.991
E''	0^+	10	1	E'	0^+	9	4	8788561	0.292E-2	-0.996
E''	0^-	10	2	E'	0^-	9	5	9456048	0.352E-2	-0.970
E'	0^-	10	1	E''	0^-	9	4	8605372	0.737E-2	-0.971
A_2''	0^-	10	0	A_2'	0^-	9	3	7767436	0.758E+0	-0.983
A_2''	0^+	10	3	A_2'	0^+	9	0	5280810	0.218E+0	-0.969
A_2'	0^-	11	3	A_2''	0^-	10	6	10906889	0.460E-2	-0.964
E''	0^-	11	2	E'	0^-	10	5	10058374	0.717E-2	-0.967
E''	0^+	11	1	E'	0^+	10	4	9392283	0.509E-2	-0.990
A_2'	0^+	11	0	A_2''	0^+	10	3	8521500	0.203E+0	-0.991
E'	0^-	11	1	E''	0^-	10	4	9213773	0.138E-1	-0.967
A_2'	0^-	11	3	A_2''	0^-	10	0	5884393	0.687E-1	-0.970
E'	0^-	12	5	E''	0^-	11	8	13229315	0.464E-2	-0.965
E''	0^-	12	4	E'	0^-	11	7	12356185	0.663E-2	-0.963
A_2'	0^-	12	3	A_2''	0^-	11	6	11498974	0.917E-2	-0.963
E'	0^+	12	2	E''	0^+	11	5	10862715	0.255E-2	-0.986
E''	0^-	12	2	E'	0^-	11	5	10651877	0.132E-1	-0.962
E''	0^+	12	1	E'	0^+	11	4	9985895	0.813E-2	-0.983
E'	0^-	12	1	E''	0^-	11	4	9813803	0.238E-1	-0.963
A_2'	0^-	12	0	A_2''	0^-	11	3	8987776	0.381E+0	-0.967
E'	0^+	12	4	E''	0^+	11	1	5706783	0.502E-2	-0.979
A_2''	0^+	12	3	A_2'	0^+	11	0	6554476	0.142E+0	-0.975

Table 6: Combination differences (CD) of the 'forbidden' ($\Delta|k-l| = 3$) and allowed ($\Delta|k-l| = 0$) transitions between the ν_3 and ground vibrational states in $H_3{}^{16}O^+$ [a].

Allowed	ν_{calc}/cm^{-1}	ν_{exp}/cm^{-1}	A/s^{-1}	Forbidden	ν_{calc}/cm^{-1}	ν_{exp}/cm^{-1}	A/s^{-1}	CD/cm^{-1}
^{r}P(3,0)$^+$	3457.025		0.390E+3	^{o}P(3,3)$^-$	3447.266		0.826E-1	9.7594
^{r}Q(3,0)$^+$	3523.544		0.964E+3	^{o}Q(3,3)$^-$	3513.785		0.189E-1	9.7594
^{r}R(3,0)$^+$	3610.441		0.530E+3	^{o}R(3,3)$^-$	3600.682		0.326E-1	9.7594
^{p}P(3,3)$^-$	3474.787		0.934E+3	^{s}P(3,0)$^+$	3484.546		0.420E-1	9.7594
^{p}Q(3,3)$^-$	3539.922		0.233E+3	^{s}Q(3,0)$^+$	3549.681		0.142E+0	9.7594
^{p}R(3,3)$^-$	3626.725		0.246E+2	^{s}R(3,0)$^+$	3636.484		0.222E+0	9.7594
^{r}R(3,3)$^-$	3564.692		0.730E+3	^{u}R(3,0)$^+$	3574.452		0.104E-1	9.7594
^{r}P(5,0)$^+$	3409.061		0.434E+3	^{o}P(5,3)$^-$	3402.343		0.543E+0	6.7184
^{r}Q(5,0)$^+$	3520.120		0.954E+3	^{o}Q(5,3)$^-$	3513.402		0.206E-1	6.7184
^{r}R(5,0)$^+$	3649.203		0.508E+3	^{o}R(5,3)$^-$	3642.485		0.558E+0	6.7184
^{p}P(5,3)$^-$	3428.386		0.577E+3	^{s}P(5,0)$^+$	3435.104		0.441E+0	6.7184
^{r}P(5,3)$^-$	3366.353		0.222E+2	^{u}P(5,0)$^+$	3373.071		0.110E-1	6.7184
^{p}Q(5,3)$^-$	3536.580		0.375E+3	^{s}Q(5,0)$^+$	3543.298		0.130E+0	6.7184
^{r}Q(5,3)$^-$	3474.807		0.274E+3	^{u}Q(5,0)$^+$	3481.525		0.153E+0	6.7184
^{p}R(5,3)$^-$	3666.517		0.650E+2	^{s}R(5,0)$^+$	3673.236		0.673E+0	6.7184
^{r}R(5,3)$^-$	3604.698		0.540E+3	^{u}R(5,0)$^+$	3611.416		0.356E+0	6.7184
^{r}P(7,0)$^+$	3359.844		0.441E+3	^{o}P(7,3)$^-$	3357.106		0.877E+1	2.7377
^{r}Q(7,0)$^+$	3515.328		0.930E+3	^{o}Q(7,3)$^-$	3512.590		0.965E+1	2.7377
^{r}R(7,0)$^+$	3685.519		0.482E+3	^{o}R(7,3)$^-$	3682.782		0.104E+2	2.7377
^{p}P(7,3)$^-$	3381.138	3385.075	0.442E+3	^{s}P(7,0)$^+$	3383.876	3387.725	0.762E+1	2.7377(2.650)
^{r}P(7,3)$^-$	3319.319	3323.231	0.664E+2	^{u}P(7,0)$^+$	3322.056	3325.884	0.111E+1	2.7377(2.653)
^{p}Q(7,3)$^-$	3531.771	3535.834	0.421E+3	^{s}Q(7,0)$^+$	3534.508	3538.495	0.205E+1	2.7377(2.661)
^{r}Q(7,3)$^-$	3470.509		0.340E+3	^{u}Q(7,0)$^+$	3473.246		0.617E+1	2.7377
^{p}R(7,3)$^-$	3704.670		0.851E+2	^{s}R(7,0)$^+$	3707.407		0.387E+1	2.7377
^{r}R(7,3)$^-$	3642.850		0.445E+3	^{u}R(7,0)$^+$	3645.587		0.903E+1	2.7377
^{r}P(9,0)$^+$	3309.424	3313.435	0.424E+3	^{o}P(9,3)$^-$	3311.889	3315.944	0.311E+2	2.4653(2.509)
^{r}Q(9,0)$^+$	3509.010	3513.136	0.833E+3	^{o}Q(9,3)$^-$	3511.475	3515.651	0.856E+2	2.4653(2.515)
^{r}R(9,0)$^+$	3719.122		0.449E+3	^{o}R(9,3)$^-$	3721.587		0.287E+2	2.4653
^{p}P(9,3)$^-$	3333.778	3337.640	0.350E+3	^{s}P(9,0)$^+$	3331.312	3335.123	0.292E+2	2.4653(2.517)
^{r}P(9,3)$^-$	3271.958	3275.802	0.946E+2	^{u}P(9,0)$^+$	3269.492	3273.280	0.752E+1	2.4653(2.522)
^{p}Q(9,3)$^-$	3525.875	3529.900	0.394E+3	^{s}Q(9,0)$^+$	3523.410	3527.384	0.540E+2	2.4653(2.516)
^{r}Q(9,3)$^-$	3465.261	3469.262	0.340E+3	^{u}Q(9,0)$^+$	3462.796	3466.750	0.241E+2	2.4653(2.512)
^{p}R(9,3)$^-$	3741.744		0.958E+2	^{s}R(9,0)$^+$	3739.278		0.351E+1	2.4653
^{r}R(9,3)$^-$	3679.393		0.375E+3	^{u}R(9,0)$^+$	3676.927		0.222E+2	2.4653
^{r}P(11,0)$^+$	3258.726		0.445E+3	^{o}P(11,3)$^-$	3266.211		0.861E+1	7.4847
^{r}Q(11,0)$^+$	3501.923		0.856E+3	^{o}Q(11,3)$^-$	3509.407		0.340E+2	7.4847
^{r}R(11,0)$^+$	3750.757		0.456E+3	^{o}R(11,3)$^-$	3758.241		0.527E+1	7.4847
^{p}P(11,3)$^-$	3286.368	3290.155	0.317E+3	^{s}P(11,0)$^+$	3278.883	3282.529	0.937E+1	7.4847(7.626)
^{r}P(11,3)$^-$	3224.017	3227.779	0.121E+3	^{u}P(11,0)$^+$	3216.532	3220.154	0.295E+1	7.4847(7.625)
^{p}Q(11,3)$^-$	3518.513		0.433E+3	^{s}Q(11,0)$^+$	3511.028		0.310E+2	7.4847
^{r}Q(11,3)$^-$	3458.662		0.353E+3	^{u}Q(11,0)$^+$	3451.178		0.502E+1	7.4847
^{p}R(11,3)$^-$	3777.943		0.975E+2	^{s}R(11,0)$^+$	3770.459		0.343E+0	7.4847
^{r}R(11,3)$^-$	3714.190		0.261E+3	^{u}R(11,0)$^+$	3706.706		0.738E-1	7.4847

[a] Experimental frequencies from Refs. [7, 8]. Experimental CD data in parentheses. Transitions with $\Delta J = -1, 0, +1$ are described using the labels P, Q, R respectively, whilst the superscript o, p, q, r, s, t, u notation corresponds to transitions with $\Delta K = -2, -1, 0, +1, +2, +3, +4$ respectively. All transitions are between states of A_2' and A_2'' symmetry, where $+(-) \rightarrow +(-)$ are allowed, and $+(-) \rightarrow -(+)$ are forbidden. See also Figure 3.

Table 7: The 'forbidden' combination differences (ν) and sensitivities (T) of the $H_3{}^{16}O^+$ and $H_3{}^{18}O^+$ ground vibrational state transitions[a] .

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	ν_{exp}/MHz	T^b	T^c
								$H_3{}^{16}O^+$			
A_2''	0^+	8	3	A_2''	0^-	8	6	2490592	2499819	-0.492	-0.490
A_2''	0^+	9	3	A_2''	0^-	9	6	2549767	2557200	-0.536	-0.534
E'	0^+	7	4	E'	0^-	7	7	3257694	3261952	-0.566	-0.565
E'	0^+	8	4	E'	0^-	8	7	3311613	3316064	-0.597	-0.596
E'	0^+	8	4	E'	0^-	8	7	3311613	3316124	-0.597	-0.596
E''	0^+	7	7	E''	0^-	5	4	2096835	2100526	-0.196	-0.196
E''	0^-	7	4	E''	0^+	7	7	6467432	6471380	-1.241	-1.240
E''	0^-	7	4	E''	0^+	7	7	6467432	6473688	-1.241	-1.239
E''	0^-	8	4	E''	0^+	8	7	6341551	6347955	-1.222	-1.221
A_1'	0^-	3	3	A_2'	0^+	3	0	292579		-6.094	
A_2'	0^-	5	3	A_2'	0^+	5	0	201415		-7.803	
A_2'	0^-	7	3	A_2'	0^+	7	0	82072	79535	-15.416	-15.907
A_2'	0^-	7	3	A_2'	0^+	7	0	82072	79445	-15.416	-15.925
A_2'	0^-	7	3	A_2'	0^+	7	0	82072	79775	-15.416	-15.859
A_2'	0^-	9	3	A_2'	0^+	9	0	73906	75308	10.518	10.322
A_2'	0^-	9	3	A_2'	0^+	9	0	73906	75608	10.518	10.281
A_2'	0^-	9	3	A_2'	0^+	9	0	73906	75458	10.518	10.302
A_2'	0^-	9	3	A_2'	0^+	9	0	73906	75428	10.518	10.306
A_2'	0^-	9	3	A_2'	0^+	9	0	73906	75218	10.518	10.344
A_2'	0^-	9	3	A_2'	0^+	9	0	73906	75398	10.518	10.310
A_2'	0^-	11	3	A_2'	0^+	11	0	224387	228592	2.508	2.462
A_2'	0^-	11	3	A_2'	0^+	11	0	224387	228622	2.508	2.461
								$H_3{}^{18}O^+$			
A_2'	0^-	3	3	A_2'	0^+	3	0	251040		-6.858	
A_2'	0^-	5	3	A_2'	0^+	5	0	159424		-9.453	
A_2'	0^-	7	3	A_2'	0^+	7	0	42250		-26.035	
A_2'	0^-	9	3	A_2'	0^+	9	0	111874		7.280	
A_1'	0^-	11	3	A_2'	0^+	11	0	263960		1.933	

[a] Experimental frequencies from Refs. [7, 8]. [b] Calculated using theoretical frequencies. [c] Calculated using experimental frequencies.

Table 8: Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $D_3{}^{16}O^+$ in the ground vibrational state.

J	K	ν_{calc}/MHz	A/s^{-1}	T	J	K	ν_{calc}/MHz	A/s^{-1}	T
1	1	461457.7	0.202E-2	-2.594	9	3	396223.5	0.262E-3	-2.532
2	1	457746.8	0.659E-3	-2.591	9	-3	396307.6	0.262E-3	-2.533
2	2	462036.6	0.271E-2	-2.595	9	4	404995.9	0.495E-3	-2.541
3	1	452238.3	0.318E-3	-2.586	9	5	416478.0	0.837E-3	-2.552
3	2	456477.0	0.131E-2	-2.590	9	6	430926.5	0.133E-2	-2.565
3	3	463624.8	0.307E-2	-2.596	9	7	448609.6	0.202E-2	-2.580
3	-3	463624.9	0.307E-2	-2.596	9	8	469861.2	0.301E-2	-2.597
4	1	445000.1	0.182E-3	-2.580	9	9	495091.4	0.441E-2	-2.617
4	2	449171.5	0.749E-3	-2.583	10	1	371355.7	0.197E-4	-2.506
4	3	456206.1	0.176E-2	-2.589	10	2	374847.8	0.811E-4	-2.510
4	-3	456205.3	0.176E-2	-2.589	10	3	380737.2	0.191E-3	-2.516
4	4	466229.2	0.333E-2	-2.597	10	-3	380588.7	0.191E-3	-2.515
5	1	436120.3	0.115E-3	-2.572	10	4	389060.1	0.361E-3	-2.525
5	2	440209.4	0.471E-3	-2.575	10	5	400099.1	0.610E-3	-2.536
5	3	447102.0	0.111E-2	-2.581	10	6	413989.0	0.968E-3	-2.549
5	-3	447105.0	0.111E-2	-2.581	10	7	430988.1	0.148E-2	-2.564
5	4	456929.3	0.209E-2	-2.590	10	8	451417.0	0.220E-2	-2.582
5	5	469861.8	0.354E-2	-2.600	10	9	475669.3	0.322E-2	-2.601
6	1	425705.7	0.765E-4	-2.562	10	10	504223.5	0.469E-2	-2.622
6	2	429698.4	0.314E-3	-2.565	11	1	355354.7	0.145E-4	-2.488
6	3	436431.4	0.739E-3	-2.572	11	2	358700.1	0.595E-4	-2.492
6	-3	436422.5	0.739E-3	-2.571	11	3	364095.1	0.140E-3	-2.497
6	4	446021.4	0.140E-2	-2.580	11	-3	364342.1	0.140E-3	-2.498
6	5	458648.4	0.236E-2	-2.590	11	4	372266.1	0.265E-3	-2.507
6	6	474539.6	0.374E-2	-2.603	11	5	382838.8	0.448E-3	-2.518
7	1	413879.5	0.529E-4	-2.550	11	6	396141.0	0.711E-3	-2.531
7	2	417762.9	0.217E-3	-2.554	11	7	412420.4	0.108E-2	-2.547
7	3	424290.4	0.511E-3	-2.560	11	8	431984.1	0.161E-2	-2.564
7	-3	424311.5	0.511E-3	-2.560	11	9	455208.5	0.237E-2	-2.584
7	4	433633.4	0.966E-3	-2.568	11	10	482551.0	0.345E-2	-2.605
7	5	445914.1	0.163E-2	-2.579	11	11	514564.3	0.500E-2	-2.629
7	6	461368.9	0.259E-2	-2.592	12	1	338716.8	0.106E-4	-2.468
7	7	480284.7	0.395E-2	-2.607	12	2	341909.8	0.438E-4	-2.472
8	1	400778.6	0.375E-4	-2.537	12	3	347292.8	0.103E-3	-2.479
8	2	404541.2	0.154E-3	-2.541	12	-3	346901.5	0.103E-3	-2.477
8	3	410886.1	0.363E-3	-2.547	12	4	354781.7	0.195E-3	-2.487
8	-3	410841.9	0.363E-3	-2.547	12	5	364869.9	0.330E-3	-2.498
8	4	419907.3	0.686E-3	-2.556	12	6	377561.1	0.524E-3	-2.512
8	5	431804.8	0.116E-2	-2.566	12	7	393092.4	0.800E-3	-2.527
8	6	446776.9	0.184E-2	-2.579	12	8	411756.9	0.119E-2	-2.545
8	7	465101.3	0.280E-2	-2.594	12	9	433913.7	0.175E-2	-2.565
8	8	487124.4	0.417E-2	-2.612	12	10	459998.3	0.255E-2	-2.587
9	1	386551.6	0.271E-4	-2.523	12	11	490536.8	0.369E-2	-2.610
9	2	390183.3	0.111E-3	-2.526	12	12	526162.6	0.535E-2	-2.635

Table 9: The frequencies (ν), Einstein coefficients (A), and sensitivities (T) of the rotation-inversion transitions in the ground vibrational state of $D_3{}^{16}O^+$.

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	A/s^{-1}	T
A_1''	0^-	1	0	A_1'	0^+	0	0	799894^a	0.703E-2	-1.919
A_2''	0^-	0	0	A_2'	0^+	1	0	122016	0.748E-4	-7.018
E'	0^-	2	1	E''	0^+	1	1	1137348	0.182E-1	-1.644
A_2''	0^-	2	0	A_2'	0^+	1	0	1135859	0.242E-1	-1.643
E''	0^+	2	1	E'	0^-	1	1	218144	0.128E-3	2.352
A_1'	0^+	2	0	A_1''	0^-	1	0	219509	0.174E-3	2.319
E''	0^-	3	2	E'	0^+	2	2	1475670	0.315E-1	-1.496
E'	0^-	3	1	E''	0^+	2	1	1471128	0.501E-1	-1.492
A_1''	0^-	3	0	A_1'	0^+	2	0	1469623	0.562E-1	-1.490
E'	0^+	3	2	E''	0^-	2	2	557156	0.170E-2	0.311
E''	0^+	3	1	E'	0^-	2	1	561143	0.278E-2	0.287
A_2'	0^+	3	0	A_2''	0^-	2	0	562464	0.315E-2	0.279
A_1'	0^-	4	-3	A_1''	0^+	3	-3	1814847	0.479E-1	-1.404
A_2'	0^-	4	3	A_2''	0^+	3	3	1814848	0.479E-1	-1.404
E''	0^-	4	2	E'	0^+	3	2	1807141	0.813E-1	-1.398
A_2''	0^+	4	3	A_2'	0^-	3	3	895017	0.574E-2	-0.183
A_1''	0^+	4	-3	A_1'	0^-	3	-3	895017	0.574E-2	-0.183
E'	0^-	4	1	E''	0^+	3	1	1802568	0.101E+0	-1.394
A_2''	0^-	4	0	A_2'	0^+	3	0	1801051	0.108E+0	-1.393
E'	0^+	4	2	E''	0^-	3	2	901493	0.101E-1	-0.203
E''	0^+	4	1	E'	0^-	3	1	905329	0.128E-1	-0.215
A_1'	0^+	4	0	A_1''	0^-	3	0	906601	0.137E-1	-0.219
E''	0^-	5	4	E'	0^+	4	4	2154875	0.675E-1	-1.342
E'	0^+	5	4	E''	0^-	4	4	1231716	0.126E-1	-0.403
A_2'	0^-	5	3	A_2''	0^+	4	3	2143872	0.119E+0	-1.334
A_1'	0^-	5	-3	A_1''	0^+	4	-3	2143874	0.119E+0	-1.334
E''	0^-	5	2	E'	0^+	4	2	2136144	0.154E+0	-1.328
A_2''	0^+	5	3	A_2'	0^-	4	3	1240564	0.230E-1	-0.423
A_1''	0^+	5	-3	A_1'	0^-	4	-3	1240564	0.230E-1	-0.423
E'	0^-	5	1	E''	0^+	4	1	2131556	0.176E+0	-1.325
A_1''	0^-	5	0	A_1'	0^+	4	0	2130034	0.183E+0	-1.324
E'	0^+	5	2	E''	0^-	4	2	1246763	0.307E-1	-0.436
E''	0^+	5	1	E'	0^-	4	1	1250435	0.354E-1	-0.443
A_2'	0^+	5	0	A_2''	0^-	4	0	1251654	0.370E-1	-0.446

[a] Experimental value of 798713.814 MHz measured in Ref. [9]. Note that states with $K = +3$ are of A_2 symmetry, whilst those with $K = -3$ are of A_1 symmetry.

Table 10: The frequencies (ν), Einstein coefficients (A), and sensitivities (T) of the strongest 'forbidden' rotation-inversion transitions in the ground vibrational state of $D_3{}^{16}O^+$.

Γ'	p'	J'	K'	Γ''	p''	J''	K''	$\nu_{\rm calc}$/MHz	A/s^{-1}	T
A_1''	0^-	9	0	A_1'	0^-	8	-3	3688528	0.170E-3	-0.989
A_1'	0^+	10	0	A_1''	0^+	9	-3	4042517	0.147E-3	-1.000
A_2''	0^-	10	0	A_2'	0^-	9	3	4016397	0.375E-3	-0.987
E'	0^-	11	1	E''	0^-	10	4	4785669	0.151E-3	-0.985
A_2'	0^+	11	0	A_2''	0^+	10	3	4368847	0.288E-3	-0.997
A_1''	0^-	11	0	A_1'	0^-	10	-3	4342344	0.754E-3	-0.985
A_1''	0^+	11	-3	A_1'	0^+	10	0	3024066	0.275E-3	-0.991
E''	0^-	12	2	E'	0^-	11	5	5551457	0.191E-3	-0.983
E'	0^-	12	1	E''	0^-	11	4	5107776	0.289E-3	-0.983
A_1'	0^+	12	0	A_1''	0^+	11	-3	4692929	0.520E-3	-0.994
A_2''	0^-	12	0	A_2'	0^-	11	3	4666233	0.140E-2	-0.983
A_2''	0^+	12	3	A_2'	0^+	11	0	3354397	0.556E-3	-0.989
A_1'	0^-	12	-3	A_1''	0^-	11	0	3347266	0.160E-3	-0.985

Note that states with $K = +3$ are of A_2 symmetry, whilst those with $K = -3$ are of A_1 symmetry.

Table 11: The 'forbidden' combination differences (ν) and sensitivities (T) of the $D_3{}^{16}O^+$ ground vibrational state transitions[a] .

Γ'	p'	J'	K'	Γ''	p''	J''	K''	$\nu_{\rm calc}$/MHz	$\nu_{\rm exp}$/MHz	T^b	T^c
A_2'	0+	8	6	A_2'	0+	7	6	2711462	2714369	-1.004	-1.003
A_2'	0+	7	6	A_2'	0+	6	6	2376103	2378622	-1.006	-1.005
E'	0+	6	4	E'	0+	5	4	2035287	2037351	-1.005	-1.004
A_2''	0+	4	3	A_2''	0+	3	3	1358641	1360071	-1.006	-1.005
A_1''	0+	4	-3	A_1''	0+	3	-3	1358642	1360071	-1.006	-1.005
E'	0+	3	2	E'	0+	2	2	1019193	1020224	-1.006	-1.005
E'	0+	5	2	E'	0+	4	2	1695934	1697704	-1.005	-1.004

[a] Experimental frequencies from Ref. [10]. [b] Calculated using theoretical frequencies. [c] Calculated using experimental frequencies.

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