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

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ABSTRACT

The mass sensitivity of the vibration–rotation–inversion transitions of $H_3{}^{16}O^+$, $H_3{}^{18}O^+$, and $D_3{}^{16}O^+$ is investigated variationally using the nuclear motion program TROVE (Yurchenko, Thiel & Jensen). The calculations utilize new high-level ab initio potential energy and dipole moment surfaces. Along with the mass dependence, frequency data and Einstein A coefficients are computed for all transitions probed. Particular attention is paid to the $\Delta|k| = 3$ and $\Delta|k - l| = 3$ transitions comprising the accidentally coinciding $|J, K = 0, v_2 = 0^+\rangle$ and $|J, K = 3, v_2 = 0^-\rangle$ rotation–inversion energy levels. The newly computed probes exhibit sensitivities comparable to their ammonia and methanol counterparts, thus demonstrating their potential for testing the cosmological stability of the proton-to-electron mass ratio. The theoretical TROVE results are in close agreement with sensitivities obtained using the non-rigid and rigid inverter approximate models, confirming that the ab initio theory used in the present study is adequate.

Key words: molecular data – cosmological parameters – infrared: ISM – submillimetre: ISM.

1 INTRODUCTION

The hydronium cation (H_3O^+) is one of the key molecular ions for inferring properties of the interstellar medium, particularly for constraining the cosmic ray ionization rate of atomic and molecular hydrogen (see Indriolo et al. 2015 and references therein). Knowledge of such parameters is of astrophysical importance, and as a result, H_3O^+ is one of the most searched for galactic and extragalactic interstellar molecules (Hollis et al. 1986; Wootten et al. 1986, 1991; Phillips, van Dishoeck & Keene 1992; Boreiko & Betz 1993; Goicoechea & Cernicharo 2001; van der Tak et al. 2006; van der Tak, Aalto & Meijerink 2008; Gerin et al. 2010; Gupta et al. 2010; Aalto et al. 2011; González-Alfonso et al. 2013; Lis et al. 2014). Since H_3O^+ formation requires presence of H_2O, and the chemical relation between H_3O^+ and H_2O is well understood, H_3O^+ can serve as an excellent proxy for H_2O, which is often hard to observe directly (Timmermann et al. 1996).

Similar to the ammonia molecule, H_3O^+ has several far-infrared and submillimetre transitions that are particularly sensitive to the proton-to-electron mass ratio μ (Kozlov & Levshakov 2011; Kozlov, Porsev & Reimers 2011). The most robust constraint on a variable μ has recently been determined using methanol absorption spectra observed in the lensing galaxy PKS1830−211 (Kanekar et al. 2015). The three measured lines possessed sensitivities differing by $\Delta T = 6.4$, where T is the sensitivity coefficient of a transition. In principle then, hydronium is capable of being used exclusively to constrain a possible variation in the proton-to-electron mass ratio, thus avoiding certain systematic errors which arise when using transitions from different molecular species (Flambaum & Kozlov 2007; Murphy et al. 2008; Henkel et al. 2009; Kanekar 2011).

A small number of pure inversion and rotation–inversion transitions in the ground vibrational state of H_3O^+ were originally investigated by Kozlov & Levshakov (2011). However the calculated sensitivity coefficients were overestimated and new values have been computed for H_3O^+, along with the isotopologues H_2DO^+, HD_2O^+, and D_3O^+ (Kozlov et al. 2011). Given the astronomical relevance of H_3O^+, and a good representative set of accurately measured experimental data (Uy, White & Oka 1997; Araki, Ozeki & Saito 1999; Tang & Oka 1999; Furuya & Saito 2005; Yu et al. 2009; Yu & Pearson 2014), we find it worthwhile to carry out a comprehensive study of hydronium, $H_3{}^{16}O^+$ (also referred to as H_3O^+),

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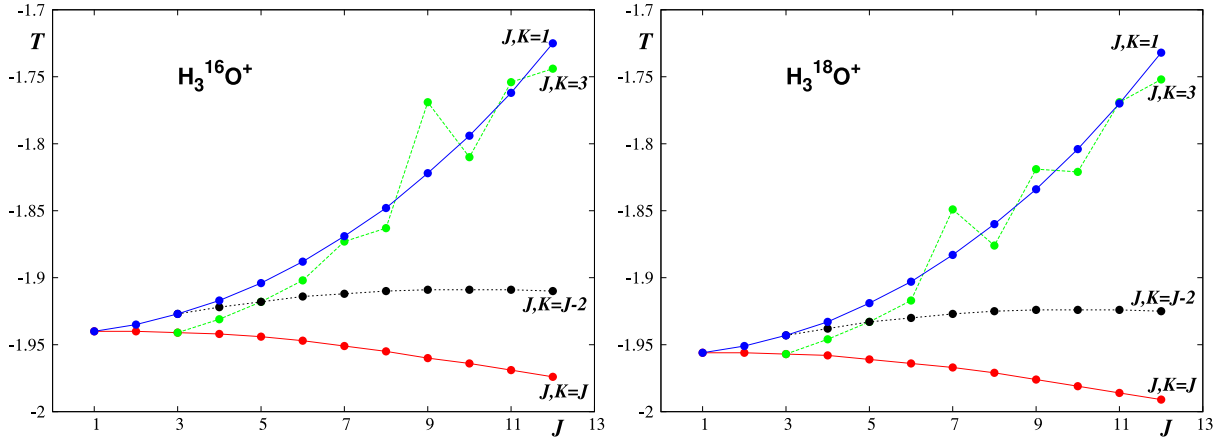
Figure 1. Rotational dependence of the sensitivities (T) of the inversion transitions in the ground vibrational states of $H_3^{16}O^+$ and $H_3^{18}O^+$.
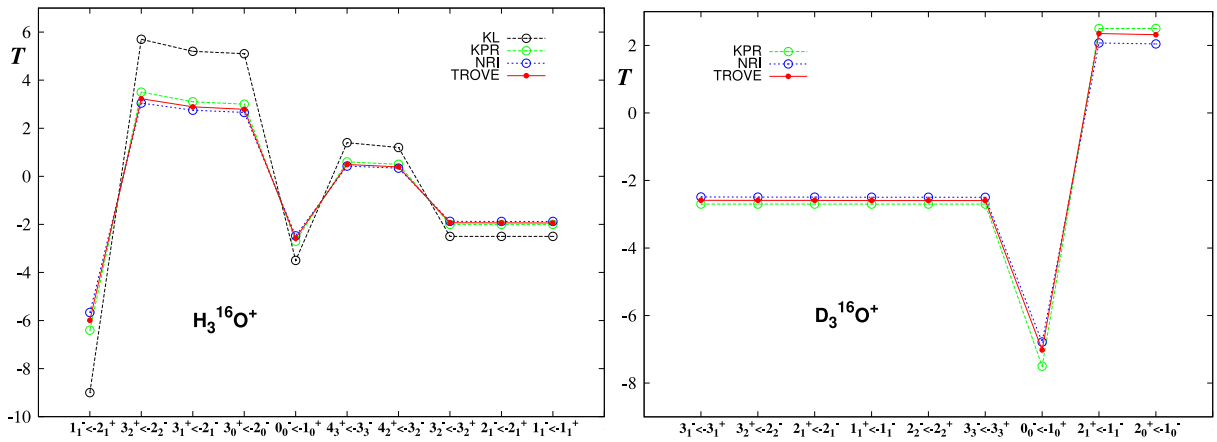
Figure 2. State dependence of the calculated sensitivities (T) of the rotation–inversion transitions in the ground vibrational states of $H_3^{16}O^+$ and $D_3^{16}O^+$. KL: calculated in Kozlov & Levshakov (2011); KPR: calculated in Kozlov et al. (2011); NRI: calculated using the NRI theory (this study); TROVE: calculated variationally (this study). States are labelled as $J_K^\pm$ on the x-axis.

and its two symmetric top isotopologues, $H_3^{18}O^+$ and $D_3^{16}O^+$. To do this we employ a highly accurate variational approach, which was recently applied to ammonia (Owens et al. 2015). Like NH_3 (Jansen, Bethlem & Ubachs 2014; Špirko 2014; Owens et al. 2015), there is a possibility to find transitions with strongly anomalous sensitivities caused by the $\Delta k = \pm 3$ interactions (see Papoušek et al. 1986), which have not yet been considered.

2 VARIATIONAL APPROACH

To calculate sensitivity coefficients we follow the same approach that was employed for ammonia (Owens et al. 2015). The key assumption is that all baryonic matter may be treated equally (Dent 2007), and so μ is assumed to be proportional to the molecular mass. One can then use suitably scaled values for the mass of hydronium and perform a series of calculations, from which numerical values of the required derivatives, $dE/d\mu$, can be obtained. The sensitivity coefficient $T_{u,1}$ is defined as

$$T_{u,1} = \frac{\mu}{E_u - E_l}\left(\frac{dE_u}{d\mu} - \frac{dE_l}{d\mu}\right), \tag{1}$$

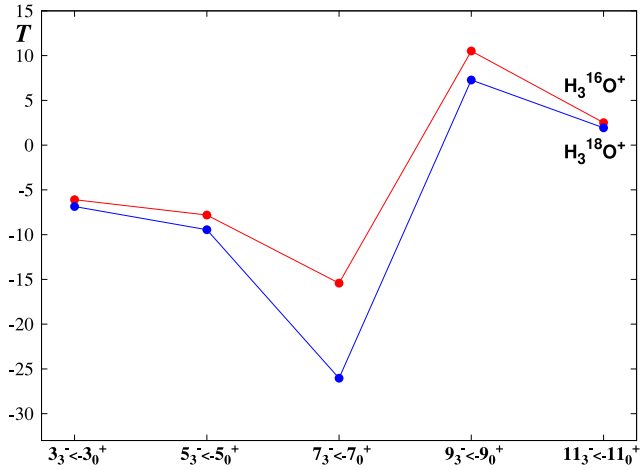where E_u and E_l refer to the energy of the upper and lower state, respectively. The resulting sensitivities can then be used to determine the induced frequency shift of a probed transition, given by
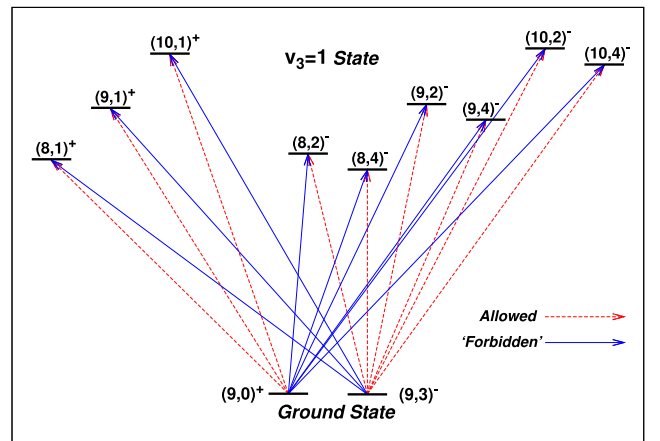
Figure 3. The $|J = 9, K = 0, v_2 = 0^+\rangle - |J = 9, K = 3, v_2 = 0^-\rangle$ combination differences of the ν_3 band of H_3O^+.

the expression

$$\frac{\Delta\nu}{\nu_0} = T_{u,1}\frac{\Delta\mu}{\mu_0}, \tag{2}$$

Figure 4. The sensitivities (T) of the most sensitive $|J, K = 0, v_2 = 0^+\rangle - |J, K = 3, v_2 = 0^-\rangle$ ($J = 3, 5, 7, 9, 11$) combination differences of $H_3^{16}O^+$ and $H_3^{18}O^+$. States are labelled as $J_K^{\pm}$ on the x-axis.

where $\Delta\nu = \nu_{obs} - \nu_0$ is the change in the frequency, and $\Delta\mu = \mu_{obs} - \mu_0$ is the change in μ, both with respect to their present-day values ν_0 and μ_0.

Calculations were carried out using the nuclear motion code TROVE (Yurchenko, Thiel & Jensen 2007). To compute ro-vibrational transitions and corresponding intensities (Yurchenko et al. 2009), TROVE requires as input a potential energy surface (PES) and dipole moment surface (DMS). For the present study, new high-level ab initio PES and DMS have been utilized. A detailed description of these will be reported elsewhere (Polyansky & Ovsyannikov, in preparation). Here we only provide a summary of the ab initio calculations used to generate the respective surfaces.

The PES was computed at the all-electron multireference config-uration interaction (MRCI) level of theory using the core–valence-weighted basis sets, aug-cc-pwCVQZ and aug-cc-pwCV5Z. A two-point formula was applied to extrapolate the electronic energy to the complete basis set limit. Additional complete-active-space and relativistic corrections were also incorporated into the PES. For the

DMS, the MRCI/aug-cc-pwCV5Z level of theory was used, which is known to produce reliable line intensities (Polyansky et al. 2015).

To demonstrate that our variational calculations are robust, we also employ a perturbative non-rigid-inverter (NRI) theory approach (Špirko 1983), which has previously been used to investigate am-monia (Špirko 2014; Owens et al. 2015). The NRI potential energy function for hydronium (Špirko & Kraemer 1989) was upgraded by fitting to a much broader set of experimental data.

3 RESULTS AND DISCUSSION

The results are illustrated in Figs 1–4, with sample tables provided for reference (Tables 1–11). Detailed tables are provided as sup-plementary material. In Fig. 1, the rotational dependence of the sensitivities for the inversion transitions in the ground vibrational state of $H_3^{16}O^+$ and $H_3^{18}O^+$ is shown. The non-smooth behaviour of the (J, $K = 3$) transitions is caused by the $\Delta k = \pm 3$ interac-tions (for details see Belov et al. 1980). For $D_3^{16}O^+$ the sensitivities display a very similar albeit smoother trend.

More encouraging are the low-J rotation–inversion transitions displayed in Fig. 2, of which a large number have been observed experimentally in both laboratory (Furuya & Saito 2005; Yu & Pear-son 2014), and astronomical (Wootten et al. 1991; Phillips et al. 1992; Goicoechea & Cernicharo 2001; van der Tak et al. 2006; González-Alfonso et al. 2013) environments. The appearance of both positive and negative sensitivities is beneficial to constrain a possible variation in the proton-to-electron mass ratio. The effective Hamiltonian model used by Kozlov et al. (2011, KPR in Fig. 2), which does not account for all centrifugal corrections, shows con-sistent agreement with both the NRI theory, and variational (TROVE) results. Thus the strongly anomalous sensitivity coefficients of the $1_{1,1}^- \leftarrow 2_{2,1}^+$, and $1_{1,0}^- \leftarrow 2_{2,0}^+$ transitions of H_2DO^+, and the $1_{0,1}^- \leftarrow 1_{1,1}^+$ transition of HD_2O^+, proposed by Kozlov et al. (2011) have real promise. As discussed previously (Kozlov et al. 2011), the re-sults of Kozlov & Levshakov (2011, KL in Fig. 2) overestimate the $H_3^{16}O^+$ sensitivities and should not be used in future studies.

The $\Delta k = \pm 3$ interactions give rise to several 'forbidden' ro-vibrational combination differences of the ν_3 band (see Fig. 3). The most sensitive of these are presented in Fig. 4. Notably the $7_3^- \leftarrow 7_0^+$

Table 1. Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3^{16}O^+$ in the ground vibrational state. The full table is available online as supplementary material.

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
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Table 2. Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3^{18}O^+$ in the ground vibrational state. The full table is available online as supplementary material.

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
...	...	...	...	...	...	...	...	...	...

Table 3. The rotation–inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3^{16}O^+$ in the ground vibrational state[a]. The full table is available online as supplementary material.

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	308 483.172	307 192.410[d]	0.556E–3	−5.992	−6.017
E'	0^+	3	2	E''	0^-	2	2	362 865.643	364 797.427[d, e]	0.432E–3	3.227	3.210
E''	0^+	3	1	E'	0^-	2	1	386 507.906	388 458.641	0.838E–3	2.891	2.876
A_2'	0^+	3	0	A_2''	0^-	2	0	394 315.581	396 272.412[f]	0.100E–2	2.788	2.775
A_2''	0^-	0	0	A_2'	0^+	1	0	985 361.418	984 711.888	0.362E–1	−2.575	−2.577
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Notes. [a]If not stated otherwise, the experimental frequencies have been taken from Yu & Pearson (2014). [b]Calculated using theoretical frequencies. [c]Calculated using experimental frequencies. [d]Also observed astronomically in van der Tak et al. (2006). [e]Also observed astronomically in Wootten et al. (1991). [f]Also observed astronomically in Phillips et al. (1992). [g]Astronomical observation from Goicoechea & Cernicharo (2001). [h]Astronomical observation from González-Alfonso et al. (2013).

Table 4. The rotation–inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3^{18}O^+$ in the ground vibrational state. The full table is available online as supplementary material.

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	939 604	0.314E–1	−2.633
E'	0^-	2	1	E''	0^+	1	1	2929 768	0.287E+0	−1.520
A_2''	0^-	2	0	A_2'	0^+	1	0	2921 121	0.379E+0	−1.518
E'	0^-	1	1	E''	0^+	2	1	263 884	0.349E–3	−6.765
E''	0^-	3	2	E'	0^+	2	2	3590 704	0.419E+0	−1.423
...	...	...	...	...	...	...	...	...	...	...

Table 5. The frequencies (ν), Einstein coefficients (A), and sensitivities (T) of the strongest 'forbidden' rotation–inversion transitions in the ground vibrational state of $H_3^{16}O^+$. The full table is available online as supplementary material.

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	6013 041	0.532E–1	−1.012
A_2'	0^-	7	3	A_2''	0^-	6	0	3320 905	0.115E–1	−0.982
A_2''	0^+	8	3	A_2'	0^+	7	0	3986 710	0.132E–1	−0.985
A_2''	0^-	8	0	A_2'	0^-	7	3	6509 745	0.713E–1	−0.980
A_2'	0^+	9	0	A_2''	0^+	8	3	7288 334	0.473E+0	−1.011
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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]. The full table is available online as supplementary material.

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}
$^rP(3,0)^+$	3457.025		0.390E+3	$^oP(3,3)^-$	3447.266		0.826E–1	9.7594
$^rQ(3,0)^+$	3523.544		0.964E+3	$^oQ(3,3)^-$	3513.785		0.189E–1	9.7594
$^rR(3,0)^+$	3610.441		0.530E+3	$^oR(3,3)^-$	3600.682		0.326E–1	9.7594
$^pP(3,3)^-$	3474.787		0.934E+3	$^sP(3,0)^+$	3484.546		0.420E–1	9.7594
$^pQ(3,3)^-$	3539.922		0.233E+3	$^sQ(3,0)^+$	3549.681		0.142E+0	9.7594
$^pR(3,3)^-$	3626.725		0.246E+2	$^sR(3,0)^+$	3636.484		0.222E+0	9.7594
$^rR(3,3)^-$	3564.692		0.730E+3	$^uR(3,0)^+$	3574.452		0.104E–1	9.7594
...	...	...	...	...	...	...	...	...

Notes. [a]Experimental frequencies from Tang & Oka (1999) and Uy et al. (1997). 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 Fig. 3.

and $9_3^- \leftarrow 9_0^+$ combination differences, for which a number of the corresponding transitions have been observed experimentally (Uy et al. 1997), have theoretically derived values of $T = -15.416$ and 10.518, respectively. The difference, $\Delta T = 25.934$, is comparable to the most stringent limit on μ obtained using methanol, which utilized transitions with $\Delta T = 31.8$ (Bagdonaite et al. 2013). However, it should be noted that this constraint has recently been deemed unreliable, and subsequently replaced by a more robust value which employed methanol transitions with $\Delta T = 6.4$ (Kanekar et al. 2015). Despite available experimental data (Araki et al. 1999), the $D_3^{16}O^+$

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]. The full table is available online as supplementary material.

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	2490 592	2499 819	-0.492	-0.490
A_2''	0^+	9	3	A_2''	0^-	9	6	2549 767	2557 200	-0.536	-0.534
E'	0^+	7	4	E'	0^-	7	7	3257 694	3261 952	-0.566	-0.565
E'	0^+	8	4	E'	0^-	8	7	3311 613	3316 064	-0.597	-0.596
E'	0^+	8	4	E'	0^-	8	7	3311 613	3316 124	-0.597	-0.596
...	...	...	...	...	...	...	...	...	...	...	...

Notes. [a]Experimental frequencies from Tang & Oka (1999) and Uy et al. (1997). [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. The full table is available online as supplementary material.

J	K	ν_{calc}/MHz	A/s^{-1}	T	J	K	ν_{calc}/MHz	A/s^{-1}	T
1	1	461 457.7	0.202E–2	-2.594	9	3	396 223.5	0.262E–3	-2.532
2	1	457 746.8	0.659E–3	-2.591	9	-3	396 307.6	0.262E–3	-2.533
2	2	462 036.6	0.271E–2	-2.595	9	4	404 995.9	0.495E–3	-2.541
3	1	452 238.3	0.318E–3	-2.586	9	5	416 478.0	0.837E–3	-2.552
3	2	456 477.0	0.131E–2	-2.590	9	6	430 926.5	0.133E–2	-2.565
...	...	...	...	...	...	...	...	...	...

Table 9. The frequencies (ν), Einstein coefficients (A), and sensitivities (T) of the rotation–inversion transitions in the ground vibrational state of $D_3{}^{16}O^+$. The full table is available online as supplementary material.

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	799 894[a]	0.703E–2	-1.919
A_2''	0^-	0	0	A_2'	0^+	1	0	122 016	0.748E–4	-7.018
E'	0^-	2	1	E''	0^+	1	1	1137 348	0.182E–1	-1.644
A_2''	0^-	2	0	A_2'	0^+	1	0	1135 859	0.242E–1	-1.643
E''	0^+	2	1	E'	0^-	1	1	218 144	0.128E–3	2.352
...	...	...	...	...	...	...	...	...	...	...

Notes. [a]Experimental value of 798 713.814 MHz measured in Furuya & Saito (2005). 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 $D_3{}^{16}O^+$. The full table is available online as supplementary material.

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	A/s^{-1}	T
A_1''	0^-	9	0	A_1'	0^-	8	-3	3688 528	0.170E–3	-0.989
A_1'	0^+	10	0	A_1''	0^+	9	-3	4042 517	0.147E–3	-1.000
A_2''	0^-	10	0	A_2'	0^-	9	3	4016 397	0.375E–3	-0.987
E'	0^-	11	1	E''	0^-	10	4	4785 669	0.151E–3	-0.985
A_2'	0^+	11	0	A_2''	0^+	10	3	4368 847	0.288E–3	-0.997
...	...	...	...	...	...	...	...	...	...	...

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

counterparts of these combination differences do not appear to be of any real use, with sensitivities around $T = -1.006$ (see supplementary material for more detail).

4 CONCLUSION

A robust variational study of the vibration–rotation–inversion transitions of $H_3{}^{16}O^+$, $H_3{}^{18}O^+$, and $D_3{}^{16}O^+$ has been carried out. We

hope that by providing theoretical frequency data and Einstein A coefficients, future laboratory and astronomical observations can be tailored to measure transitions which possess sizeable sensitivities. The astrophysical importance of hydronium suggests that this is a realistic prospect. Emphasis should be placed on the 'forbidden' combination differences of the ν_3 band, since several of the corresponding transitions have already been experimentally measured (Uy et al. 1997). The $7_3^- \leftarrow 7_0^+$ and $9_3^- \leftarrow 9_0^+$ combination

Table 11. The 'forbidden' combination differences (ν) and sensitivities (T) of the $D_3{}^{16}O^+$ ground vibrational state transitions[a]. The full table is available online as supplementary material.

Γ'	p'	J'	K'	Γ''	p''	J''	K''	ν_{calc}/MHz	ν_{exp}/MHz	T^b	T^c
A_2'	0+	8	6	A_2'	0+	7	6	2711 462	2714 369	−1.004	−1.003
A_2'	0+	7	6	A_2'	0+	6	6	2376 103	2378 622	−1.006	−1.005
E'	0+	6	4	E'	0+	5	4	2035 287	2037 351	−1.005	−1.004
A_2''	0+	4	3	A_2''	0+	3	3	1358 641	1360 071	−1.006	−1.005
A_1''	0+	4	−3	A_1''	0+	3	−3	1358 642	1360 071	−1.006	−1.005
...	...	...	...	...	...	...	...	...	...	...	...

Notes. [a]Experimental frequencies from Araki et al. (1999). [b]Calculated using theoretical frequencies. [c]Calculated using experimental frequencies.

differences are separated by $\Delta T = 25.934$. This is around four times larger than the ΔT of the methanol transitions recently used to determine the most reliable constraint on a possible variation in the proton-to-electron mass ratio (Kanekar et al. 2015).

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SUPPORTING INFORMATION

Additional Supporting Information may be found in the online version of this paper:

Table 1. Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{16}O^+$ in the ground vibrational state.
Table 2. Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{18}O^+$ in the ground vibrational state.
Table 3. The rotation–inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{16}O^+$ in the ground vibrational state[a].
Table 4. The rotation–inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $H_3{}^{18}O^+$ in the ground vibrational state.
Table 5. The frequencies (ν), Einstein coefficients (A), and sensitivities (T) of the strongest 'forbidden' rotation–inversion transitions in the ground vibrational state of $H_3{}^{16}O^+$.
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].
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].
Table 8. Inversion frequencies (ν), Einstein coefficients (A), and sensitivities (T) of $D_3{}^{16}O^+$ in the ground vibrational state.

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

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

Table 11. The 'forbidden' combination differences (ν) and sensitivities (T) of the $D_3{}^{16}O^+$ ground vibrational state transitions[a]. (http://www.mnras.oxfordjournals.org/lookup/suppl/doi: 10.1093/mnras/stv2023/-/DC1).

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