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Line lists for BH isotopologues

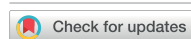
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Abstract

The decision by the International Thermonuclear Experimental Reactor to use boron coated tungsten walls puts an emphasis on the spectroscopy of boron hydride, Boron hydride (BH), whose emissions can be used to monitor wall erosion. An accurate spectroscopic model for all six isotopologues of BH (^{11}BH , ^{10}BH , ^{11}BD , ^{10}BD , ^{11}BT and ^{10}BT) is constructed and used to compute line lists for these species. These line lists, named AX, can be used to simulate both the $\text{A } ^1\Pi\text{—X } ^1\Sigma^+$ system in the 400 nm region and infrared transitions within the $\text{X } ^1\Sigma^+$ ground. A MARVEL (Measured Active Rotation Vibration Energy Levels) study of observed ^{11}BH high resolution spectra produces a list of 204 empirical energy levels which are used to tune potential energy curves used in the model, which results in root-mean-square errors between the calculated and empirical energy levels of 0.037 cm^{-1} for the $\text{A } ^1\Pi$ state and 0.025 cm^{-1} for the $\text{X } ^1\Sigma^+$ state. The revised T_e value between these states is 23151.78 cm^{-1} . The MARVEL energy levels are also used explicitly to improve the energy levels and transition wavenumbers. Comparisons of our calculations with measured lifetimes and observed spectra give excellent agreement for ^{11}BH . Our model is found to be good but less accurate for other isotopologues, but further improvements will require input from laboratory measurements. The line lists are made freely available on the ExoMol website (www.exomol.com).

1. Introduction

The International Thermonuclear Experimental Reactor (ITER) is leading developments in magnetic fusion reactor technology. In October 2023, ITER decided to change the material of the first wall panels in the reactor from beryllium to tungsten due to its greater resilience to disruptions and lower dust production (Loarte 2023). Additionally, the tungsten will be coated with a layer of boron through a process known as boronization to ‘maintain good vacuum conditions’, by removing impurities from the plasma (Winter 1996). A year earlier, Kawate *et al* (2022) demonstrated that when boron is introduced in a fusion plasma reactor, Boron hydride (BH) and BH^+ molecules form and distribute themselves over the divertor region. In particular, Kawate *et al* (2022) observed the clear spectral signature of the $\text{A } ^1\Pi\text{—X } ^1\Sigma^+$ of BH near 433 nm. The spectra of the various BH isotopologues can therefore provide a key diagnostic on the of involving higher disposition of boron in the plasma. By analogy, we note that analysis of high-resolution visible spectra of the beryllium hydride isotopologues (BeH , BeD , BeT) observed in the beryllium-walled JET fusion reactor has provided powerful insights into plasma-surface interactions (Pawelec *et al* 2024). The analysis of beryllium hydride spectra was based on computed line lists (Darby-Lewis *et al* 2018) which used the same methodology as we employ here.

BH isotopologues refer to the family of molecules that contain one boron atom, either ^{10}B or ^{11}B , and one hydrogen atom, which can be either hydrogen (H), deuterium (D) or tritium (T). There are a number of high resolution spectroscopic studies of the BH isotopologues (Thunberg 1936, Almy and Horsfall 1937, Johns *et al* 1967, Pianalto *et al* 1988, Fernando and Bernath 1991, Clark *et al* 2001) focusing on $\text{A } ^1\Pi\text{—X } ^1\Sigma^+$ rovibronic spectra and vibration-rotation spectra plus a number of studies

involving higher electronic states (Douglas 1941, Bauer *et al* 1964, Johns *et al* 1967) which we will not consider here. Other spectroscopic studies of BH included measurements of radiative lifetimes of states within the A $^1\Pi$ manifold (Smith 1971, Dufayard and Nedelec 1978). It should be noted, however, that most of these spectroscopic data recordings focus on $^{10/11}\text{BH}$, with only a few considering BD (Thunberg 1936, Fernando and Bernath 1991) and none involving work on tritiated boron hydride, BT.

Besides fusion, studies of BH are important for other areas of research, including chemical lasers (Benard *et al* 1994, Benard and Boehmer 1994), laser cooling (Hendricks *et al* 2014, Gao and Gao 2015), pain management (Liu *et al* 2024) and sunspots, where the tentative detection of BH (Engvold 1970) is hard to confirm due overlap of its spectrum with those of several other species (Karthikeyan *et al* 2009).

The structure of BH molecules is one of the simplest in nature, consisting of just two nuclei and six electrons, which allows for calculations at high levels of *ab initio* theory (Meier *et al* 2011). For this reason, extensive theoretical work has been done on BH, including *ab initio* calculations of the potential energy curves (PECs) for the electronic levels A $^1\Pi$, X $^1\Sigma^+$ and B $^1\Sigma^+$ (Jaszuński *et al* 1981, Pederson *et al* 1994, Xie *et al* 2005, Wang *et al* 2009, Gagliardi *et al* 1997, Koput 2015) and semi-empirical PECs (Luh and Stwalley 1983). Additionally, in some of these studies, dipole and dipole transition moment functions were calculated for the X $^1\Sigma^+$ state (Pederson *et al* 1994, Koput 2015), the A $^1\Pi$ state (Pederson *et al* 1994), and the A $^1\Pi$ —X $^1\Sigma^+$ transition (Pederson *et al* 1994).

In this paper we used methods developed as part of the ExoMol project (Tennyson and Yurchenko 2012, 2024) to compute line lists for all six isotopologues of BH. In the following section we describe our methodology. Section 3 presents our results and compares them to available laboratory data. Section 4 presents our conclusions.

2. Methodology

The PECs of the BH isotopologues were fitted using the Duo program, which solves the Schrödinger equation for the motion of diatomic nuclei using the variational principle (Yurchenko *et al* 2016). The input to Duo consists of potential energy and dipole moment curves plus appropriate coupling terms, either in the form of a function or grid points. If, as here, Duo is to be used to improve PECs by fitting to experimental energies, these energies also form part of the inputs. The resulting line lists can then be used as an input to the ExoCross (Yurchenko *et al* 2018) or PyExoCross (Zhang *et al* 2024) post-processing program to generate spectral graphs, compute radiative lifetimes, and determine partition functions.

2.1. MARVEL analysis

The MARVEL (Measured Active Vibration Rotation Energy Levels) procedure provides energy levels from a given network of measured and assigned transition wavenumbers and associated uncertainties (Furtenbacher *et al* 2007, Tóbiás *et al* 2019). As a first step we gathered the available high-resolution spectroscopic data involving transitions within and between the X $^1\Sigma^+$ and A $^1\Pi$ state (Johns *et al* 1967, Pianalto *et al* 1988, Clark *et al* 2001). This provided a dataset of 519 measured transitions, see table 1. This MARVEL input file is provided as part of the supplementary material. Rather unusually for MARVEL studies, all transitions were validated; to obtain a well-behaved network it was only necessary to increase the stated uncertainty slightly for the oldest source, 67JoGrPo (Johns *et al* 1967) from 0.03 cm^{-1} to 0.05 cm^{-1} for most transitions and to 0.1 cm^{-1} for those transitions marked as diffuse.

The transitions formed a single network, again somewhat unusually, with no unattached transitions. This network gave 204 empirical energy levels which are depicted in figure 1. The MARVEL energy file is provided as part of the supplementary material.

2.2. Potential energy curves

The empirical energies for ^{11}BH derived using MARVEL were used as input in fits performed with Duo. In the fits, the uncertainties for each empirical energy level were used to determine its weight in the fit. The weight of the lowest energy level (X $^1\Sigma^+$, $v = 0$, $J = 0$), with energy set to zero here, is fixed at 500.

Figure 2 shows our fitted PECs for the X $^1\Sigma^+$ and A $^1\Pi$ states with the dissociation level set at 29420 cm^{-1} . While the ground state PEC has a fairly standard shape, the $^1\Pi$ PEC has a maximum at large internuclear separations (R) which arises from the crossing of attractive and repulsive valence states (Jaszuński *et al* 1981); this feature considerably complicates the representation of this state. We note that this behavior is similar to that shown by several other diatomic hydrides such as AlH (Yurchenko *et al* 2024), NH (Uhlíková *et al* 2025, Perri *et al* 2026) and CH (Sokolov *et al* 2026).

Table 1. Experimental sources of high resolution transitions, denoted with unique tags, used to construct the spectroscopic network for ^{11}BH . Given are the wavenumber range (Range) of each source, the number of actual (A) and validated (V) transitions, plus uncertainty (unc.) statistics, in cm^{-1} : the stated (initial) uncertainty adopted and the final average uncertainty adopted.

Segment tag	Reference	Range/ cm^{-1}	V/A	Initial unc.	Final unc.
88PiOBKeBe	Pianalto <i>et al</i> (1988)	1911–2455	45/45	0.002	0.002
91FeBe	Fernando and Bernath (1991)	22 133–23 545	168/168	0.002	0.002
67JoGrPo	Johns <i>et al</i> (1967)	21 767–25 329	286/286	0.03	0.051
01ClKoZhGr	Clark <i>et al</i> (2001)	26 872–27 066	20/20	0.2	0.2

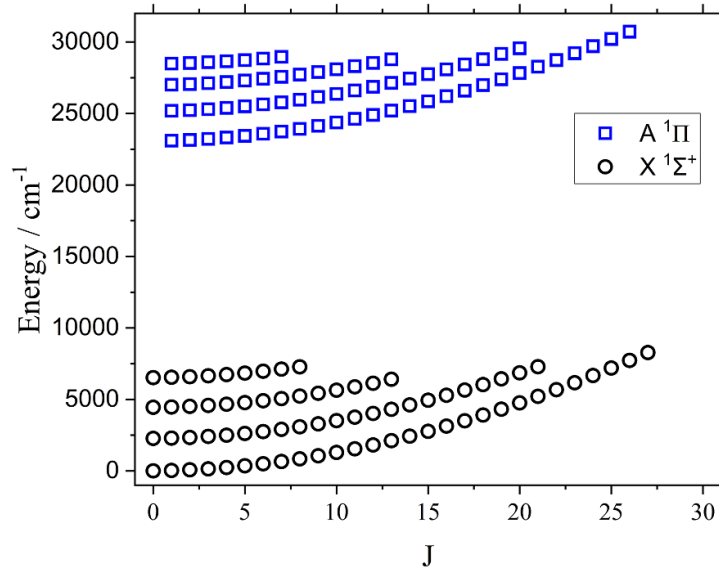


Figure 1. Experimentally derived energy levels for ^{11}BH from MARVEL.

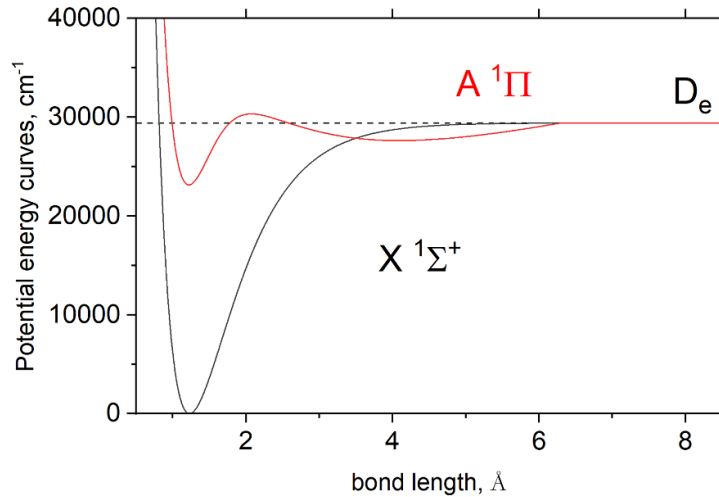


Figure 2. Potential energy curves derived in this work with the dissociation limit indicated by the dashed line.

Luh and Stwalley (1983) provided PECs for the $A\ ^1\Pi$ and $X\ ^1\Sigma^+$ states generated using the Rydberg–Kelvin–Rees (RKR) approach. These curves gave good initial values for the vibrational levels of the system, but it proved difficult to adapt the $A\ ^1\Pi$ curve to show the right behavior at larger R . This is unsurprising since the maximum at larger R is due to avoided crossing and therefore difficult to model using a single curve. We therefore decided to adopt the approach used by Yurchenko *et al* (2024) for AlH (and AlD) and fit the $A\ ^1\Pi$ as the lowest member of the coupled two-state system.

For the $X\ ^1\Sigma^+$ ground electronic state, the selected analytical function form was the extended Morse oscillator (EMO) (Lee *et al* 1999). This choice was made because the EMO function ensures an accurate

dissociation limit and allows flexibility in the degree of the polynomial around the equilibrium inter-nuclear separation (R_e), thereby improving the flexibility of the fit. The potential $V(R)$ of the EMO is given by

$$V(R) = V_e + (A_e - V_e) [1 - \exp(-\beta_{\text{EMO}}(R)(R - R_e))]^2 \quad (1)$$

$$\beta_{\text{EMO}}(R) = \sum_{n=1}^N a_n \gamma_p(R)^n \quad (2)$$

$$\gamma_p(R) = \frac{R^p - R_{\text{ref}}^p}{R^p + R_{\text{ref}}^p} \quad (3)$$

where V_e is the minimum of the PEC, which for the $X^1\Sigma^+$ state is set to zero; $(A_e - V_e)$ is the dissociation energy; N is the expansion order parameter; β_{EMO} is the distance dependent expansion coefficient; $\gamma_p(R)$ is the so-called Surkus variable (Surkus *et al* 1984) and p is an integer parameter that varies depending on the particular case of the potential energy function used. For the $X^1\Sigma^+$ state, we used β_{EMO} expanded as a sixth order polynomial ($N=6$).

Attempts to fit the $A^1\Pi$ electronic state by morphing the RKR curve of Luh and Stwalley (1983) did not give satisfactory results. We therefore used a diabatic-like scheme, inspired by work on the AlH molecule (Yurchenko *et al* 2024), taking the A-state curve as the lower eigenvalue (V_l) of the matrix:

$$\begin{pmatrix} V_1(R) & W(R) \\ W(R) & V_2(R) \end{pmatrix}, \quad (4)$$

where $V_1(R)$ is described by an EMO, equation (1) and $V_2(R)$ is a simple repulsive inverse polynomial form whose long-range limit was set to the dissociation limit of $A^1\Pi$.

$$V_2(R) = A_e + \frac{b_1}{R} + \frac{b_2}{R^2} + \frac{b_3}{R^3} + \frac{b_8}{R^8} + \frac{b_{10}}{R^{10}}. \quad (5)$$

The coupling function, $W(R)$ was modeled by an inverted EMO curve with a long range limit of zero

$$W(R) = W_0 [1 - \exp(-\gamma(R)(R - R_0))]^2 \quad (6)$$

where W_0 denotes the maximum coupling which occurs at separation R_0 .

Additionally, due to the shape of the $A^1\Pi$ PEC, see figure 2, some quasi-bound states exist above the dissociation level. While these states are included in Duo calculations, they are ignored in our line lists, and only bound states are considered. Specifically, the $A^1\Pi$ $v=3$ vibrational state energy levels lie above the dissociation limit and are labeled as $v=4$ in the Duo calculation, the states labeled $v=3$ being quasi-continuum states. We note that our representation of the $A^1\Pi$ shows a secondary minimum at large internuclear separation. While there is no experimental evidence for this feature, the large *ab initio* calculations of Miliordos and Mavridis (2008) show a similar feature. We did not explore the consequences of this feature on our spectrum.

For both the $X^1\Sigma^+$ and $A^1\Pi$ PECs, Born–Oppenheimer breakdown (BOB) effects are considered in the form of a decaying polynomial expansion

$$F(R) = \sum_{k=0}^n B_k z^k (1 - \zeta_p) + \zeta_p B_\infty \quad (7)$$

where z is taken as the damped coordinate, given by

$$z = (R - R_e) \exp\left(-\beta_2 (R - R_e)^2 - \beta_4 (R - R_e)^4\right) \quad (8)$$

where β_2 and β_4 are damping factors. A second-order decaying polynomial ($n=2$) was used for the $X^1\Sigma^+$ and a first-order polynomial ($n=1$) was used for the $A^1\Pi$ state, as increasing the order of the function did not improve the overall accuracy of the fit.

To account for the Λ -doubling of energy levels in the $A^1\Pi$ state which splits the e and f parity states (Yurchenko *et al* 2018), a Λ -doubling function and an electronic angular momentum coupling function between the $X^1\Sigma^+$ and $A^1\Pi$ states were included. These functions both took the form of third-order polynomial expansions in a Surkus variable, see equation (3).

To generate spectra we require an $X^1\Sigma^+$ permanent dipole moment curve and an $X^1\Sigma^+$ to $A^1\Pi$ states transition dipole moment curve. These were taken from the *ab initio* calculations of Koput (2015) and Pederson *et al* (1994), respectively.

Table 2. Comparison of the T_e values for the A $^1\Pi$ states from this work and previous experimental studies.

Reference	T_e / cm^{-1}
Huber and Herzberg (1979)	23 135.8
Fernando and Bernath (1991)	23 135.4376
Clark <i>et al</i> (2001)	23 105.1004
This work	23 151.78

3. Results and discussion

3.1. Potential energy curves

The PECs were fit using the variational nuclear motion program Duo. The Duo calculations used a sinc-DVR basis of 501 points to span $0.55 \leq R \leq 3.0 \text{ \AA}$. As a first step, Duo solves the $J=0$ vibrational states for each, uncoupled electronic state. These solutions provide the vibrational basis for the subsequent full calculation; 30 vibrational basis states were retained for both the X and A state to form the basis in the final calculations.

The PECs were fit to the MARVEL energies with dissociation limit set to $29\,420 \text{ cm}^{-1}$ as given by Persico (1994). The root-mean-square (rms) error measures the quality of our fit by quantifying the discrepancy between the observed energy levels from the MARVEL data and the calculated energy levels from the fitted PEC. The rms error for the X $^1\Sigma^+$ state is 0.025 cm^{-1} , while the rms for the A $^1\Pi$ state was 0.037 cm^{-1} . This fit gave an electronic excitation energy, T_e value of $23\,151.78 \text{ cm}^{-1}$, which is close to but differs from the values determined experimentally, see table 2. Given that our analysis is based on essentially the same transition data as the studies quoted in table 2, our slightly higher value of T_e almost certainly comes from our more accurate treatment of the zero point energies and hence vibrational motion in the system. Unlike the other treatments, we make no assumptions about motion being (quasi-)harmonic.

The expected general trends for the X $^1\Sigma^+$ and A $^1\Pi$ PECs are accurately reproduced by our fitted PECs, including the local maxima in the A $^1\Pi$ state. The only significant differences between our curves and those of Luh and Stwalley (1983) occur in regions well away from the potential energy well where the curves are poorly determined by the semi-empirical procedures used by both Luh & Stwalley and us. However, it is notable that our A $^1\Pi$ curve dips below the dissociation level at $3 \text{ \AA}$, giving a local minimum at large R as was also found for the AlH molecule (Yurchenko *et al* 2024) a feature not given by to Luh & Stwalley's PEC. Regardless of whether the local minima is accurate, the energy levels are close to those determined using MARVEL; however, they are fairly insensitive to the geometry of the curve beyond the potential energy barrier, so the nature of the PEC beyond $2 \text{ \AA}$ will have to be confirmed by further work.

The curves representing BOB corrections, electronic angular momentum coupling and Λ -doubling parity splitting of the levels are shown in figure 3. The parameters used in the fitting of the PECs and other curve corrections can be found in the Duo input files attached in the supplementary information section.

3.2. Line lists

Line lists were generated for each of the six isotopologues of BH, see table 3. Each line list is stored in standard ExoMol format (Tennyson *et al* 2013, 2024); that is each line list is divided into states and transitions files, see tables 4 and 5, respectively. The AX line lists are available from the ExoMol website, www.exomol.com

For $^{11}\text{B}^1\text{H}$ the MARVEL energy levels were used instead of those computed by Duo where possible. For these levels the MARVEL uncertainty was adopted. For other levels of $^{11}\text{B}^1\text{H}$ and all levels of the other isotopologues the associated uncertainty, in cm^{-1} , was conservatively estimated using the formulae:

$$\delta E = 0.05\nu + 0.003J(J+1) \quad (9)$$

for the X $^1\Sigma^+$ state and

$$\delta E = 2.0 + 0.003J(J+1) \quad (10)$$

for the A $^1\Pi$ state.

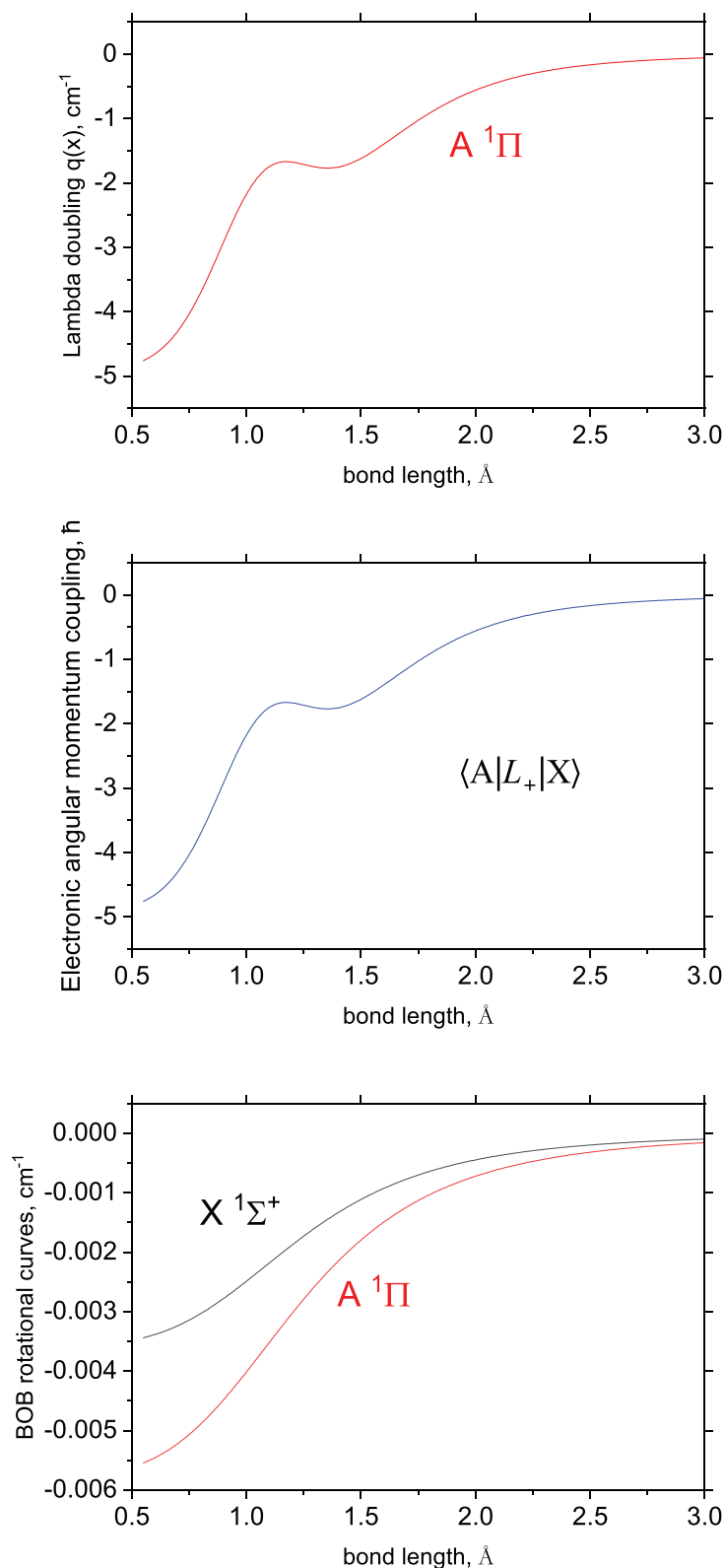


Figure 3. Coupling curves used in our spectroscopic model for BH; Upper panel: Lambda-q coupling, middle panel: electronic angular momentum coupling; lower panel Born–Oppenheimer breakdown corrections for the $X\ ^1\Sigma^+$ and $A\ ^1\Pi$ states.

These are supported by a partition function file. The states, trans and partition function files are available on the ExoMol website, www.exomol.com.

3.3. Radiative lifetimes

Radiative lifetimes for each state were computed using the Einstein A coefficients (Tennyson *et al* 2016) using program ExoCross (Yurchenko *et al* 2018) and included in the state file, as is the ExoMol policy.

Table 3. Summary of our BH line lists: g_I is the nuclear spin degeneracy factor, $\nu_{\max}$ and $J_{\max}$ are the maximum vibrational and rotational state, and N_{state} and N_{trans} are the number of states and transitions which make up each line list; $N(X)$ and $N(A)$ give the number of states in the $X^1\Sigma^+$ and $A^1\Pi$ states, respectively.

isotopologue	g_I	$\nu_{\max}$	$J_{\max}$	N_{state}	$N(X)$	$N(A)$	N_{trans}
^{11}BH	8	11	56	508	384	124	5530
^{10}BH	14	11	56	505	381	124	5473
^{11}BD	12	15	60	850	636	214	12 713
^{10}BD	21	15	60	838	628	210	12 433
^{11}BT	8	29	60	1108	818	290	20 739
^{10}BT	14	29	60	1090	804	286	19 792

The lifetimes for states belonging to the $A^1\Pi$ states of ^{11}BH are given in figure 4. Vibrational-averaged lifetimes for a few of the states have been measured; our predictions are compared with these measurements in table 6. The agreement is excellent: all our calculated lifetimes agree with experiment within the experimental uncertainties. This gives strong support for the reliability of the $A^1\Pi-X^1\Sigma^+$ transition dipole due to Pederson *et al* (1994) which we adopt and suggests that our predicted transition intensities should also be accurate.

3.4. Partition functions

Partition functions were computed for each isotopologue by direct summation of energy levels in 1 K steps up to 5000 K. ExoMol follows the HITRAN convention (Gamache *et al* 2025) and includes the nuclear spin degeneracy factor, g_I , in the partition function. These factors are given for each isotopologue in table 3. For ^{11}BH our partition function can be compared to the one provided by Barklem and Collet (2016) once allowance is made for the nuclear spin factor which they do not include. The agreement is very good, with Barklem & Collet's value being just 0.7% higher at 3000 K, the highest temperature for which there is a common data point.

3.5. Line spectra

Figure 5 shows the ^{11}BH spectra at 300 and 3000 K; Doppler profiles were applied to account for temperature-dependent line broadening effects.

Fernando and Bernath (1991) obtained Q branch emission spectra for the $A^1\Pi-X^1\Sigma^+$ (0,0) band for both BH and BD, figures 6 and 7 respectively, both of which present a comparison with those generated using our AX line lists. Our emission spectrum was computed assuming a temperature of 2000 K and using a Gaussian profile with a HWHM of 0.07 cm^{-1} as this gave the best fit by eye to the observations. Due to the naturally high abundance of ^{10}B , it is reasonable to assume that features due to both ^{10}BH and ^{10}BD are present in these spectra. Included in the overall spectra; therefore, ^{10}BH and ^{10}BD were incorporated into the AX ^{11}BH and ^{11}BD spectra, respectively. This was done assuming ^{11}B and ^{10}B natural abundances of 80.10% and 19.90%, respectively. We note that the observed spectra only give relative intensities and, indeed, the distribution of rotational states may not be thermal; the intensity scales given in the figures therefore come from our calculations.

Figure 6 demonstrates strong agreement between our calculated ^{11}BH spectrum and that of Fernando and Bernath (1991). However for ^{10}BH , which is based on computed energy levels rather than those provided by MARVEL, the agreement is less good. As shown in the lower panel, there appears to be a systematic shift of approximately 0.40 cm^{-1} for ^{10}BH in our computed ^{10}BH transition wavenumbers.

Figure 7 shows that our calculations reproduce the shape and structure of the observations but show a systematic shift of approximately 3 cm^{-1} to the red relative to the spectrum (Fernando and Bernath 1991). This shift is almost certainly due to our inability to fully account for non-Born–Oppenheimer effects in the system. The need to shift the ^{10}BH by 0.04 cm^{-1} to improve the BH spectral representation suggests that similar non-Born–Oppenheimer effects may also be present in ^{10}BH . Our model does include a BOB correction term; removing this significantly worsens the agreement between the observed and calculated spectra. We note that for the rather similar AlH/AlD system the ExoMol line lists are based on separate spectroscopic models for the two isotopologues (Yurchenko *et al* 2024). Unfortunately, the very limited experimental data for BD, largely concerning Q-branch transitions, does not provide enough information for us to construct separate models for deuterated (and triterated) boron hydride.

Table 4. First 7 rows of the ^{11}BH states file.

N	E	g	J	Unc	τ	Parity	p	State	ν	Λ	Σ	Ω	Label	E_{Ca}
1	0.000 000	8	0	0.000 000	Inf	+	e	X1Sigma+	0	0	0	0	Ma	0.000 000
2	2269.254 639	8	0	0.060 000	4.2508×10^{-03}	+	e	X1Sigma+	1	0	0	0	Ma	2269.222 547
3	4443.034 180	8	0	0.004 000	2.2651×10^{-03}	+	e	X1Sigma+	2	0	0	0	Ma	4443.032 149
4	6523.607 422	8	0	0.064 000	1.6183×10^{-03}	+	e	X1Sigma+	3	0	0	0	Ma	6523.606 735
5	8518.791 996	8	0	0.100 000	1.2979×10^{-03}	+	e	X1Sigma+	4	0	0	0	Ca	8518.791 996
6	10 440.250 436	8	0	0.100 000	1.1065×10^{-03}	+	e	X1Sigma+	5	0	0	0	Ca	10 440.250 436
7	12 292.787 533	8	0	0.100 000	9.8442×10^{-04}	+	e	X1Sigma+	6	0	0	0	Ca	12 292.787 533

N : state index,

E : energy level in cm^{-1} ,

g : total statistical weight $= (2J + 1)g_l$,

J : total angular momentum,

Unc: energy level uncertainty in cm^{-1} ,

τ : state lifetime in s,

Parity: total parity (+/−),

p : rotationless parity (*e/f*) (Brown *et al* 1975),

State: electronic state,

ν : vibrational quantum number,

Λ : projection of electronic angular momentum,

Σ : projection of electronic spin,

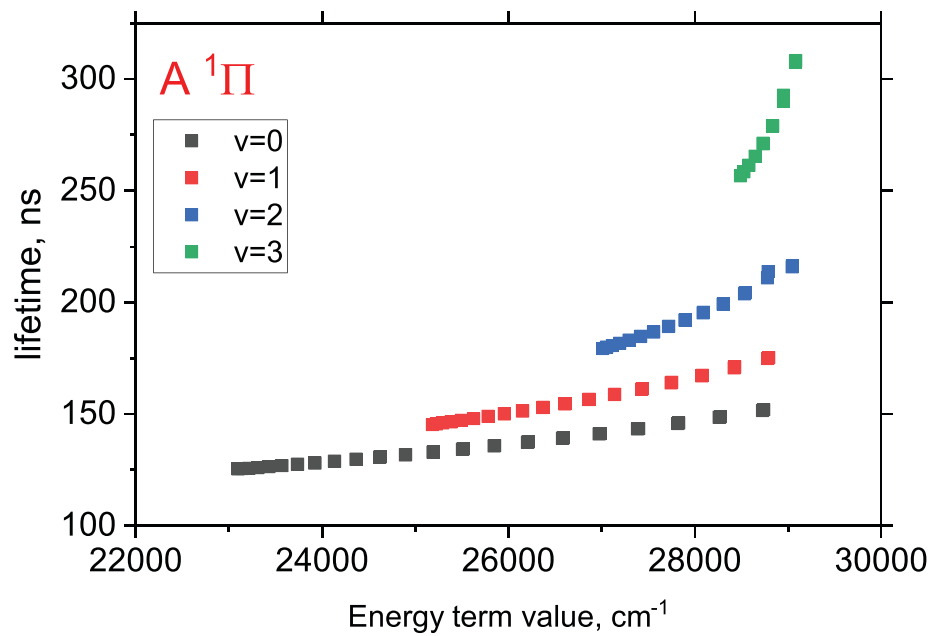
Ω : projection of total angular momentum.

Label: Ma, energy level from MARVEL; Ca, energy level calculated (McKemmish *et al* 2024),

E_{Ca} : the calculated energy level in cm^{-1} .

Table 5. Snapshot of the ^{11}BH transition file.

f	i	A_{fi}/s^{-1}	ν/cm^{-1}
38	1	8.5598E+01	2292.019 829
49	1	5.2973E+06	23 097.835 904
50	1	6.7571E+04	25 183.218 435
39	2	1.5832E+02	2195.790 039
49	2	3.5312E+04	20 828.613 357
50	2	4.5109E+06	22 913.995 888
51	2	3.1244E+05	24 743.456 651

 f : Upper state index, i : Lower state index, A : Einstein A coefficient, ν : transition wavenumber.**Figure 4.** Computed radiative lifetimes for the lowest five $A\ ^1\Pi$ vibrational states; lifetimes generally increase with increasing rotational excitation, J .**Table 6.** Comparison of observed and calculated $A\ ^1\Pi$ state radiative lifetimes.

v	J	$\tau_{\text{obs}}/\text{ns}$	$\tau_{\text{calc}}/\text{ns}$
0	1	125 ± 5^a	125.4
0	2	125 ± 5^a	125.5
0	7	125 ± 5^a	127.5
1	3	146 ± 12^b	145.9
2	3	172 ± 14^b	180.3

^a Dufayard and Nedelec (1978)^b Douglass *et al* (1989)

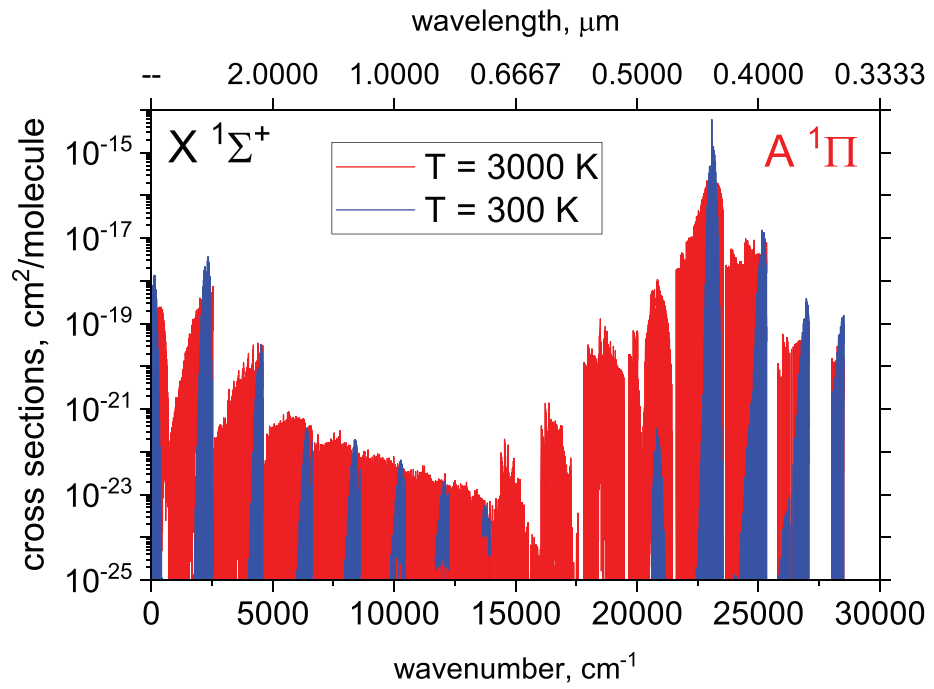


Figure 5. Computed absorption spectra for ^{11}BH at 300 and 3000 K.

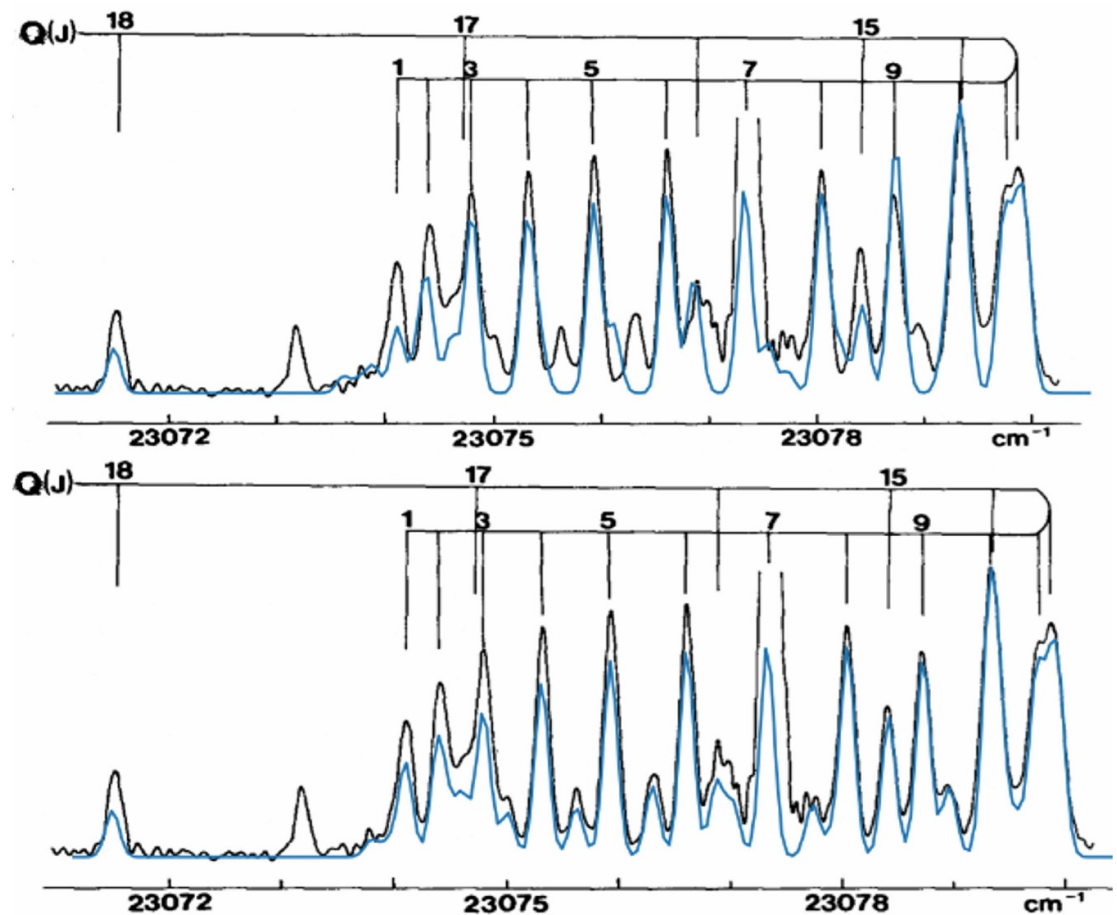
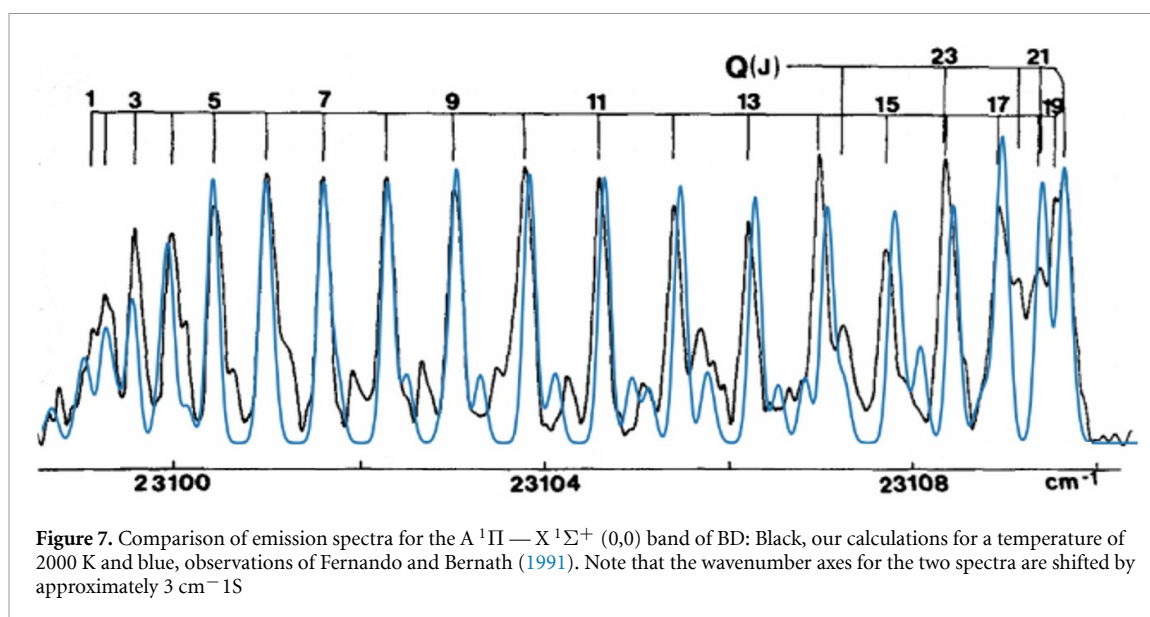


Figure 6. Comparison of emission spectra for the $A^1\Pi - X^1\Sigma^+$ (0,0) of BH: Blue, our calculations for a temperature of 2000 K using both ^{11}BH and ^{10}BH line lists assuming natural abundance; black, observations of Fernando and Bernath (1991). In the lower panel, features due to ^{10}BH are shifted by 0.40 cm^{-1} to the blue. Note the observed feature near 23073 cm^{-1} is not due to BH.



4. Conclusion

We present comprehensive line lists for the isotopologues of BH which can be used to simulate absorption and emission spectra of these molecules for rotation-vibration transitions and the $A\ ^1\Pi - X\ ^1\Sigma^+$ band system over a wide range of temperatures. The line lists, which we call AX, are available from the ExoMol website, www.exomol.com.

Comparisons with laboratory data suggest that our results for the ^{11}BH parent isotopologue are highly accurate both in terms of line positions and, as judged from our computed vibrational state lifetimes and transition intensities. The agreement in line positions for the other isotopologues for which laboratory data are available, namely ^{10}BH and BD , is less satisfactory. At present, it is difficult to improve these line lists due to the paucity of available experimental data. However, we note that we have started exploring methods that use machine learning to improve isotopologue energy levels, and hence transition wavenumbers, starting from accurate predictions of the corresponding energy levels of the parent isotopologue (Barnfield *et al* 2026); hopefully, this approach can be used to improve the line lists in the future.

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Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: www.exomol.com.

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References

- Almy G and Horsfall R 1937 *Phys. Rev.* **51** 491–500
- Barklem P S and Collet R 2016 *Astron. Astrophys.* **588** A96
- Barnfield M G, Polyansky O L, Yurchenko S N and Tennyson J 2026 *J. Mol. Spectrosc.* **418–419** 112084
- Bauer S, Herzberg G and Johns J 1964 *J. Mol. Spectrosc.* **13** 256–80
- Benard D and Boehmer E 1994 *Appl. Phys. Lett.* **65** 1340–2
- Benard D, Boehmer E, Michels H and Montgomery J 1994 *J. Phys. Chem.* **98** 8952–8
- Brown J M, Hougen J T, Huber K P, Johns J W C, Kopp I, Lefebvre-Brion H, Merer A J, Ramsay D A, Rostas J and Zare R N 1975 *J. Mol. Spectrosc.* **55** 500–3
- Clark J, Konopka M, Zhang L and Grant E 2001 *Chem. Phys. Lett.* **340** 45–54
- Darby-Lewis D, Tennyson J, Lawson K D, Yurchenko S N, Stamp M F, Shaw A and Brezinsek S (JET Contributor) 2018 *J. Phys. B: At. Mol. Opt. Phys.* **51** 185701
- Douglas A E 1941 *Can. J. Phys.* **19** 27–31
- Douglas C H, Nelson H H and Rice J K 1989 *J. Chem. Phys.* **90** 6940–8
- Dufayard J and Nedelec O 1978 *J. Chem. Phys.* **69** 4708–9
- Engvold O 1970 *Sol. Phys.* **11** 183–97
- Fernando W and Bernath P 1991 *J. Mol. Spectrosc.* **145** 392–402
- Furtenbacher T, Császár A G and Tennyson J 2007 *J. Mol. Spectrosc.* **245** 115–25
- Gagliardi L, Bendazzoli G and Evangelisti S 1997 *Mol. Phys.* **98** 861–71
- Gamache R R, Vispoel B, Tennyson J, Yurchenko S N, Polyansky O L, Gordon I E, Hargreaves R J and Huang X 2025 *J. Quant. Spectrosc. Radiat. Transf.* **345** 109568
- Gao Y and Gao T 2015 *Phys. Chem. Chem. Phys.* **17** 10830–7
- Hendricks R J, Holland D A, Truppe S, Sauer B E and Tarbutt M R 2014 *Front. Phys.* **2** 51
- Huber K and Herzberg G 1979 *Molecular Spectra and Molecular Structure: IV. Constants of Diatomic Molecules* (Van Nostrand Reinhold)
- Jaszuński M, Roos B O and Widmark P O 1981 *J. Chem. Phys.* **75** 306–14
- Johns J, Grimm F and Porter R 1967 *J. Mol. Spectrosc.* **22** 435–51
- Karthikeyan B, Bagare S P, Rajamanickam N and Raja V 2009 *Astropart. Phys.* **31** 6–12
- Kawate T *et al* 2022 *Nucl. Fusion* **62** 126052
- Koput J 2015 *J. Comput. Chem.* **36** 2219–27
- Lee E G, Seto J Y, Hirao T, Bernath P F and Le Roy R J 1999 *J. Mol. Spectrosc.* **194** 197–202
- Liu Y *et al* 2024 *Angew. Chem.* **63** e202405131
- Loarte A 2023 STAC committee reviews new plans for construction and operation ITER (available at: www.iter.org/node/20687/stac-committee-reviews-new-plans-construction-and-operation) (Accessed 24 February 2025)
- Luh W T and Stwalley W C 1983 *J. Mol. Spectrosc.* **102** 212–23
- McKemmish L K, Bowesman C A, Kefala K, Perri A N, Syme A M, Yurchenko S N and Tennyson J 2024 *RAS Tech. Instr.* **3** 565–83
- Meier P, Neff M and Rauhut G 2011 *J. Chem. Theory Comput.* **7** 148–52
- Miliordos E and Mavridis A 2008 *J. Chem. Phys.* **128** 144308
- Pawelec E, Borodin D, Brezinsek S, Dittmar T, Douai D, Mazur D, Meigs A, Shaw A and Thomas B (JET Contributors and EUROfusion Tokamak Exploitation Team) 2024 *Phys. Plasmas* **31** 042516
- Pederson L, Hetttema H and Yarkony D 1994 *J. Phys. Chem.* **98** 11069–74
- Perri A N, Uhlíková T U, Kim G S, Yurchenko S N and Tennyson J 2026 *Mon. Not. R. Astron. Soc.* **548** stag744
- Persico M 1994 *Mol. Phys.* **81** 1463–71
- Pianalto F, O'Brien L, Keller P and Bernath P 1988 *J. Mol. Spectrosc.* **129** 348–53
- Smith W H 1971 *J. Chem. Phys.* **54** 1384–6
- Sokolov A, Yurchenko S N and Tennyson J 2026 *Phys. Chem. Chem. Phys.* **28** 7484–93
- Šurkus A, Rakauskas R and Bolotin A 1984 *Chem. Phys. Lett.* **105** 291–4
- Tennyson J *et al* 2024 *J. Quant. Spectrosc. Radiat. Transfer* **326** 109083
- Tennyson J, Hill C and Yurchenko S N 2013 6th international conference on atomic and molecular data and their applications ICAMDATA-2012 *AIP Conf. Proc.* vol 1545 pp 186–95
- Tennyson J, Hulme K, Naim O K and Yurchenko S N 2016 *J. Phys. B: At. Mol. Opt. Phys.* **49** 044002
- Tennyson J and Yurchenko S N 2012 *Mon. Not. R. Astron. Soc.* **425** 21–33
- Thunberg S 1936 *Z. Phys.* **100** 471–7
- Tóbiás R, Furtenbacher T, Tennyson J and Császár A G 2019 *Phys. Chem. Chem. Phys.* **21** 3473–95
- Uhlíková T, Yurchenko S N, Perri A N, Tennyson J and Kim G S 2025 *J. Chem. Phys.* **162** 144108
- Wang X Q, Yang C L, Su T and Wang M S 2009 *Acta Phys. Sin.* **58** 6873–8
- Winter J 1996 *Plasma Phys. Control. Fusion* **38** 1503
- Xie A, Shi D, Zhu Z and Zhu Z 2005 *Acta Phys.-Chim. Sin.* **21** 658–62

- Yurchenko S N, Al-Refaie A F and Tennyson J 2018 *Astron. Astrophys.* **614** A131
- Yurchenko S N, Lodi L, Tennyson J and Stolyarov A V 2016 *Comput. Phys. Commun.* **202** 262–75
- Yurchenko S N, Szajna W, Hakalla R, Semenov M, Sokolov A, Tennyson J, Pavlenko Y and Schmidt M R 2024 *Mon. Not. R. Astron. Soc.* **527** 9736–56
- Yurchenko S N, Williams H, Leyland P C, Lodi L and Tennyson J 2018 *Mon. Not. R. Astron. Soc.* **479** 1401–11
- Zhang J, Tennyson J and Yurchenko S N 2024 *RAS Tech. Instr.* **3** 257–87