ExoMol line lists XXXII: The rovibronic spectrum of MgO

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ABSTRACT

Line lists for magnesium oxide are computed and extensive comparisons are made with existing experimental spectra. The LiTY line lists cover all ro-vibration transitions within the five lowest-lying electronic states (X $^1\Sigma^+$, a $^3\Pi$, A $^1\Pi$, B $^1\Sigma^+$ and b $^3\Sigma^+$) and five isotopologues: $^{24}\text{Mg}^{16}\text{O}$, $^{25}\text{Mg}^{16}\text{O}$, $^{26}\text{Mg}^{16}\text{O}$, $^{24}\text{Mg}^{17}\text{O}$, $^{24}\text{Mg}^{18}\text{O}$, $^{24}\text{Mg}^{17}\text{O}$ and $^{24}\text{Mg}^{18}\text{O}$. The calculation use potential energy curves, spin-orbit and electronic angular momentum couplings curves determined by fitting to empirical energy levels; these levels are reproduced to within 0.01 cm$^{-1}$ in most cases. Computed nuclear-motion wavefunctions are combined with $ab$ initio dipole moment curves to give transition intensities and excited state radiative lifetimes which are compared with laboraroty measurements. The $^{24}\text{Mg}^{16}\text{O}$ line list comprises 186 842 ($J \leq 320$) ro-vibronic states and 72 833 173 transitions with angular momenta, $J$, up to 300 and covering wavenumbers up to 33 000 cm$^{-1}$ ($\lambda > 0.3$ µm). The line lists are suitable for temperatures up to about 5000 K. They are relevant to astrophysical studies of exoplanet atmospheres, cool stars and brown dwarfs, and are made available in electronic form at the CDS and ExoMol databases.

Key words: molecular data; opacity; astronomical data bases: miscellaneous; planets and satellites: atmospheres; stars: low-mass

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1 INTRODUCTION

Magnesium oxide (MgO) is a metal oxide formed from the cosmically abundant elements of magnesium and oxygen. MgO is a major constituent of chondritic meteorites (Maatouk et al. 2010). It was observed in the exosphere of Mercury by the first and second flyby of the MESSENGER spacecraft (Killen et al. 2010; Sarantos et al. 2011). The observed distribution suggests temperatures of tens of thousands Kelvin. The quantity of MgO in the lunar surface was estimated using X-ray fluorescence observations made by the Chandrayaan-1 X-ray Spectrometer (Weider et al. 2012). The strongest singlet band ($B^1\Sigma^+ - X^1\Sigma^+$) present in the lunar exosphere were analysed during the 2009 Perseid meteor shower (Berezhnoy et al. 2014).

MgO is also thought to be a major component of interstellar dust (Yoneda & Grossman 1995; Nozawa et al. 2003; Rietmeijer 2009). Attempts to detect MgO in the gas phase in the interstellar medium (ISM) have so far proved inconclusive (Turner & Steimle 1985) or negative (Sakamoto et al. 1998), suggesting that Mg is heavily depleted onto grains (Sakamoto et al. 1998). The discovery of hot, rocky exoplanets has led to suggestions that the many compounds usually in the condensed phase, and in particular MgO (Coppari et al. 2013), should be present in significant concentrations in the gas phases (Schaefer et al. 2012; Tennyson & Yurchenko 2018). The detection of us such species would require lists of key spectroscopic transitions and here we provide line lists for MgO isotopologues which should be valid over an extended range of temperatures.

MgO has a very characteristic electronic spectrum which should be amenable to observations. In particular, the two singlet systems ($B^1\Sigma^+ - A^1\Pi$ and $B^1\Sigma^+ - X^1\Sigma^+$), called the red and green band systems respectively, have long been studied in the laboratory (Mahanti 1932; Lagerqvist & Uhler 1949). Experimental studies of MgO spectra initially used grating spectrographs and more recently laser spectroscopy which allowed experiments to be performed on the low lying states as well as some higher states such as the $E^1\Sigma^+$ and $F^1\Pi$ states (Bellert et al. 2003; Wang et al. 2004). A full survey of high resolution spectroscopic studies of MgO is given in the next section.

The most recent and comprehensive ab initio study of MgO is by Bauschlicher & Schwenke (2017), who presented a high level study for a large number of electronic states of this molecule using the SA-CASSCF/IC-MRCI/aug-cc-pV5Z level of theory. They reported high level ab initio potential energy and (transition) dipole moment curves as well as lifetimes.
for a number of electronic bands. We have adopted these \textit{ab initio} curves for the present study. Another recent and accurate \textit{ab initio} study of MgO, also relevant to our work, is by Maatouk et al. (2010), who used the MRCI/cc-pV5Z method to compute potential energy, spin-orbit and transition dipole moment curves for the valence and valence-Rydberg electronic states of MgO. Earlier, but also comprehensive, \textit{ab initio} studies of MgO were performed by Thommel et al. (1989b) and Thommel et al. (1989a) using the MRDCI method for various states. None of these works reported the electronic angular momenta of MgO.

Limited work have been performed on the construction of MgO line lists. While studies have reduced the observed spectra into spectroscopic constants (Pyykkö et al. 1987; Thommel et al. 1989b; Daily et al. 2002), the only source of astronomical transition data is the JPL list of 44 pure rotational transitions associated with the \(v = 0\) and \(v = 1\) vibrational states of the \(X^1\Sigma^+\) electronic ground state (Pickett et al. 1998). These data are designed for detecting MgO in the interstellar medium but do not provide the information required to study the spectra of hotter sources.

The ExoMol project aims to provide a catalogue of spectroscopic transitions for molecular species which may be present in the atmospheres of the exoplanets, brown dwarfs and cool stars (Tennyson & Yurchenko 2012). The ExoMol database (Tennyson et al. 2016) currently contains 52 molecules ranging from diatomic to polyatomic molecules and ions (Tennyson & Yurchenko 2018). However, there are only a handful of metal oxides available, namely CaO (Yurchenko et al. 2016), VO (McKemmish et al. 2016), AlO (Patrascu et al. 2015) and SiO (Barton et al. 2013); an updated line list for TiO has just been completed (McKemmish et al. 2019). Such line lists are also important for analysing and modelling spectra in laser induced plasmas (Woods et al. 2012; De Giacomo et al. 2014; Parigger et al. 2015).

Here we present new extensive line lists for MgO covering the spectroscopy of its five lowest electronic states, \(X^1\Sigma^+, A^1\Pi, B^1\Sigma^+, a^3\Pi\) and \(b^3\Sigma^+\). The line list are computed using nuclear-motion program DUO (Yurchenko et al. 2016a) using a combination of empirical and \textit{ab initio} potential energy curves (PECs), spin-orbit curves (SOCs) and electronic angular momentum curves (EAMCs) in conjunction with high level \textit{ab initio} (transition) dipole moment curves (T)DMCs. The \textit{ab initio} curves were taken from the literature, where available, or were computed as part of this work. Given the astronomical interest in MgO, the line lists are produced to cover an extensive energy and spectroscopic range, up to 37 250 cm\(^{-1}\) and should be applicable for temperatures up to at least 5000 K. Line lists are generated for the three stable isotopes of Mg and three stable isotopes of O.
Table 1. Experimental sources and maximal values of $J$, $v$ and energy term values (cm$^{-1}$) of high resolution spectroscopic data of MgO used in this work.

| Source                          | Method       | State$'$ | State$''$ | $v'$ | $v''$ | $J'$ | $J''$ | $E_{\text{max}}'$ | $E_{\text{max}}''$ |
|--------------------------------|--------------|----------|-----------|------|-------|------|-------|-------------------|-------------------|
| Kagi & Kawaguchi (2006)        | Microwave    | $a^3\Pi$ | $a^3\Pi$  | 0    | 0     | 12   | 7     | 13                | 13                |
|                               |              | $X^1\Sigma^+$ | $X^1\Sigma^+$ | 1 | 1 | 12 | 7 | 14 | 14 |
|                               |              |          |           | 2 | 2 | 12 | 7 |         | 7 |
|                               |              |          |           | 3 | 3 | 12 | 7 |         | 7 |
| Brewer et al. (1962)          | Grating     | $C^1\Sigma^-$ | $A^1\Pi$  | 0 | 0 | 80 | 4 | 26414 | 26544 |
|                               |              |          |           | 1 | 1 | 65 | 21 |         | 21 |
| Trajmar & Ewing (1965)        | Grating     | $G^1\Sigma^-$ | $A^1\Pi$  | 1 | 1 | 60 | 9 | 26387 | 26769 |
|                               |              |          |           | 1 | 1 | 43 | 4 |         | 4 |
| Singh (1973)                  | Ebert       | $G^1\Pi$ | $A^1\Pi$  | 0 | 1 | 40 | 14 | 36388 | 39870 |
|                               |              |          |           | 0 | 1 | 40 | 16 |         | 16 |
| Singh (1973)                  | Ebert       | $G^1\Pi$ | $X^1\Sigma^+$ | 0 | 0 | 38 | 16 |         | 16 |
| Antic-Jovanovic et al. (1976) | Grating     | $E^1\Sigma^+$ | $A^1\Pi$  | 0 | 0 | 36 | 36 | 34304 | 34173 |
| Azuma et al. (1994)           | LIF         | $B^1\Sigma^+$ | $X^1\Sigma^+$ | 0 | 0 | 40 | 0 | 19971 | 20602 |
|                               |              |          |           | 1 | 1 | 56 | 0 |         | 0 |
| Civis et al. (1991)           | DLFR        | $X^1\Sigma^+$ | $X^1\Sigma^+$ | 1 | 0 | 32 | 6 | 766 | 792 |
|                               |              |          |           | 2 | 1 | 28 | 7 |         | 7 |
| Ip et al. (1991)              | LIF         | $B^1\Sigma^+$ | $a^3\Pi$  | 0 | 0 | 48 | 4 | 16735 | 27256 |
|                               |              |          |           | 1 | 1 | 48 | 6 |         | 6 |
|                               |              |          |           | 1 | 1 | 17 | 1 |         | 1 |
| Kagi et al. (1994)            | FTS         | $A^1\Pi$ | $X^1\Sigma^+$ | 1 | 0 | 56 | 0 | 2644 | 5452 |
|                               |              |          |           | 2 | 0 | 67 | 3 |         | 3 |
|                               |              |          |           | 3 | 0 | 58 | 3 |         | 3 |
|                               |              |          |           | 2 | 1 | 31 | 11 |         | 11 |
|                               |              |          |           | 0 | 1 | 37 | 8 |         | 8 |

Microwave = Microwave spectroscopy
Grating = Grating spectrograph
Ebert = Ebert spectrograph
DLFR = Diode-laser flame spectrometer
LIF = Laser-induced fluorescence spectroscopy
FTS = Fourier Transform Spectrometer

2 METHOD

2.1 Experimental data

Experimental transitions frequencies for $^{24}$Mg$^{16}$O involving a total nine different electronic states were collected from various papers which are summarised in Table 1. The MARVEL technique (Measured Active Rotational-Vibrational Energy Levels) (Furtenbacher et al. 2007; Furtenbacher & Császár 2012; Tóbiás et al. 2019) was used to determine empirical energy levels. A total of 2457 transitions were collected from the listed sources and validated yielding 757 distinct empirical energy levels. The MARVEL transitions and energy files are given as part of the supplementary data. The MARVEL energy levels together with the experimental transitions were used as DUO inputs to refine our spectroscopic model (PECs, SOCs and EAMCs).
2.2 Spectroscopic model

As with other metal oxides studied within the ExoMol projects, the procedure used here to calculate the line list for MgO is to refine the \textit{ab initio} PECs, SOCs and EAMCs using available experimental data (Tennyson 2011).

Our model of MgO consists of five PECs, $X \,^1\Sigma^+$, $A \,^1\Pi$, $B \,^1\Sigma^+$, $a \,^3\Pi$ and $b \,^3\Sigma^+$ which are shown in Figure 1. They are augmented by five SOCs, $X \,^1\Sigma^-$, $a \,^1\Sigma^-$, $A \,^1\Pi$, $B \,^1\Sigma^-$ and $a \,^3\Pi$, which are shown in Figure 2, and two EAMCs $X \,^1\Pi$ and $a \,^3\Pi$, the $x$ components of which are shown in Figure 3. The initial, \textit{ab initio}, PECs were taken from Bauschlicher & Schwenke (2017). The SOCs and EAMCs were obtained \textit{ab initio} using the MOLPRO electronic structure package (Werner et al. 2012) at the multi-reference configuration interaction (MRCI) level of theory in conjunction with the aug-cc-pwCVQZ basis sets with relativistic, core-correlation effects and Davidson correction, as part of this study. The active space is given by $(8,4,4,0)$. The states-averaged CASSCF (SA-CASSCF) comprised $(3,2,1,1)$ states of symmetries $\Sigma^+$, $\Pi$, $\Delta$ and $\Sigma^-$, respectively. All electron were correlated. The relativistic correction was estimated using the Douglas-Kroll method.

The nuclear motion program DUO (Yurchenko et al. 2016b) is used to solve the fully-coupled Schrödinger equation for the five lowest bound electronic states of MgO. DUO calculations used a grid-based sinc DVR basis of 501 points spanning 0.02 to 8 Å to obtain
vibrational basis functions by solving five independent $J = 0$ problems for the corresponding electronic state. The final vibrational basis set comprised 100, 62, 100, 57, and 70 lowest vibrational eigenfunctions of the $X, a, A, B$ and $b$ states, respectively. These numbers were chosen to include all vibrational states below the corresponding dissociation limits (see be-
low). A detailed description of the methodology is given by Yurchenko et al. (2016b) and Tennyson et al. (2016).

In order to facilitate the refinement of the experimental model, the four lowest PECs (X, a A, and B) were represented using an extended Morse oscillator (EMO) (Lee et al. 1999) potentials with the form:

\[ V(R) = V_e + (A_e - V_e) \left[ 1 - \exp \left( -\sum_{k=0}^{N} B_k \xi^k (r - r_e) \right) \right]^2, \]  

(1)

where \( D_e = A_e - V_e \) is the dissociation energy, \( r_e \) is an equilibrium distance of the PEC, and \( \xi \) is the Šurkus variable (Šurkus et al. 1984). The Šurkus variable is defined as:

\[ \xi = \frac{r_p - r_{ref}}{r_p + r_{ref}}, \]  

(2)

where \( p \) is a non-zero real number parameter, \( r_{ref} \) is a reference position and \( r_{ref} = r_e \) in this case. The b state \textit{ab initio} PEC was not used in the refining procedure and therefore did not need to be represented analytically. The \textit{ab initio} points values were interpolated on the DUO grid using the cubic splines Yurchenko et al. (2016a).

The lowest dissociation limit from MgO is to the \( a^3 \Pi \) asymptote (Mg\(^1S\) and O\(^3P\)), which Bauschlicher & Schwenke (2017) estimated as lying at 2.7±0.1 eV. Their adiabatic dissociation energy for the \( X^1 \Sigma^+ \) state is 4.65 eV, which is similar to the value obtained using the atomic asymptotic separation to O\(^1D\), 4.67 eV. This is also the asymptote as for the \( A^1 \Pi \) state. Adding the atomic separation of O\(^3P\) and Mg\(^3P\) to this limit gives the asymptote for the \( B^1 \Sigma^+ \) state of 5.4 eV. These asymptotes were adopted for the values of \( A_e \) in Eq. (1) used in this work.

We did not represent the \textit{ab initio} SOCs and EAMCs analytically directly. Instead, in order to allow for their refinement, the morphing procedure (Meuwly & Hutson 1999; Skokov et al. 1999; Patrascu et al. 2014) was used. According to this procedure, as implemented in DUO, the \textit{ab initio} SOCs and EAMCs are multiplied by a morphing function \( F(z) \) represented by following expansion:

\[ F(z) = \sum_{k=0}^{N} B_k z^k (1 - z) + z B_\infty, \]  

(3)

where \( z \) is either taken as a damped-coordinate (for the \( a-S \) SOC) given by:

\[ z = (r - r_{ref}) e^{-\beta_2 (r - r_{ref})^2 - \beta_4 (r - r_{ref})^4}, \]  

(4)

see also Prajapat et al. (2017) and Yurchenko et al. (2018), or as the Šurkus variable \( z = \xi \) (all other SOCs and EAMCs). Here \( r_{ref} \) is a reference position equal to \( r_e \) by default and \( \beta_2 \)
and $\beta_4$ are damping factors. When used with morphing, the parameter $B_\infty$ is usually fixed to 1.

EAMCs give rise to the $\Lambda$ doubling (parity doubling) for states with $\Lambda$ (projection of the electronic angular momentum) greater than 0.

The PECs, SOCs and EAMCs, representing the final, refined spectroscopic model are shown in Figs. 1-3 and given as part of the supplementary material inside the DUO input file.

MgO is an ionic system. This leads to large permanent dipole moments which vary strongly with $r$ and, because the degree of charge separation changes strongly between excited states, large transition dipoles. Similar behaviour was observed in the previous ExoMol study on CaO (Yurchenko et al. 2016). The diagonal DMCs ($X - X$, $a - a$, $A - A$, $b - b$) as well as the transition DMC for $B - A$ are taken from the ab initio work of Bauschlicher & Schwenke (2017) who used an MRCI calculation with an aug-cc-pV5Z. All other TDMCs ($A - X$, $B - X$, $a - c$) were computed ab initio as part of the present work. The corresponding electronic transition dipole moments are shown in Fig. 4. All (T)DMCs except for $B - B$, $B - A$, $b - b$ were represented analytically using the damped-$z$ expansion in Eq. (3). This was done in order to reduce the numerical noise in the calculated intensities for high overtones, see recommendations by Medvedev et al. (2016). The corresponding expansion parameters as well as their grid representations can be found in the DUO input files provided as supplementary data. Büsener et al. (1987) reported experimental electric dipole moments for the $X^1\Sigma^+$ and $A^1\Pi$ states ($v = 0$) using Stark quantum-beat spectroscopy, 6.2(6) D and 5.94(24) D, respectively. Our values of the vibrationally ($v = 0$) averaged dipole moments based on the ab initio dipole moment of Bauschlicher & Schwenke (2017) are 5.99 D and 5.68 D, respectively, which agree well with these experimental value. The dipole moment curves (DMCs) are shown in Figure 4.

DUO input files which fully specify our final spectroscopic model are given as part of the supplementary data.

3 RESULTS

4 ACCURACY OF THE FITS

The ab initio PECs ans SOCs were refined by fitting to the 2457 experimental transition frequencies (see Table 1) augmented with 756 MARVEL term values for $^{24}$Mg$^{16}$O. The data
Figure 4. Dipole moment curves and transition dipole moments due to Bauschlicher & Schwenke (2017) (X − X, A − A, a − a, B − B, A − X, B − X) and Maatouk et al. (2010) (A − X) presented as a function of the nuclear separation.

Table 2. Selections of the Obs.−Calc. residuals, in cm\(^{-1}\), for the microwave transition frequencies (X, \(v' = v''\), \(R(J)\)) of the three isotopologues of Mg\(^{16}\)O. The Obs. term values are from Töring & Hoeft (1986).

| Iso     | J  | \(v'\) | Obs    | Calc   | Obs.-Calc. |
|---------|----|--------|--------|--------|------------|
| \(^{26}\)MgO 1 0 | 2.217914 | 2.217857 | 0.000057 |
| \(^{26}\)MgO 2 0 | 3.326801 | 3.326716 | 0.000085 |
| \(^{26}\)MgO 2 1 | 3.396283 | 3.396159 | 0.000124 |
| \(^{26}\)MgO 7 0 | 8.869430 | 8.869204 | 0.000226 |
| \(^{25}\)MgO 2 0 | 3.377244 | 3.377161 | 0.000083 |
| \(^{24}\)MgO 1 0 | 2.288127 | 2.288066 | 0.000061 |
| \(^{24}\)MgO 1 1 | 2.266805 | 2.266722 | 0.000083 |
| \(^{24}\)MgO 2 0 | 3.432117 | 3.432026 | 0.000091 |
| \(^{24}\)MgO 2 1 | 3.400133 | 3.400008 | 0.000125 |
| \(^{24}\)MgO 2 2 | 3.368112 | 3.368431 | -0.000319 |
| \(^{24}\)MgO 7 0 | 9.150138 | 9.149896 | 0.000242 |
| \(^{24}\)MgO 7 1 | 9.064847 | 9.064513 | 0.000334 |
| \(^{24}\)MgO 7 2 | 8.979447 | 8.980309 | -0.000856 |

used in the fit are provided as part of the spectroscopic model. The root mean square (RMS) errors as observed minus calculated (Obs. – Calc.) residues are 0.029 cm\(^{-1}\) for all transition wavenumbers, or 0.009 cm\(^{-1}\), 0.002 cm\(^{-1}\), 0.016 cm\(^{-1}\) and 0.04 cm\(^{-1}\) for the X, a, A and B states, respectively. The MARVEL term values are reproduced with an RMS error of 0.05 cm\(^{-1}\). Figure 5 gives an overview of the Obs. – Calc. residues with more detailed results given in Tables 3, 4 and 5.

Line lists for the other isotopologues of MgO were generated using the curves with no allowance for any failure of the Born-Oppenheimer approximation. This means that while we expect these line lists to still be accurate, some loss of accuracy is to be expected. The pure rotational frequencies of \(^{25}\)Mg\(^{16}\)O and \(^{26}\)Mg\(^{16}\)O do show excellent agreement with experiment, see Table 2.
Table 3. Selections of the Obs.−Calc. residuals, in cm$^{-1}$, for the $X$ state and $a$ states ($v = 0$) for the refined model of $^{24}\text{Mg}^{16}\text{O}$. The Obs. term values are represented by our MARVEL values.

| $J$ | Obs  | Calc  | Obs.-Calc. | $J$ | Obs  | Calc  | Obs.-Calc. |
|-----|------|-------|------------|-----|------|-------|------------|
| 1   | 1.1441 | 1.1441 | 0.0001 | 1   | 2551.297 | 2551.290 | 0.007 |
| 5   | 17.1596 | 17.1597 | -0.0001 | 5   | 2556.295 | 2556.297 | -0.008 |
| 7   | 32.0276 | 32.0296 | -0.0020 | 7   | 2560.319 | 2560.326 | -0.006 |
| 9   | 51.4667 | 51.4724 | -0.0057 | 9   | 2565.293 | 2565.309 | -0.015 |
| 11  | 75.4784 | 75.4860 | -0.0076 | 11  | 2571.361 | 2571.365 | -0.004 |
| 13  | 104.6584 | 104.0679 | -0.0095 | 13  | 2578.322 | 2578.324 | -0.002 |
| 15  | 137.2076 | 137.2153 | -0.0077 | 15  | 2586.413 | 2586.416 | -0.003 |
| 17  | 174.9176 | 174.9246 | -0.0070 | 17  | 2595.338 | 2595.342 | -0.005 |
| 19  | 217.1868 | 217.1919 | -0.0051 | 19  | 2605.470 | 2605.477 | -0.007 |
| 21  | 264.0096 | 264.0129 | -0.0033 | 21  | 2616.352 | 2616.360 | -0.008 |
| 23  | 315.3829 | 315.3826 | 0.0003 | 23  | 2628.539 | 2628.545 | -0.007 |
| 25  | 371.2966 | 371.2959 | 0.0007 | 25  | 2641.369 | 2641.376 | -0.006 |
| 27  | 431.7481 | 431.7467 | 0.0014 | 27  | 2655.606 | 2655.617 | -0.011 |
| 29  | 496.7330 | 496.7299 | 0.0040 | 29  | 2670.374 | 2670.386 | -0.012 |
| 31  | 566.2387 | 566.2358 | 0.0029 | 31  | 2686.657 | 2686.689 | -0.032 |
| 33  | 640.2592 | 640.2601 | -0.0009 | 33  | 2703.360 | 2703.387 | -0.027 |
| 35  | 718.7909 | 718.7940 | -0.0031 | 35  | 2721.727 | 2721.757 | -0.030 |
| 37  | 801.8280 | 801.8294 | -0.0014 | 37  | 2740.350 | 2740.375 | -0.026 |
| 39  | 889.3578 | 889.3576 | 0.0002 | 39  | 2760.792 | 2760.815 | -0.023 |

Table 4. Selections of the Obs.−Calc. residuals, in cm$^{-1}$, for the $A$ and $B$ term values ($v = 0$, $+$) for the refined model of $^{24}\text{Mg}^{16}\text{O}$. The Obs. term values are represented by our MARVEL values.

| $A$ $^1\Sigma^+$, $v = 0$, $+ \Omega = 1$ | $B$ $^1\Pi$, $v = 0$, $\Omega = 1$ |
|-----|-------|-----|-------|-----|-----|-----|-----|-----|-----|-----|
| $J$  | Obs  | Calc  | Obs.-Calc. | $J$  | Obs  | Calc  | Obs.-Calc. |
| 9   | 3548.585 | 3548.563 | 0.022 | 0   | 20003.59 | 20003.593 | 0.002 |
| 11  | 3569.710 | 3569.685 | 0.025 | 2   | 20007.07 | 20007.073 | 0.003 |
| 13  | 3594.843 | 3594.825 | 0.018 | 4   | 20015.19 | 20015.194 | 0.004 |
| 15  | 3623.999 | 3623.980 | 0.020 | 6   | 20027.95 | 20027.954 | 0.002 |
| 17  | 3657.260 | 3657.146 | 0.113 | 12  | 20094.05 | 20094.057 | -0.006 |
| 19  | 3694.343 | 3694.321 | 0.022 | 16  | 20161.27 | 20161.290 | -0.011 |
| 21  | 3735.522 | 3735.500 | 0.021 | 20  | 20201.84 | 20201.845 | -0.006 |
| 23  | 3775.646 | 3775.634 | 0.011 | 22  | 20296.81 | 20296.818 | -0.001 |
| 25  | 3804.825 | 3804.819 | 0.007 | 26  | 20410.24 | 20410.238 | 0.002 |
| 27  | 3833.089 | 3832.851 | 0.018 | 28  | 20473.85 | 20473.854 | 0.001 |
| 29  | 3865.002 | 3855.996 | 0.006 | 30  | 20542.08 | 20542.065 | 0.019 |
| 31  | 3883.034 | 3883.012 | 0.022 | 32  | 20614.86 | 20614.864 | 0.000 |
| 33  | 3911.167 | 3911.159 | 0.007 | 34  | 20692.23 | 20692.245 | -0.009 |
| 35  | 3940.174 | 3940.157 | 0.018 | 36  | 20774.18 | 20774.200 | -0.011 |
| 37  | 4001.292 | 4001.277 | 0.014 | 38  | 20860.71 | 20860.721 | -0.007 |
| 39  | 4053.413 | 4053.422 | -0.009 | 40  | 20951.81 | 20951.800 | 0.009 |
| 41  | 4147.411 | 4147.428 | -0.019 | 42  | 21047.41 | 21047.428 | -0.019 |
Table 5. Selections of Obs. - Calc. residuals, in cm$^{-1}$, showing the vibrational accuracy of the refined model. The Obs. term values are represented by our MARVEL values.

| $J$ | parity | State | $v$ | $\Omega$ | Obs   | Calc   | Obs.-Calc. |
|-----|--------|-------|----|---------|-------|--------|------------|
| 1   | -      | $X$   | 0  | 0       | 1.144 | 1.144  | 0.0001     |
| 6   | +      | $X$   | 2  | 0       | 1562.7462 | 1562.715 | 0.0314    |
| 1   | +      | $a$   | 0  | 0       | 2551.2967 | 2551.29  | 0.0068    |
| 3   | +      | $a$   | 1  | 0       | 3193.0857 | 3193.105 | 0.0190    |
| 7   | -      | $A$   | 0  | -1      | 3539.537 | 3539.509 | 0.0280    |
| 1   | -      | $A$   | 1  | -1      | 4160.8965 | 4160.902 | 0.0058    |
| 3   | +      | $A$   | 2  | 1       | 4814.6699 | 4814.617 | 0.0527    |
| 3   | +      | $A$   | 3  | 1       | 5455.8189 | 5455.807 | 0.0123    |
| 0   | +      | $B$   | 0  | 0       | 20033.5941 | 20033.59 | 0.0016    |
| 0   | +      | $B$   | 1  | 0       | 20818.1573 | 20818.14 | 0.0126    |

Figure 5. The Obs. - Calc. residuals on different states as a function of the wavenumber.

4.1 Partition function

Partition functions, $Q(T)$, were computed with DUO in steps of 1 K by explicit summation of the calculated energy levels. ExoMol always produces partition functions according to the HITRAN convention (Gamache et al. 2017) which explicitly includes the full atomic nuclear spin degeneracy, $g_{ns}$. Since the nuclear spins of $^{24}\text{Mg}$ and $^{16}\text{O}$ are both zero, therefore the nuclear statistical weight is 1. There is no need to scale the Sauval & Tatum (1984) or Barklem & Collet (2016) partition functions for comparison. The nuclear spins of $^{26}\text{Mg}$ and $^{18}\text{O}$ are also zero, while the $^{25}\text{Mg}$ and $^{17}\text{O}$ have the nuclear spins of $5/2$, which result in the nuclear spin statistical factor of 6 for $^{25}\text{Mg}^{16}\text{O}$ and $^{24}\text{Mg}^{17}\text{O}$.

At 300 K we obtain a value of $Q = 374.651$ which is in excellent agreement with the value.
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Figure 6. Partition function of $^{24}$Mg$^{16}$O produced from the ExoMol line list compared with Sauval & Tatum (1984) and Barklem & Collet (2016).

of 374.621 used in the JPL database (Pickett et al. 1998). Figure 6 plots our temperature-dependent partition function and compared with those computed by Sauval & Tatum (1984) and by Barklem & Collet (2016). All three data sets agree very well below 3500 K with the ExoMol results being higher than Barklem & Collet or Sauval & Tatum. We believe our energies to be more complete which should explain why our partition function is higher. However, above about 5000 K electronically excited states of MgO, not considered in this calculation, will become increasingly thermally occupied. For this reason and because the abundance of MgO is likely to small in this temperature region we used a 5000 K upper temperature limit in this study.

The partition functions for all isotopologues are given in the supplementary data.

4.2 Lifetimes

Lifetimes for the states are provided as part of the DUO calculations, detailed methodology is given by Tennyson et al. (2016). Lifetimes of the excited states have only been studied experimentally for the $B^{1}\Sigma^+$ state and in this case there is disagreement between previous studies on the lifetime of the $v = 0$ state. The lifetime was measured to be 32.7±1.7 ns by Diffenderfer et al. (1983) using fluorescence decay, 22.5±1.5 ns by Büsener et al. (1987)
Figure 7. Lifetimes of the four low-lying states of $^{24}\text{Mg}^{16}\text{O}$ computed by summation of the Einstein-A coefficients.

$(J = 1)$ using Stark quantum-beat spectroscopy, and 21.5±1.8 ns by Naulin et al. (1991) $(J = 70)$ also using fluorescence decay. Maatouk et al. (2010) calculated the $J = 0$ and $J = 70$ lifetimes as 33.3 and 22.0 ns, respectively suggesting a significant decrease in lifetime with rotational excitation.

Our lifetimes ($B^{1}\Sigma^+, v = 0$) for $J = 0$ and $J = 70$ are 21.8 ns and 21.7 ns, respectively, in agreement with the measurements of Büsener et al. (1987) and Naulin et al. (1991). An overview of the lifetimes of MgO for the four lowest electronic states is presented in Figure 7. The shortest-lived states are from $B^{1}\Sigma^+$. The lowest states ($v = 0$, small $J$) of $X^{1}\Sigma^+$ and $a^{3}\Pi$ have very long lifetime.

4.3 Line lists

Line lists were generated by consider all lower states up to 24 000 cm$^{-1}$, upper states up to 37 500 cm$^{-1}$ and rotationally excited states up to $J = 300$. These parameters are sufficient for completeness up to temperatures of 5000 K and wavenumbers up to 33 000 cm$^{-1}$ or wavelengths longer than 0.3 µm, although at higher temperatures the line lists will be not quite complete for the highest wavenumbers.

The line list for $^{24}\text{Mg}^{16}\text{O}$ contains 72 833 173 transitions between 186 842 states. The line list have been formatted into the ExoMol format (transition files and state files) (Tennyson 2018 RAS, MNRAS 000, 1–24).
Table 6. Extract from the states file for $^{24}$Mg$^{16}$O.

| $i$ | $E$ (cm$^{-1}$) | $g_i$ | $J$ | $\tau$ (s$^{-1}$) | $g$ | $+/-$ | $e/f$ | State | $v$ | $\Lambda$ | $\Sigma$ | $\Omega$ |
|-----|-----------------|-------|-----|-------------------|-----|--------|--------|--------|-----|--------|--------|-------|
| 636 | 1.144048        | 3     | 1   | 1.7793E+05        | 0.000000 | - | e      | X1Sigma+ | 0   | 0      | 0      | 0     |
| 637 | 775.871080      | 3     | 1   | 1.3597E+00        | 0.000000 | - | e      | X1Sigma+ | 1   | 0      | 0      | 0     |
| 638 | 1540.259721     | 3     | 1   | 6.3338E-01        | 0.000000 | - | e      | X1Sigma+ | 2   | 0      | 0      | 0     |
| 639 | 2294.147145     | 3     | 1   | 3.9856E-01        | 0.000000 | - | e      | X1Sigma+ | 3   | 0      | 0      | 0     |
| 640 | 2551.292291     | 3     | 1   | 8.2303E-02        | 0.527645 | - | e      | a3Pi    | 0   | -1     | 0      | -1    |
| 641 | 2622.22505      | 3     | 1   | 2.5848E-02        | -0.027585 | - | e      | a3Pi    | 0   | -1     | 1      | 0     |
| 642 | 3038.170256     | 3     | 1   | 2.2267E-01        | 0.000236 | - | e      | X1Sigma+ | 4   | 0      | 0      | 0     |
| 643 | 3193.107760     | 3     | 1   | 3.2736E-02        | 0.526013 | - | e      | a3Pi    | 1   | -1     | 0      | -1    |
| 644 | 3265.98397      | 3     | 1   | 2.0885E-02        | -0.026155 | - | e      | a3Pi    | 1   | -1     | 1      | 0     |
| 645 | 3504.293682     | 3     | 1   | 1.0652E-04        | 0.499992 | - | e      | A1Pi    | 0   | 1      | 0      | -1    |
| 646 | 3771.346664     | 3     | 1   | 9.6921E-02        | 0.002761 | - | e      | X1Sigma+ | 5   | 0      | 0      | 0     |
| 647 | 3824.775932     | 3     | 1   | 2.0612E-02        | 0.520372 | - | e      | a3Pi    | 2   | -1     | 0      | -1    |
| 648 | 3901.850493     | 3     | 1   | 1.8291E-02        | -0.023039 | - | e      | a3Pi    | 2   | -1     | 1      | 0     |
| 649 | 4160.902293     | 3     | 1   | 7.4729E-02        | 0.499992 | - | e      | A1Pi    | 1   | -1     | 0      | -1    |
| 650 | 4446.228208     | 3     | 1   | 1.5176E-02        | 0.538037 | - | e      | a3Pi    | 3   | -1     | 0      | -1    |
| 651 | 4479.741149     | 3     | 1   | 2.3166E-02        | -0.028181 | - | e      | a3Pi    | 3   | -1     | 1      | 0     |
| 652 | 4544.158030     | 3     | 1   | 2.7766E-02        | -0.009762 | - | e      | X1Sigma+ | 6   | 0      | 0      | 0     |
| 653 | 4809.732662     | 3     | 1   | 5.8409E-05        | 0.499993 | - | e      | A1Pi    | 2   | -1     | 0      | -1    |
| 654 | 5057.431336     | 3     | 1   | 1.2102E-02        | 0.530620 | - | e      | a3Pi    | 4   | -1     | 0      | -1    |
| 655 | 5117.344124     | 3     | 1   | 1.2082E-02        | -0.030073 | - | e      | a3Pi    | 4   | -1     | 1      | 0     |
| 656 | 5239.189020     | 3     | 1   | 7.8093E-02        | -0.000452 | - | e      | X1Sigma+ | 7   | 0      | 0      | 0     |
| 657 | 5450.913256     | 3     | 1   | 4.8307E-05        | 0.499994 | - | e      | A1Pi    | 3   | -1     | 0      | -1    |
| 658 | 5658.311999     | 3     | 1   | 1.0135E-02        | 0.528937 | - | e      | a3Pi    | 5   | -1     | 0      | -1    |

$i$: State counting number.
$E$: State energy in cm$^{-1}$.
$g_i$: Total statistical weight, equal to $g_{ns} (2J + 1)$.
$J$: Total angular momentum.
$\tau$: Lifetime (s$^{-1}$).
$g$: Landé $g$-factors.
$+/−$: Total parity.
$e/f$: Rotationless parity.
State: Electronic state.
$v$: State vibrational quantum number.
$\Lambda$: Projection of the electronic angular momentum.
$\Sigma$: Projection of the electronic spin.
$\Omega$: Projection of the total angular momentum, $\Omega = \Lambda + \Sigma$.

et al. 2013] with lifetimes of each state quoted. A extract of the states file is shown in Table 6 and a extract of the transition file is shown in Table 7. The line lists for isotopologues have comparable sizes.

5 SIMULATED SPECTRA

Absorption spectra at different temperatures are presented in Figure 8. The contribution of each band is shown in Figure 9. The green ($B − X$) and red ($B − A$) singlet band systems are the strongest bands and show a significant overlap at visible wavelengths. All spectral simulations employed the ExoCross code [Yurchenko et al. 2018].

Comparisons with the previous experimental works have been made to assess the quality of our computed line list. The rotational X band in the form of a stick spectrum is shown in Figure 10, where it is compared to the experimentally determined transitions from the JPL.
Figure 8. Simulated absorption spectra of MgO at 5 different temperatures. The spectrum becomes increasingly flat with increasing temperature; the difference with temperature is most marked around 20000 cm$^{-1}$.

Figure 9. Contribution of each band to the simulated absorption spectra of MgO at 2000 K.
Table 7. Extract from the transitions file for $^{24}\text{Mg}^{16}\text{O}$.

| $f$ | $i$ | $A_{fi}$ (s$^{-1}$) | $\tilde{\nu}$ (cm$^{-1}$) |
|-----|-----|--------------------|-----------------|
| 36757 | 37183 | 7.7028E-12 | 0.098041 |
| 32237 | 31809 | 2.1383E-14 | 0.098067 |
| 32909 | 32497 | 1.0981E-11 | 0.098167 |
| 90382 | 90758 | 2.8824E-13 | 0.098189 |
| 98009 | 98376 | 3.5386E-14 | 0.098192 |
| 49202 | 49606 | 1.5586E-12 | 0.098197 |
| 123918 | 124241 | 1.7154E-15 | 0.098208 |
| 91640 | 91262 | 4.8358E-13 | 0.098261 |
| 83152 | 82769 | 9.9825E-15 | 0.098285 |
| 7957 | 8392 | 4.4448E-11 | 0.098298 |
| 101679 | 102046 | 5.2911E-14 | 0.098322 |
| 82876 | 83259 | 2.4564E-18 | 0.098324 |

$f$ = state number of final state  
$i$ = state number of initial state  
$A_{fi}$ = Einstein-A coefficient  
$\tilde{\nu}$ = transition wavenumber

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure10.png}
\caption{Comparison of the ExoMol spectrum and JPL.}
\end{figure}

database (Pickett et al. 1998). The JPL spectrum is based on the dipole moment of 6.88 D taken from an old ab initio calculation due to Fowler & Sadlej (1991). Our vibrational averaged ($v = 0$) value is 5.99 D, which is the same as given by Bauschlicher & Schwenke (2017). We expect this new value to be represent an improvement which suggests that the current JPL intensities are about 30% too strong and, correspondingly, the observational upper limits for the ISM (Turner & Steimle 1985; Sakamoto et al. 1998) to be about 30% too low.
5.1 The red band

Dreyer et al. (2001) made excitation scans using the Laser-induced fluorescence excitation spectroscopy for the $B - A$ transitions. For the 588 nm to 632 nm range there is overall agreement as shown in Figure 11. The $(0, 0)$ and $(0, 1)$ bandheads give a good match, whereas the bandheads for the higher state are not as clear as the lower ones.

Figure 12 shows a spectrum for the 16115 cm$^{-1}$ to 16150 cm$^{-1}$ region from Dreyer et al. (2001). The main peaks for the $(0, 1)$ lines generally agree whereas the magnitudes can differ, see Figure 13. The $(0, 1)$ bandhead region cannot be resolved between 1584 nm and 1586 nm otherwise the resolved peaks agree with experiment within 0.1 nm. This figure shows the individual contributions from all three major isotopologues assuming the terrestrial abundance (0.79/0.10/0.11 for $^{24}\text{Mg}^{16}\text{O}/^{25}\text{Mg}^{16}\text{O}/^{26}\text{Mg}^{16}\text{O}$, respectively).

Red band studies made by Pasternack et al. (1978) also show good agreement with the ExoMol data around the $(1, 1)$ band; Figure 14 gives a comparison of the emission spectrum simulated using the ExoMol line list with the laser-induced fluorescence of MgO in acetylene-air flames (Pasternack et al. 1978). In order to match the experiment, the vacuum wavelength was re-scaled to the air-acetylene wavelength using the refractive indexes from Ciddor (1996) assuming a 45:55 mixture. This ratio was adjusted to match the experimental spectrum.

5.1.1 The green band

For the 495 nm to 501 nm region of the $B - X$ transitions, Figure 15 compares our data with the laser-induced fluorescence spectrum of Pasternack et al. (1978). The shapes, which are largely determined by bandheads, of the two spectra are similar. The same wavelength calibration (vacuum to air-acetylene) as above was applied. The ExoMol spectrum agrees very well also with the higher resolution experimental data from the same region, measured between 499.7 nm and 500.1 nm using Stark quantum-beat spectroscopy by Büsener et al. (1987), see Figure 16, where no calibration was required. For these simulations the non-LTE model was assumed based on two temperatures, rotational $T_{\text{rot}}$ and vibrational $T_{\text{vib}}$, as implemented in Duo. The temperatures selected to match the experimental emission spectra were 1000 K and 2500 K, respectively.

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1 The refractive index data are taken from M. N. Polyanskiy’s “Refractive index database”, https://refractiveindex.info.
Figure 11. Comparison of the ExoMol spectrum (lower) and experimental spectrum from Dreyer et al. (2001) (upper) in the range of 588 nm to 633 nm. The (0,0) and (0,1) bandheads agree whereas the other bandheads cannot be clearly distinguished from each other.

6 CONCLUSION

Accurate and complete line lists, known as LiTY, for $^{24}$Mg$^{16}$O, $^{25}$Mg$^{16}$O, $^{26}$Mg$^{16}$O are computed using high level ab initio DMCs as well as a spectroscopically refined DUO model. Our work displays good agreement with the most theoretical and experimental studies made in the past. The lifetimes computed for ($B^{1}\Sigma^{+}, v = 0$) are 2.18 ns for $J = 0$ and 2.17 ns for $J = 70$, partially matching prior studies which disagree with each other. The partition functions agree with other theoretical studies for the temperature up to 5000 K.

With a valid temperature range up to 5000 K, the strong red and green bands between
Figure 12. Comparison of the ExoMol emission (2300 K) and experimental spectra from Dreyer et al. (2001) in the range of 16115 cm$^{-1}$ to 16150 cm$^{-1}$ using the Voigt profile with $\gamma = 1.1$ cm$^{-1}$ combined from the contributions from three main isotopologues, also shown, assuming the terrestrial abundance (0.79/0.10/0.11 for 24/25/26, respectively).

Figure 13. Comparison of the ExoMol absorption spectrum and experimental spectrum from Dreyer et al. (2001) in the range of 15840 cm$^{-1}$ to 15960 cm$^{-1}$ for the (1,0) band using the Gaussian line profile of HWHM=1 cm$^{-1}$ at $T = 2300$ K.

15000 and 20000 cm$^{-1}$ (0.66 to 0.5 $\mu$m) should be useful for detecting MgO in the atmospheres of cool stars, brown dwarfs and some exoplanets.

The LiTY line lists can be downloaded from the CDS, via ftp://cdsarc.u-strasbg.fr/pub/cats/J/MNRAS/, or http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/MNRAS/ or from www.exomol.com.

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Figure 14. Comparison of the ExoMol emission spectrum and experimental spectrum from Pasternack et al. (1978) around the (1,1) bandhead using the Voigt profile with $\gamma = 1.1 \text{ cm}^{-1}$ at $T = 2500$ K. The vacuum wavelength was re-calibrated to the acetylene-air wavelength to match the experiment.

Figure 15. Comparison of the Exomol emission spectrum and experimental spectrum from Pasternack et al. (1978) in the range of 495 nm to 501 nm. The ExoMol spectrum was generated using the Voigt profile with $\gamma = 1.1 \text{ cm}^{-1}$ at $T = 2500$ K. The vacuum wavelength was re-calibrated to the acetylene-air wavelength to match the experiment.

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Figure 16. Comparison of the absorption ExoMol spectrum and experimental spectrum from Büsener et al. (1987) in the range of 499.7 nm to 500.1 nm in the green band using the Gaussian line profile of HWHM=1 cm$^{-1}$, at $T_{\text{rot}} = 1000$ K and $T_{\text{rot}} = 2500$ K.

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