

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 rovibration 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: $^{24}\text{Mg}^{16}\text{O}$, $^{25}\text{Mg}^{16}\text{O}$, $^{26}\text{Mg}^{16}\text{O}$, $^{24}\text{Mg}^{17}\text{O}$ and $^{24}\text{Mg}^{18}\text{O}$. The calculations use potential energy curves, spin-orbit and electronic angular momentum coupling 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 laboratory measurements. The $^{24}\text{Mg}^{16}\text{O}$ line list comprises 186 842 ($J \leq 320$) rovibronic states and 72 833 173 transitions with angular momenta, J , up to 300 and covering wavenumbers up to $33\,000\text{ cm}^{-1}$ ($\lambda > 0.3\ \mu\text{m}$). 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 in the CDS and ExoMol databases.

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

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 of Kelvin. The quantity of MgO at 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 was analysed during the 2009 Perseid meteor shower (Berezhnaya 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 on to grains (Sakamoto et al. 1998). The discovery of hot, rocky exoplanets has led to suggestions that the many compounds usually in the condensed phase, in particular MgO (Coppari et al. 2013), should be present in significant concentrations in the gas phases (Schaefer, Lodders & Fegley 2012; Tennyson & Yurchenko 2018). The detection of 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 *ab initio* curves for the present study. Another recent and accurate *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, *ab initio* studies of MgO were performed by Thommel, Klotz & Peyerimhoff (1989b) and Thommel, Klotz & Peyerimhoff (1989a) using the Multi-

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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''	\bar{E}'_{max}	\bar{E}''_{max}
Kagi & Kawaguchi (2006)	Microwave	$a^3\Pi$	$a^3\Pi$	0	0	12	7	7	13
		$X^1\Sigma^+$	$X^1\Sigma^+$	1	1	12	7	7	14
				2	2	12	7		
				3	3	12	7		
Brewer, Trajmar & Berg (1962)	Grating	$C^1\Sigma^-$	$A^1\Pi$	0	0	80	4	26414	26544
				1	1	65	21		
Trajmar & Ewing (1965)	Grating	$C^1\Sigma^-$	$A^1\Pi$	1	1	60	9	26387	26769
		$D^1\Delta$	$A^1\Pi$	0	0	61	1		
Singh (1973)	Ebert	$G^1\Pi$	$A^1\Pi$	1	1	43	4		
		$G^1\Pi$	$X^1\Sigma^+$	0	1	40	14	36388	39870
				0	0	38	16		
Singh (1973)	Ebert	$F^1\Pi$	$X^1\Sigma^+$	0	1	40	16		
				0	0	83	14	37686	37896
Antic-Jovanovic, Bojovic & Pesic (1976)	Grating	$E^1\Sigma^+$	$A^1\Pi$	0	0	56	36	34304	34173
Azuma et al. (1984)	LIF	$B^1\Sigma^+$	$X^1\Sigma^+$	0	0	40	0	19971	20062
Civis, Hedderich & Blom (1991)	DLFR	$X^1\Sigma^+$	$X^1\Sigma^+$	1	1	56	0		
				1	0	32	6	766	792
Ip et al. (1991)	LIF	$B^1\Sigma^+$	$a^3\Pi$	2	1	28	7		
				0	0	48	4	16735	27256
		$D^1\Delta$	$a^3\Pi$	1	1	48	6		
Kagi et al. (1994)	FTS	$A^1\Pi$	$X^1\Sigma^+$	0	0	33	1		
				1	1	17	1	2644	5452
				2	0	67	3		
				3	0	58	3		
				2	1	31	11		
				0	1	37	8		

Notes. Microwave = Microwave spectroscopy

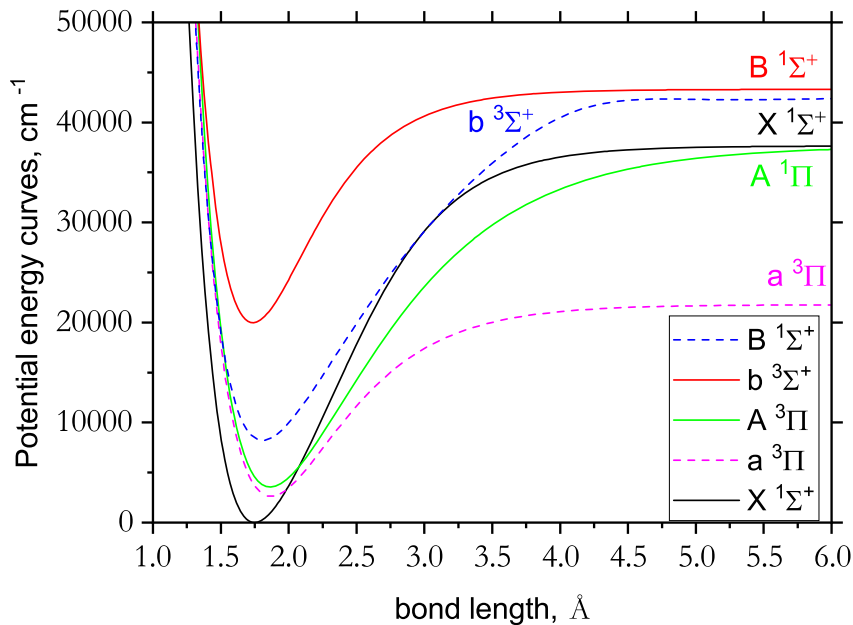
Grating = Grating spectrograph

Ebert = Ebert spectrograph

DLFR = Diode-laser flame spectrometer

LIF = Laser-induced fluorescence spectroscopy

FTS = Fourier Transform Spectrometer

**Figure 1.** Refined potential energy curves (PECs) of MgO used to produce the line list as part of the final spectroscopic model.

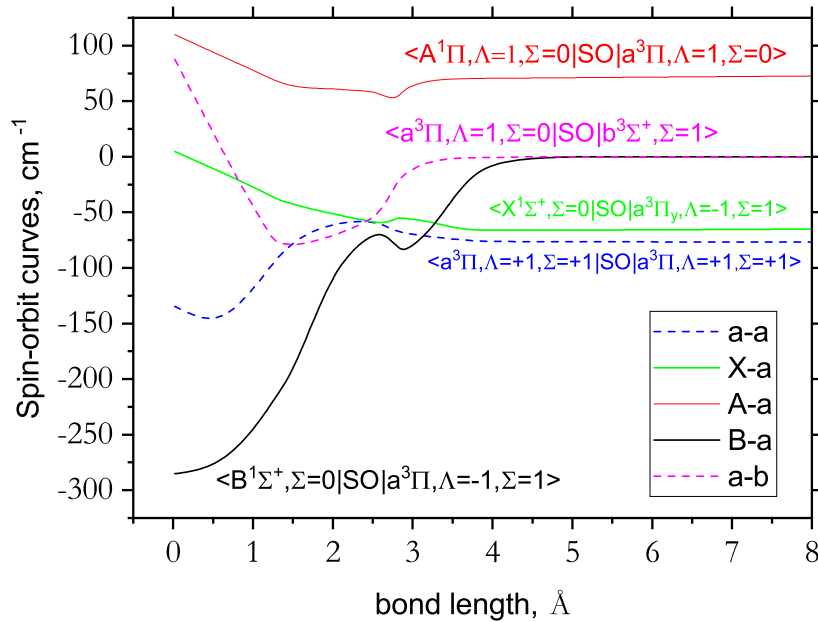


Figure 2. Empirical spin-orbit (SO) couplings (*ab initio* values morphed by DUO) in the spherical representation.

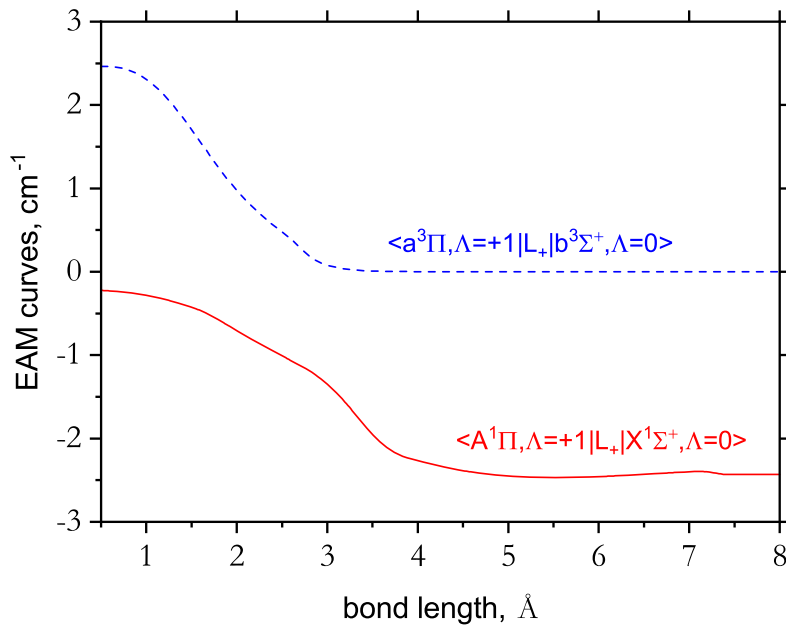


Figure 3. Empirical electronic angular momentum (*ab initio* values morphed by DUO) in the spherical representation.

reference double configuration interaction (MRDCI) method for various states. None of these works reported the electronic angular momenta of MgO.

Limited work has 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 that may be present in the atmospheres of exoplanets, brown dwarfs and cool stars (Tennyson & Yurchenko 2012). The ExoMol database (Tennyson et al. 2016a) currently contains 52 molecules, ranging from diatomic to polyatomic molecules and ions (Tennyson & Yurchenko 2018). However, only a handful of metal oxides are available, namely CaO (Yurchenko et al. 2016c), VO (McKemmish, Yurchenko & Tennyson 2016), AlO (Patrascu, Tennyson & Yurchenko 2015) and

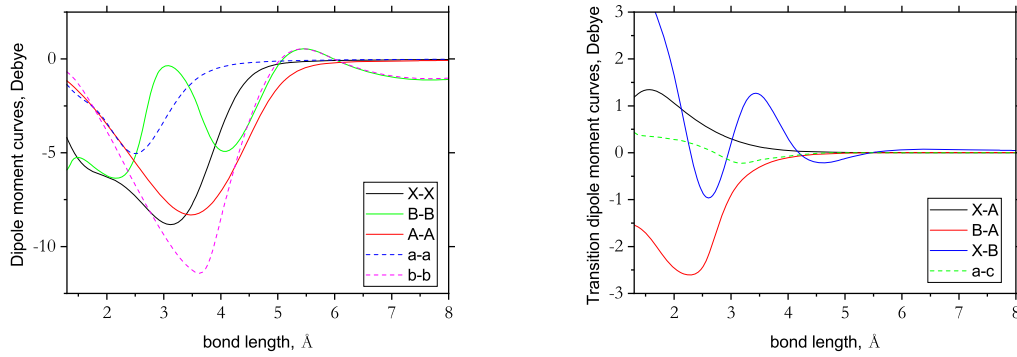


Figure 4. Dipole moment curves and transition dipole moments due to Bauschlicher & Schwenke (2017) ($X-X$, $A-A$, $a-a$, $b-b$, $B-B$, $A-B$, $B-X$, $a-c$) and Maatouk et al. (2010) ($A-X$) presented as a function of nuclear separation.

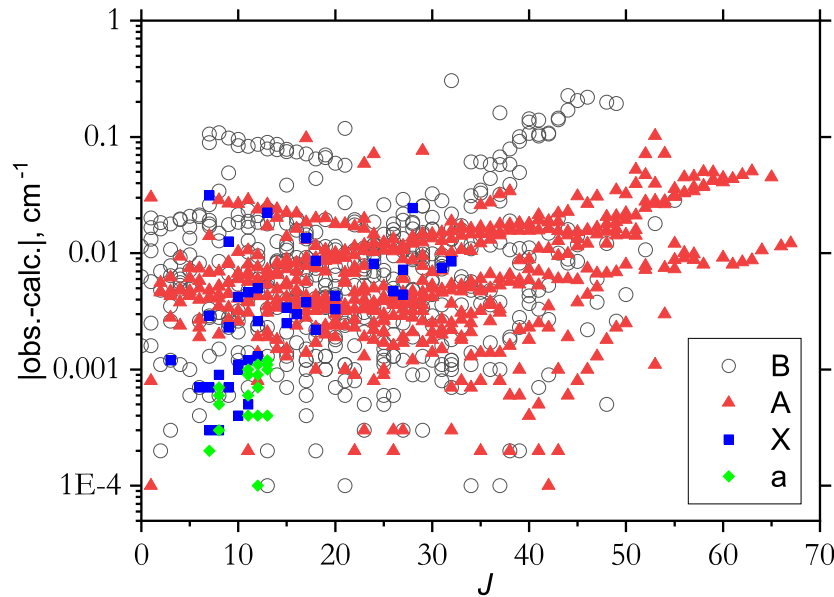


Figure 5. The Obs. – Calc. residuals for different states as a function of wavenumber.

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 Törring & Hoefl (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	3.296283	3.296159	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	8.980303	-0.000856

SiO (Barton, Yurchenko & Tennyson 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, Parigger & Hornkohl 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 lists are computed using the nuclear-motion program DUO (Yurchenko et al. 2016a), using a combination of empirical and *ab initio* potential energy curves (PECs), spin-orbit curves (SOCs) and electronic angular momentum curves (EAMCs) in conjunction with high-level *ab initio* (transition) dipole moment curves (TDMCs). The *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 $37\,250\text{ cm}^{-1}$, 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 3. Selection of Obs. – Calc. residuals, in cm^{-1} , for the X 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.

$X^1\Sigma^+, v = 0$				$a^3\Pi, v = 0, \Omega = 1$			
J	Obs	Calc	Obs. – Calc.	J	Obs	Calc	Obs. – Calc.
1	1.1441	1.144	0.0001	1	2551.297	2551.290	0.007
3	6.8671	6.8641	0.0030	2	2553.290	2553.300	–0.010
5	17.1596	17.1597	–0.0001	3	2556.289	2556.297	–0.008
7	32.0276	32.0296	–0.0020	4	2560.319	2560.326	–0.006
9	51.4667	51.4724	–0.0057	5	2565.293	2565.309	–0.015
11	75.4784	75.486	–0.0076	6	2571.361	2571.365	–0.004
13	104.0584	104.0679	–0.0095	7	2578.322	2578.324	–0.002
15	137.2076	137.2153	–0.0077	8	2586.413	2586.416	–0.003
17	174.9176	174.9246	–0.0070	9	2595.338	2595.342	–0.005
19	217.1868	217.1919	–0.0051	10	2605.470	2605.477	–0.007
21	264.0096	264.0129	–0.0033	11	2616.352	2616.360	–0.008
23	315.3829	315.3826	0.0003	12	2628.539	2628.545	–0.007
25	371.2966	371.2959	0.0007	13	2641.369	2641.376	–0.006
27	431.7481	431.7467	0.0014	14	2655.606	2655.617	–0.011
29	496.733	496.729	0.0040	15	2670.374	2670.386	–0.012
31	566.2387	566.2358	0.0029	16	2686.657	2686.689	–0.032
33	640.2592	640.2601	–0.0009	17	2703.360	2703.387	–0.027
35	718.7909	718.794	–0.0031	18	2721.727	2721.757	–0.030
37	801.828	801.8294	–0.0014	19	2740.350	2740.375	–0.026
39	889.3578	889.3576	0.0002	20	2760.792	2760.815	–0.023
41	981.3724	981.3695	0.0029				
43	1077.8619	1077.856	0.0064				
45	1178.8162	1178.805	0.0108				
47	1284.2229	1284.209	0.0142				
49	1394.0739	1394.054	0.0195				
51	1508.3514	1508.331	0.0205				
53	1627.0503	1627.026	0.0240				
55	1750.1546	1750.128	0.0266				
57	1877.6509	1877.623	0.0279				
59	2009.5313	2009.498	0.0333				
61	2145.7752	2145.739	0.0362				
61	2145.7752	2145.739	0.0362				

2 METHOD

2.1 Experimental data

Experimental transition frequencies for $^{24}\text{Mg}^{16}\text{O}$ involving a total of nine different electronic states were collected from various articles and are summarized in Table 1. The Measured Active Rotational-Vibrational Energy Levels (MARVEL) technique (Furtenbacher, Császár & Tennyson 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 *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 Fig. 1. They are augmented

by five SOCs, $X-a$, $a-a$, $A-a$, $B-a$ and $a-b$, which are shown in Fig. 2, and two EAMCs, $X-A$ and $a-b$, the x -components of which are shown in Fig. 3. The initial, *ab initio*, PECs were taken from Bauschlicher & Schwenke (2017). The SOCs and EAMCs were obtained *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 state-averaged complete active space self-consistent field (CASSCF) (SA-CASSCF) comprised (3,2,1,1) states of symmetries Σ^+ , Π , Δ and Σ^- , respectively. All electrons were correlated. The relativistic correction was estimated using the Douglas–Kroll method.

The nuclear motion program DUO (Yurchenko et al. 2016a) 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 0.02–8 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 below). A detailed

Table 4. Selection of 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.

$A^1\Pi, v = 0, \Omega = 1, +$				$B^1\Sigma^+, v = 0, +$			
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
14	3608.936	3608.919	0.017	6	20027.95	20027.954	0.002
15	3623.999	3623.980	0.020	8	20045.35	20045.353	0.001
16	3640.197	3640.085	0.111	10	20067.38	20067.388	–0.007
17	3657.260	3657.146	0.113	12	20094.05	20094.057	–0.006
18	3675.277	3675.263	0.014	14	20125.34	20125.359	–0.013
19	3694.343	3694.321	0.022	16	20161.27	20161.290	–0.011
20	3714.460	3714.447	0.013	18	20201.84	20201.845	–0.006
21	3735.522	3735.500	0.021	20	20247.01	20247.023	–0.005
22	3757.646	3757.634	0.011	22	20296.81	20296.818	–0.001
23	3780.699	3780.678	0.021	24	20351.22	20351.224	0.004
24	3804.825	3804.819	0.007	26	20410.24	20410.238	0.002
25	3829.869	3829.851	0.018	28	20473.85	20473.854	0.001
26	3856.002	3855.996	0.006	30	20542.08	20542.065	0.019
27	3883.034	3883.012	0.022	32	20614.86	20614.864	0.000
28	3911.167	3911.159	0.007	34	20692.23	20692.245	–0.009
29	3940.174	3940.157	0.018	36	20774.18	20774.200	–0.011
31	4001.292	4001.277	0.014	38	20860.71	20860.721	–0.007
32	4033.413	4033.422	–0.009	40	20951.81	20951.800	0.009
				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	Ω	Obs	Calc	Obs. – Calc.
1	–	X	0	0	1.1441	1.144	0.0001
1	–	X	1	0	775.8723	775.8711	0.0012
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	20003.5941	20003.59	0.0016
0	+	B	1	0	20818.1573	20818.14	0.0126

description of the methodology is given by Yurchenko et al. (2016a) and Tennyson et al. (2016c).

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) potential with the form

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

where $D_e = A_e - V_e$ is the dissociation energy, r_e is the equilibrium distance of the PEC and ξ is the Šurkus variable (Šurkus, Rakauskas & Bolotin 1984). The Šurkus variable is defined as

$$\xi = \frac{r^p - r_{\text{ref}}^p}{r^p + r_{\text{ref}}^p}, \quad (2)$$

where p is a non-zero real number parameter, r_{ref} is a reference position and $r_{\text{ref}} = r_e$ in this case. The b -state *ab initio* PEC was not used in the refining procedure and therefore did not need

to be represented analytically. The *ab initio* point values were interpolated on the DUO grid using cubic splines (Yurchenko et al. 2016a).

The lowest dissociation limit from MgO is to the $a^3\Pi$ asymptote ($\text{Mg}(^1S)$ and $\text{O}(^3P)$), 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 $\text{O}(^1D)$, 4.67 eV. This is also the asymptote as for the $A^1\Pi$ state. Adding the atomic separation of $\text{O}(^3P)$ and $\text{Mg}(^3P)$ 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 equation (1) used in this work.

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

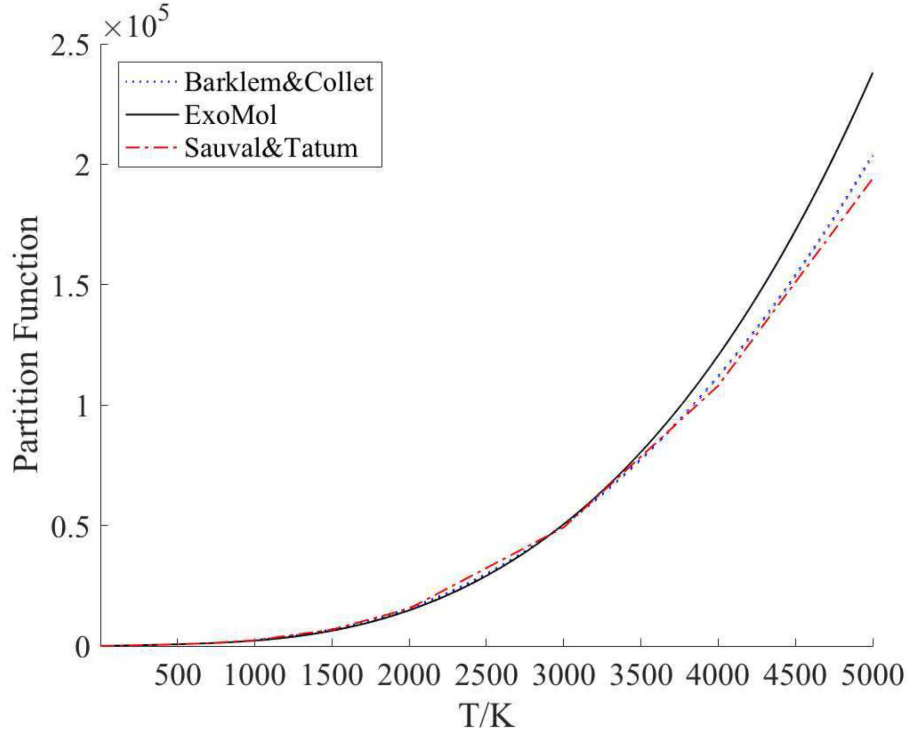


Figure 6. Partition function of $^{24}\text{Mg}^{16}\text{O}$ produced from the ExoMol line list compared with the results of Sauval & Tatum (1984) and Barklem & Collet (2016).

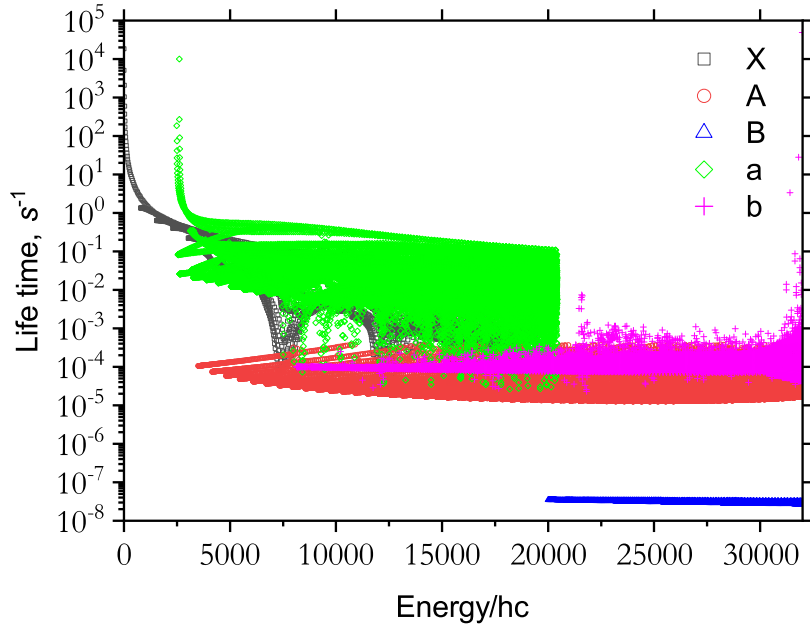


Figure 7. Lifetimes of the four low-lying states of $^{24}\text{Mg}^{16}\text{O}$ computed by summation of the Einstein A coefficients.

expansion:

$$F(z) = \sum_{k=0}^N B_k z^k (1-z) + z B_\infty, \quad (3)$$

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

$$z = (r - r_{\text{ref}}) e^{-\beta_2(r-r_{\text{ref}})^2 - \beta_4(r-r_{\text{ref}})^4} \quad (4)$$

(see also Prajapat et al. 2017; Yurchenko et al. 2018a) or as the Šurkus variable $z = \xi$ (all other SOCs and EAMCs). Here, r_{ref} is a reference position equal to r_c by default and β_2 and β_4 are damping factors. When used with morphing, the parameter B_∞ is usually fixed at 1.

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

Table 6. Extract from the state file for $^{24}\text{Mg}^{16}\text{O}$.

i	\tilde{E}	g_i	J	τ	g	+/-	elf	State	v	Λ	Σ	Ω
636	1.144048	3	1	1.77983E+05	0.000000	-	e	X1Sigma+	0	0	0	0
637	775.871080	3	1	1.35976E+00	0.000000	-	e	X1Sigma+	1	0	0	0
638	1540.259721	3	1	6.33385E-01	0.000002	-	e	X1Sigma+	2	0	0	0
639	2294.147145	3	1	3.98566E-01	0.000034	-	e	X1Sigma+	3	0	0	0
640	2551.292291	3	1	8.23030E-02	0.527645	-	e	a3Pi	0	-1	0	-1
641	2622.222505	3	1	2.58488E-02	-0.027585	-	e	a3Pi	0	-1	1	0
642	3038.170256	3	1	2.22267E-01	0.000236	-	e	X1Sigma+	4	0	0	0
643	3193.107760	3	1	3.27360E-02	0.526013	-	e	a3Pi	1	-1	0	-1
644	3265.983987	3	1	2.08686E-02	-0.026155	-	e	a3Pi	1	-1	1	0
645	3504.293682	3	1	1.05523E-04	0.499992	-	e	A1Pi	0	-1	0	-1
646	3771.346664	3	1	9.69221E-02	0.002761	-	e	X1Sigma+	5	0	0	0
647	3824.775932	3	1	2.06126E-02	0.520372	-	e	a3Pi	2	-1	0	-1
648	3901.850493	3	1	1.82913E-02	-0.023039	-	e	a3Pi	2	-1	1	0
649	4160.902293	3	1	7.47291E-05	0.499992	-	e	A1Pi	1	-1	0	-1
650	4446.228208	3	1	1.51760E-02	0.538037	-	e	a3Pi	3	-1	0	-1
651	4479.741149	3	1	2.31664E-02	-0.028181	-	e	a3Pi	3	-1	1	0
652	4544.158030	3	1	2.77669E-02	-0.009762	-	e	X1Sigma+	6	0	0	0
653	4809.732862	3	1	5.84090E-05	0.499993	-	e	A1Pi	2	-1	0	-1
654	5057.431336	3	1	1.21026E-02	0.530620	-	e	a3Pi	4	-1	0	-1
655	5117.344124	3	1	1.20824E-02	-0.030073	-	e	a3Pi	4	-1	1	0
656	5239.189020	3	1	7.80934E-02	-0.000452	-	e	X1Sigma+	7	0	0	0
657	5450.913256	3	1	4.83072E-05	0.499994	-	e	A1Pi	3	-1	0	-1
658	5658.311999	3	1	1.01359E-02	0.528937	-	e	a3Pi	5	-1	0	-1

Notes. i : state counting number

\tilde{E} : state energy in cm^{-1}

g_i : total statistical weight, equal to $g_{ns}(2J + 1)$

J : total angular momentum

τ : lifetime (s^{-1})

g : Landé g -factors

+/-: total parity

elf : rotationless parity

State: electronic state

v : state vibrational quantum number

Λ : projection of the electronic angular momentum

Σ : projection of the electronic spin

Ω : projection of the total angular momentum, $\Omega = \Lambda + \Sigma$

Table 7. Extract from the transition file for $^{24}\text{Mg}^{16}\text{O}$.

f	i	$A_{fi}(\text{s}^{-1})$	$\bar{\nu}(\text{cm}^{-1})$
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

Notes. f : state number of final state

i : state number of initial state

A_{fi} : Einstein A coefficient

$\bar{\nu}$: transition wavenumber

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 that 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. 2016b). 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 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 equation (3). This was done in order to reduce the numerical noise in the calculated intensities for high overtones; see the 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, Heinrich & Hese (1987) reported experimental electric dipole moments for the $X^1\Sigma^+$ and $A^1\Pi$ states ($v = 0$) using

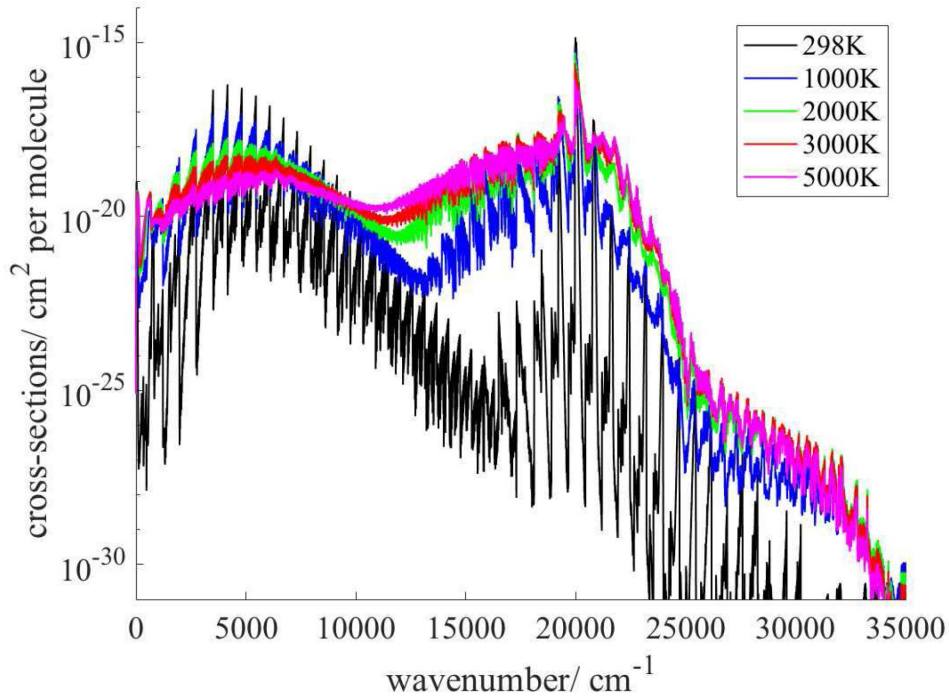


Figure 8. Simulated absorption spectra of MgO at five different temperatures. The spectrum becomes increasingly flat with increasing temperature: the difference with temperature is most marked around 20 000 cm^{-1} .

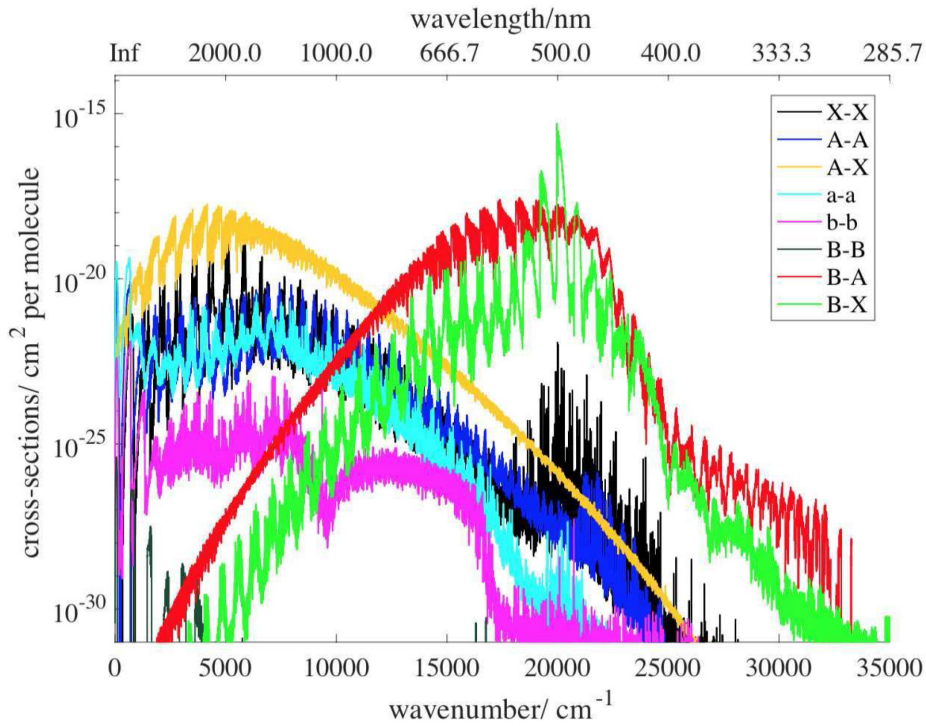


Figure 9. Contribution of each band to the simulated absorption spectra of MgO at 2000 K.

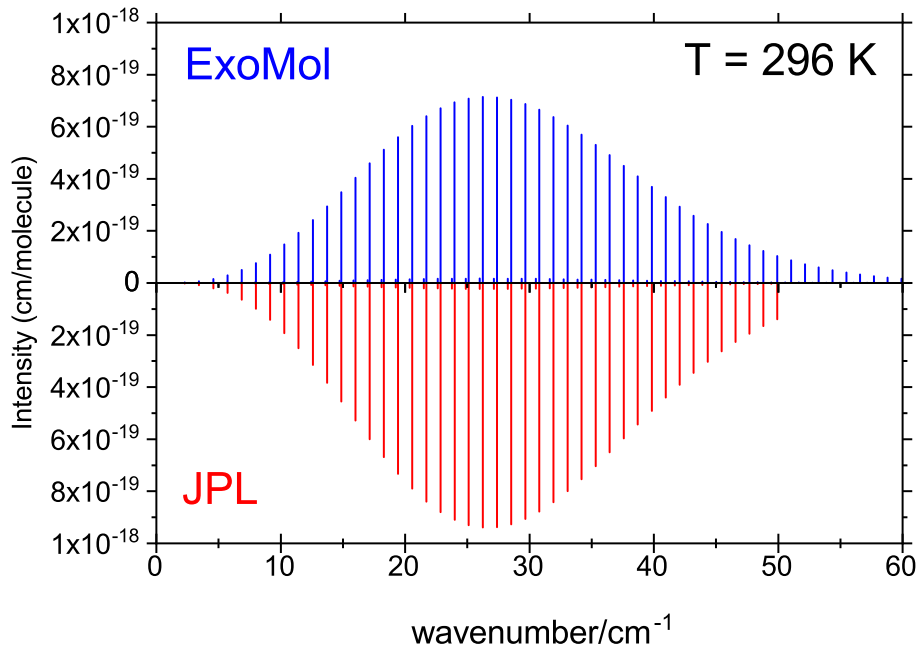


Figure 10. Comparison of the ExoMol spectrum and JPL.

Stark quantum-beat spectroscopy of 6.2(6) D and 5.94(24) D (where D denotes Debye), 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 the experimental values. The dipole moment curves (DMCs) are shown in Fig. 4.

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

3 RESULTS

3.1 Accuracy of the fits

The *ab initio* PECs and SOCs were refined by fitting to 2457 experimental transition frequencies (see Table 1), augmented with 756 MARVEL term values for $^{24}\text{Mg}^{16}\text{O}$. The data 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, 0.002, 0.016 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} . Fig. 5 gives an overview of the Obs. – Calc. residues, with more detailed results given in Tables 2, 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 still to be accurate, some loss of accuracy is to be expected. The pure rotational frequencies of $^{25}\text{Mg}^{16}\text{O}$ and $^{26}\text{Mg}^{16}\text{O}$ do show excellent agreement with experiments: see Table 2.

3.2 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}Mg and ^{16}O are both zero, 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}Mg and ^{18}O are also zero, while ^{25}Mg and ^{17}O have nuclear spins of 5/2, which results 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 of 374.621 used in the JPL database (Pickett et al. 1998). Fig. 6 plots our temperature-dependent partition function compared with those computed by Sauval & Tatum (1984) and Barklem & Collet (2016). All three data sets agree very well below 3500 K, with the ExoMol results being higher than those of 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 be 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.

3.3 Lifetimes

Lifetimes for the states are provided as part of the DUO calculations; a detailed methodology is given by Tennyson et al. (2016b). 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 $32.7 \pm 1.7\text{ ns}$ by Diffenderfer, Yarkony & Dagdigian (1983) using fluorescence decay, $22.5 \pm 1.5\text{ ns}$ by Büsener et al. (1987) ($J = 1$) using Stark quantum-beat spectroscopy and $21.5 \pm 1.8\text{ ns}$ by Naulin et al. (1991) ($J = 70$) also using fluorescence decay. Maatouk et al. (2010) calculated the $J = 0$ and

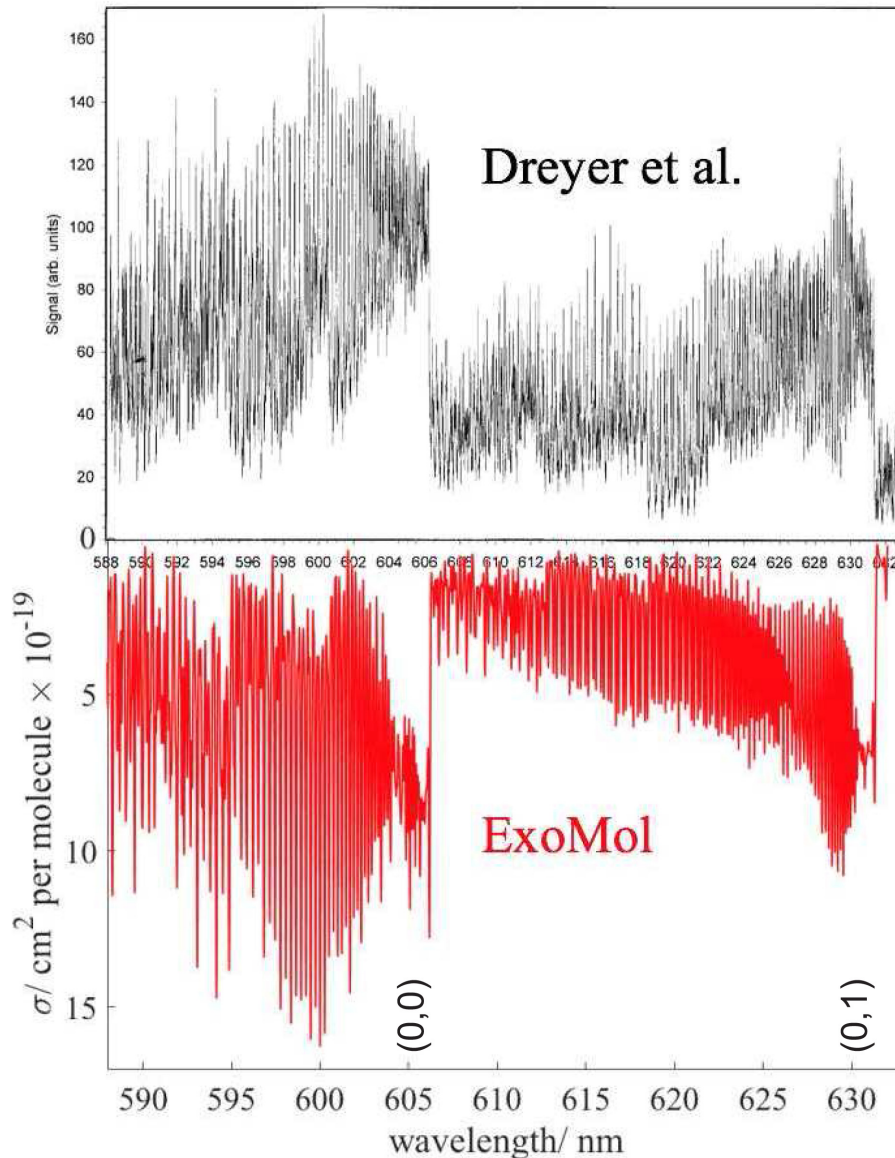


Figure 11. Comparison of the ExoMol spectrum (lower) and experimental spectrum from Dreyer et al. (2001) (upper) in the range 588–633 nm. The (0,0) and (0,1) bandheads agree, whereas the other bandheads cannot be distinguished clearly from each other.

$J = 70$ 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 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 Fig. 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 lifetimes.

3.4 Line lists

Line lists were generated by considering 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 lists have been formatted into ExoMol format (transition files and state files: Tennyson, Hill & Yurchenko 2013), with lifetimes of each state quoted. An extract of the state file is shown in Table 6 and an extract of the transition file is shown in Table 7. The line lists for isotopologues have comparable sizes.

4 SIMULATED SPECTRA

Absorption spectra at different temperatures are presented in Fig. 8. The contribution of each band is shown in Fig. 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, Al-Refaie & Tennyson 2018b).

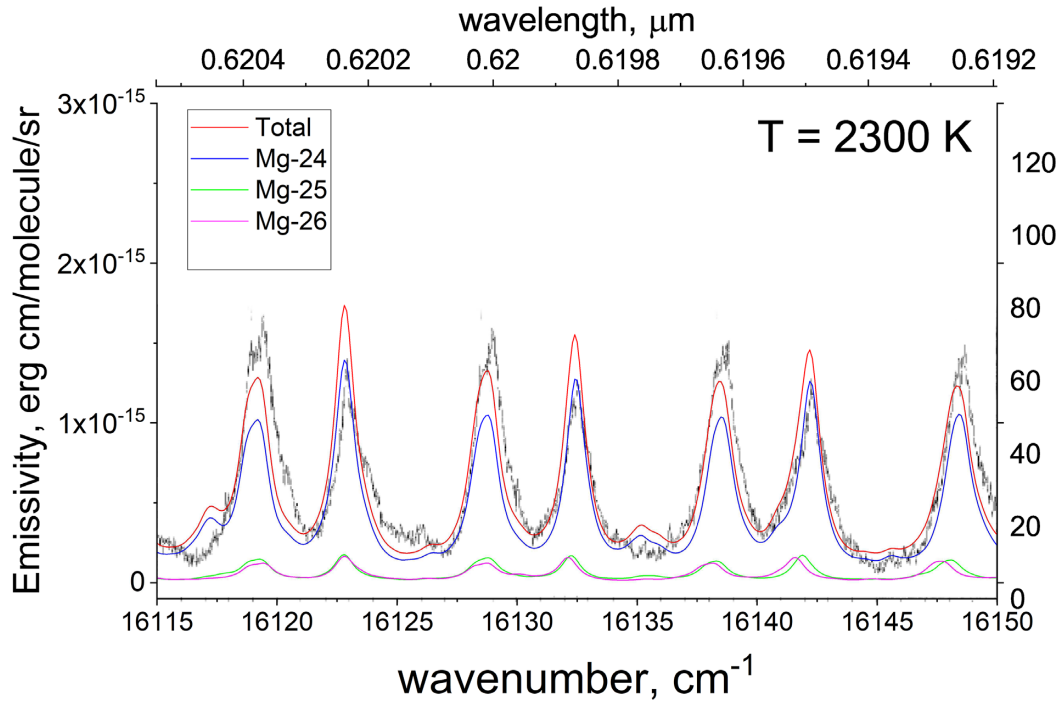


Figure 12. Comparison of the ExoMol emission (2300 K) and experimental spectra from Dreyer et al. (2001) in the range 16 115–161 50 cm^{-1} using the Voigt profile with $\gamma = 1.1 \text{ cm}^{-1}$ from the combined contributions of the three main isotopologues, also shown, assuming the terrestrial abundance (0.79/0.10/0.11 for 24/25/26, respectively).

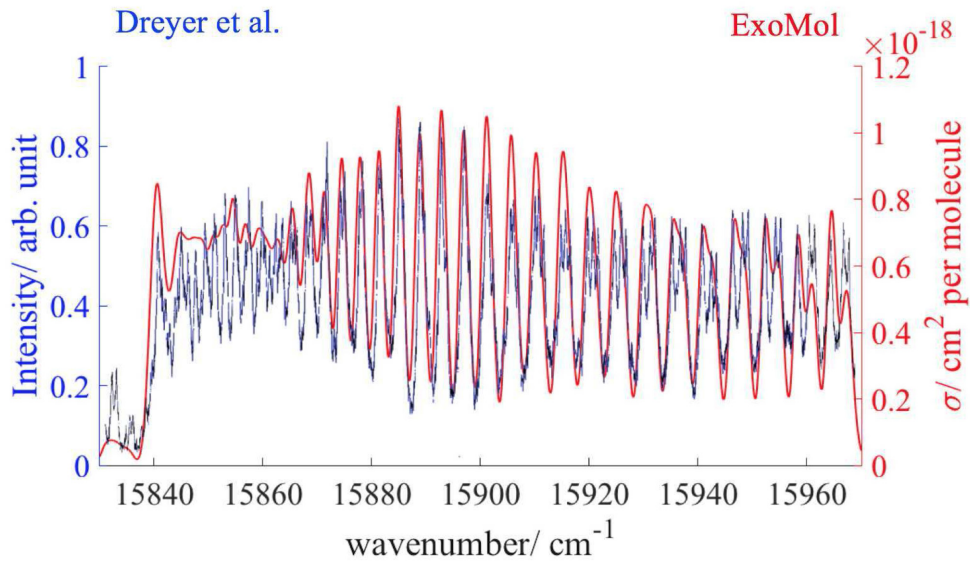


Figure 13. Comparison of the ExoMol absorption spectrum and experimental spectrum from Dreyer et al. (2001) in the range 15 840–15 960 cm^{-1} for the (1,0) band using the Gaussian line profile with half-width at half maximum (HWHM)=1 cm^{-1} at $T = 2300 \text{ K}$.

Comparisons with the previous experimental work 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 Fig. 10, where it is compared with the experimentally determined transitions from the JPL 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 represent an improvement, which suggests that the current JPL intensities are about 30 per cent

too strong and, correspondingly, the observational upper limits for the ISM (Turner & Steimle 1985; Sakamoto et al. 1998) are about 30 per cent too low.

4.1 The red band

Dreyer et al. (2001) made excitation scans using laser-induced fluorescence excitation spectroscopy for the $B - A$ transitions. For the 588–632 nm range, there is overall agreement, as shown in

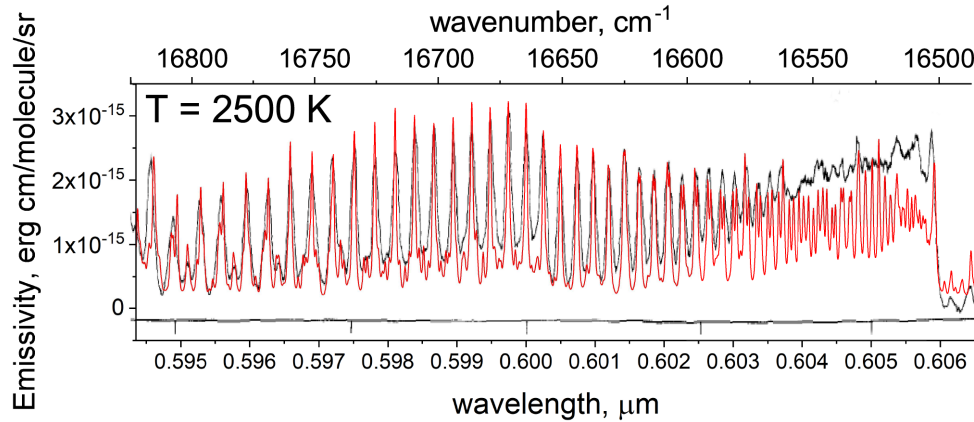


Figure 14. Comparison of the ExoMol emission spectrum and experimental spectrum from Pasternack et al. (1978) around the (1,1) bandhead using the Voigt profile with $\gamma = 1.1 \text{ cm}^{-1}$ at $T = 2500 \text{ K}$. The vacuum wavelength was re-calibrated to the acetylene–air wavelength to match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

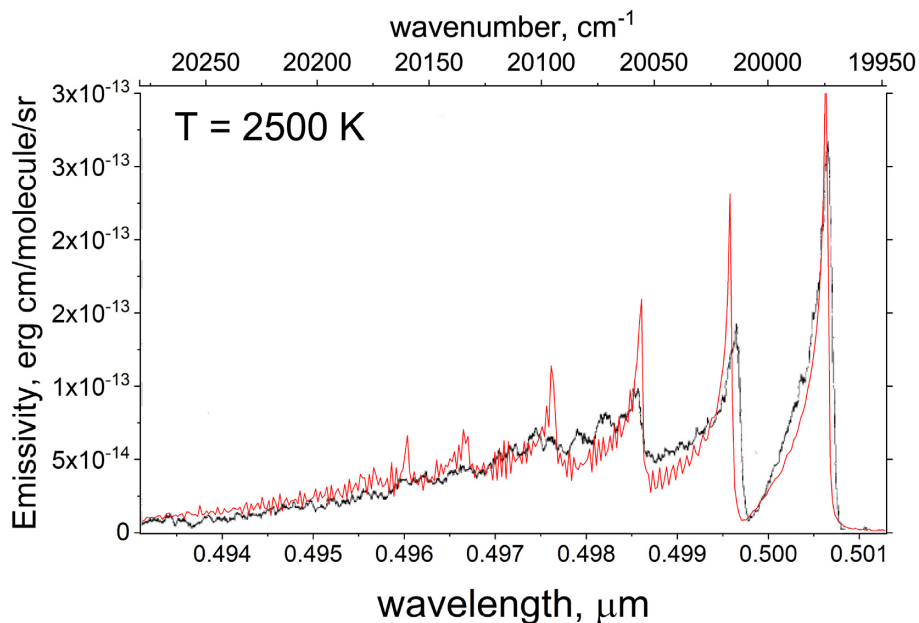


Figure 15. Comparison of the ExoMol emission spectrum and experimental spectrum from Pasternack et al. (1978) in the range 495–501 nm. The ExoMol spectrum was generated using the Voigt profile with $\gamma = 1.1 \text{ cm}^{-1}$ at $T = 2500 \text{ K}$. The vacuum wavelength was re-calibrated to the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

Fig. 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.

Fig. 12 shows a spectrum for the $16\,115\text{--}16\,150 \text{ cm}^{-1}$ region from Dreyer et al. (2001). The main peaks for the (0,1) lines generally agree, whereas the magnitudes can differ; see Fig. 13. The (0,1) bandhead region cannot be resolved between 1584 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, Baronavski & McDonald (1978) also show good agreement with the ExoMol data around the (1,1) band; Fig. 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 refrac-

tive indexes from Ciddor (1996) and Loria (1909)¹ assuming a 45:55 mixture. This ratio was adjusted to match the experimental spectrum.

4.2 The green band

For the 495–501 nm region of the $B - X$ transitions, Fig. 15 compares our data with the laser-induced fluorescence spectrum of Pasternack et al. (1978). The shapes, which are largely determined by the bandheads, of the two spectra are similar. The same wavelength calibration (vacuum to air–acetylene) as above was applied. The ExoMol spectrum also agrees very well with the higher resolution experimental data from the same region,

¹The refractive index data are taken from M. N. Polyanskiy’s “Refractive index database”, <https://refractiveindex.info>.

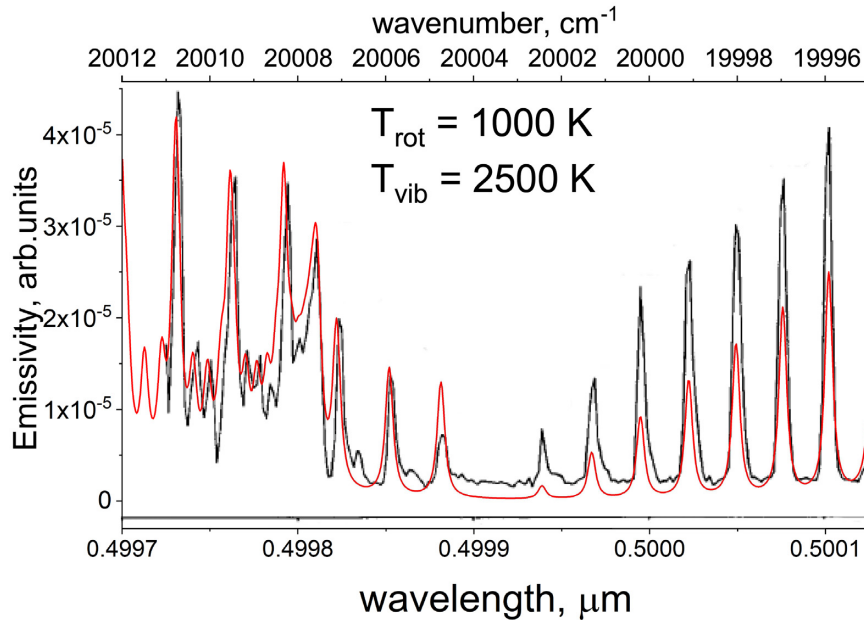


Figure 16. Comparison of the absorption ExoMol spectrum and experimental spectrum from Büsener et al. (1987) in the range 499.7–500.1 nm in the green band using the Gaussian line profile with $\text{HWHM}=1 \text{ cm}^{-1}$, at $T_{\text{rot}} = 1000$ and 2500 K .

measured between 499.7 and 500.1 nm using Stark quantum-beat spectroscopy by Büsener et al. (1987); see Fig. 16, where no recalibration was required. For these simulations, the non-local thermodynamic equilibrium (non-LTE) model was assumed based on two temperatures, rotational T_{rot} and vibrational T_{vib} , as implemented in DUO. The temperatures selected to match the experimental emission spectra were 1000 and 2500 K, respectively.

5 CONCLUSION

Accurate and complete line lists, known as LiTY, for $^{24}\text{Mg}^{16}\text{O}$, $^{25}\text{Mg}^{16}\text{O}$, $^{26}\text{Mg}^{16}\text{O}$ are computed using high-level *ab initio* DMCs as well as a spectroscopically refined DUO model. Our work displays good agreement with 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 temperatures up to 5000 K.

With a valid temperature range up to 5000 K, the strong red and green bands between 15 000 and 20 000 cm^{-1} (0.66–0.5 μm) 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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SUPPORTING INFORMATION

Supplementary data are available at *MNRAS* online.

Containing the following (a) A spreadsheet with MARVEL transitions file and resulting energy levels; (b) A Duo input file for $^{24}\text{Mg}^{16}\text{O}$ containing all parameters fitted for the refined PECs, SOCs and EAMS, and the DMSs; (c) partition function files for $^{24}\text{Mg}^{16}\text{O}$, $^{25}\text{Mg}^{16}\text{O}$, $^{26}\text{Mg}^{16}\text{O}$, $^{24}\text{Mg}^{18}\text{O}$ and $^{24}\text{Mg}^{17}\text{O}$

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