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Einstein A coefficients for rovibronic lines of the $A^2\Pi \rightarrow X^2\Sigma^+$ and $B'^2\Sigma^+ \rightarrow X^2\Sigma^+$ transitions of MgH

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ABSTRACT

Einstein A coefficients have been calculated for rovibronic lines of the $A^2\Pi \rightarrow X^2\Sigma^+$ and $B'^2\Sigma^+ \rightarrow X^2\Sigma^+$ transitions of ^{24}MgH . Using the experimentally determined analytic potential energy curve for the $X^2\Sigma^+$ state, and the Rydberg–Klein–Rees potentials for the $A^2\Pi$ and $B'^2\Sigma^+$ states, combined with the most recent ab initio transition dipole moments, rovibronic transition moments were computed. The rovibronic transition frequencies were obtained accurately by subtracting the published term values of the $X^2\Sigma^+$, $A^2\Pi$ and $B'^2\Sigma^+$ states. Using the rovibronic transition dipole moments, transition frequencies and the Hönl–London factors, the *Einstein A* coefficients were calculated individually for $\sim 30\,000$ rovibronic lines of the $A^2\Pi \rightarrow X^2\Sigma^+$ and $B'^2\Sigma^+ \rightarrow X^2\Sigma^+$ transitions of ^{24}MgH .

Key words: molecular data – stars: late-type – subdwarfs.

1 INTRODUCTION

MgH has been the subject of extensive studies due to its importance in a variety of astrophysical environments. Lines of the $A^2\Pi - X^2\Sigma^+$ system of ^{24}MgH have been detected and analysed in the spectra of various stellar regions including the solar photosphere (Grevesse & Sauval 1973), sunspots (Richardson 1931; Webber 1971; Sotirovski 1972), late-type stars (Joy 1926; Öhman 1936; Davis 1937) and nearby galaxies (Spinrad & Taylor 1971). Moreover, these bands have been found in the spectra of four nearby L dwarfs and subdwarfs (Cottrell 1978; Reid et al. 2000). Recently, Wallace et al. have observed and identified the $v' = 0$ and $v' = 1$ progressions of the $B'^2\Sigma^+ \leftarrow X^2\Sigma^+$ bands of MgH in sunspot umbral spectra (Wallace et al. 1998, 1999).

Because of the importance of Mg atoms in the ionization balance of interstellar clouds (Oppenheimer & Dalgarno 1974), several studies have been carried out to calculate the abundance of ^{24}MgH and its isotopologues since the 1970s. Line intensities of the $A^2\Pi \leftarrow X^2\Sigma^+$ bands of ^{25}MgH and ^{26}MgH have been compared with those of ^{24}MgH to obtain relative abundance estimates for magnesium isotopes in sunspot and late-type stars (Boesgaard 1968; Branch 1970; Boyer 1971; Boyer, Henoux & Sotirovski 1971). Using the 0–0 band of the $A^2\Pi - X^2\Sigma^+$ system of MgH, isotope abundance ratios $^{24}\text{Mg}:^{25}\text{Mg}:^{26}\text{Mg}$ were derived for Arcturus (Tomkin & Lambert 1976), for five dwarfs (Tomkin & Lambert 1980) and for various cool and red giant stars (Gay & Lambert 2000; Yong, Lambert & Ivans 2003; Yong, Aoki & Lambert 2006). In addition to the $A - X$ band system, the $B'^2\Sigma^+ \rightarrow X^2\Sigma^+$ bands have been used to

measure the solar isotope ratio, which is in good agreement with the much better determined terrestrial ratio (Wallace et al. 1999). Magnesium abundance derived from a combination of Mg I and MgH is also used to determine surface gravities of Arcturus and cool giant stars (Bell, Edvardsson & Gustafsson 1985; Bonnell & Bell 1993).

The first laboratory spectrum of ^{24}MgH was photographed more than a century ago (Fowler 1907, 1909). In the 1970s, Balfour and co-workers studied the absorption and emission spectra of MgH and MgD extensively, and discovered the $B'^2\Sigma^+ - X^2\Sigma^+$ transitions (Balfour & Cartwright 1975b). They analysed both the $A - X$ and $B' - X$ systems (Balfour 1970a,b; Balfour & Cartwright 1976a; Balfour & Lindgren 1978) and used their spectroscopic data to estimate the dissociation energy of ground and low-lying states (Balfour & Cartwright 1975a, 1976b; Balfour 1980). A few years later, the emission spectrum of the $A^2\Pi \rightarrow X^2\Sigma^+$ system of ^{24}MgH was recorded at high resolution using a Fourier transform spectrometer, and the pure rotational transitions of the $X^2\Sigma^+$ ground state were predicted (Bernath, Black & Brault 1985). The vibration–rotation and pure rotational spectra of MgH were recorded subsequently (Leopold et al. 1986; Lemoine et al. 1988; Ziurys, Barclay & Anderson 1993). Recently, Shayesteh et al. (2004, 2007) recorded the infrared and visible emission spectra of MgH at high resolution and reported a detailed analysis of the $X^2\Sigma^+$ ground state and the $A^2\Pi$ and $B'^2\Sigma^+$ excited states. Moreover, deperturbation analysis of both $A - X$ and $B' - X$ systems have been carried out by fitting the spectroscopic data for the $v = 0$ to 3 levels of the $A^2\Pi$ state and the $v = 0$ to 4 levels of the $B'^2\Sigma^+$ state simultaneously (Shayesteh & Bernath 2011).

Parallel to the experimental work on MgH, several theoretical studies have been carried out since the 1970s (Popkie 1971; Meyer

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& Rosmus 1975). The $X^2\Sigma^+$, $A^2\Pi$ and $B'^2\Sigma^+$ potential curves, equilibrium internuclear distances, dipole moment functions, vibrational frequencies and spectroscopic constants of MgH have been calculated (Sink et al. 1976; Saxon, Kirby & Liu 1978; Sink & Bandrauk 1979; Saxon, Kirby & Liu 1983). In addition, a complete line list has been computed for the ground and two low-lying excited states (Skory et al. 2003; Weck et al. 2003; Yadin et al. 2012). Recently, potential energy curves of the ground and excited states of MgH have been calculated at high levels of theory (Mestdagh et al. 2009; Guitou, Spielfiedel & Feautrier 2010), and ab initio transition dipole moments have been reported (Mostafanejad & Shayesteh 2012).

In this paper, we report *Einstein A* coefficients for rovibronic transitions of the $A^2\Pi \rightarrow X^2\Sigma^+$ and $B'^2\Sigma^+ \rightarrow X^2\Sigma^+$ systems of MgH, calculated using a combination of spectroscopic data and ab initio transition dipole moments. Calculation of absolute line intensities of molecular species has important applications in astrophysics and atmospheric science (Tatum 1967; Bernath 2009).

2 THEORY AND CALCULATIONS

Line intensities of rovibronic transitions are related to *Einstein A* coefficients (Bernath 2005):

$$A_{v',J' \rightarrow v'',J''} = \frac{16\pi^3 \nu^3}{3\epsilon_0 \hbar c^3} \left| \langle \psi_{v',J'} | \mathbf{R}_e(r) | \psi_{v'',J''} \rangle \right|^2 \left(\frac{S_{J'}^{\Delta J}}{2J' + 1} \right). \quad (1)$$

According to equation (1), $A_{v',J' \rightarrow v'',J''}$ depends on transition frequency ν , the Hönl–London factor $S_{J'}^{\Delta J}$, and the electronic transition dipole moment, $\mathbf{R}_e(r)$, which is a function of internuclear distance r (Bernath 2005). The electronic transition dipole moment, $\mathbf{R}_e(r)$, is usually calculated theoretically and is defined by

$$\mathbf{R}_e(r) = \int \psi_{el}^*(\mathbf{r}_i; r) \boldsymbol{\mu}(\mathbf{r}_i; r) \psi_{el}(\mathbf{r}_i; r) d\tau_{el}, \quad (2)$$

with \mathbf{r}_i representing the electronic coordinates. *Einstein A* coefficients are related to excited state lifetimes, which can be measured experimentally. However, the lifetime is related only to the overall rate of radiative decay of an excited state i to all lower states j :

$$\tau_i = \left(\sum_j A_{i \rightarrow j} \right)^{-1}. \quad (3)$$

The most accurate method for calculating *Einstein A* coefficients for small molecules is to combine experimental potential curves and energy levels with high-quality ab initio transition dipole moments. Electronic transition dipole moments of the $A^2\Pi \rightarrow X^2\Sigma^+$ and $B'^2\Sigma^+ \rightarrow X^2\Sigma^+$ systems have been computed recently using high-level ab initio calculations (Mostafanejad & Shayesteh 2012). The program LEVEL (Le Roy 2007) takes a diatomic potential energy curve and solves the following one-dimensional radial Schrödinger equation numerically to find all bound and quasi-bound rovibrational energy levels ($E_{v,J}$) and the corresponding wavefunctions $\psi_{v,J}(r)$:

$$-\frac{\hbar^2}{2\mu} \frac{d^2 \psi_{v,J}(r)}{dr^2} + V_J(r) \psi_{v,J}(r) = E_{v,J} \psi_{v,J}(r). \quad (4)$$

The effective one-dimensional potential $V_J(r)$ in equation (4), is a sum of the rotationless (electronic) potential $V(r)$ and a centrifugal term that depends on J . For the normal problem of a diatomic

molecule in a singlet electronic state rotating in three dimensions, $V_J(r)$ is given by the following equation:

$$V_J(r) = V(r) + \frac{\hbar^2}{2\mu r^2} [J(J+1) - \Omega^2], \quad (5)$$

in which Ω is equal to 0 and 1 for $^1\Sigma^+$ and $^1\Pi$ states, respectively. In addition, when two potential energy curves and the electronic transition dipole moments, $\mathbf{R}_e(r)$, are provided as input, the program LEVEL finds $\psi_{v',J'}$ and $\psi_{v'',J''}$, and calculates the rovibronic transition dipole moment integral ($M_{v',J' \rightarrow v'',J''}$) numerically for each individual rovibronic transition:

$$M_{v',J' \rightarrow v'',J''} = \langle \psi_{v',J'} | \mathbf{R}_e(r) | \psi_{v'',J''} \rangle. \quad (6)$$

The *Einstein A* coefficient $A_{v',J' \rightarrow v'',J''}$ can then be calculated from the transition frequency (ν), the rovibronic transition dipole moment ($M_{v',J' \rightarrow v'',J''}$) and the Hönl–London factor ($S_{J'}^{\Delta J}$) using equation (1).

3 RESULTS AND DISCUSSION

Accurate potential energy curves and term values for the $X^2\Sigma^+$, $A^2\Pi$ and $B'^2\Sigma^+$ states of MgH have been determined experimentally in recent years (Shayesteh et al. 2007, 2011). An analytical Morse–Long–Range (MLR) potential curves exists for the $X^2\Sigma^+$ state, and Rydberg–Klein–Rees (RKR) potentials are available for the $A^2\Pi$ and $B'^2\Sigma^+$ states.

Table 1. Hönl–London factors $S_{J'}^{\Delta J}$ for $^2\Pi \rightarrow ^2\Sigma^+$ and $^2\Sigma^+ \rightarrow ^2\Sigma^+$ transitions.^a

$^2\Pi \rightarrow ^2\Sigma^+$	
Branch	$\lambda = \frac{A}{B} \quad U = [\lambda^2 - 4\lambda + (2J' + 1)^2]^{-1/2}$
P_{11}	$\frac{(2J'+1)^2 + (2J'+1)U(4J'^2 + 4J' - 7 + 2\lambda)}{8(J'+1)}$
P_{21}	$\frac{(2J'+1)^2 - (2J'+1)U(4J'^2 + 4J' - 7 + 2\lambda)}{8(J'+1)}$
P_{12}	$\frac{(2J'+1)^2 - (2J'+1)U(4J'^2 + 4J' + 1 - 2\lambda)}{8(J'+1)}$
P_{22}	$\frac{(2J'+1)^2 + (2J'+1)U(4J'^2 + 4J' + 1 - 2\lambda)}{8(J'+1)}$
Q_{11}	$\frac{(2J'+1)[(4J'^2 + 4J' - 1) + U(8J'^3 + 12J'^2 - 2J' - 7 + 2\lambda)]}{8J'(J'+1)}$
Q_{21}	$\frac{(2J'+1)[(4J'^2 + 4J' - 1) - U(8J'^3 + 12J'^2 - 2J' - 7 + 2\lambda)]}{8J'(J'+1)}$
Q_{12}	$\frac{(2J'+1)[(4J'^2 + 4J' - 1) - U(8J'^3 + 12J'^2 - 2J' + 1 - 2\lambda)]}{8J'(J'+1)}$
Q_{22}	$\frac{(2J'+1)[(4J'^2 + 4J' - 1) + U(8J'^3 + 12J'^2 - 2J' + 1 - 2\lambda)]}{8J'(J'+1)}$
R_{11}	$\frac{(2J'+1)^2 + (2J'+1)U(4J'^2 + 4J' + 1 - 2\lambda)}{8J'}$
R_{21}	$\frac{(2J'+1)^2 - (2J'+1)U(4J'^2 + 4J' + 1 - 2\lambda)}{8J'}$
R_{12}	$\frac{(2J'+1)^2 - (2J'+1)U(4J'^2 + 4J' - 7 + 2\lambda)}{8J'}$
R_{22}	$\frac{(2J'+1)^2 + (2J'+1)U(4J'^2 + 4J' - 7 + 2\lambda)}{8J'}$
$^2\Sigma^+ \rightarrow ^2\Sigma^+$	
P_{11}, P_{22}	$\frac{4(J'+1)^2 - 1}{4(J'+1)}$
R_{11}, R_{22}	$\frac{4J'^2 - 1}{4J'}$
Q_{12}, Q_{21}	$\frac{2J' + 1}{4J'(J'+1)}$

^aIn this table, J' is the upper state total angular momentum quantum number. The λ values for the vibrational levels of the $A^2\Pi$ state were calculated using the band constants (A_v and B_v) reported by Shayesteh & Bernath (2011); λ 's were determined to be 5.744, 5.933, 6.137 and 6.360 for the $v' = 0, 1, 2$ and 3 levels, respectively.

Table 2. Einstein A coefficients (in s⁻¹) for the A²Π → X²Σ⁺ and B'²Σ⁺ → X²Σ⁺ band systems of ²⁴MgH.^a

X ² Σ ⁺		A ² Π				B' ² Σ ⁺				
	Line	v' = 0	v' = 1	v' = 2	v' = 3	v' = 0	v' = 1	v' = 2	v' = 3	v' = 4
v'' = 0	R ₁₁ (0) ^b	8.345(6)	4.385(5)	7.619(1)	8.109(1)	8.183(1)	7.354(2)	3.243(3)	9.316(3)	1.953(4)
	R ₁₁ (10)	1.076(7)	5.181(5)	3.861(-1)	1.041(2)	1.218(2)	1.079(3)	4.726(3)	1.360(4)	2.889(4)
	R ₁₁ (20)	1.079(7)	4.589(5)	1.931(3)*. ^c	1.048(2)	1.551(2)	1.298(3)	4.268(3)*	1.550(4)	
	R ₁₁ (30)	1.072(7)	3.875(5)			2.618(2)	1.945(3)	7.485(3)	1.985(4)	
	R ₁₁ (40)	1.040(7)				7.123(2)	4.246(3)			
v'' = 1	R ₁₁ (0)	4.878(5)	7.043(6)	7.824(5)	3.655(-1)	1.620(3)	1.130(4)	3.868(4)	8.610(4)	1.395(5)
	R ₁₁ (10)	5.977(5)	9.319(6)	9.371(5)	3.090(2)	2.437(3)	1.668(4)	5.644(4)	1.253(5)	2.039(5)
	R ₁₁ (20)	5.853(5)	9.366(6)	9.457(5)*	1.999(3)	3.163(3)	2.015(4)	1.271(5)*	1.392(5)	
	R ₁₁ (30)	5.832(5)	9.261(6)			5.493(3)	3.012(4)	8.631(4)	1.705(5)	
	R ₁₁ (40)	5.811(5)				1.557(4)	6.423(4)			
v'' = 2	R ₁₁ (0)	3.046(4)	8.704(5)	5.862(6)	1.030(6)	1.432(4)	7.188(4)	1.737(5)	2.637(5)	2.747(5)
	R ₁₁ (10)	3.627(4)	1.090(6)	7.971(6)	1.249(6)	2.182(4)	1.069(5)	2.545(5)	3.847(5)	4.032(5)
	R ₁₁ (20)	3.599(4)	1.064(6)	6.609(6)*	1.062(6)	2.885(4)	1.290(5)	1.273(6)*	4.153(5)	
	R ₁₁ (30)	3.824(4)	1.048(6)			5.117(4)	1.877(5)	3.583(5)	4.598(5)	
	R ₁₁ (40)	4.368(4)				1.486(5)	3.576(5)			
v'' = 3	R ₁₁ (0)	2.215(3)	8.599(4)	1.149(6)	4.803(6)	7.500(4)	2.433(5)	3.570(5)	2.879(5)	1.137(5)
	R ₁₁ (10)	2.595(3)	1.047(5)	1.472(6)	6.720(6)	1.155(5)	3.624(5)	5.211(5)	4.171(5)	1.671(5)
	R ₁₁ (20)	2.670(3)	1.039(5)	3.597(5)*	6.777(6)	1.545(5)	4.261(5)	1.801(6)*	4.079(5)	
	R ₁₁ (30)	3.146(3)	1.100(5)			2.738(5)	5.592(5)	5.663(5)	3.239(5)	
	R ₁₁ (40)	4.407(3)				7.734(5)	7.075(5)			
v'' = 4	R ₁₁ (0)	1.872(2)	8.894(3)	1.601(5)	1.329(6)	2.566(5)	4.437(5)	2.776(5)	3.740(4)	2.314(4)
	R ₁₁ (10)	2.176(2)	1.069(4)	1.995(5)	1.741(6)	3.973(5)	6.514(5)	3.899(5)	4.881(4)	3.527(4)
	R ₁₁ (20)	2.370(2)	1.108(4)	5.198(5)*	1.681(6)	5.272(5)	6.939(5)	2.676(4)*	2.026(4)	
	R ₁₁ (30)	3.220(2)	1.319(4)			8.900(5)	6.447(5)	1.446(5)	6.057(3)	
	R ₁₁ (40)	5.879(2)				2.009(6)	1.924(4)			
v'' = 5	R ₁₁ (0)	1.821(1)	1.018(3)	2.221(4)	2.458(5)	5.856(5)	3.426(5)	8.470(3)	1.040(5)	1.966(5)
	R ₁₁ (10)	2.116(1)	1.220(3)	2.741(4)	3.145(5)	9.023(5)	4.664(5)	5.833(3)	1.643(5)	2.818(5)
	R ₁₁ (20)	2.506(1)	1.355(3)	5.645(4)*	3.139(5)	1.141(6)	3.337(5)	2.685(1)*	2.365(5)	
	R ₁₁ (30)	4.106(1)	1.920(3)			1.613(6)	1.700(4)	1.584(5)	3.141(5)	
v'' = 6	R ₁₁ (0)	2.026(0)	1.323(2)	3.344(3)	4.399(4)	8.548(5)	1.028(4)	1.900(5)	1.892(5)	8.668(3)
	R ₁₁ (10)	2.371(0)	1.593(2)	4.147(3)	5.586(4)	1.280(6)	1.999(3)	3.048(5)	2.509(5)	6.065(3)
	R ₁₁ (20)	3.171(0)	1.940(2)	8.183(4)*	5.895(4)	1.397(6)	8.095(4)	3.065(5)*	1.454(5)	
	R ₁₁ (30)	6.511(0)	3.321(2)			1.014(6)	1.300(6)	2.377(4)	3.076(3)	
v'' = 7	R ₁₁ (0)	2.604(-1)	1.995(1)	5.652(2)	8.558(3)	6.840(5)	3.905(5)	1.533(5)	1.174(4)	1.580(5)
	R ₁₁ (10)	3.080(-1)	2.447(1)	7.116(2)	1.098(4)	9.338(5)	7.411(5)	1.485(5)	3.577(4)	2.350(5)
	R ₁₁ (20)	4.820(-1)	3.358(1)	8.605(3)*	1.258(4)	6.328(5)	1.444(6)	3.935(4)*	1.049(5)	
v'' = 8	R ₁₁ (0)	4.034(-2)	3.555(0)	1.111(2)	1.875(3)	1.782(5)	9.369(5)	2.708(5)	1.028(5)	6.025(3)
	R ₁₁ (10)	4.817(-2)	4.502(0)	1.430(2)	2.464(3)	1.682(5)	1.320(6)	6.850(5)	6.490(4)	1.916(3)
	R ₁₁ (20)	8.037(-2)	6.360(0)	4.760(5)*	2.767(3)	7.080(2)	4.972(5)	9.141(5)*	2.770(5)	
v'' = 9	R ₁₁ (0)	7.816(-3)	7.482(-1)	2.561(1)	4.621(2)	5.580(2)	1.280(5)	9.680(5)	5.639(5)	1.416(2)
	R ₁₁ (10)	9.077(-3)	9.477(-1)	3.247(1)	5.966(2)	9.771(3)	3.429(4)	9.955(5)	1.191(6)	7.423(4)
v'' = 10	R ₁₁ (0)	1.579(-3)	1.550(-1)	5.645(0)	1.054(2)	1.610(3)	4.460(4)	3.294(4)	1.435(5)	5.130(5)
v'' = 11	R ₁₁ (0)	2.335(-4)	2.300(-2)	8.536(-1)	1.608(1)	3.628(2)	5.635(3)	5.740(2)	4.467(4)	7.937(4)

^aThe number in parentheses following an entry is the power of 10 by which the entry is to be multiplied.

^bThe lines are marked as R₁₁(N'') where N'' is the rotational quantum number of the lower state (X²Σ⁺).

^cThe numbers marked with asterisks (*) belong to perturbed upper state levels, and have been calculated using PGOFFER.

First, using experimental term values of the X²Σ⁺ ground state and the A²Π and B'²Σ⁺ excited states (Shayesteh et al. 2007), a complete list of rovibronic transition wavenumbers (and frequencies) were calculated. Then, we used the experimental potential energy curves of the X²Σ⁺, A²Π and B'²Σ⁺ states of ²⁴MgH (Shayesteh & Bernath 2011) and the ab initio electronic transition dipole moments **R_e**(r) (Mostafanejad & Shayesteh 2012) in the

LEVEL program to calculate $M_{v',J' \rightarrow v'',J''}$ for all possible rovibronic transitions, including v' = 0, 1, 2, 3 of the A²Π state, v' = 0–9 of the B'²Σ⁺ state and v'' = 0–11 of the X²Σ⁺ state.

The A²Π – X²Σ⁺ bands consist of 12 branches: P₁₁, Q₁₁, R₁₁, P₂₂, Q₂₂, R₂₂, P₁₂, Q₁₂, R₁₂, P₂₁, Q₂₁ and R₂₁. The B'²Σ⁺ → X²Σ⁺ system involves four strong branches, i.e. P₁₁, R₁₁, P₂₂, R₂₂, and two satellite branches: Q₁₂ and Q₂₁. Because the program

LEVEL is limited to singlet states, we introduced the X , A and B' states as if they are $^1\Sigma^+$, $^1\Pi$ and $^1\Sigma^+$ states, respectively, in order to obtain $M_{v',J' \rightarrow v'',J''}$ values for P , Q and R branches. The Hönl–London factors for $^2\Pi \rightarrow ^2\Sigma^+$ (Earls 1935) and $^2\Sigma^+ \rightarrow ^2\Sigma^+$ transitions (Herzberg 1950) were used to calculate the J dependence of rovibronic transition intensities. Following Li et al. (2012), we multiplied the Hönl–London factors reported by Earls (1935) by four (Table 1), in order to make them consistent with the PGOPHER program (Western 2010).

It should be noted that the $B' ^2\Sigma^+ \rightarrow X ^2\Sigma^+$ transition intensities depend strongly on the rotational quantum number N . For example, Franck–Condon factors for rovibronic transitions belonging to the 1–6 band change drastically from $N = 0$ to $N = 25$ (Wallace et al. 1999). In other words, the *Einstein A* coefficients of the $B' ^2\Sigma^+ \rightarrow X ^2\Sigma^+$ system are very sensitive to the rotational quantum number and for this reason, we calculated $M_{v',J' \rightarrow v'',J''}$ for each rovibronic transition separately. Table 2 lists the *Einstein A* coefficients for several lines of the R_{11} branches of the $A ^2\Pi \rightarrow X ^2\Sigma^+$ and $B' ^2\Sigma^+ \rightarrow X ^2\Sigma^+$ bands, and displays how the A values change with the ground state rotational quantum number (N'').

There are several perturbations between the $A ^2\Pi$ and $B' ^2\Sigma^+$ states of ^{24}MgH that have been analysed recently (Shayesteh & Bernath 2011). Hamiltonian operators for rotation and spin–orbit coupling (\hat{H}_{Rot} and \hat{H}_{SO}) have off-diagonal matrix elements between $^2\Sigma_{1/2}^+$, $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ basis functions. As a result, the wavefunctions of some rovibrational levels of the $A ^2\Pi$ and $B' ^2\Sigma^+$ states are mixed, and this causes significant changes in line intensities and *Einstein A* coefficients for transitions originating from these levels. Shayesteh & Bernath (2011) have listed the rotational quantum numbers (N') of the perturbed levels in table 1 of their article. We used the program PGOPHER (Western 2010) to simulate the $A ^2\Pi \rightarrow X ^2\Sigma^+$ and $B' ^2\Sigma^+ \rightarrow X ^2\Sigma^+$ transitions only for the N' values at which perturbations were severe. This program can take spectroscopic constants of the upper and lower vibronic states along with the transition dipole moment of the corresponding band ($M_{v' \rightarrow v''}$) to calculate line positions and intensities. For the perturbed lines of ^{24}MgH , we used the $M_{v',J' \rightarrow v'',J''}$ values from LEVEL along with the band constants of the $X ^2\Sigma^+$, $A ^2\Pi$ and $B' ^2\Sigma^+$ states and the perturbation matrix elements (Shayesteh & Bernath 2011) in the PGOPHER program. The *Einstein A* coefficients calculated using this program have been marked with asterisks in Table 2. A comprehensive list of $\sim 30\,000$ *Einstein A* coefficients for the $A ^2\Pi \rightarrow X ^2\Sigma^+$ and $B' ^2\Sigma^+ \rightarrow X ^2\Sigma^+$ band systems, including $v' = 0-3$ of the $A ^2\Pi$ state, $v' = 0-9$ of $B' ^2\Sigma^+$ state and $v'' = 0-11$ of the $X ^2\Sigma^+$ state, is provided as a supplementary file (available online as Supplementary Information).

4 CONCLUSIONS

The experimentally determined analytic potential energy curve for the $X ^2\Sigma^+$ state, and the RKR potentials for the $A ^2\Pi$ and $B' ^2\Sigma^+$ states of MgH were combined with the most recent ab initio transition dipole moments, in order to compute rovibronic transition moments. The rovibronic transition frequencies were obtained accurately by subtracting the published term values of the $X ^2\Sigma^+$, $A ^2\Pi$ and $B' ^2\Sigma^+$ states of ^{24}MgH . Using the rovibronic transition dipole moments, transition frequencies and Hönl–London factors, the *Einstein A* coefficients were calculated individually for $\sim 30\,000$ rovibronic lines of the $A ^2\Pi \rightarrow X ^2\Sigma^+$ and $B' ^2\Sigma^+ \rightarrow X ^2\Sigma^+$ transitions of ^{24}MgH .

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SUPPORTING INFORMATION

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

Table 3. Transition wavenumbers and Einstein A coefficients for the A-X bands of MgH.

Table 4. Transition wavenumbers and Einstein A coefficients for the B'-X bands of MgH (<http://mnras.oxfordjournals.org/lookup/suppl/doi:10.1093/mnras/stt510/-/DC1>).

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