

Predicted Landé g -factors for open shell diatomic molecules



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ABSTRACT

The program Duo (Yurchenko et al., 2016) provides direct solutions of the nuclear motion Schrödinger equation for the (coupled) potential energy curves of open shell diatomic molecules. Wavefunctions from Duo are used to compute Landé g -factors valid for weak magnetic fields; the results are compared with the idealized predictions of both Hund's case (a) and Hund's case (b) coupling schemes. Test calculations are performed for AlO, NO, CrH and C₂. The computed g_j 's both provide a sensitive test of the underlying spectroscopic model used to represent the system and an indication of whether states of the molecule are well-represented by the either of the Hund's cases considered. The computation of Landé g -factors is implemented as a standard option in the latest release of Duo.

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1. Introduction

The lifting of the degeneracy of the energy levels in a molecule by a magnetic field is a well-known and well-studied phenomenon. Thus it has spawned experimental techniques such as laser magnetic resonance spectroscopy [1,2], magnetic rotation spectroscopy [3], and optical Zeeman spectroscopy [4,5]. These techniques, for example, use the Zeeman effect to tune transitions in and out resonance by changing the applied magnetic field [6]. Zeeman effects can also be probed directly using standard spectroscopic techniques to study molecules in magnetic fields [7–9]. In a similar fashion, Zeeman effects are increasingly being used to form, probe and trap molecules at ultra-cold temperatures [10] for example by use of magnetically tunable Feshbach resonances [11].

Spectral shifts and splittings provide a remote sensing technique with which to study the Universe. Zeeman splitting of molecular spectra are actively being used to probe magnetic fields in a variety of astronomical environments including sunspots [12–14], starspots [15], white dwarfs [16,17] M-dwarfs [18] and potentially exoplanets [19].

The Zeeman splitting patterns of the spectrum of an open shell diatomic molecule can be calculated in a straightforward fashion provided that the quantum numbers characterizing states in question are known and are conserved. However, there are circumstances, such as resonance interactions between nearby states via spin-orbit or other couplings, where the quantum numbers used

to specify the electronic state associated with a given level are not precisely conserved. In this case evaluation of Zeeman splitting as represented by the Landé g -factor is not straightforward and requires a numerical treatment. It is such a treatment which is the focus of the present article.

The important advantage of the Zeeman effect is that the associated splitting can be made large enough to separate otherwise degenerate spin-components (Λ -doublet). Moreover, the measurement of the g values can be more accurate than the energy spacing [20].

The Zeeman methodology for diatomics was introduced by Schade [21]. Stolyarov et al. [22] investigated the perturbations in the calculation of the Landé factors caused by interactions with other electronic states. In very recent theoretical work Borkov et al. [23] presented a numerical model of Zeeman splitting based on the use of effective molecular Hamiltonians.

Le Roy's LEVEL [24] has become the program of choice for solving the diatomic nuclear motion problem. However, LEVEL can only treat open shell molecules in limited circumstances [25,26] and does not consider the coupling between states by spin-orbit and related effects which can have an important effect of the g -factors. For this reason we have written our own diatomic nuclear motion code Duo [27]. Duo explicitly treats open shell systems and can allow for coupling between the various states involved. In this context, of particular interest to us are the many open-shell diatomic molecules which are known to be present, or may be present, in hot astronomical atmospheres such as those found in cool stars and exoplanets. Such species are being studied as part of the ExoMol project [28]. Zeeman splittings in these

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molecules can provide useful information on the magnetic fields present in these distant bodies. So far ExoMol has created spectroscopic models for a number of open shell diatomic species [26,29–36].

In this paper we present extension to Duo which allows Landé g -factors to be computed for individual states of open shell systems. As initial examples we focus on four systems studied by ExoMol, namely AlO [29], NO [37], CrH [33] and C₂ [38,39]. These systems were selected as ones of interest for ExoMol and for which there are laboratory Zeeman spectra. These laboratory studies are discussed below.

2. Theory

Discussions of the underlying theory and methodology used in Duo is given elsewhere [27,40,41] so only key points are considered below. Duo solves the diatomic nuclear motion problem using a Hund's case (a) basis. This does not represent an approximation even for molecules poorly represented by Hund's case (a) since a complete set of angular momentum functions are used for a given total angular momentum, J . We note that the same choice has been adopted by others [42,43].

The basis set used by Duo can be written as

$$|n\rangle = |\text{state}, J, \Omega, \Lambda, S, \Sigma, \nu\rangle = |\text{state}, \Lambda, S, \Sigma\rangle |J, \Omega, M\rangle |\text{state}, \nu\rangle, \quad (1)$$

where Λ is the projection of electron angular momentum on the molecular axis; S is the electron spin quantum number with projection Σ along the molecular axis and Ω is corresponding projection of J . The vibrational quantum number is given by ν and the label 'state' is used to denote the electronic state which is required for both the state-dependent angular momenta and the vibrational state. M is the projection of the total angular momentum along the laboratory axis Z and is therefore the magnetic quantum number which quantizes the splitting of the levels in a weak magnetic field. Finally, $|n\rangle$ is simply a compound index representing the various quantum numbers. These basis functions are symmetrized to give a definite parity, τ . Only J and τ are conserved quantum numbers with the addition of u/g for homonuclear molecules.

Duo obtains the wavefunctions for a given nuclear motion problem by diagonalizing a coupled-states Hamiltonian. These wavefunctions, $\phi_\lambda^{J\tau}$, are then given by

$$\phi_\lambda^{J\tau} = \sum_n C_{\lambda n}^{J\tau} |n\rangle, \quad (2)$$

where λ denotes the electronic state.

In the case of weak magnetic fields, the Zeeman splitting can be approximated by

$$\Delta E_B = g_J M \mu_0 B, \quad (3)$$

where ΔE_B is the shift in energy of a state with total angular momentum J and projection of J along the field direction is M , g_J is the Landé factor, μ_0 is the Bohr magneton, B is the magnetic field. Within a Hund's case (a) representation, the Landé g -factor is given by [20,44]:

$$g_J^{(a)} = \frac{(g_L \Lambda + g_S \Sigma) \Omega}{J(J+1)} \quad (4)$$

where g_S and g_L are the standard electron spin and orbital g -factors respectively. If Λ and Σ are conserved quantities for a given rovibronic state then this expression is analytic; below this will be known as the QN(a) approximation meaning good quantum numbers in Hund's case (a).

The good-quantum number approximation has been also introduced and used in the case of the NiH spectroscopy by Gray et al. [20]. Here we used g_J as a total Landé factor which includes all

other contributions from the electron spin and orbital angular momenta; this is different from the definition conventionally used in Zeeman experimental studies, see, for example, Gray et al. [20].

The corresponding expression for the Hund's case (b) Landé factor can be approximated by Solanki [44]

$$g_J^{(b)} = \frac{g_L}{2J(J+1)} \left\{ \frac{\Lambda^2 [J(J+1) + N(N+1) - S(S+1)]}{N(N+1)} \right\} + \frac{g_S}{2J(J+1)} [J(J+1) - N(N+1) + S(S+1)], \quad (5)$$

where N is the rotational quantum number. If Λ and N are conserved quantities for a given rovibronic state then this expression is analytic; below this will be known as the QN(b) approximation meaning good quantum numbers in Hund's case (b).

The intermediate (and more general) case can be modeled using the \underline{G} matrix with the following matrix elements [44]:

$$G_{\Sigma, \Sigma} = \frac{(g_L \Lambda + g_S \Sigma) \Omega}{J(J+1)}, \quad (6)$$

$$G_{\Sigma, \Sigma \pm 1} = g_S \frac{\sqrt{S(S+1) - \Sigma(\Sigma \pm 1)} \sqrt{J(J+1) - \Omega(\Omega \pm 1)}}{2J(J+1)} \delta_{\nu, \nu'} \delta_{\Lambda, \Lambda'} \delta_{S, S'}. \quad (7)$$

In practice Λ and Σ are not generally conserved when spin-orbit and other curve coupling effects are taken into account. In this case one can use the Duo wavefunctions to compute g_J for a given rovibronic state by averaging over the corresponding wavefunction as given by

$$G_{\Sigma, \Sigma}^{\text{Duo}} = \sum_n |C_{\lambda n}^{J\tau}|^2 \frac{(g_L \Lambda_n + g_S \Sigma_n) \Omega_n}{J(J+1)}, \quad (8)$$

$$G_{\Sigma, \Sigma \pm 1}^{\text{Duo}} = \sum_n \sum_{n'} C_{\lambda n}^{J\tau} C_{\lambda n'}^{J\tau} \delta_{\nu, \nu'} \delta_{\Lambda, \Lambda'} \delta_{S, S'} \times g_S \frac{\sqrt{S_n(S_n + 1) - \Sigma_n(\Sigma_n \pm 1)} \sqrt{J(J+1) - \Omega_n(\Omega_n \pm 1)}}{2J(J+1)}, \quad (9)$$

where S_n , Λ_n and Σ_n are the values of S , Λ and Σ taken in basis function $|n\rangle$ and $\Omega_n = \Lambda_n + \Sigma_n$, case (a). In the following we also assume $g_L = 1$ and $g_S = 2.0023$.

To help interpret our results we define the difference between g_J 's evaluated using Duo wavefunctions and using the QN approximation as given by.

$$\Delta g_J^{(x)} = g_J^{\text{Duo}} - g_J^{(x)}. \quad (10)$$

where (x) is (a) or (b) as appropriate.

3. Results

3.1. AlO

As an initial test case Landé g -factors were computed for aluminum oxide (AlO). The spectroscopic model used for AlO is due to Patrascu et al. [29,40] which is based on *ab initio* curves tuned to reproduce the extensive set of experimental spectra. The model comprises three electronic states: X ²Σ⁺, A ²Π and B ²Σ⁺. The latter two states lie, respectively, 5,406 and 20,688 cm⁻¹ above the ground states. The closeness of the X and A states leads to significant mixing. A recent study of radiative lifetime [45] using this model showed strong effects due to X – A mixing but that the B state appeared largely unperturbed.

Fig. 1 shows the difference between g_J 's evaluated using Duo wavefunctions and using the QN approximations. These results show systematic effects. Firstly, it would appear that the g_J -factors for the X ²Σ⁺ and B ²Σ⁺ are significantly better represented in the Hund's case (b) than case (a). Secondly, the A ²Π appears closer to Hund's case (a), although in this case the

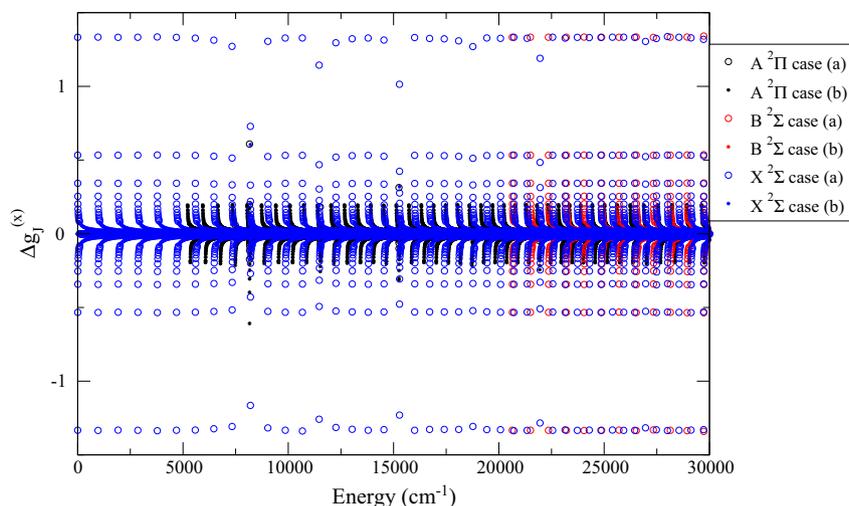


Fig. 1. Difference between Landé g -factors obtained for AIO using Duo wavefunctions and the QN approximations.

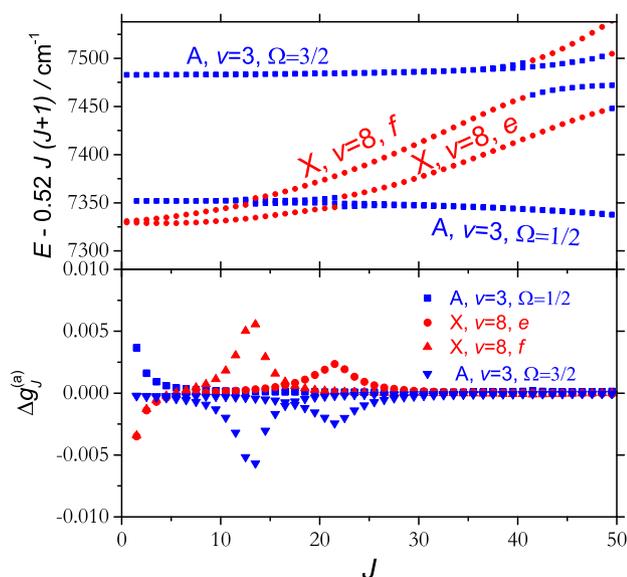


Fig. 2. Reduced energy term values of AIO in the region of the crossing between X, $\nu = 8$ and A, $\nu = 3$ (upper display) and difference between Landé g -factors obtained for AIO using Duo wavefunctions and the QN Hund's case (a) approximation.

differences are smaller. Finally, there are a number perturbations caused by a coupling between levels in the X and A states. Such interactions have been noted before [45].

Changes due to the X – A state coupling appearing as well pronounced structures in Fig. 1 suggest that the B state g -factors are largely unchanged from the idealized values. In order to illustrate how the coupling between different states affect the values of the Landé factors in Fig. 2 we show energy crossings between the X ($\nu = 8$) and A ($\nu = 3, \Sigma = 1/2$ and $\Sigma = 3/2$) rovibronic states (upper display). The spikes in the J progressions of the Landé factors (lower display) appear at the same J values (13.5 and 21.5) as the two crossings. This is where the wavefunctions are extremely mixed and the quantum number approximation, Eq. (4), becomes very poor. The net effect from the Duo model even in case of strongest couplings of AIO is still relatively small, of the order of 10^{-2} for $J = 50$ see Fig. 3.

Fig. 3 shows the g_J values computed using the three methods: Duo wavefunctions, Hund's case (a) and Hund's case (b) approxi-

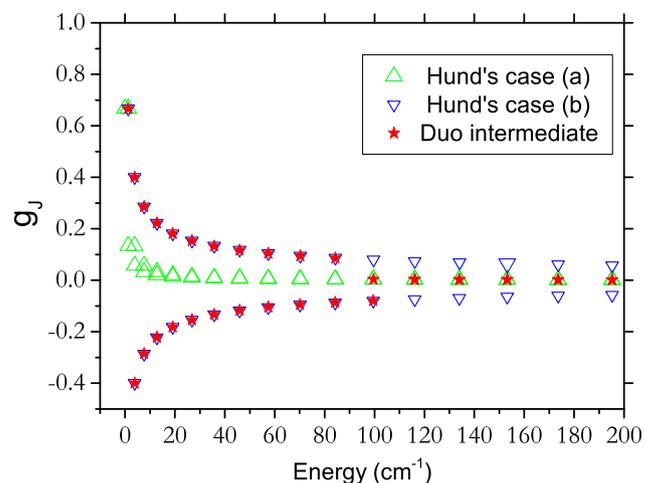


Fig. 3. Landé g -factors of AIO obtained using Duo wavefunctions with Eqs. (8), (9) and the QN approximation, Hund's cases (a) and (b).

mations for the X ($\nu = 0$) state. The character of g_J changes from (b) to (a) as energy increases, illustrating importance of the proper modelling of the Zeeman effect.

We should note the study by Gilka et al. [46], where the effects of couplings between orbital- and spin-angular momenta of the X and A states on the g_5 values were also studied in their *ab initio* calculations of the g -tensor of AIO.

3.2. NO

The nitric oxide (NO) molecule provides a rather simple test of our methodology. McConkey et al. [37] recently constructed a spectroscopic model and generated the associated line list for NO considering only the X $^2\Pi$ electronic ground state. McConkey et al. consider all 6 major isotopologues of the system; here we restrict ourselves to $^{14}\text{N}^{16}\text{O}$ for which there are some limited, experimental studies on the behavior of its ground state ro-vibrational transitions in a magnetic field, albeit a relatively strong one [47]. These observations have been subject of recent models [23] which show that for most of the field strengths considered it was necessary to move beyond the linear Zeeman effect considered here. We note the Zeeman effect in NO has also been used to ascertain the distribution of NO in the Martian atmosphere [48].

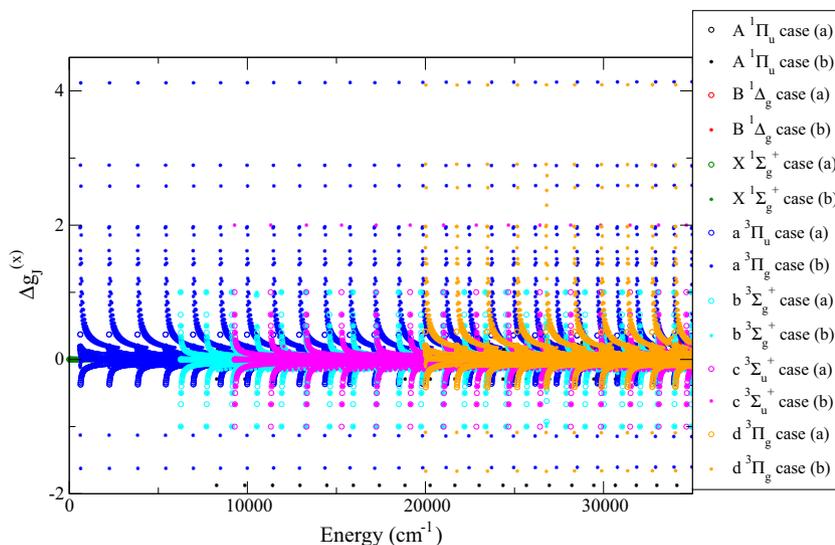


Fig. 4. Difference between Landé g -factors obtained for C_2 using Duo wavefunctions and the QN approximation.

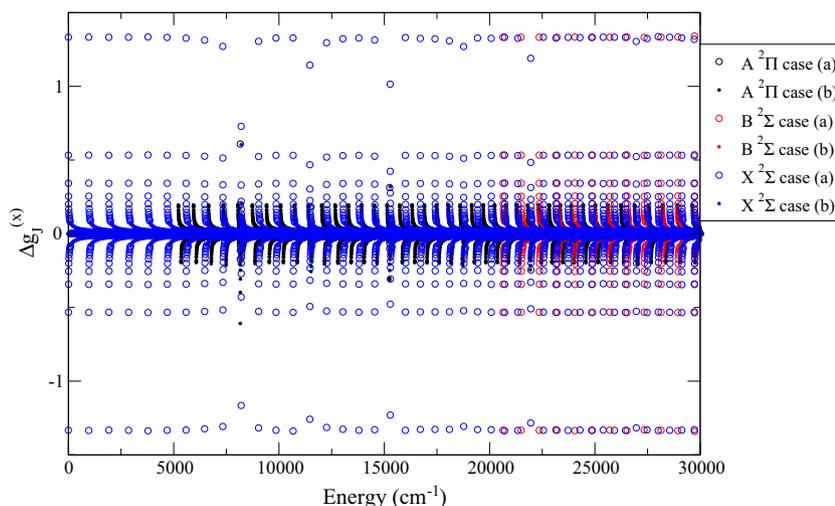


Fig. 5. Difference between Landé g -factors obtained for CrH using Duo wavefunctions and the QN approximation.

The spectroscopic model of McConkey et al. [37] made extensive use of experimental data in determining both the shape of the $X^2\Pi$ potential energy curve and the various coupling terms. However even with a high quality fit their model does not predict transition frequencies with the accuracy required for studying the relatively small Zeeman splittings. We therefore follow McConkey et al. and adopt as our zero-field energy levels the empirical values they determine.

The experimental study of Ionin et al. [47] only considered in detail the splitting of the $^2\Pi_{3/2}$ Q(2.5) fundamental transition at 1875.7228 cm^{-1} as a function of magnetic field. Their strategy was to use the magnetic field to tune the transition into resonance with CO laser lines. Ionin et al. observed 3 components of this transition, namely the (M', M'') ones associated with $(1/2, -1/2)$, $(3/2, 1/2)$ and $(5/2, 3/2)$ which they observed using the CO laser line $9 \rightarrow 8$ P(15) which lies at 1876.30 cm^{-1} . Bringing the lines into resonance required magnetic fields of approximately 3.8, 4.2 and 5.6 T respectively. Strong fields are required since the g factors for the ground and first excited vibrational states are fairly similar so the transition frequency only depends weakly on B .

If the Zeeman splittings were linear then the three lines considered would all lie at the same frequency. In practice this is only true up to about 2 T and for fields above this value the quadratic Zeeman effects become increasingly important [47,23]. The previous studies suggest that only the $(M', M'') = (1/2, -1/2)$ transition frequency varies approximately linearly with field strength in the 2–6 T region. Our calculations place this transition at 1876.29 cm^{-1} for a field of 3.8 T, in excellent agreement with the observations. This values are obtained from our calculated g_J factors of 0.316625 and 0.316857 for the $^2\Pi_{3/2}$ $J = 2.5$ state of $v = 0$ and $v = 1$ respectively.

3.3. C_2

The carbon dimer is a very well studied system [38,49] whose spectrum is widely used for studying astronomical and terrestrial plasmas. The many systems of C_2 electronic bands are well-known to have many perturbations due to couplings between states, something that should be reflected in the Landé g -factors.

The ExoMol model for C_2 considers the eight lowest electronic states of C_2 : $X^1\Sigma_g^+$, $A^1\Pi_u$, $B^1\Delta_g$, $B'^1\Sigma_g^+$, $a^3\Pi_u$, $b^3\Sigma_g^-$, $c^3\Sigma_u^+$, and

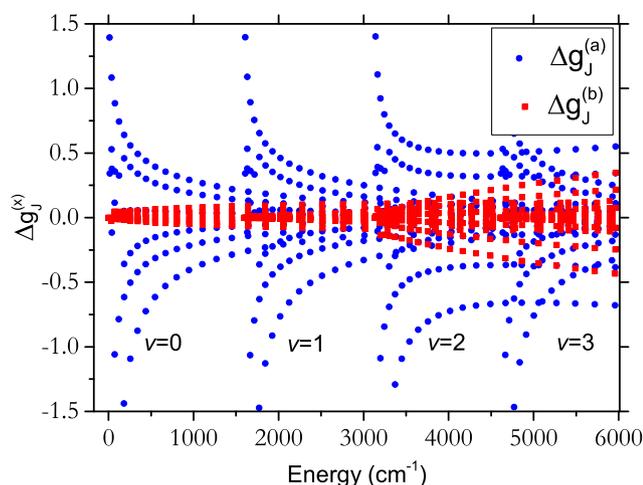


Fig. 6. Difference between Landé g -factors obtained for CrH using Duo wavefunctions, the QN case (a) and (b) approximations.

$d^3\Pi_g$. Due to strong interactions between rovibronic states in this system especially at high rotational excitations, the approximate quantum numbers cease to be meaningful and therefore very difficult to correlate between Hund's cases. Therefore we restrict ourselves to states with $J \leq 35$ and energies up to $35,000 \text{ cm}^{-1}$.

Fig. 4 gives an overview of our computed Landé g -factors for C_2 . It is clear that for this system the changes caused by coupling between states are large.

Apart from the characteristic spikes as in the case of AlO, these Landé factors show that these deviated values also build well defined horizontal patterns. These patterns should indicate a deviation of the C_2 spectra from Hund's case (a). The transition from Hund's cases (a) and (b) for different J is a well-known issue in the analysis of the rovibronic spectra of C_2 , see, for example, [50].

4. CrH

As a final example we consider the CrH molecule, another astronomically important species. The ExoMol model [33] for this system considers the lowest 8 electronic states: $X^6\Sigma^+$, $a^4\Sigma^+$, $A^6\Sigma^+$, $B^6\Pi$, $b^4\Pi$, $C^6\Delta$, $c^4\Delta$ and the lowest dissociative $8\Sigma^+$ state. Here we consider states with $J \leq 35$ and energies up to $35,000 \text{ cm}^{-1}$. As the model used does not consider electronic states with thresholds above $20,000 \text{ cm}^{-1}$, where new states become increasingly dense, it is likely that our calculations will underestimate the perturbation of the g -factors in this region. However even below $10,000 \text{ cm}^{-1}$, where the states all belong to $X^6\Sigma^+$ electronic state the perturbations are fairly large.

Fig. 5 gives an overview of our computed Landé g -factors for the lowest two sextet states of CrH compared to the QN approximations. Clearly there are lots of structures. For the singlet X state, QN (a) appears a poor approximation in all cases (see Fig. 6); QN (b) does better but still shows pronounced structures starting at about 4000 cm^{-1} . Above about $14,000 \text{ cm}^{-1}$ all X state g_j factors appear highly perturbed. This is also true for the singlet A state.

Chen et al. [6] measured effective g values for a few levels in CrH; Table 1 compares these measurements ($A^6\Sigma^+$, $v=1$) with our results. This table also shows that the Hund's case (b) approximation to g_j is more appropriate than case (a). Chen et al. [6] also reported an averaged g value for the $A^6\Sigma^+$, $v=0$ state over the measured values for four states $J=3/2, N=1, J=5/2, N=0, J=5/2, N=1, J=7/2, N=1$ of $2.0081(20)$. Using the Duo g_j

Table 1

Comparison between measured values of g_j for CrH due to Chen et al. [6] and our calculated values using the Duo wavefunction approach, Hund's cases (a) and (b) approximations.

State	[6]	Duo	QN(a)	QN(b)
$N=0, J=5/2$	1.7468(17)	1.9781	0.0571	2
$N=1, J=3/2$	1.8760(30)	2.8168	0.1333	2.8
$N=1, J=5/2$	1.7208(28)	1.7433	0.0571	2
$N=1, J=7/2$	1.9123(25)	1.4221	1.4286	1.7714

values to produce the same averaging we obtained 1.9976, which is in very close agreement to the experiment. The agreement for other levels is not as good, suggesting that our model for CrH needs further improvement.

5. Conclusion

We have developed a numerical procedure for evaluating Landé g -factors for diatomic molecules without making any assumptions about conserved quantum numbers. This method is tested for four molecules AlO, NO, C_2 and CrH. It would seem that besides making predictions for g -factors, the comparison between our computed value and the value predicted under the assumption of particular Hund's case gives a clear means of distinguishing those levels which are best represented by Hund's case (a) from those which are approximately Hund's case (b)-like.

The accuracy of our predicted g_j factors depend on a number of factors: (a) the accuracy of the underlying spectroscopic model used and, in particular, its ability to reproduce coupling between different electronic states, (b) our ability to solve this model by, for instance, converging the basis set representation and (c) any assumptions made about angular momentum couplings within the system. Although our procedure is based on a Hund's case (a) coupling scheme, our general formulation means that no actual approximations are made by adopting a (complete) basis formulated within this scheme. Similarly it is relatively easy, and computationally cheap, to use large vibrational basis sets when converging the problem. This means that the choice of spectroscopic model is likely to be the major source of uncertainty in our calculations or, conversely, that available measurements of Landé g -factors have the potential to be used to improve the spectroscopic model. In addition we note that our formulation is only appropriate when the changes depend linearly with the magnetic field. Inclusion of non-linear effects require a more sophisticated treatment which we plan to study in future work.

It is our plan to routinely compute Landé g -factors for all open shell diatomic species studied as part of the ExoMol project from now on. To this end, the new ExoMol data format [51] has been adjusted to include the computed values of g_j for each state as part of the states file made available for each isotopologue studied.

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