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MARVEL Analysis of barium oxide (BaO): Generation of magnetic field Landé g-factors.

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Introduction

In this poster we present progress on developing “magnetic line lists” for the diatomic molecule BaO which are a function of an external weak magnetic field (Zeeman effect).

This is a development to the work done within the ExoMol group which began in 2011 with the aims of developing line lists (lists of wavelengths with corresponding intensities) for molecules of interest in exoplanets which are unperturbed by magnetic fields.

Diatomic molecules in sunspots

It has been known since the early 19th century that diatomic molecules are present in sunspots (Richardson 1931, Babcock 1945, Broida & Moore 1957, Moore-Sitterly 1967, Wöhl 1971). Since then, various authors (Bagare, Balachandrakumar, Brault, Chaturvedi, Engvold, Karthikeyan, Raja, Rajamanickam, Sangeetha, Shanmugapriya, Shanmugavel, Sriramachandran, Viswanathan) have searched for and tentatively detected molecules in sunspots and, for those positively identified identified and calculated effective temperatures.

Interest in the study of using molecules as magnetic field probes in sunspots has more recently been heightened with the proposition that the formation of diatomic molecules play a crucial role in the evolution of the magnetic fields within sunspots (Jaeggli et al. 2011).

The existence of the diatomic molecule BaO was confirmed by Shanmugapriya et al. (2015) who analysed the rotational lines of the $A^1\Sigma^+ - X^1\Sigma^+$ and $A^1\Pi - X^1\Sigma^+$ systems and evaluated rotational temperature.

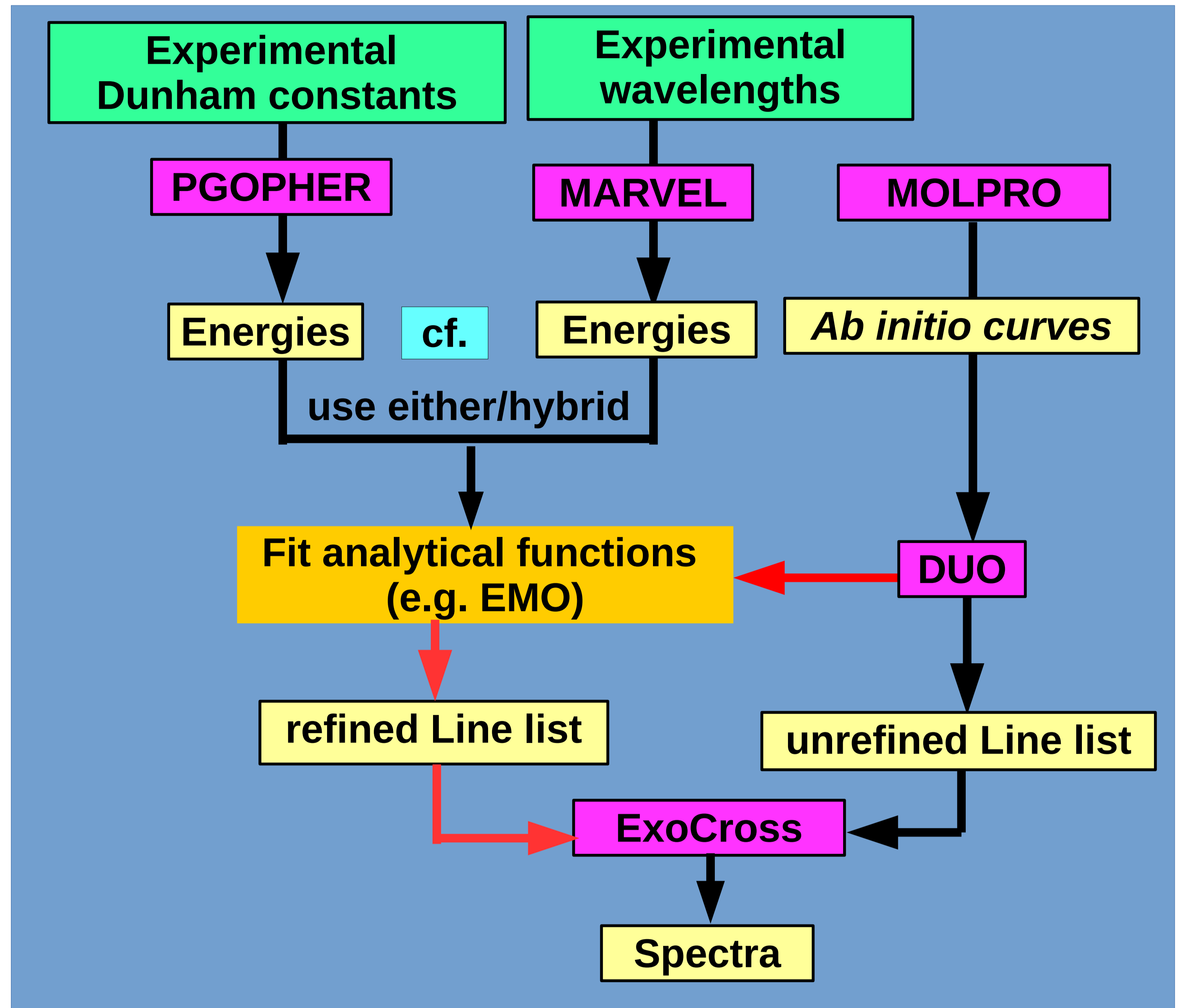


Figure 1. Schematic of calculation of refined line list (ExoMol process).

Study	System	Vibrational coverage	J range
Mahanti (1934)	$A^1\Sigma^+ - X^1\Sigma^+$	(0, 2), (0, 3), (1, 1), (1, 2), (2, 1)	0 - 59
Lagerqvist, Lind & Barrow (1950)		(0, 2), (0, 3), (1, 1), (1, 2), (2, 1), (2, 0), (3, 0), (3, 1), (0, 4), (4, 0), (5, 0)	0 - 83
Furio & Pruett (1989)		(10, 0), (11, 0).....(15, 0), (16, 1), (17, 1)	0 - 58
Shanmugapriya et al. (2015)		(0, 2), (0, 3)	0 - 83
Pruett & Zare (1975)	$A^1\Pi - X^1\Sigma^+$	(12, 0), (17, 0), (18, 0)	13 - 54
Furio & Pruett (1989)		(10, 0), (11, 0).....(17, 0)	3 - 47
Shanmugapriya et al. (2015)		(12, 0)	14 - 55

Table 1. Overview of experimental data inputted into MARVEL in order to construct a list of self-consistent energy levels which can be used to produce a (zero field) refined line list.

Compilation and analysis of experimental data

Referring to Table 1, a “MARVEL” analysis of the available experimental measurements for the $A^1 - X$ and $A-X$ systems has been undertaken.

MARVEL stands for “Measured Active Rotational-Vibrational Energy Levels” and is a program which converts lists of transitions into a self-consistent list of energy levels taking into experimental uncertainties.

Additionally, experimental Dunham constants have been gathered and a Dunham expansion performed for the X , A^1 and A states of BaO. The list of energies produced has been compared to the “MARVEL” energies and shows a satisfactory match.

Calculation of magnetic line lists

The process for the calculation of a line list in the absence of an external field is shown in Figure 1. The format of the outputted line list is as follows:

States file: contains energy level, quantum labels, lifetime, Landé g-factor, “counting number”.

Trans file: transition frequency, intensity and two “counting numbers” corresponding to energy states which transition is between.

At present code is in development which, for a given magnetic field, calculates the new rovibronic states (using the Landé g-factors) and the transitions by using the magnetic field selection rules. For a given state and magnetic field, the perturbation to a single energy level is given as:

$$\Delta E_{\text{Zeeman}} = g_J M \mu_0 B$$

where

- g_J is the Landé g-factor,
- M is the projection of the magnetic field along the field axis ($-J, -J+1, \dots, J-1, J$),
- B is the applied external magnetic field and
- μ_0 is the Bohr magneton.

$$E_5 = E_1 + \lambda_{13} + \lambda_{35} \text{ or}$$

$$E_5 = E_1 + \lambda_{12} + \lambda_{23} + \lambda_{35} \text{ or}$$

$$E_5 = E_1 + \lambda_{12} + \lambda_{24} + \lambda_{45}$$

$$E_4 = E_1 + \lambda_{12} + \lambda_{24} \text{ or}$$

$$E_4 = E_1 + \lambda_{13} + \lambda_{35} - \lambda_{45}$$

$$E_3 = E_1 + \lambda_{13} \text{ or}$$

$$E_3 = E_1 + \lambda_{12} + \lambda_{23}$$

$$E_2 = E_1 + \lambda_{12} \text{ or}$$

$$E_2 = E_1 + \lambda_{13} - \lambda_{23}$$

$$E_1 = 0.00$$

Figure 2. Schematic demonstrating how the MARVEL process works. Given experimentally measured wavelengths, the MARVEL program will assign one state to have energy $E_1 = 0.00$ and then from there build a network of self-consistent energy levels taking into account all possible “routes” between energy levels.