

Synthetic spectra of BeH, BeD and BeT for modelling of emission from the JET plasma

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In order to predict the erosion of the Be first wall in fusion devices such as ITER, an understanding of the release and transport of Be is an essential requirement. A study of the molecular spectra, such as those for BeH, BeD and BeT can provide valuable input to codes used for modelling these processes. To this end, synthetic spectra have been derived from potential energy curves (PECs) and *ab initio* dipole curves. Assigned synthetic spectra for BeD are presented alongside high resolution BeD spectra taken from recent JET pulses. Accurate experimental transition data for the X $^2\Sigma^+$, A $^2\Pi$, and C $^2\Sigma^+$ states of BeH, BeD and BeT are run through a program which calculates the relative positions of the energy levels from the assigned experimental transitions (Marvel Online [1]). These energy levels are then used to produce a fitted PEC for the upper states including a spin-orbit (LS) coupling term, for the Π state, a state to state (A-X states) coupling term, and Born-Oppenheimer breakdown (BOB) terms. These, along with the fitted curve of Dattani [2], including BOB terms, and (*ab initio*) dipole curves from Pitarch-Ruiz et al [3], are used to generate vibrational-rotational wavefunctions, transition energies, A-values and Franck-Condon factors. From the PECs and dipole curves, accurate assigned synthetic spectra for BeH and any of its isotopologues can be obtained. These results can also be combined with geometry resolved R-matrix calculations to determine non-Boltzmann populations and more accurate estimations of electron temperatures.

^aLitaudon et al, Overview of the JET results in support to ITER, accepted for publication in Nuclear Fusion

References

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