

R-Matrix Calculations of Electron Impact Electronic Excitation of BeH

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We present *ab initio* results of electron scattering calculations from beryllium mono-hydride (BeH) for the purpose of detecting and monitoring the transport of BeH in fusion devices such as JET and ITER [1]. Several target and scattering models have been considered, many of which failed to produce sufficiently accurate results with the UKRMol suite [2]. The final chosen model is a close coupling (CC) frozen core full configuration interaction (FC-FCI) calculation. The scattering calculation is carried out using the R-matrix method and a new version of the UK R-Matrix codes. The standard UKRMol suite uses Gaussian Type Orbitals (GTOs) for the continuum functions; we show this method has numerical problems for the present case. A new B-spline – GTO hybrid continuum function code, implemented in the UKRMol+ suite, gives good results. This new code allows the use of larger R-matrix spheres and avoids issues with linear dependence occasionally encountered with the GTOs continuum functions. The UKRMol+ code will be used to generate new results for BeH collisions including uncertainty quantification. The results from these calculations are to be used in modeling processes in JET [3].

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