

Synthetic spectra of BeH, BeD and BeT using vibronically resolved R-Martrix data for modelling of emission from the JET plasma

Daniel Darby-Lewis,¹; J. Tennyson, UCL; K. D. Lawson, CCFE, Abingdon; S. N. Yurchenko, UCL; M. F. Stamp, A. Shaw, CCFE, Abingdon; JET Contributors²

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. BeD release was shown to contribute more than 50% to the total erosion in certain cases of JET D plasma.³ 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.⁴ To this end, transition energies and A-values have been derived from fitted potential energy curves (PECs)^{5,6,7} and *ab initio* dipole curves.⁸

Ab initio R-matrix data provides electron electronic-excitation cross sections,^{9,10} which along with electron temperature dependent energy distributions can be used to calculate state to state transition rates. Geometry resolved R-matrix calculations will be rotationally-vibrationally averaged to determine vibronic transition rates. These calculations can lead to a non-Boltzmann fitting for the population of states and more accurate estimations for electron temperatures.

¹daniel.darby.11@ucl.ac.uk

²See Litaudon et al, Overview of the JET results in support to ITER, accepted for publication in Nuclear Fusion

³S. Brezinsek, M. F. Stamp, D. Nishijima, D. Borodin, S. Devaux, K. Krieger, S. Marsen, M. O'Mullane, C. Bjoerkas, A. Kirschner, and JET EFDA contributors, Nuclear Fusion 54,103001 (2014)

⁴D. Darby-Lewis, K. Lawson, S. Yurchenko, M. Stamp, A. Shaw, and J. Tennyson, To Be Published. J. Phys. B: At. Mol. Opt. Phys (2017)

⁵T. Furtenbacher, A. G. Császár, and J. Tennyson, J. Mol. Struct. (Theochem) 245, 115–125 (2007)

⁶J. M. Brown, and A. Carrington, Rotational Spectroscopy of Diatomic Molecules (Cambridge Molecular Science), Cambridge University Press, 2003, ISBN 0511814801

⁷S. N. Yurchenko, L. Lodi, J. Tennyson, and A. V. Stolyarov, Computer Phys. Comm. 202, 262–275 (2016)

⁸J. Pitarch-Ruiz, J. Sánchez-Marin, and A. M. Velasco, J. Comput. Chem. 29, 523–532 (2007)

⁹J. M. Carr, P. G. Galiatsatos, J. D. Gorfinkiel, A. G. Harvey, M. A. Lysaght, D. Madden, Z. Mašín, M. Plummer, and J. Tennyson, Eur. Phys. J. D 66, 58 (2012)

¹⁰D. Darby-Lewis, Z. Masin, and J. Tennyson, J. Phys. B: At. Mol. Opt. Phys. 50, 175201 (2017)