Abstract for ICAMDATA05, Meudon, France October 15–19, 2006

Breit-Pauli calculation of Mg V transitions among $2s^22p^4$, $2s2p^5$, $2p^6$ and $2s^22p^33\ell$ levels

N.C.Deb and A.Hibbert

School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

n.deb@qub.ac.uk

Domain : Astrophysics

A full Breit-Pauli calculation of oxygen-like magnesium fine-structure levels belonging to $2s^22p^4$, $2s2p^5$, $2p^6$ and $2s^22p^3({}^4S, {}^2D, {}^2P)3\ell$ configurations will be presented. We have used the CIV3 program of Hibbert [1,2] in this work. Atomic orbitals up to 8*d* are chosen carefully to account for important correlation effects among various configurations. The 3*s*, 3*p* and 3*d* orbitals are optimised on the energies of real states and remaining orbitals are chosen either as a correction type or as correlation type. At the LS stage we have thus used 380,559 configurations including up to three-electron promotions from the ground configuration. At the LSJ stage we retained 120,736 of them whose eigenvector strengths are ≥ 0.001 for the calculation of 86 fine-structure levels belonging to the above configurations. We then apply our fine-tuning procedure to bring the energies in line with the observed values wherever available: we adjust by a small amount the diagonal elements of the Hamiltonian matrix. Oscillator strengths, radiative rates and line strengths for all the E1 transitions among these 86 levels are then calculated.

Results are compared with a similar energy adjusted calculation of Fischer [3], the most recent calculation of Bhatia *et al* [4] and the recommended data of NIST [5]. It is found that present results show excellent agreement with the MCDF calculation of Fischer [3] for most of the transitions. The results of Bhatia *et al* [4] are consistantly higher by 20 to 50%.

[1] A.Hibbert, Comp. Phys. Commun. 9 (1975) 141

[2] R.Glass and A.Hibbert, Comp. Phys. Commun. 16 (1978) 19

[3] C.F.Fischer, http://atoms.vuse.vanderbilt.edu/

[4] A.K.Bhatia, E.Landi and W.Eissner, At. Data Nucl. Data Tables 92 (2006) 105

[5] NIST, http://physics.nist.gov/cgi-bin/AtData/levels_form