§26. Construction of Neutral Transport Code for LHD

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We have been developing a 3D neutral-transport code for hydrogen and helium species in order to investigate LHD plasmas. Collisional-radiative models for the species are indispensable parts of the neutral-transport code to calculate effective reaction rate coefficients of the atoms and molecules. As a revision of the molecular hydrogen collisional-radiative model [1, 2], which includes electronic and vibrational states, we are developing a model that also includes rotational states. This model will provide more precise effective reaction rate coefficients of the molecule.

In the revised model, assuming Hund's (b) case, the levels are labeled by the principal quantum number of the united atom n, and Λ , N, and J. The number of 2131 levels for $n \leq 4$, listed in Ref. [3] is included in the model (Table I).

Table I: Levels in the model.

$X^1\Sigma_q^+$	1-301	$O^1\Sigma_q^+$	642-661	$d^3 \Pi_u^-$	1244 - 1372
$\mathrm{E}^{1}\Sigma_{q}^{+}$	302-333	$\mathrm{B}^{"1}\Sigma_{u}^{+}$	662-676	$d^3 \Pi_u^+$	1373 - 1438
$\mathrm{B}^{1}\Sigma_{u}^{+}$	334 - 423	$\mathrm{D}^{,1}\Pi_u^-$	677 - 692	$g^3 \Sigma_g^+$	1439 - 1523
$C^1 \Pi_u^-$	424 - 454	$\mathrm{D}^{,1}\Pi^+_u$	693-708	$i^3 \Pi_g^{-}$	1524 - 1598
$C^1 \Pi^+_u$	455 - 470	$P^1\Sigma_q^+$	709-716	$i^3 \Pi_q^+$	1599 - 1661
$\mathrm{H}^{1}\Sigma_{g}^{+}$	471 - 484	$\mathrm{R}^{1}\Pi_{g}^{-}$	717 - 725	$j^3 \Delta_g^{-}$	1662 - 1724
$\mathrm{B}^{,1}\Sigma_u^+$	485 - 512	$R^1\Pi_g^+$	726-727	$j^3\Delta_g^+$	1725 - 1784
$D^1\Pi_u^-$	513 - 530	$S^1 \Delta_g^-$	728 - 730	$f^3 \Sigma_u^+$	1785 - 1810
$\mathrm{D}^{1}\Pi_{u}^{+}$	531 - 542	$S^1 \Delta_q^+$	731-733	$k^3 \Pi_u^-$	1811 - 1912
$G^1\Sigma_g^+$	543 - 577	$a^3 \Sigma_g^{+}$	734-881	$k^3 \Pi_u^+$	1913 - 1930
$I^1 \Pi_g^{-}$	578 - 597	$c^3 \Pi_u^{-}$	882-965	$r^3 \Pi_g^-$	1931 - 1999
$I^1\Pi_g^+$	598-617	$c^3 \Pi_u^+$	969 - 1049	$r^3\Pi_g^+$	2000-2062
$J^1 \Delta_g^-$	618-632	$h^3 \Sigma_g^+$	1050 - 1093	$s^3 \Delta_g^{-}$	2063 - 2098
$J^1 \Delta_q^+$	633-641	$e^{3}\Sigma_{u}^{+}$	1094 - 1243	$s^3 \Delta_q^+$	2099 - 2131

Spontaneous transition probabilities $e^{3}\Sigma_{u}^{+} \rightarrow a^{3}\Sigma_{g}^{+}$, $d^{3}\Pi_{u} \rightarrow a^{3}\Sigma_{g}^{+}$, $i^{3}\Pi_{g} \rightarrow c^{3}\Pi_{u}$, $j^{3}\Delta_{g} \rightarrow c^{3}\Pi_{u}$, $I^{1}\Pi_{g} \rightarrow C^{1}\Pi_{u}$, and $J^{1}\Delta_{g} \rightarrow C^{1}\Pi_{u}$ in Ref. [4] are included in the model. The values for other transitions are calculated according to Ref. [5]. Transition probabilities to continuum states are also calculated. The vibrationally resolved excitation cross section from the electronic ground state to $B^{1}\Sigma_{u}^{+}$, $B^{\prime 1}\Sigma_{u}^{+}$, $C^{1}\Pi_{u}$, $D^{1}\Pi_{u}$, $D^{\prime 1}\Pi_{u}$ in Ref. [6] are included in the model; for the excitation to other states, data in Ref. [7,8] are included. Currently, there is not enough information to derive vibrationally and rotationally resolved cross sections. Tentatively, for an optically allowed transition, we assume that the rate coefficients are proportional to Franck-Condon and Hönl-London factors. For an optically forbidden transition, we use the Franck-Condon factor to obtain vibrationally resolved data and divide them evenly for rotational states. Excitation cross sections between excited states are estimated from united atom helium cross sections. Processes which affect the vibrational and rotational population of the ground electronic state are included in the model. Figure 1 shows an example of the calculated population.

We can calculate emission line intensities of hydrogen molecules in plasmas using the neutral transport code which includes the revised collisional-radiative model. Molecular hydrogen spectra observed in LHD will be analyzed with the code.



Fig. 1: Calculated population (see Table I).

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