Supplemental Information for:

"Description of Quantum Interference Using Mixed Quantum/Classical Theory of Inelastic Scattering"

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1. Additional figures for publication

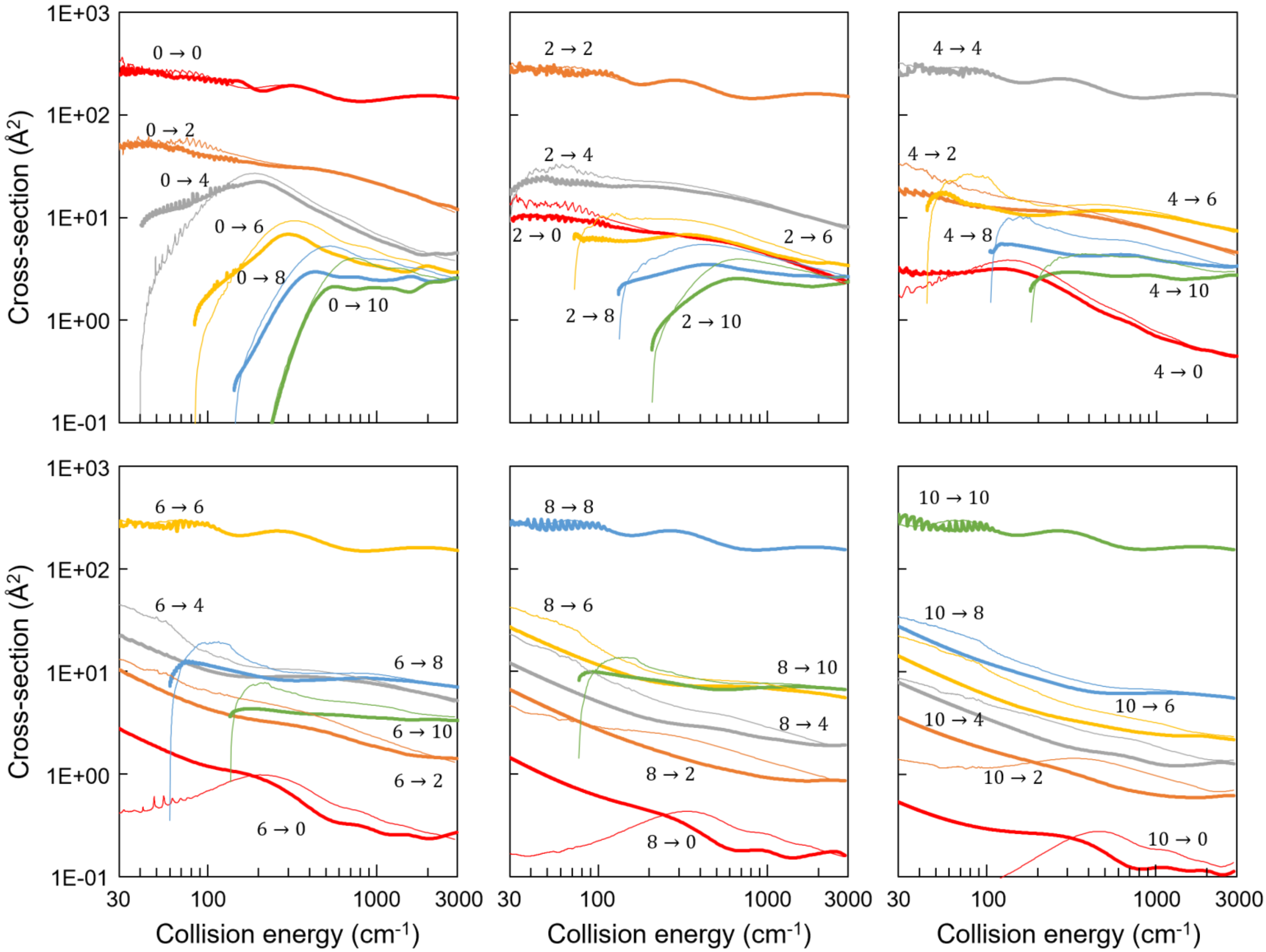

Figure S1: State-to-state transition cross sections from several initial states $0 \le j \le 10$ to several final states j' using Π PES for $N_2 + O$ system. Thick lines correspond to MQCT results, whereas thin lines are MOLSCAT results.

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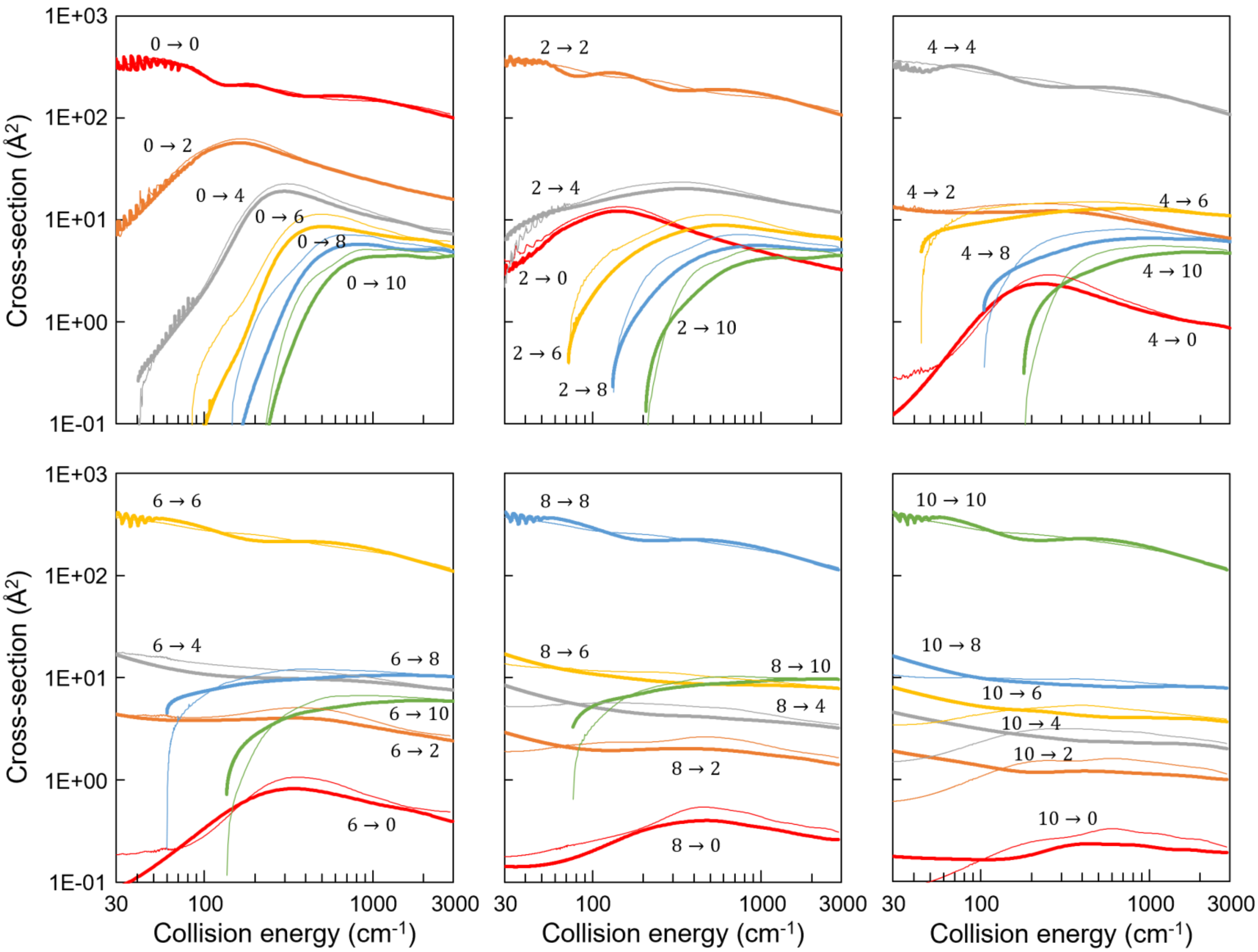


Figure S2: Same as in Fig. S1 but using Σ PES for N_2 + O system.

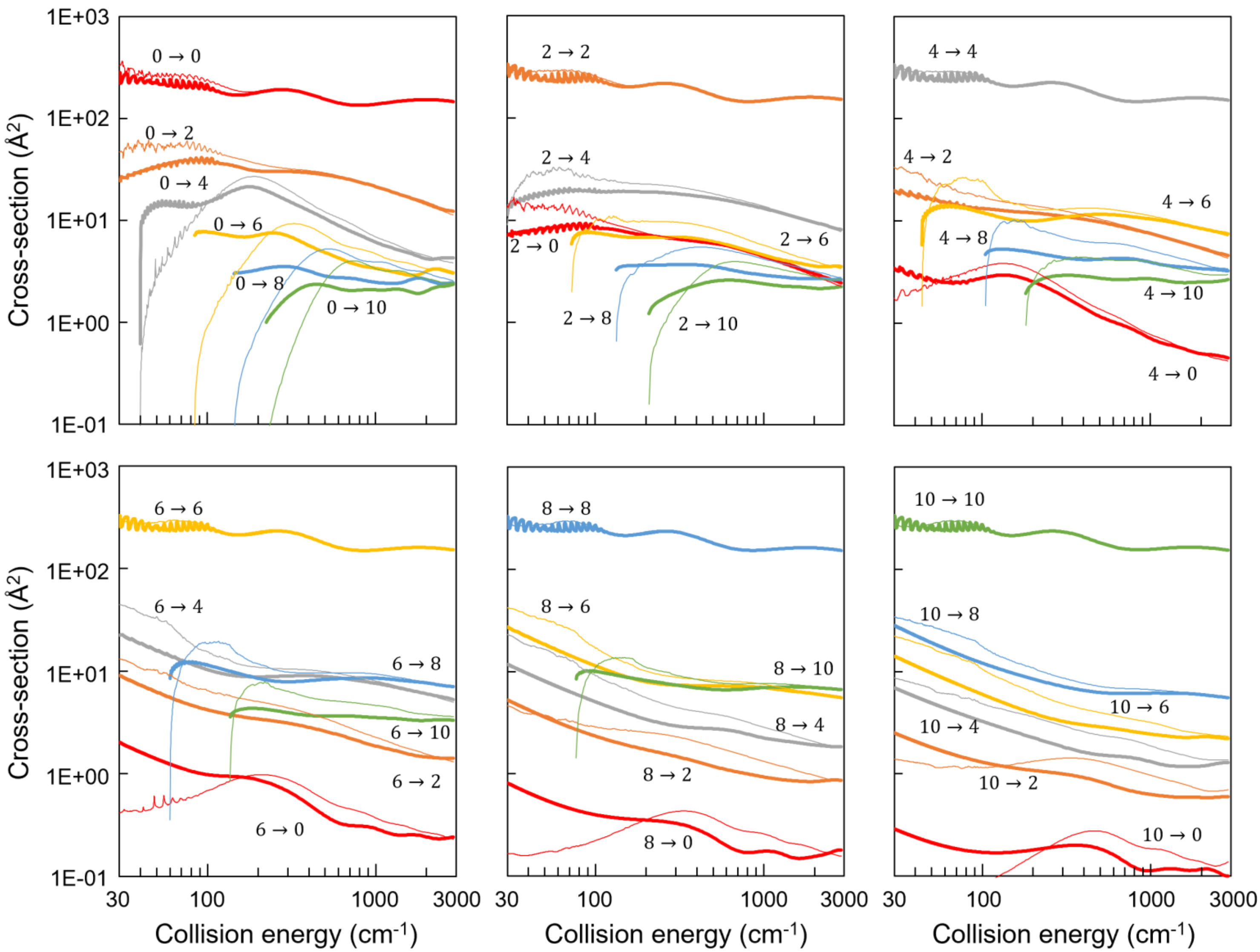


Figure S3: State-to-state transition cross sections from several initial states $0 \leq j \leq 10$ to several final states j' using Π PES for N_2 + O system. Thick lines correspond to AT-MQCT results, whereas thin lines are MOLSCAT results.

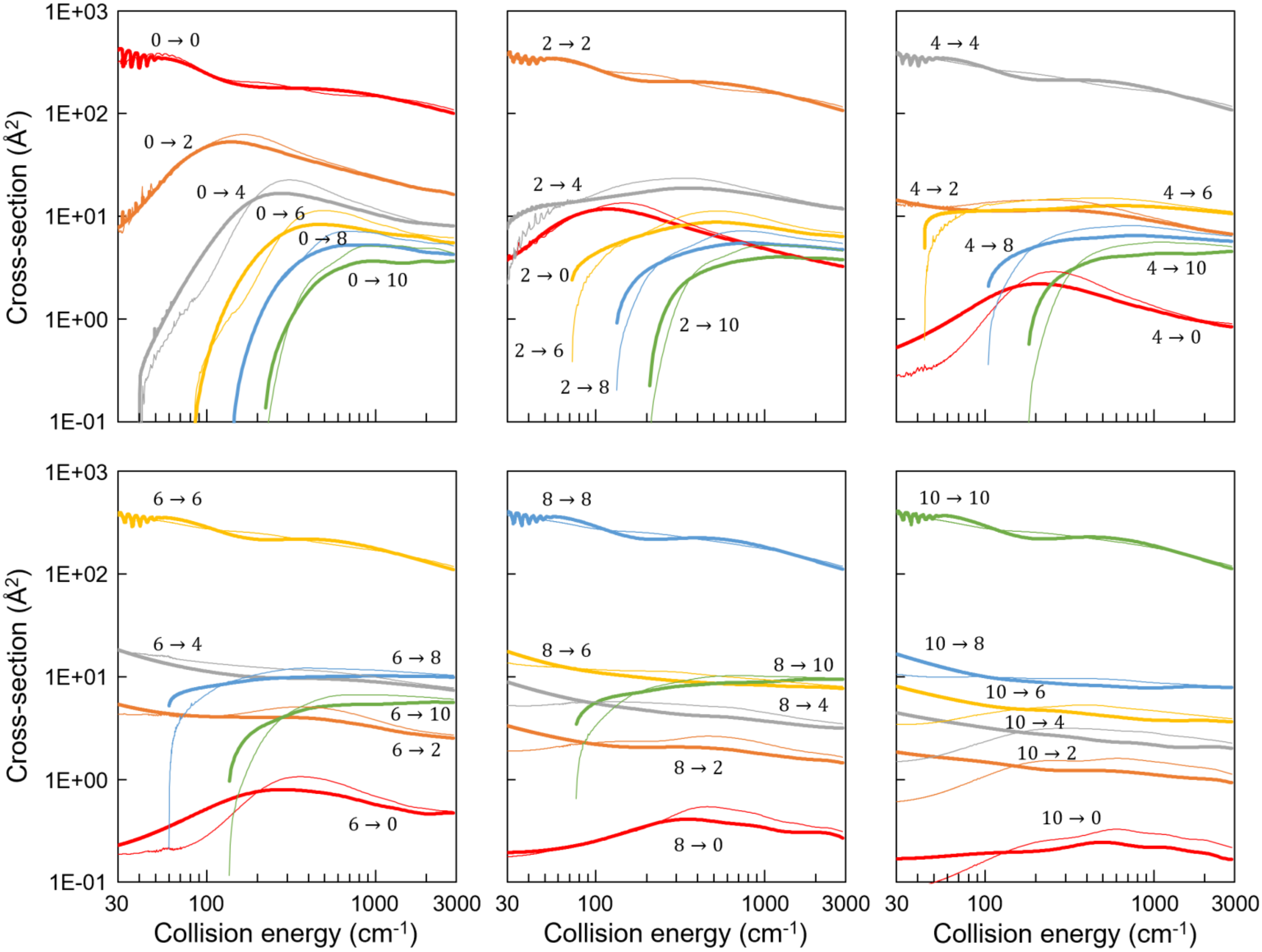


Figure S4: Same as in Fig. S3 but using Σ PES for N_2 + O system.

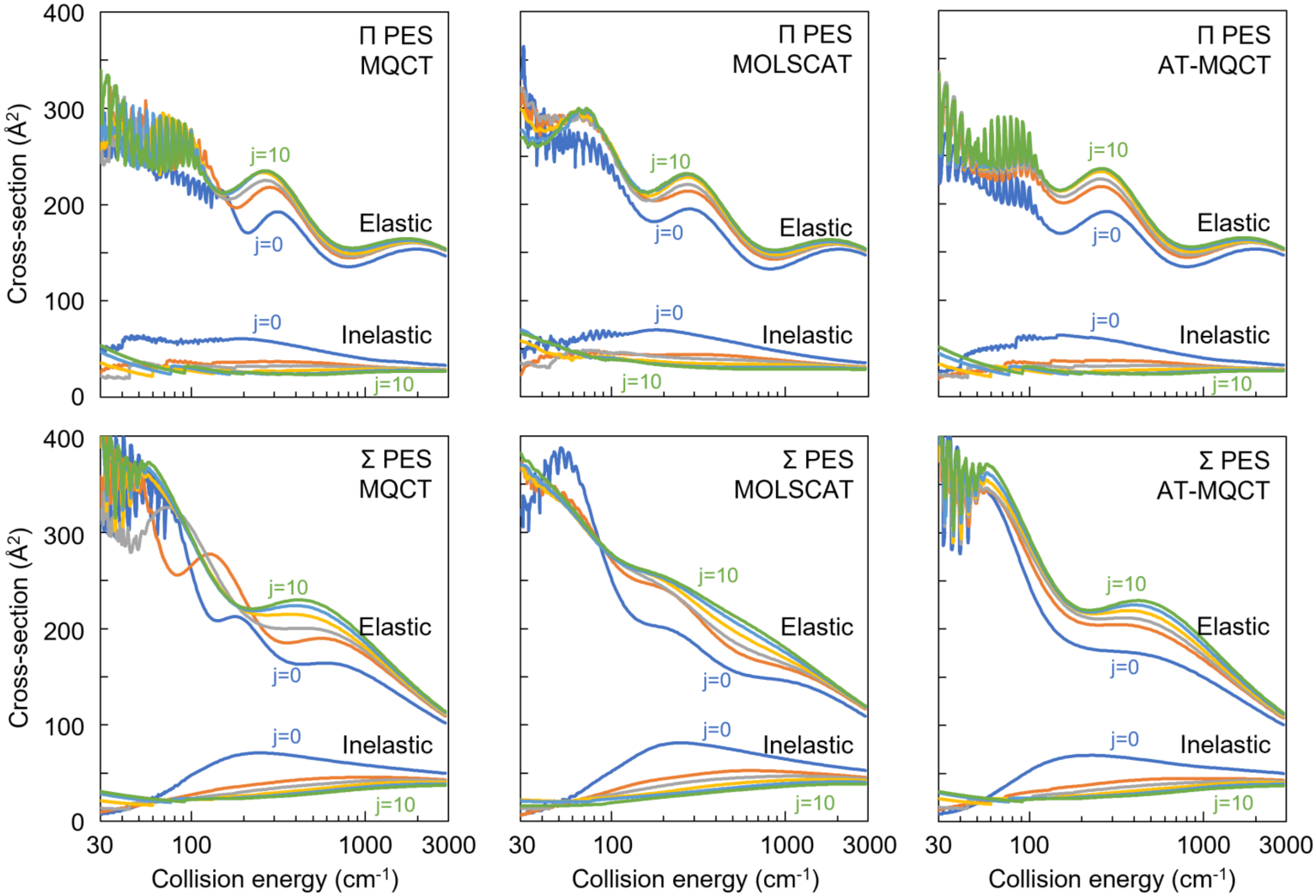


Figure S5: Elastic and inelastic cross sections as a function of collision energy computed using three different methods (MOLSCAT, MQCT, AT-MQCT) for several initial states of N_2 + O system indicated by color: $j = 0$ is blue, $j = 2$ is orange, $j = 4$ is gray, $j = 6$ is yellow, $j = 8$ is turquoise and $j = 10$ is green. Upper row of figures corresponds to Π PES, while lower row corresponds to Σ PES.

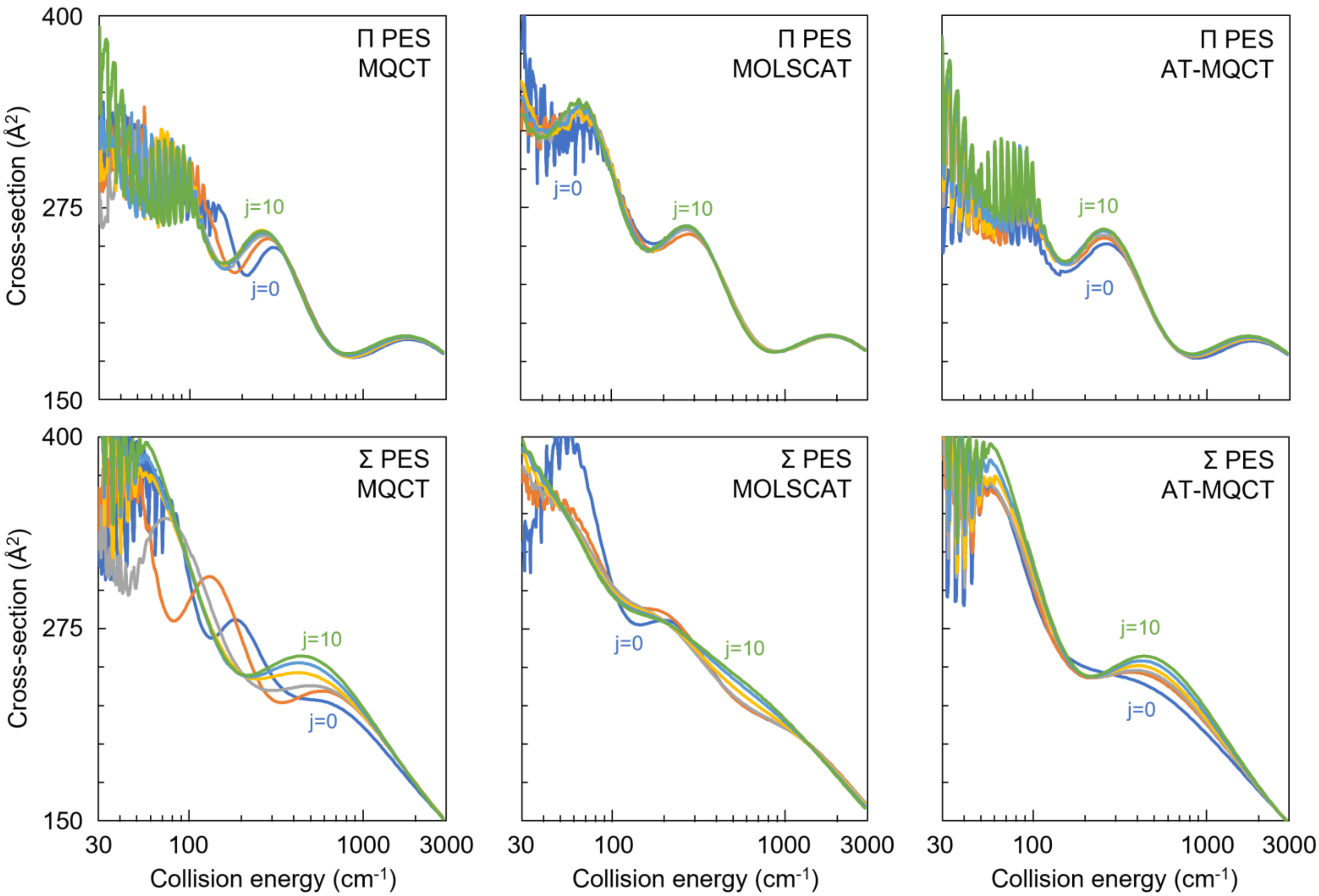


Figure S6: Total cross sections (elastic + inelastic) as a function of collision energy computed using three different methods (MOLSCAT, MQCT, AT-MQCT) for N_2 + O system. Colors corresponds to different initial states $0 \leq j \leq 10$ as indicated in Fig. S5.

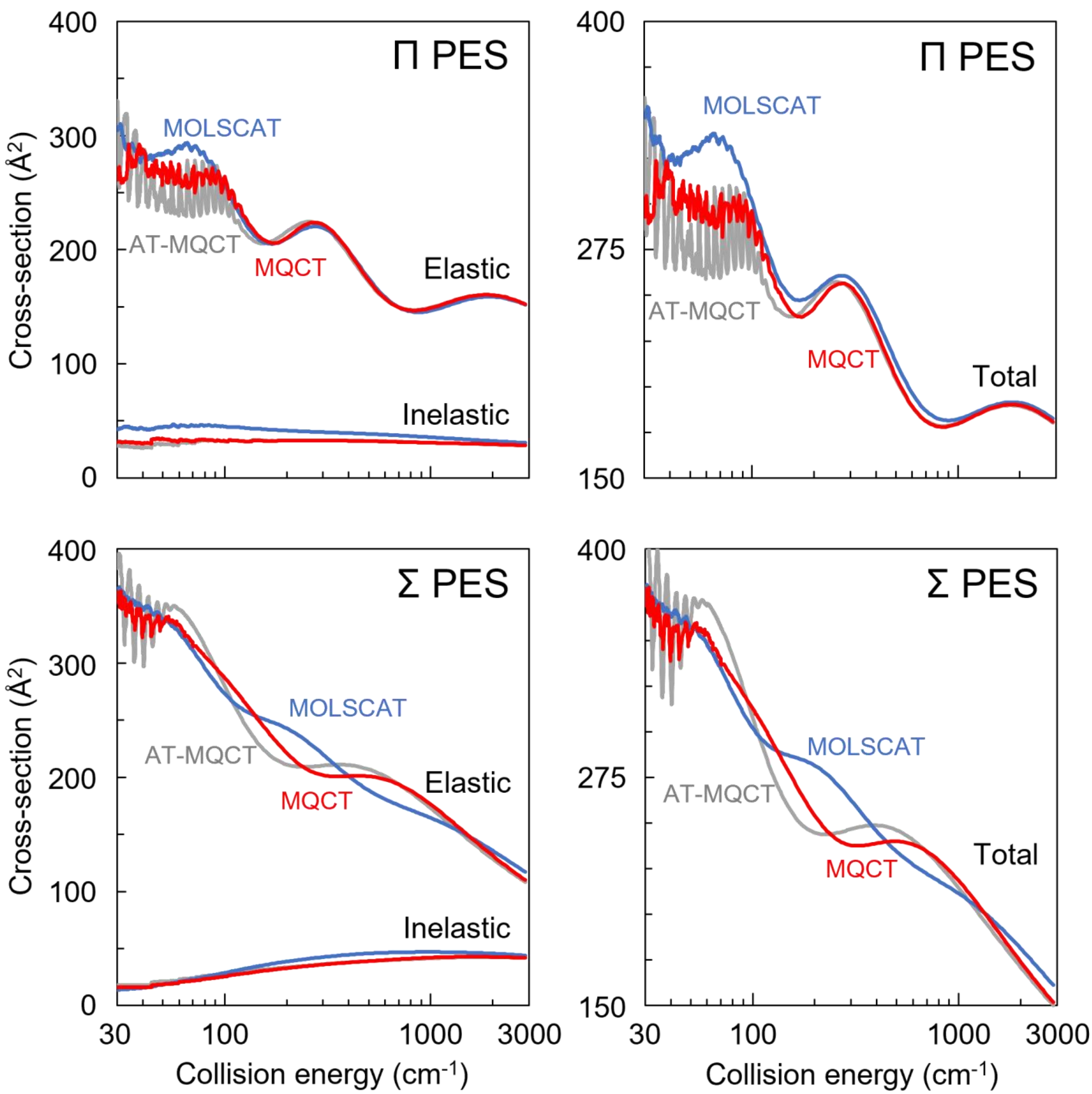


Figure S7: Thermally averaged cross sections for N_2 + O system at T = 90 K as a function of collision energy. Left frames give elastic and inelastic contributions separately, while right frames give the total scattering cross section. Upper and lower rows are for Π and Σ PESs, respectively. Results of three different methods (MOLSCAT, MQCT, AT-MQCT) are indicated by color.

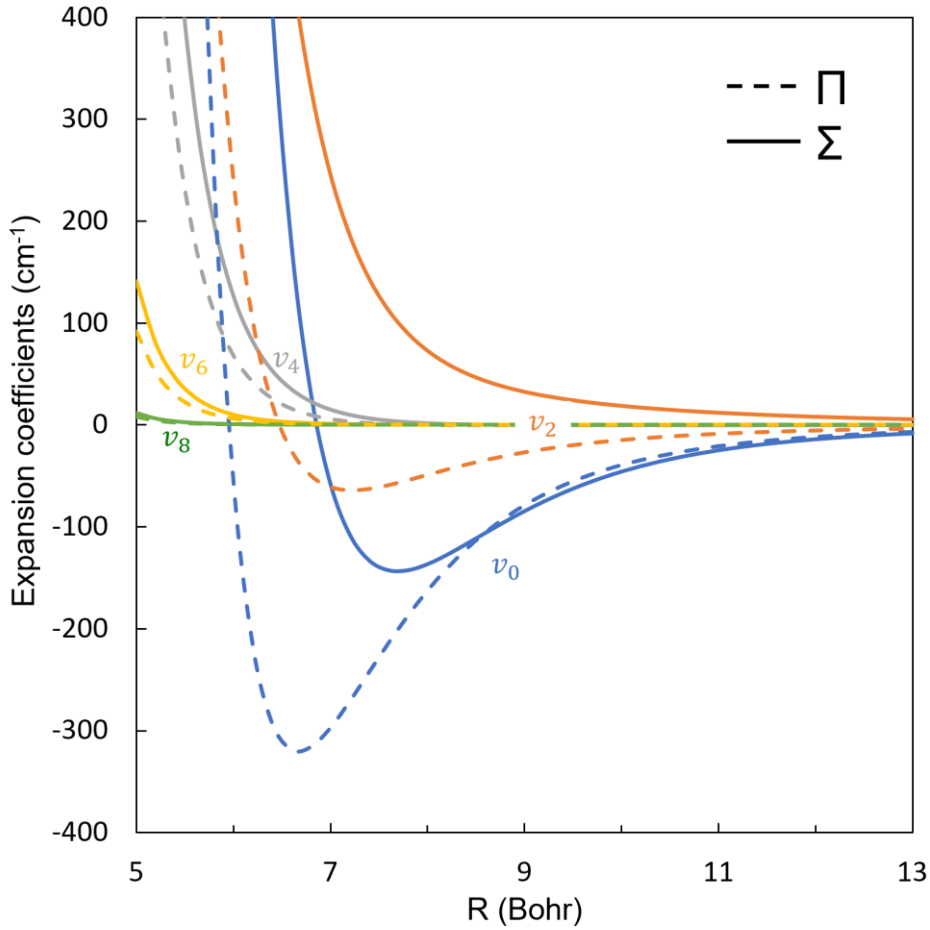


Figure S8: Radial dependence of expansion coefficients $v_\lambda(R)$ for even $0 \le \lambda \le 8$ for Π (dashed lines) and Σ (solid lines) PESs of N_2 + O system.

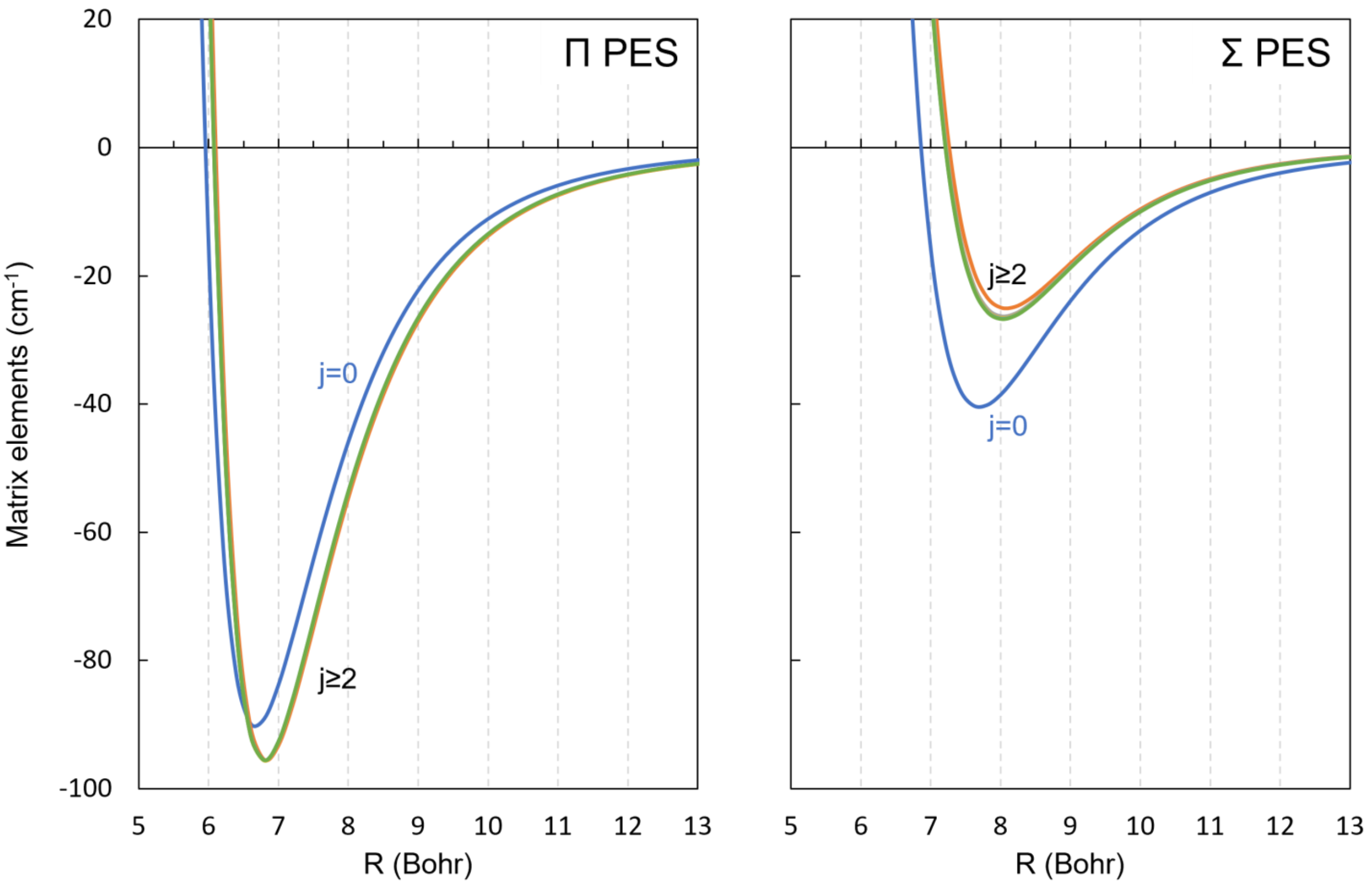


Figure S9: Radial dependence of diagonal matrix elements $M_{j,m}^{j}$ for various j-states of N_2 + O system, $0 \leq j \leq 10$, using Π and Σ PESs. Only $m = 0$ components are shown here ($m > 0$ components are shown in Fig. S10 below).

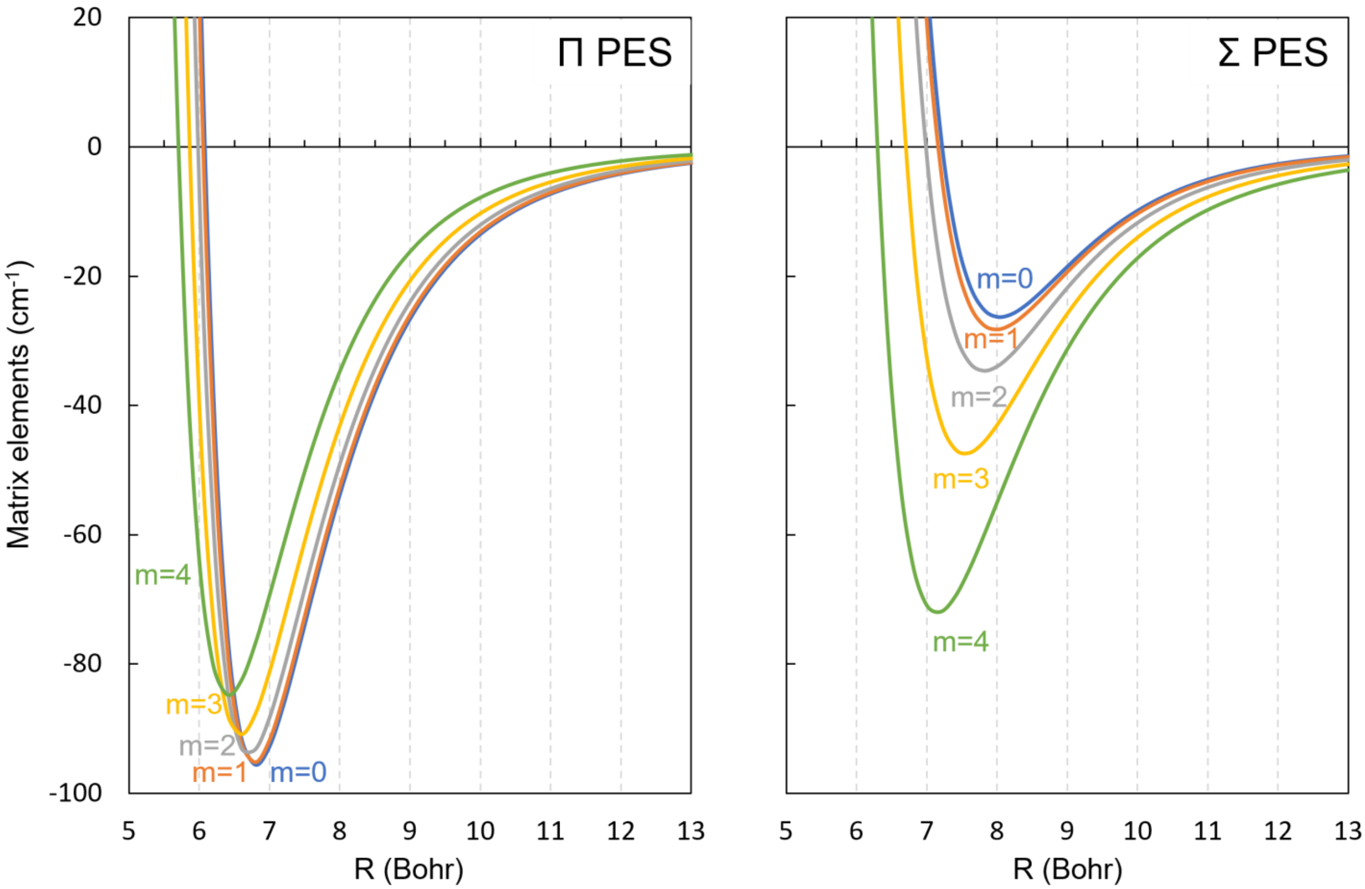


Figure S10: Radial dependence of diagonal matrix elements $M_{j,m}^{j}$ for various m-components of $j = 4$ state for Π and Σ PESs of N_2 + O system. The cases of non-negative values of m are shown (negative values give matrix elements of the same magnitude as positive once).

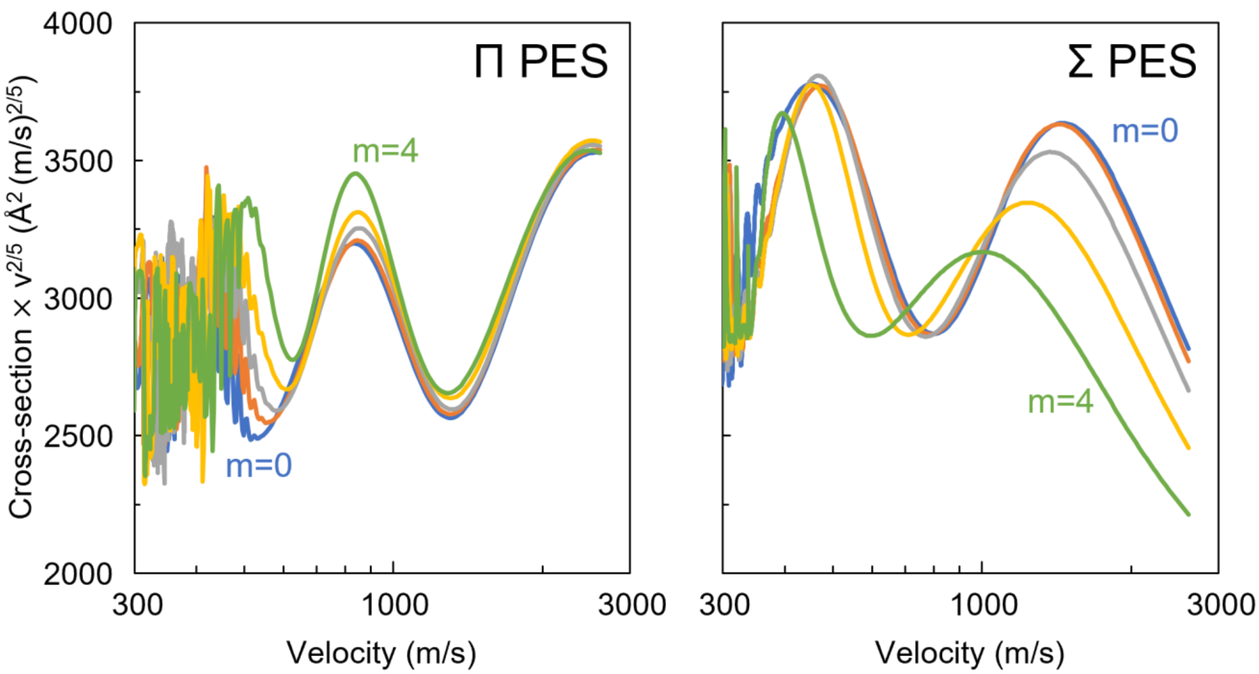


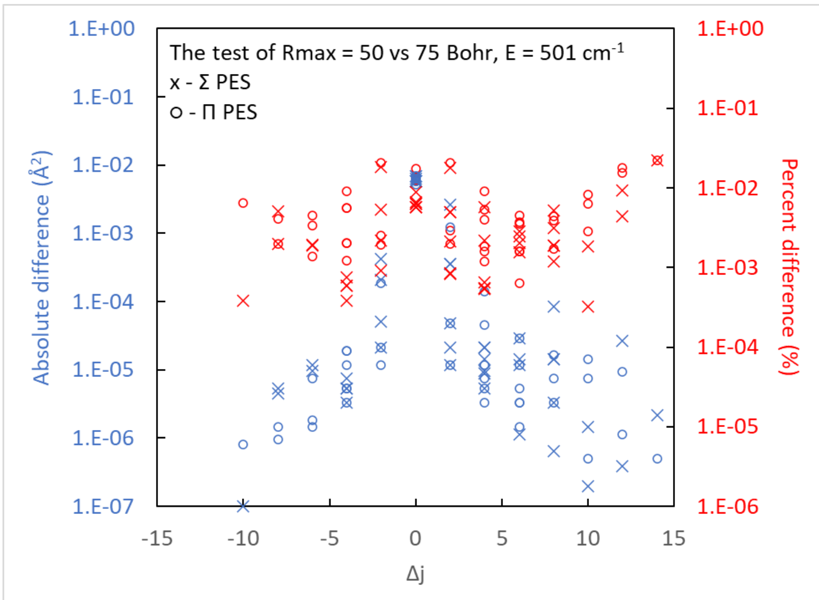
Figure S11: Velocity scaled cross sections as a function of average collision velocity for various m-components of $j = 4$ state for Π and Σ PESs of N_2 + O system.

2. Details of MOLSCAT convergence studies

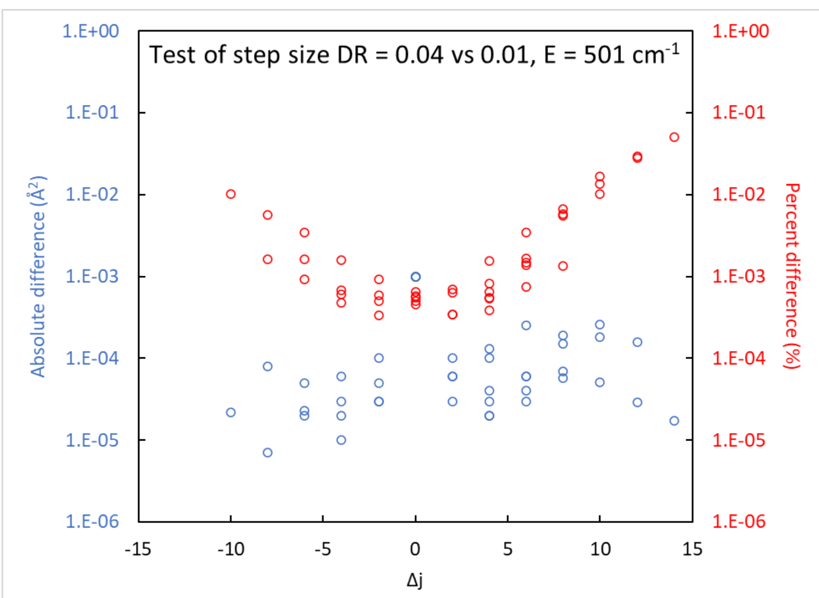
Here we summarized our convergence studies with respect to seven convergence parameters in MOLSCAT calculations: the distance Rmax, radial grid density DR, angular grid size NPT, number of angular expansion terms MXLAM, rotational basis set size NLEVEL (and the inclusion of excited vibrational state), and the maximum value of total angular momentum JTOTU.

All the figures below show Absolute (left axis) and Percent (right axis) differences of cross sections (plotted as a function of Δj) for a pair of calculations that represent a variation of all convergence parameters.

The following figure demonstrates that the difference between Rmax = 50 and 75 Bohr, for both PESs, is less than 0.1%.



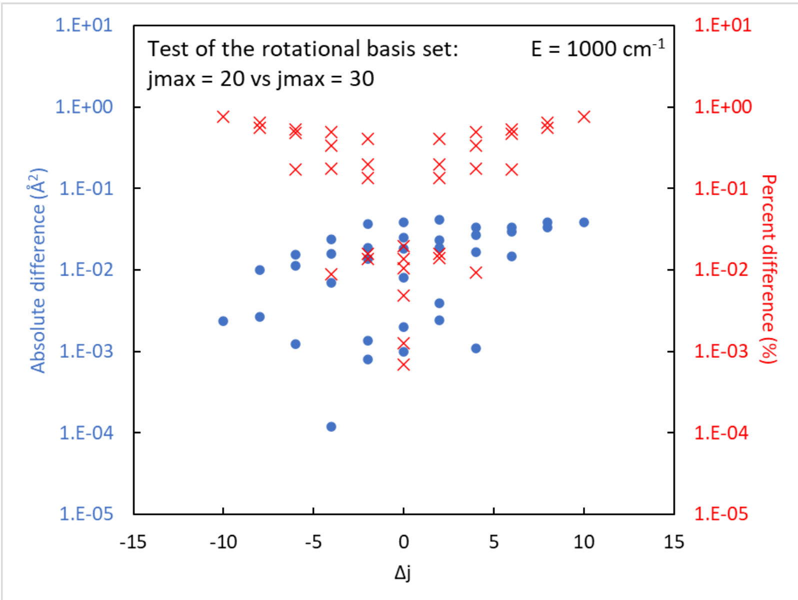
The next figure shows the convergence with respect to step size DR, where the difference between DR = 0.04 and 0.01 (the densest grid tested) is less than 0.1%.



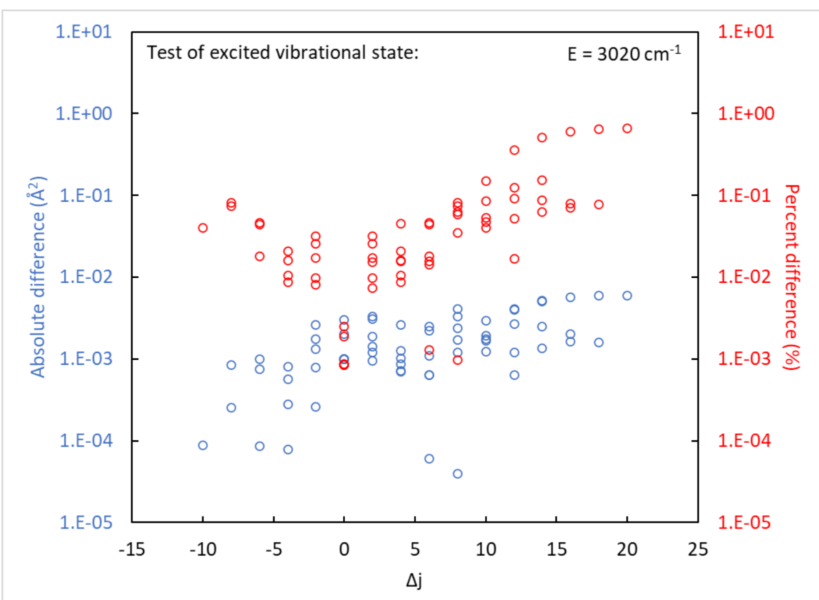
For the test of NPT, we did calculations with 41 and 21 points (which is the smallest possible value in this case) and found no difference in cross sections whatsoever.

Same for the test of the number of lambda terms MXLAM. We did calculations with 11 (even terms up to λ_{max}=20) and with 16 (even terms up to λ_{max}=30) expansion terms and found no difference of cross sections at all.

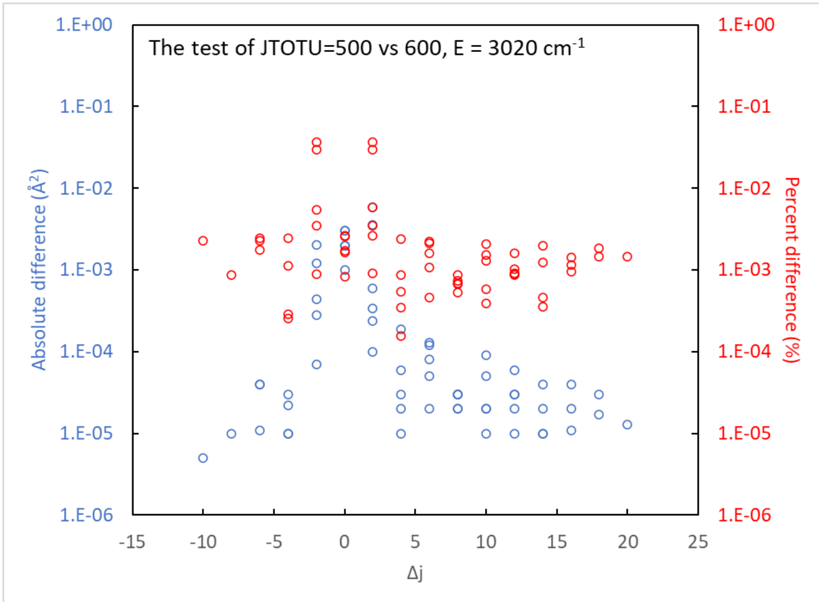
The next convergence test was done with respect to the rotational basis set size. We tried to increase rotational basis by adding 5 more even rotational states (up to jmax = 30) to our reported basis. The calculation was carried out for energy E = 1000 cm^{-1} (which is in the upper part of the experimental range) and the difference between two results is less than 1%.



Next, we checked the effect of excited vibrational state at collision energy E = 3020 cm^{-1} (the highest energy included in the paper) by adding v=1 vibrational state with 6 associated rotational states (up to jmax = 8). The differences with calculations reported in the paper were found to be within 1% for large Δj (when cross sections are small, not even reported in the paper), and is within 0.1% for larger cross sections, as presented in the figure below.



This figure below displays the percent difference between JTOTU = 500 and 600 for the total energy E = 3020 cm^{-1} (the highest energy included in our calculations). According to this figure, agreement between results is within 0.1%.



Therefore, we conclude that our results are converged with respect to all input parameters.