FINAL TECHNICAL REPORT

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"Cross Section Calculations of Astrophysical Interest"

Submitted by

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Our investigations on the subject grant were performed for a period of one year, starting September 1972. The research was carried out by Dr. Farhad Faisal, postdoctoral Research Associate working full time, under the direction of the Principal Investigator who devoted a portion of his time to this project. No publications resulted from the investigations undertaken.

In the remainder of this final technical report, we describe the conclusions which can be drawn from our efforts on this grant. To help make our discussion meaningful, it is useful first to remind the reader of the tasks we proposed to undertake. In our original proposal, we wrote:

"It is our intent to work on problems of immediate great astrophysical interest. Thus, we are proposing to compute cross sections for rotational excitation associated with current theories of the absorption and emission lines from molecules in interstellar space. In particular, we wish to compute the cross sections for excitation of rotational levels in H_2CO, CO and OH by collisions with neutral particles, such as H, H_2 and He. Although rotational excitation and deexcitation unquestionably is an important mechanism in the cooling of interstellar molecules,[1,2] rotational excitation via collisions with neutrals has been examined quantum theoretically comparatively rarely in the past. A notable exception in this regard is the work of Thaddeus[3] (see below). There have been many quantum mechanical calculations of rotational excitation by electrons[4]. In addition, some classical or semi-classical calculations of rotational excitation by neutrals have been performed[5]. However, it is difficult to evaluate the validity of such approaches without the aid of reliable quantum mechanical calculations; it does seem doubtful that classical or semi-classical approximations will be accurate for the low rotational quantum numbers and the low

colliding energies (<60°K) of interest for the observed interstellar molecule rotational transitions. In any event, these classical and semi-classical calculations have employed highly approximate and idealized interactions, e.g., hard sphere potentials.

"The quantum mechanical calculations by Thaddeus[3] also have employed dubiously oversimplified interactions. Nevertheless, these calculations by Thaddeus[3] provide the presently most sophisticated treatment of rotational excitation by neutrals. These calculations, which are very relevant to the whole problem of interstellar molecular lines, compute the cross sections for rotational excitation of H_2CO by H_2 using the so-called adiabatic method of Chase[6]. In these calculations, Thaddeus has examined successively more complicated models, and in so doing has given strong arguments for the validity of the adiabatic method he employs. Thus, Thaddeus's conclusions that the collisional cooling postulated by Townes and Cheung[5] does not occur must be taken very seriously. In fact, Thaddeus's results would be more consistent with hitherto unobserved maser action in H_2CO clouds. However, as mentioned above (and as Thaddeus himself recognizes) his calculations do make a number of not obviously inconsequential assumptions, including use of hard sphere interactions and neglect of multiple scattering (of the incident plane projectile wave) from successive atoms in the H_2CO molecule. Because of these assumptions, Thaddeus's conclusions can be questioned, and in fact have not yet been accepted by Townes[7]. On the other hand, with present theoretical techniques and computing machines, it probably is not possible to perform convincingly accurate calculations on collisions as complicated as H_2-H_2CO. Variational calculations closely related to close-coupling calculations[8] presently are being attempted by

Professor Townes' group[7], but no results have been reported as yet. In any case, such close-coupling calculations--when and if completed--surely also will be inconclusive, because they are too arduous to include the large numbers of rotational levels required to make the close-coupling expansion reasonably complete. Furthermore, some of Thaddeus's results[3] suggest that use of Chase's adiabatic method is justified for the hard sphere interactions employed by Townes and Cheung[5] as well as by Thaddeus; if the adiabatic method is valid, close-coupling calculations are an extremely arduous unnecessary elaboration.

"For these reasons, we are proposing to examine the sensitivity of Thaddeus's H_2CO calculations to changes in the form of the assumed interaction. Specifically, we propose to compute H_2CO rotational excitation by neutrals using:

a. Soft sphere interactions

b. Long range forces of various kinds

c. Available interatomic potentials, e.g., available H-H and $H-H_2$ interactions[9]

d. Combinations of the above.

In addition, we propose to compute CO and OH excitations cross sections via interactions such as a-d above. For these calculations, as well as for H_2CO, we are particularly interested in determining the possible effects of long range forces, e.g., the r^{-4} potentials between permanent dipoles and quadrupoles.

"In the proposed calculations described above, we are intending to employ the Chase adiabatic method used by Thaddeus. As discussed previously, the only present alternative to the Chase method--short of the impossible feat of solving the Schrodinger equation ab initio, without

approximation--is the very arduous and probably not more reliable close--coupling method. However, we do intend to obtain some idea of the expected relationship between adiabatic and close-coupling results in neutral-neutral rotational excitation collisions by treating $H-H_2$ rotational excitation, wherein the results of close-coupling calculations using believable interactions have been reported[10]. In this connection it is noteworthy that the close-coupling results of Hayes, Wells and Kouri[10] differ very markedly from earlier close-coupling results by Dalgarno, Henry and Roberts[11], apparently because of differences in the assumed interaction, although the interaction employed by Dalgarno, Henry and Roberts also was believable. We add that accurate knowledge of these $H-H_2$ rotational excitation cross sections is itself of astrophysical interest[2]."

In our investigations we began by examining the H_2CO items a-c listed on previous page; toward the end of the year we expended considerable effort on the $H-H_2$ computations described above. The main difficulty preventing attainment of publishable results was the very large amount of computer programming and computing that proved necessary, even after considerable analytic reduction of the complicated expressions from which we started in, e.g., the Chase adiabatic approximation. For the $H-H_2$ rotational excitation calculations we attempted to secure the cooperation of groups having working close coupling rotational excitation codes (notably groups at Rice Institute and at Argonne National Laboratories), because we did not feel we could devote the time needed to develop such a working code; however, none of the groups whose cooperation we solicited were themselves able to spare the time needed to reprogram these (essentially central potentials) codes to the two-center $H-H_2$ calculations we had in mind.

Although the possibility of very tedious computational tasks certainly had been anticipated in the original proposal, nevertheless the principal investigator was very disappointed with the lack of substantial output during the year. Therefore, especially since Dr. Faisal was returning to Bangladesh in October 1973, it was decided not to request renewal of the grant; accordingly, work on the problem under investigation was terminated in September 1973. No publications resulted from the researches undertaken, because no definite phase of the task was completed. It is the principal's investigator's opinion that the original proposal was quite well conceived, and that the proposed research remains important and worth doing. However, successful completion of the research probably requires a larger effort than could be supported on the subject grant, namely one Research Associate under the part-time direction of the Principal Investigator.

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