THEORETICAL INVESTIGATION OF LOW TEMPERATURE PRESSURE BROADENING BY DIAGNOSTIC CALCULATION

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The theory of molecule-atom collisions at low energy predicts significant resonant features in collision cross sections. These resonances correspond to the formation of short-lived, quasi-bound complexes. At low temperatures, this capture is made possible by the shallow attractive well of the intermolecular potential. In contrast, at ambient temperatures, collision cross sections result from "action at a distance" mechanisms. The shape and position of the resonances in the low energy pressure broadening cross sections depend strongly on both the well depth of the intermolecular potential and on the rotational energy level separation of the molecule. We have performed diagnostic calculations on the well-studied CO-He system, in which we have investigated the behavior of the resonances by changing the well depth of the intermolecular potential and the rotational constant of the molecule. Generalizations to other molecule-atom systems have been made.