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Photodissociation and Predissociation of Heavy Molecular Ions[1]

SVETLANA KOTOCHIGOVA, ALEXANDER PETROV, Temple University —

In support of experimental efforts to sympathetically cool heavy $BaCl^+$ molecular ions we investigated a detection mechanism of these ions by developing a quantum mechanical model of photodissociation and predissociation to ionic Ba^+ and neutral Cl atoms. Photodissociation occurs when the absorption of a photon leads to a transition from the ground electronic state to a repulsive inner wall of an excited potential. Alternatively, photon absorption leads to a transition to a bound state of an excited state followed by predissociation into a third electronic state. We first calculated the ground X and excited A and B potentials and transition dipole moments of the $BaCl^+$ molecule, using CASPT2 method. We then evaluated matrix elements of the dipole moment operator between the initial rovibrational states vJM of the X potential and final scattering states in the repulsive A potential. The photodissociation cross-section is proportional to the square of these matrix elements. We assumed a thermal distribution over rovibrational states of the X potential in order to compare with available experimental data. We then used a coupled channel calculation that involved the B and and A excited electronic states coupled by a coriolis interaction to obtain predissociation rates.

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Svetlana Kotochigova
Temple University

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