Analysis of the nuclear motion in a HeNe* transient molecule

CRISTIAN BAHRIM, JOSEPH HUNT, Department of Chemistry and Physics, Lamar University - Texas — Based on a model potential for describing the interaction between He and Ne* atoms during a collision [1] we predict a series of vibrational states within several electronic adiabatic potential wells of the HeNe* system for internuclear distances $R < 6 \, a_0$. The identification of vibrational states suggests the formation of a HeNe* temporary molecule. In our study two theoretical approaches are employed: (1) the harmonic approximation is based on the assumption that during a collision (which is considered as being one period of vibration) the nuclear motion is harmonic, and (2) the anharmonic approximation which uses the best fit of the electronic adiabatic potential wells with a Morse anharmonic function, as is typically done for stable molecules [2]. A set of vibrational-electronic transitions which can be measured using IR spectroscopy is proposed. The relative population of Ne* atoms after collisions and successful IR photo-absorption is predicted for experimental testing of the dominant character of the nuclear motion: whether is harmonic or anharmonic. The existence of a HeNe* transient molecule could have a positive impact on improving the performance of He-Ne lasers. [1] Bahrim C, Kucal H and Masnou-Seeuws F 1997 Phys. Rev. A 56 1305. [2] Bahrim C and Hunt J 2006 J. Phys. B 39 4683.

Cristian Bahrim
Department of Chemistry and Physics, Lamar University - Texas

Date submitted: 19 Nov 2007

Electronic form version 1.4