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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

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