P15

Bound and resonant states of the imidogen (NH) radical : An R-matrix study

R. Ghosh,[1,*] K. Chakrabarti,[2] and B. S. Choudhury[1]

[1] *Department of Mathematics, Indian Institute of Engineering Science and Technology, Shibpur, Howrah 711103, India*
[2] *Department of Mathematics, Scottish Church College, 1 & 3 Urquhart Sq., Kolkata 700006, India*

The NH imidogen radical is a common component in nitrogen chemical reactions that take place in the atmosphere and interstellar medium(ISM). Its existence was first observed in the 1990s in diffuse clouds[1], although it had been previously identified in the sun's atmosphere[2], stellar atmospheres and comet tails[3]. NH is also likely to be present and is a precursor to ammonia formation in the ISM [4].

NH and NH^+ are also produced during the combustion of nitramine compounds in rocket propellants, explosives, and emergency escape devices. Many nitrogen plasmas contain NH^+ and NH, therefore, the dynamics calculations and kinetic modeling of these products require electronic structure data and collision data in the form of potential energy curves, reaction rate coefficients and cross-sections[5].

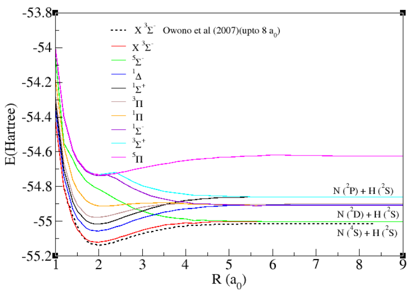

FIG. 1. Potential energy curves of the ground and eight lowest bound states of NH.

Using the R-matrix method, low-energy electron collision calculations have been performed on NH^+ at its equilibrium geometry after building a suitable model to represent the target ion[6]. Scattering calculations are performed to obtain NH bound states for $^3\Sigma^-, ^3\Pi, ^3\Sigma^+, ^1\Pi, ^1\Delta, ^1\Sigma^-, ^1\Sigma^+, ^5\Sigma^-, ^5\Pi$ symmetrices and resonance parameters for $^1\Sigma^-, ^1\Pi$ and $^3\Pi$ symmetrices as a function of geometry ranging from 1-9 a_0 on a moderately dense grid of 61 points. To illustrate the relative position of the low-lying states, we present the potential energy curves (PECs) of the ground state and the eight lowest excited states of NH in figure 1. We also compare our ground state with the work of Owono *et al* [7]. It is clear that there is a good agreement. Numerous resonances are characterised by the characteristic oscillations in the eigenphase sums of $^1\Sigma^-, ^1\Pi$ and $^3\Pi$ overall symmetrices of the $e+$ NH^+ system. It has been observed that many resonances occur in a series characterized by their effective quantum numbers ν [6]. Many of these resonances have very narrow widths and may be close to crossing an NH^+ ion curve from above. To obtain an accurate representation, we are processing a detailed construction of the potential energy curves for the ion NH^+ and resonant states as the inter-nuclear distance R varies. Other collisional calculations should benefit from these resonant states, particularly the Dissociative Recombination of the NH^+ ion.

[1] D. M. Meyer and K. C.Roth, Astrophys. J. Lett. **376**, L49 (1991).
[2] H. D. Babcock, Astrophys. J. **102**, 154 (1945).
[3] R. Meier, D. Wellnitz, S. J. Kim, and M. F. A'Hearn, Icarus **136**, 268 (1998).
[4] E. T. Galloway and E. Herbst, Astron. Astrophys. **211**, 413 (1989).
[5] G. F. Adams and R. W. Shaw, Jr., Annu. Rev. Phys. Chem. **43**, 311 (1992).
[6] R. Ghosh, K. Chakrabarti, and B. S. Choudhury, Plasma Sources Sci. Technol. **31**, 065005 (2022).
[7] L. C. O. Owono, N. Jaidane, M. G. K. Njock, and Z. B. Lakhdar, J. Chem. Phys. **126**, 244302 (2007).

* rajughosh152@gmail.com