ACCURATE POTENTIAL ENERGY CURVES FOR THE GROUND ELECTRONIC STATES OF NeH⁺ AND ArH⁺

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All available microwave and infrared spectroscopic line positions for the ground electronic states of the molecular cations NeH⁺ and ArH⁺ were employed in a direct potential fitting procedure to determine compact analytical potential curves and radial functions describing breakdown of the Born-Oppenheimer approximation. For NeH⁺, 17 adjustable parameters were required to represent a total of 183 line positions for 4 isotopologues, whereas for ArH⁺, 23 adjustable parameters were required to represent 440 line positions for 6 isotopologues. The MLR3 potential energy functional form was employed, taking full account of the proper $1/r^4$ limiting long-range dependence of the ion-atom dispersion energy interactions. Accurate vibrational energies, rotational constants and centrifugal distortion constants have been calculated for both diatomic cations.