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Testing theoretical ion-atom interaction potentials by precise measurements of gas-phase ionic mobilities RAINER JOHNSEN, University of Pittsburgh, LARRY VIEHLAND, Chatham University, TIMOTHY WRIGHT, University of Nottingham — High-level computations now predict ion-atom potentials over a wide range of inter-atomic distances, from the potential minimum up to the dissociation asymptote. Hence, their reliability needs to be tested by experiments that probe the potentials over a commensurate range of distances, which often exceeds the range accessible to spectroscopy. In a collaborative project, the authors have recently tested several theoretical potentials by comparing measured gas-phase ionic mobilities to those derived from computed potentials and state-of-the-art ion transport theory. Here we present results on the ion-atom systems O^+-He, O^+-Ne, O^+-Ar, as well as He^+-Ne and Ne^+-He. A selected-ion drift tube mass spectrometer was used that determines mobilities with an accuracy of about 2 to 3 %, after corrections for "end-effects". While the calculated mobilities agree quite well with their measured values over a wide range of E/n (the electric-field to gas-density ratio), more accurate mobility measurements (at the 1% level) are needed to test for finer details of the interaction, e.g. effects arising from spin-orbit coupling. We plan to (a) further improve the accuracy and (b) to incorporate a laser-ablation source in order to study metal-ion/molecule pairs that are of interest for molecular structure calculations.

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