METAL ION CHEMISTRY IN COLD INTERSTELLAR AND CIRCUMSTELLAR ENVIRONMENTS

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Ions of abundant metals, including Na^+, K^+, Mg^+, Ca^+ and Fe^+, are likely to play an important role in the chemical evolution of metal-containing interstellar and circumstellar environments. The ionic reaction networks include a variety of efficient radiative association, ligand-switching, clustering and recombination processes. High-level ab initio calculations, using the CP-dG2thaw method and related approaches, are combined here with VTST computations of reaction kinetics to explore the reactivity of the atomic metal ions and metal-containing molecular ions with abundant neutrals. The likely composition of the metal-containing populations and the accompanying formation of neutral species like MNC, MCN and MC_3N are examined for three different C-rich environments, typified by the cold dark interstellar cloud TMC-1, the outer circumstellar envelope of the AGB star IRC+10216 and the post-AGB object CRL 618, and are discussed with reference to molecular detections within these three objects.